



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:31 PM UTC

PDB ID : 6QA9 / pdb_00006qa9
EMDB ID : EMD-4482
Title : Isolated complex I class refinement from Ovine respiratory supercomplex I+III2
Authors : Letts, J.A.; Sazanov, L.A.
Deposited on : 2018-12-19
Resolution : 4.10 Å(reported)
Based on initial model : 1PPJ

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:

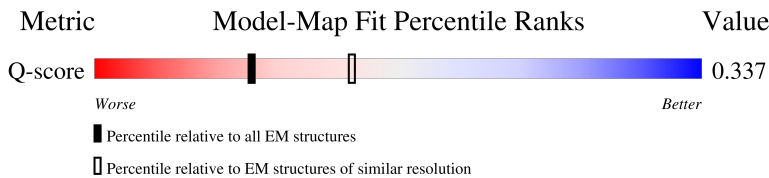
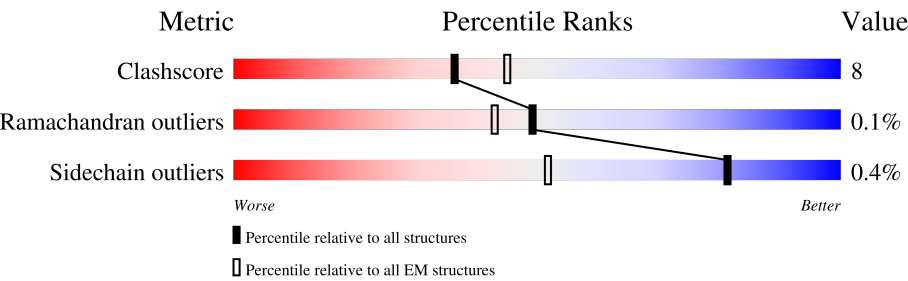
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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 $\leq 5\%$. 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	18% 73% 23% ..
2	V2	217	24% 79% 18% .
3	S1	704	21% 75% 22% .
4	S2	430	25% 78% 21% .

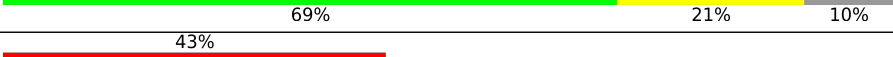
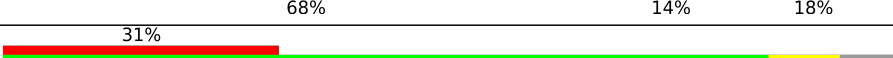
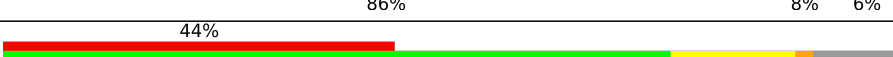
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Mol	Chain	Length	Quality of chain
5	S3	228	
6	S7	179	
7	S8	176	
8	V3	75	
9	S6	96	
10	S4	133	
11	A9	338	
12	A2	98	
13	A5	115	
14	A6	127	
15	A7	112	
16	AL	145	
17	AA	88	
17	AB	88	
18	D3	115	
19	D1	318	
20	D6	175	
21	4L	98	
22	D5	606	
23	D4	459	
24	D2	347	
25	AK	140	
26	B5	143	
27	A8	171	
28	BJ	175	

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Mol	Chain	Length	Quality of chain
29	AJ	320	
30	S5	105	
31	A3	83	
32	B3	97	
33	C2	120	
34	B4	128	
35	AM	143	
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	V1	500	-	-	X	-

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 65403 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
1	V1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

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

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

- Molecule 4 is a protein called NDUF52.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S2	427	Total	C	N	O	S	0	0
			3436	2194	589	628	25		

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

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

- Molecule 6 is a protein called NDUF57.

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

- Molecule 7 is a protein called NDUF8S.

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	40	Total	C	N	O	S	0	0
			335	209	60	65	1		

- Molecule 9 is a protein called NDUF86.

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	290	Total	C	N	O	S	0	0
			2321	1483	423	410	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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A5	111	Total	C	N	O	S	0	0
			902	583	151	166	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
			970	619	180	167	4		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A7	94	Total	C	N	O	S	0	0
			752	470	143	136	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	143	Total	C	N	O	S	0	0
			1192	768	214	206	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 NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D3	97	Total	C	N	O	S	0	0
			787	538	112	132	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D1	299	Total	C	N	O	S	0	0
			2390	1618	364	389	19		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D6	171	Total	C	N	O	S	0	0
			1308	878	187	230	13		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4L	98	Total	C	N	O	S	0	0
			748	489	112	132	15		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 8.

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

- Molecule 28 is a protein called NDUFB10.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

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

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

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

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

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

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

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

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

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

- Molecule 35 is a protein called NDUFA13.

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B6	96	Total	C	N	O	S	0	0
			815	536	139	139	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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	65	Total	C	N	O	S	0	0
			563	372	93	97	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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

11, mitochondrial.

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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

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

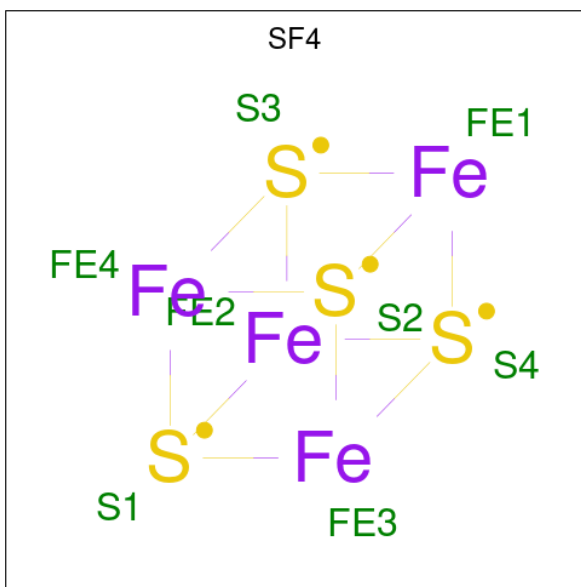
There are 3 discrepancies between the modelled and reference sequences:

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.

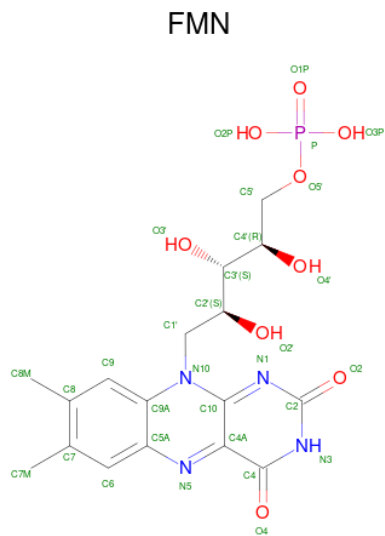
Mol	Chain	Residues	Atoms					AltConf	Trace
44	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



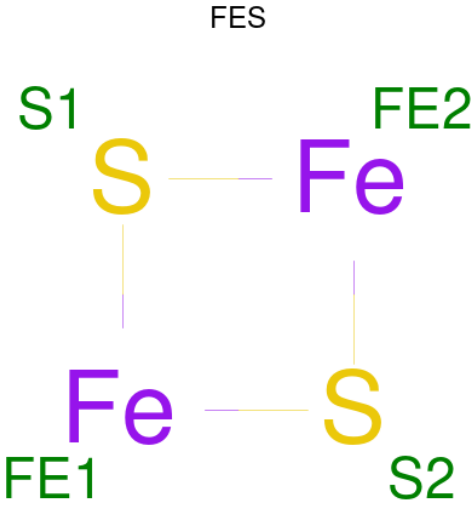
Mol	Chain	Residues	Atoms			AltConf
45	V1	1	Total	Fe	S	0
			8	4	4	
45	S1	1	Total	Fe	S	0
			8	4	4	
45	S1	1	Total	Fe	S	0
			8	4	4	
45	S7	1	Total	Fe	S	0
			8	4	4	
45	S8	1	Total	Fe	S	0
			8	4	4	
45	S8	1	Total	Fe	S	0
			8	4	4	

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



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

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

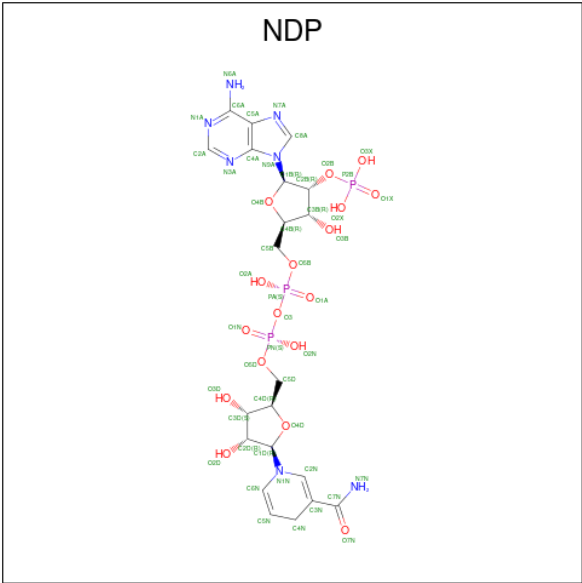


Mol	Chain	Residues	Atoms			AltConf
47	V2	1	Total 4	Fe 2	S 2	0
47	S1	1	Total 4	Fe 2	S 2	0

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

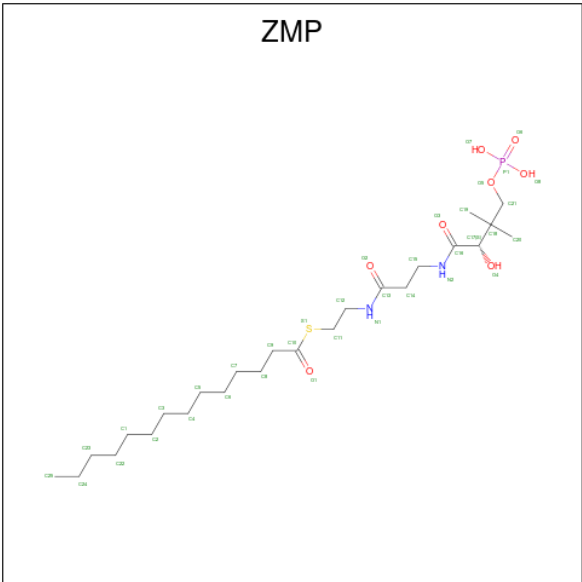
Mol	Chain	Residues	Atoms		AltConf
48	S6	1	Total	Zn	0
			1	1	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



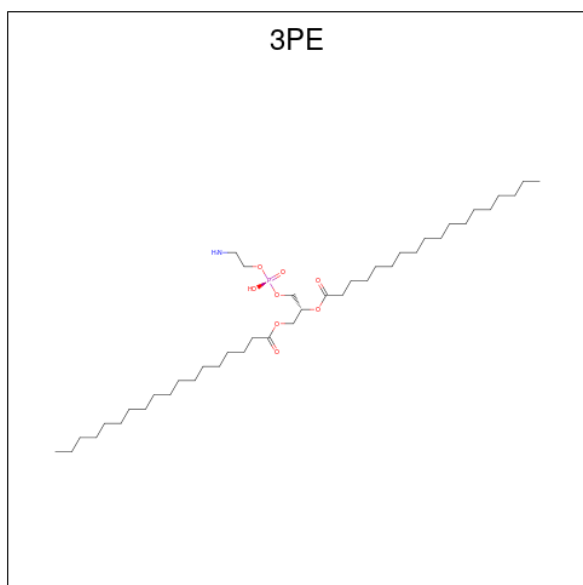
Mol	Chain	Residues	Atoms					AltConf
49	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



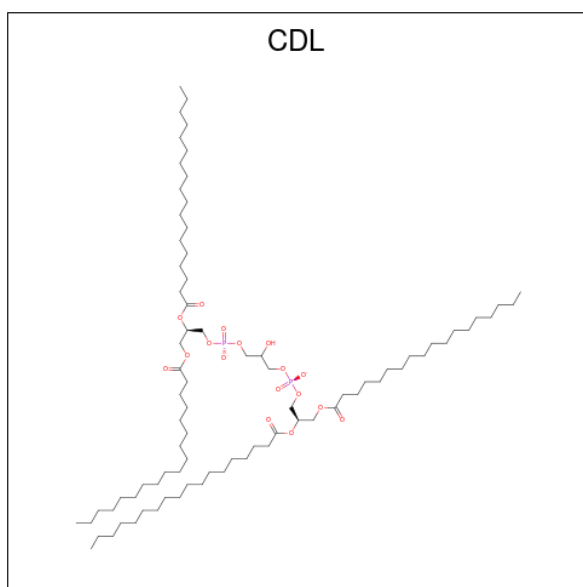
Mol	Chain	Residues	Atoms						AltConf
50	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
50	B9	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



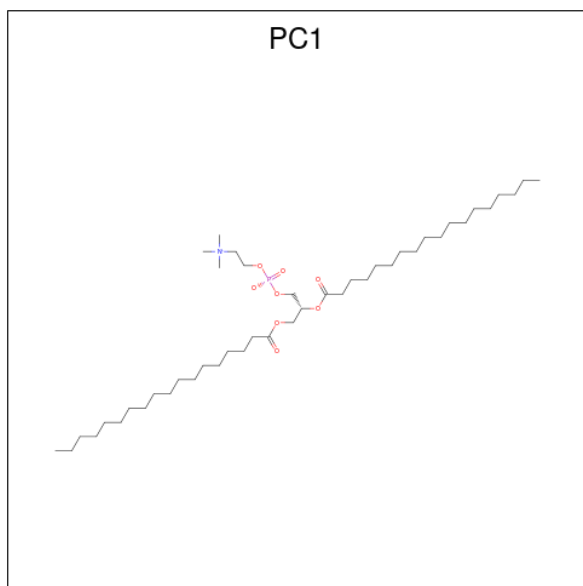
Mol	Chain	Residues	Atoms					AltConf
51	D1	1	Total	C	N	O	P	0
			19	9	1	8	1	
51	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	
51	D4	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	A8	1	Total	C	N	O	P	0
			25	15	1	8	1	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
52	D5	1	36	17	17	2	0

- Molecule 53 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	D4	1	28	18	1	8	1	0

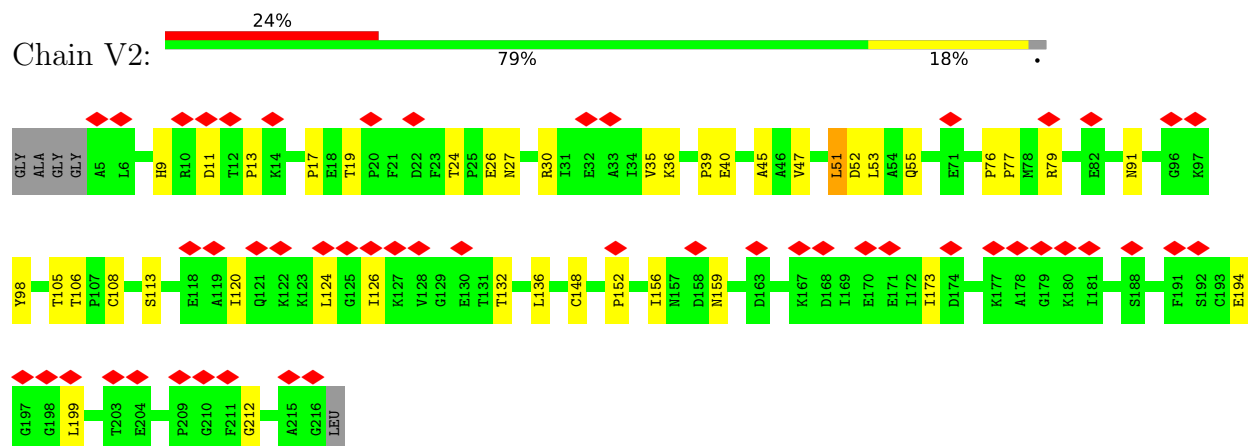
3 Residue-property plots

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.

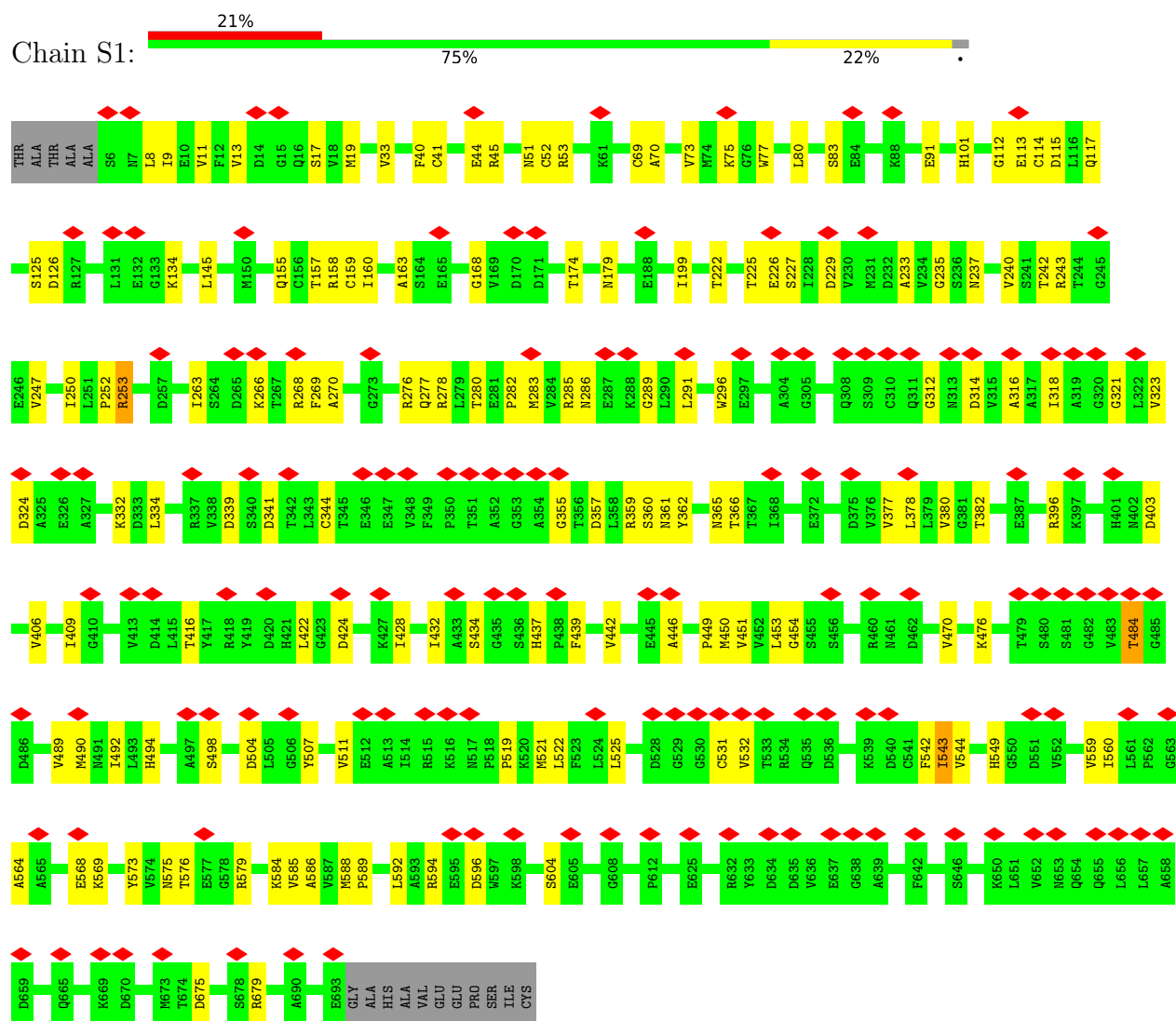
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



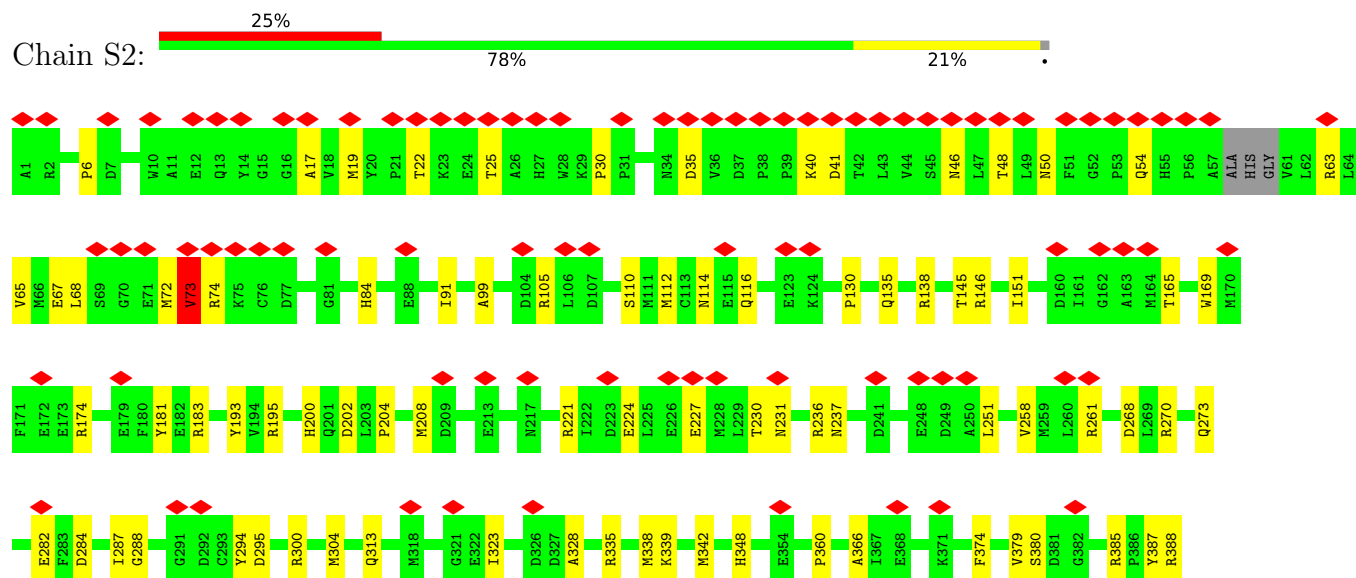
- Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

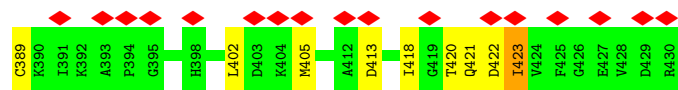


• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

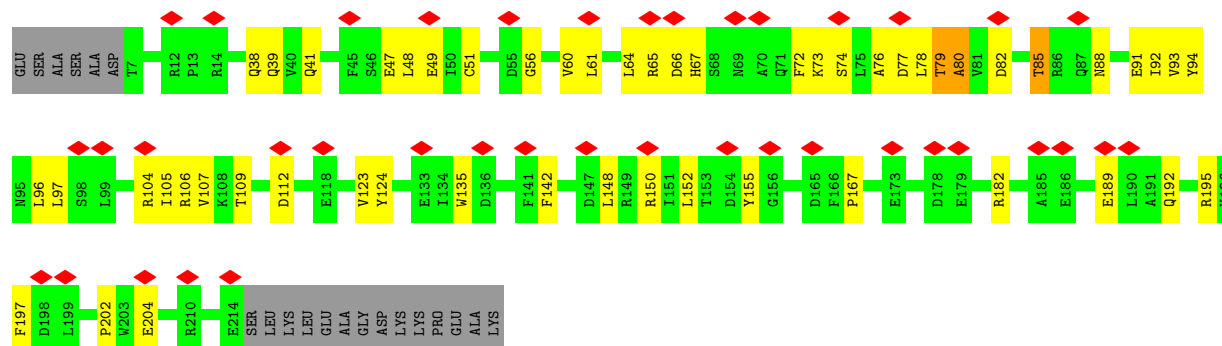


• Molecule 4: NDUF52

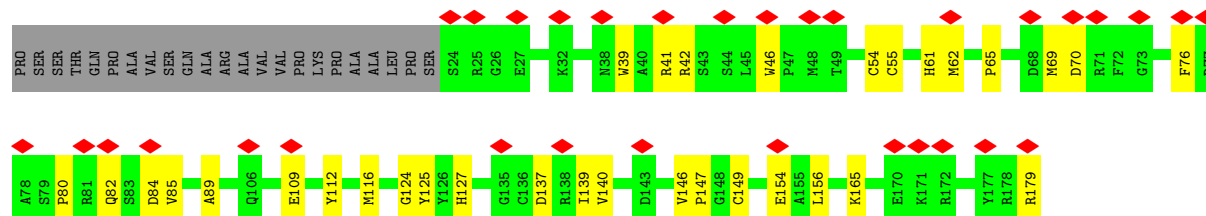




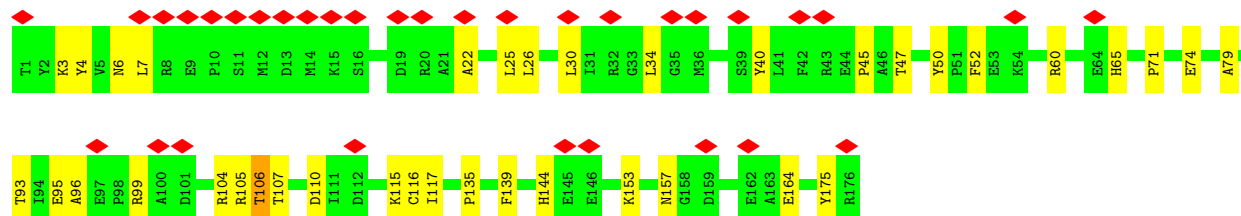
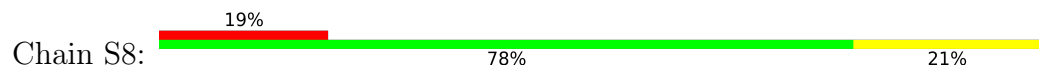
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3



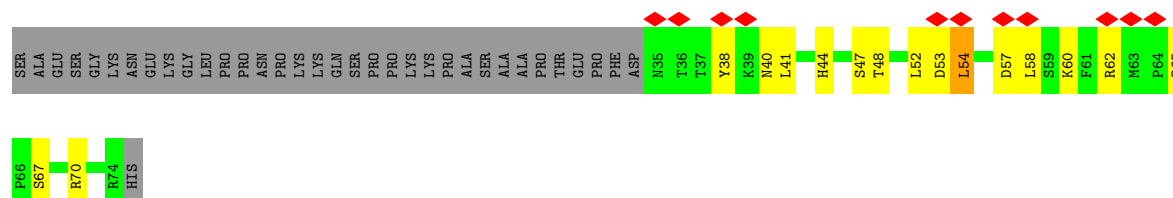
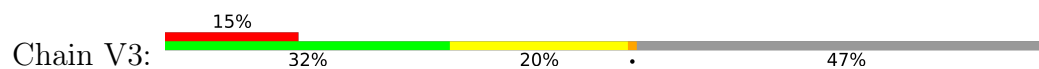
• Molecule 6: NDUFS7



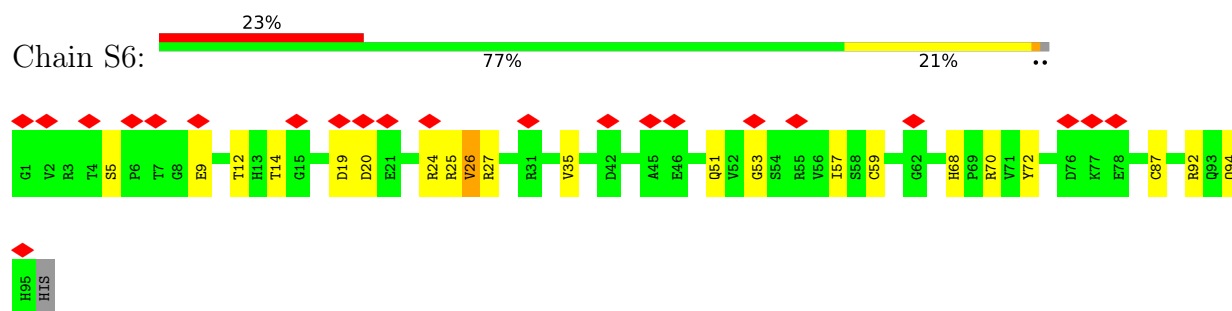
• Molecule 7: NDUFS8



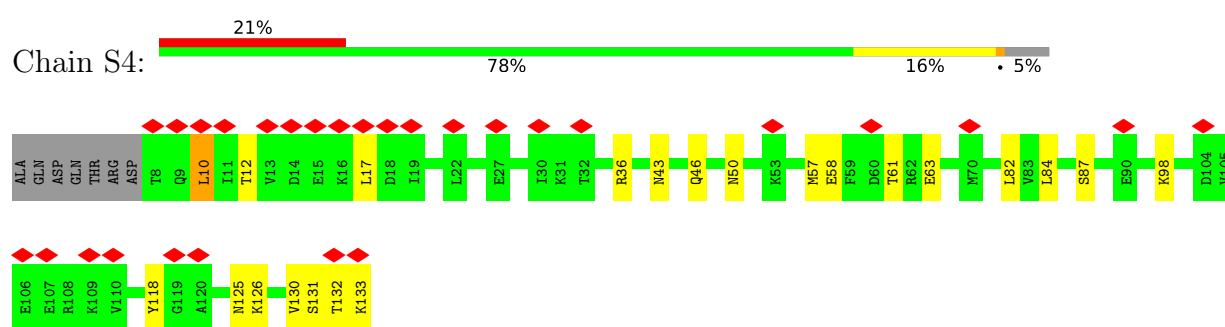
• Molecule 8: NDUFV3



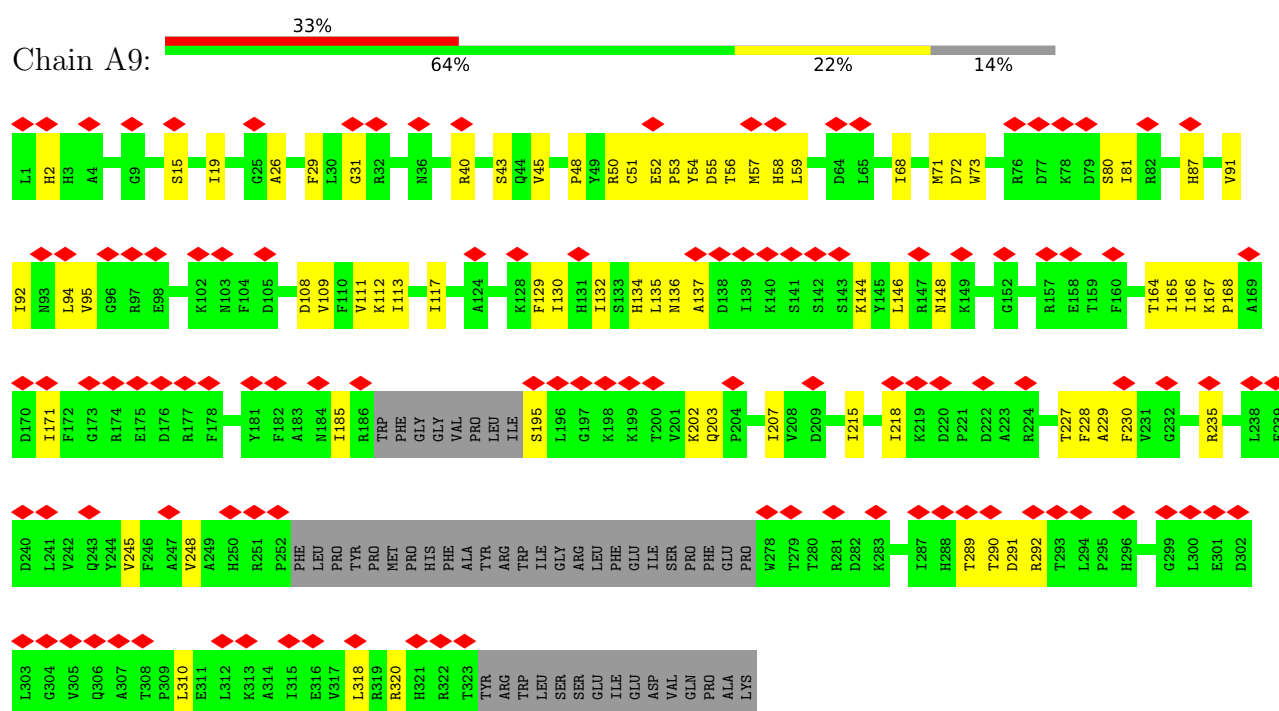
- Molecule 9: NDUFS6



- Molecule 10: NADH:ubiquinone oxidoreductase subunit S4

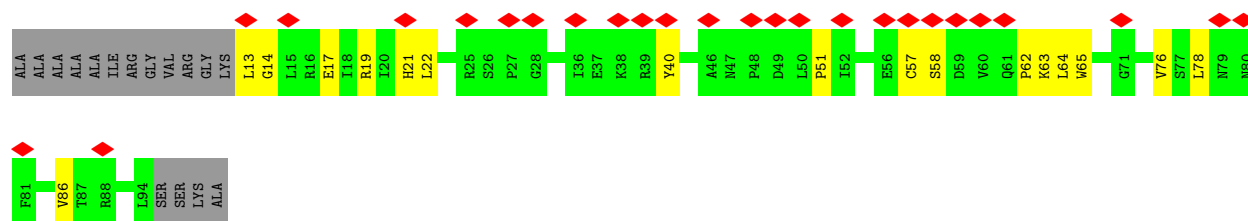


- Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

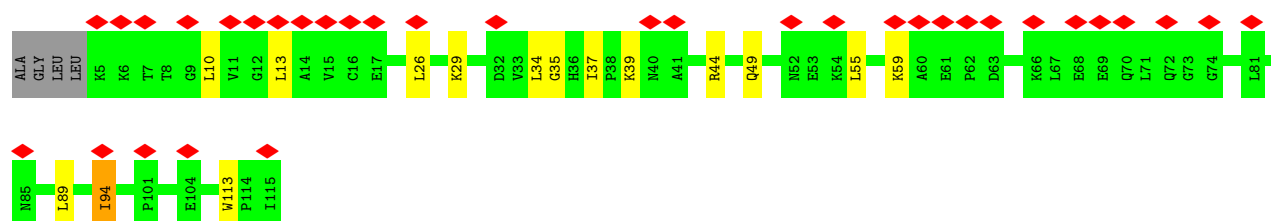
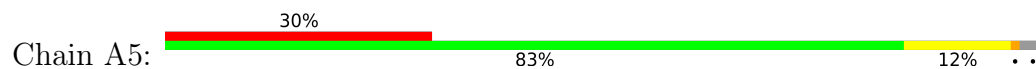


- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

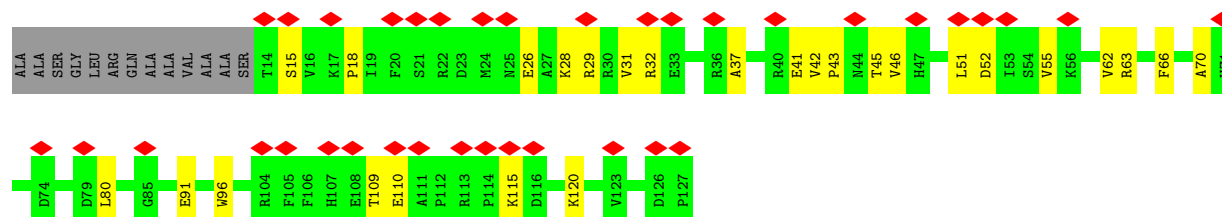




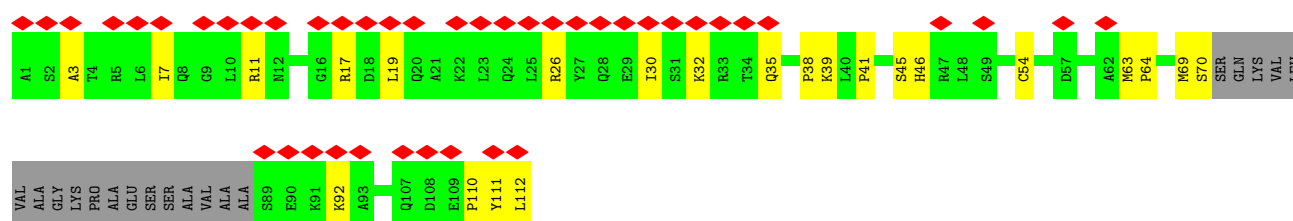
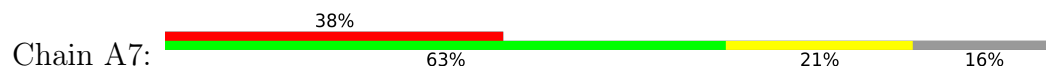
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



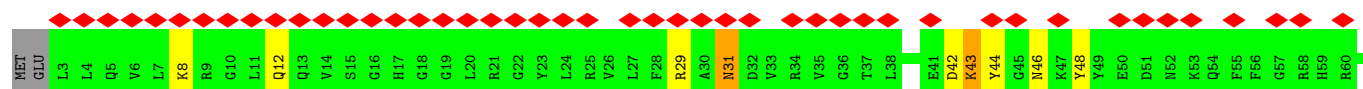
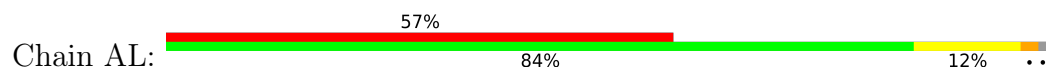
- Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

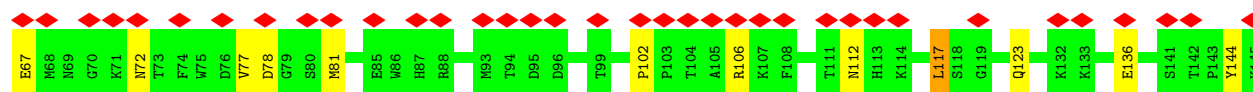


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

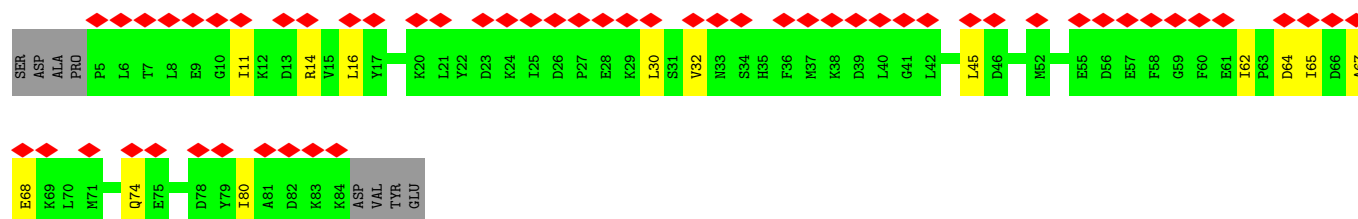
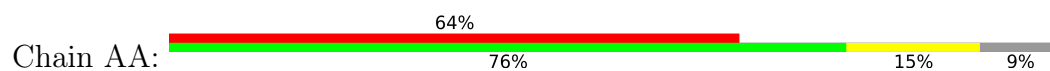


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

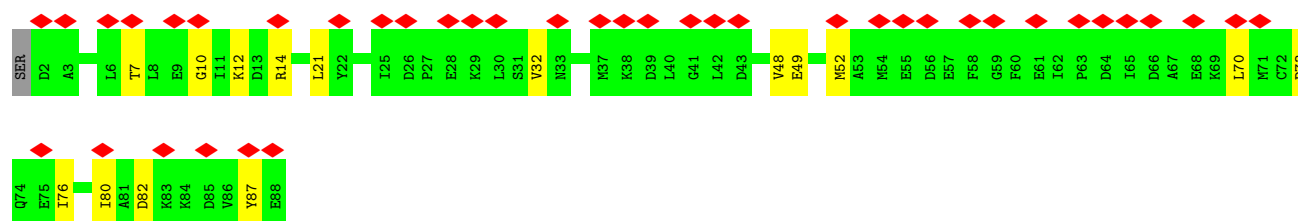
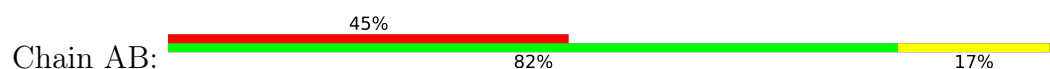




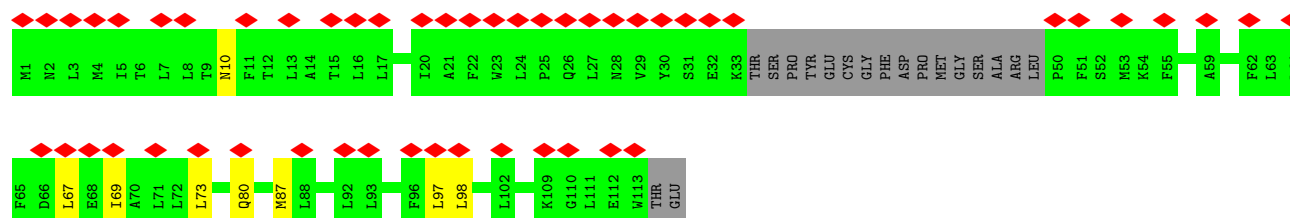
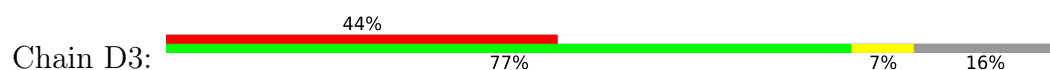
• Molecule 17: Acyl carrier protein



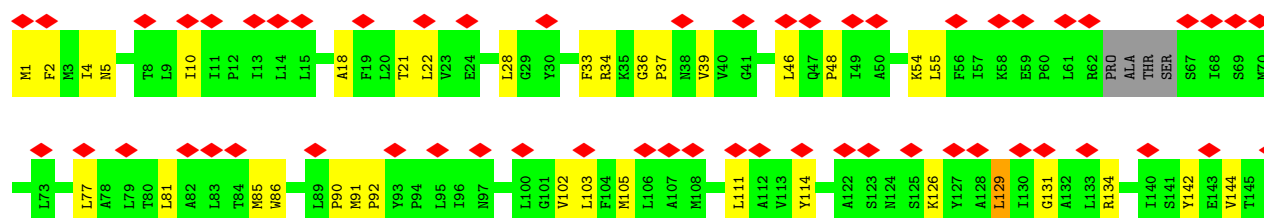
• Molecule 17: Acyl carrier protein

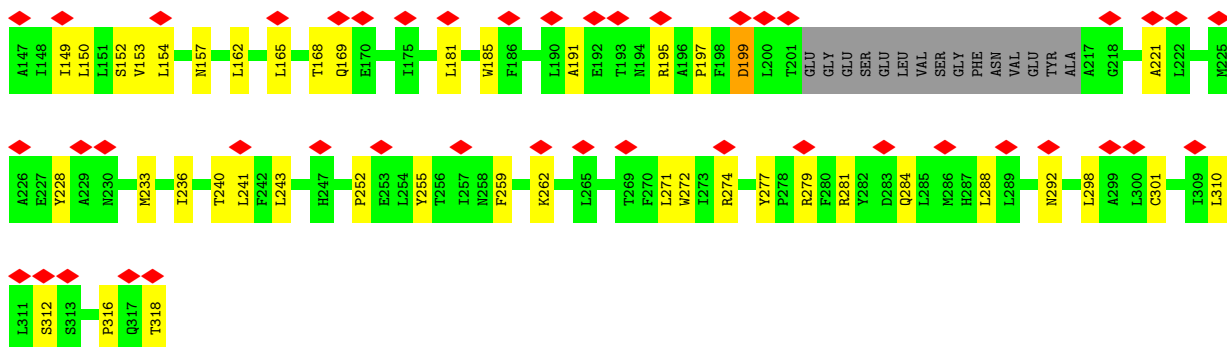


• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

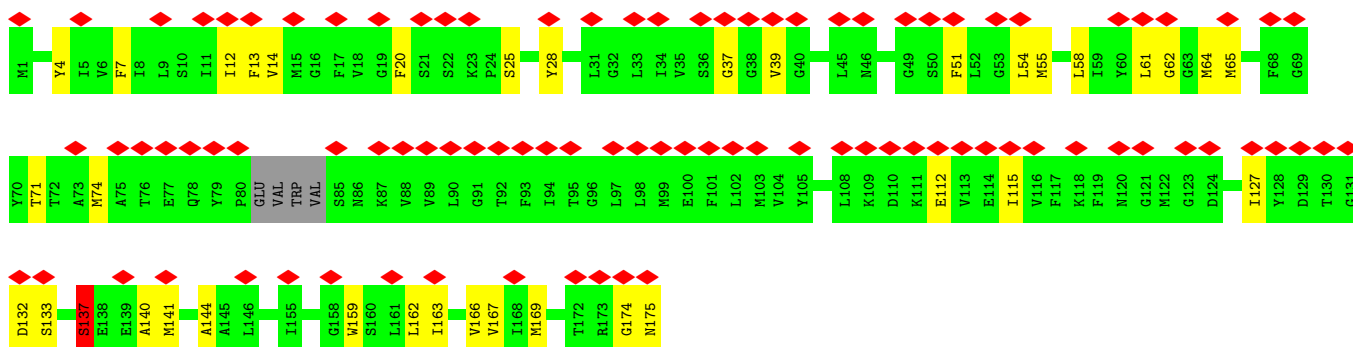
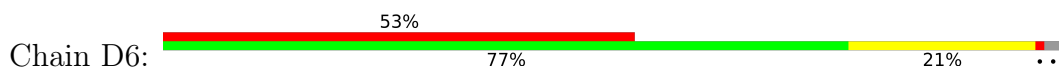


• Molecule 19: NADH-ubiquinone oxidoreductase chain 1

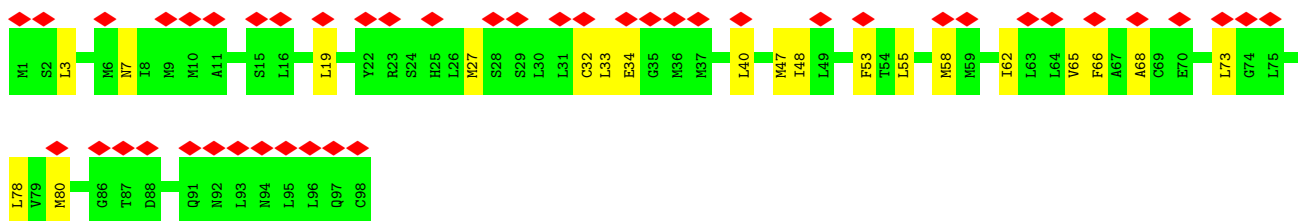
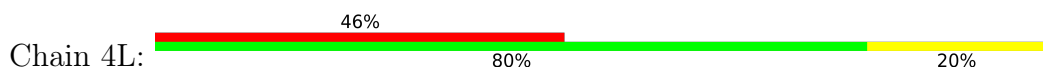




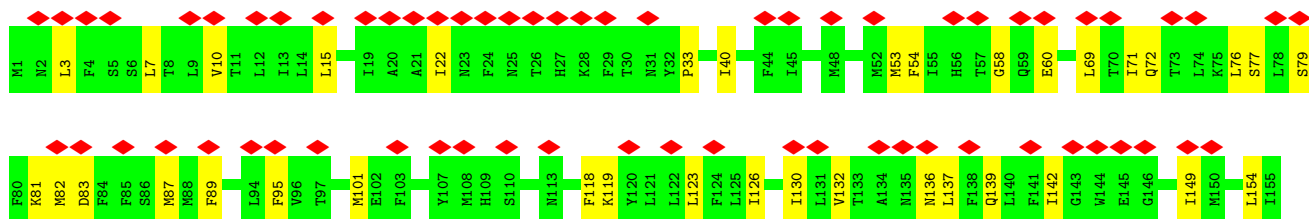
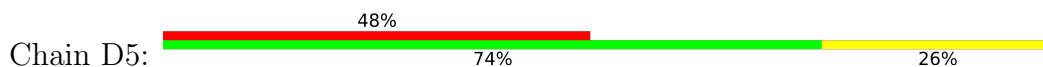
• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

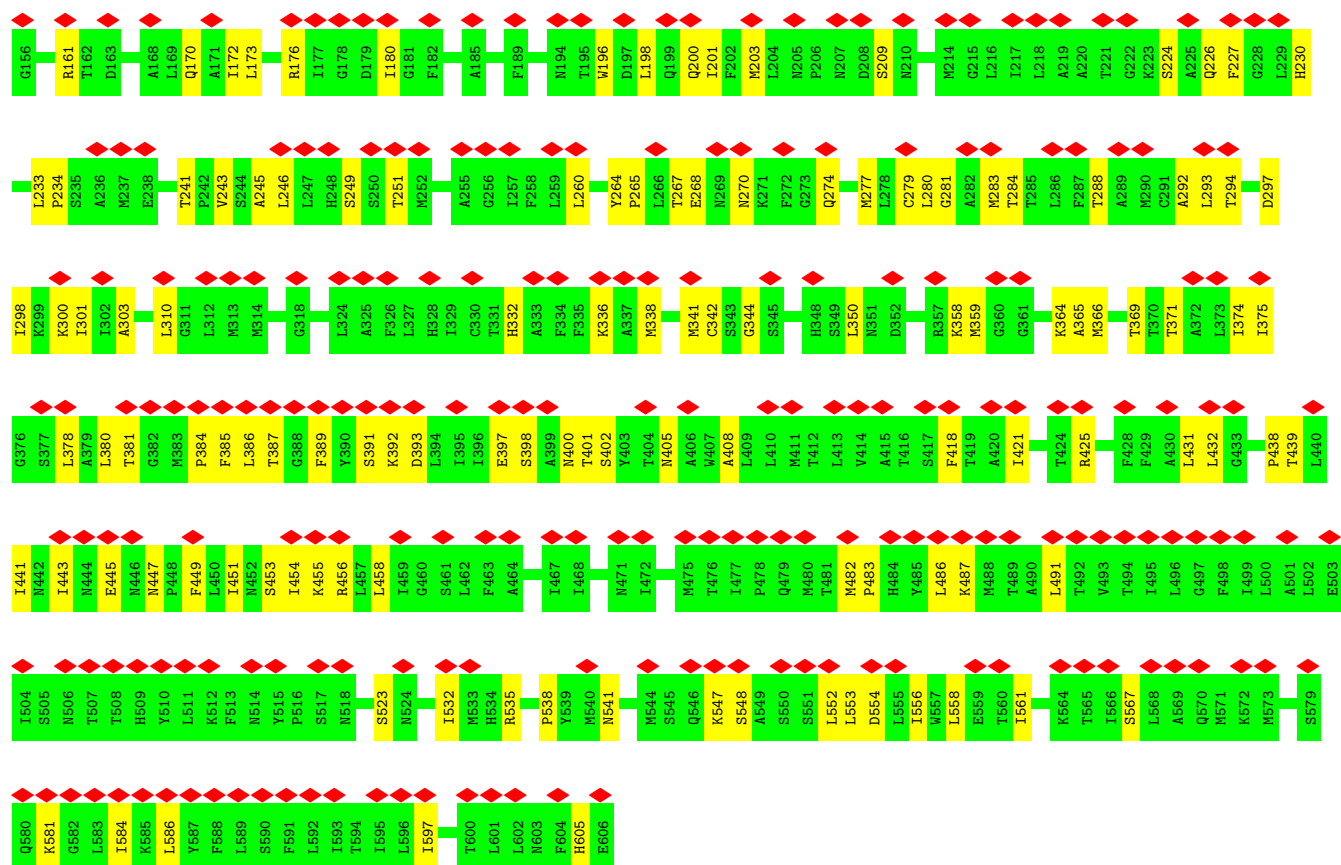


• Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

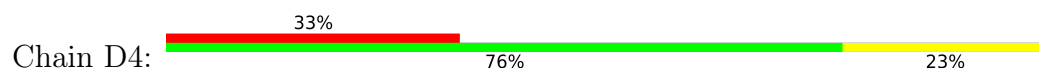


• Molecule 22: NADH-ubiquinone oxidoreductase chain 5

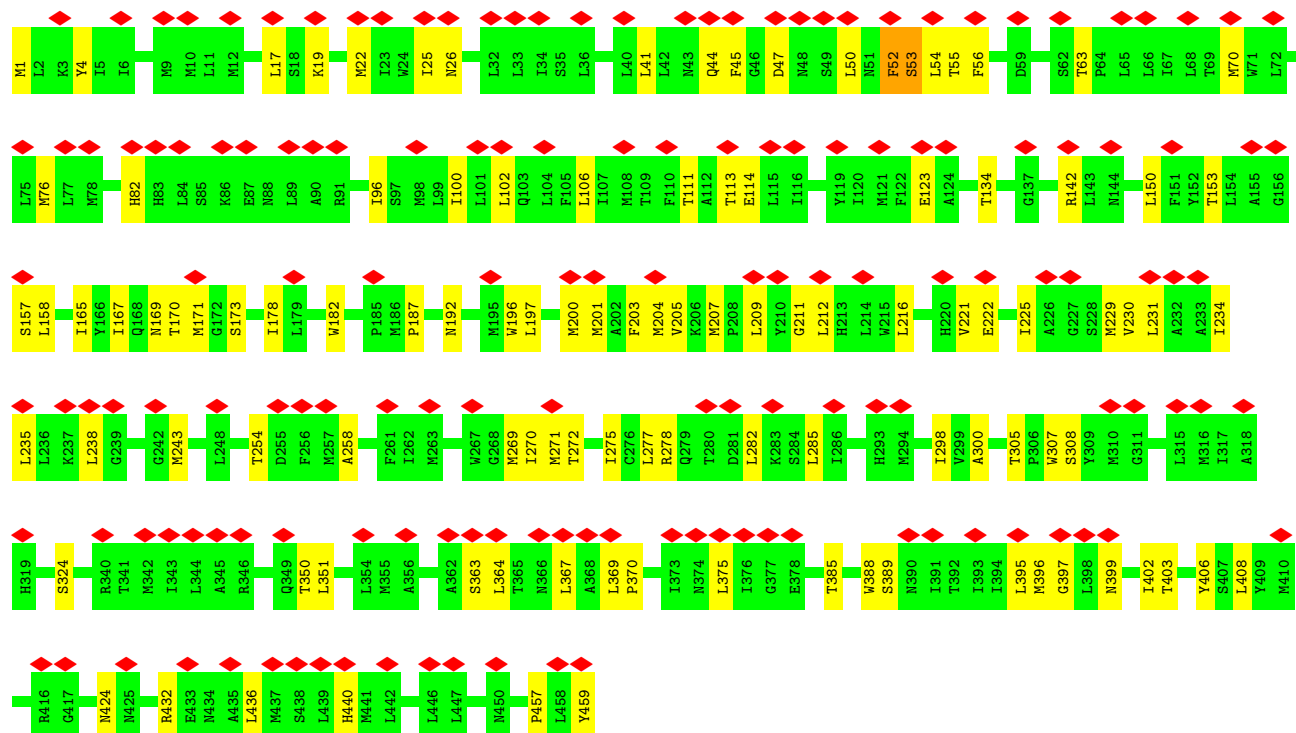




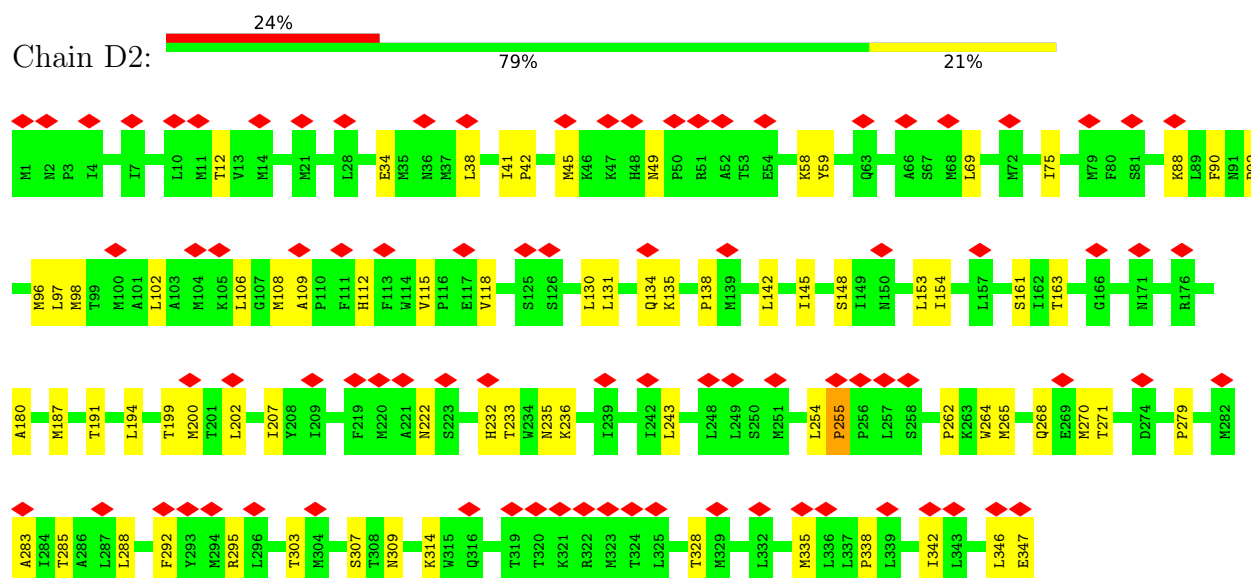
• Molecule 23: NADH-ubiquinone oxidoreductase chain 4



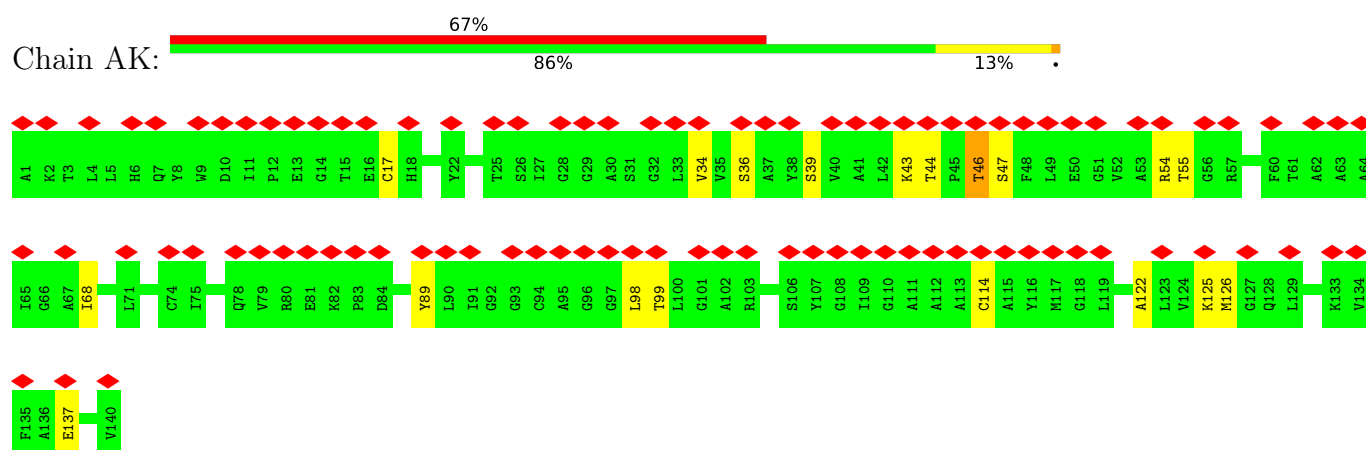
Chain D4:



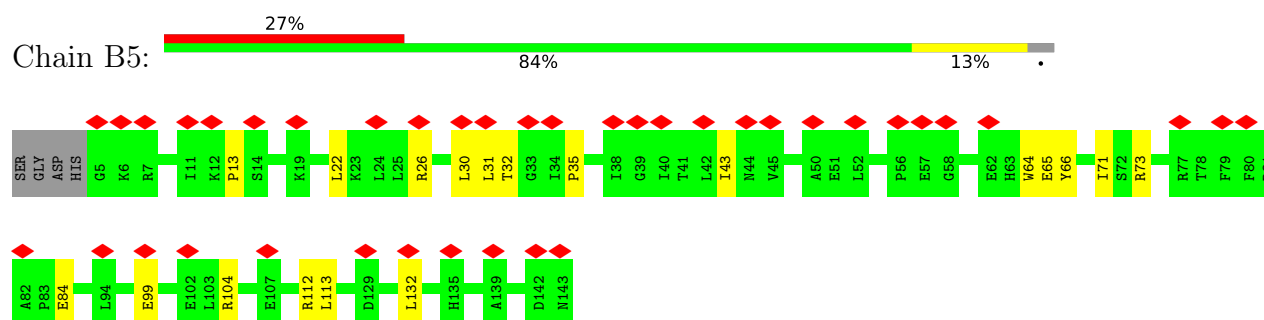
- Molecule 24: NADH-ubiquinone oxidoreductase chain 2



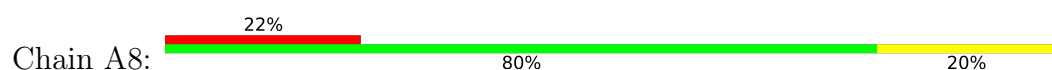
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

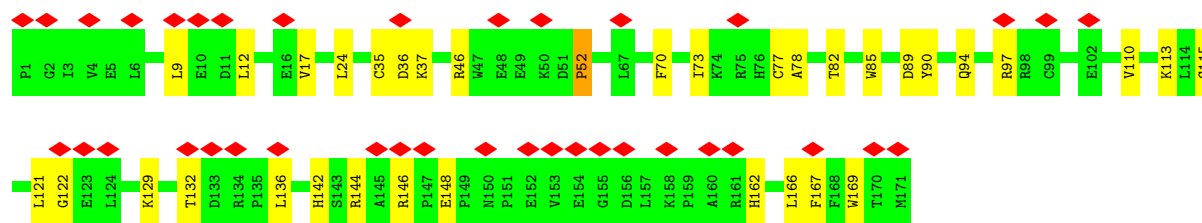


- Molecule 26: NADH:ubiquinone oxidoreductase subunit B5

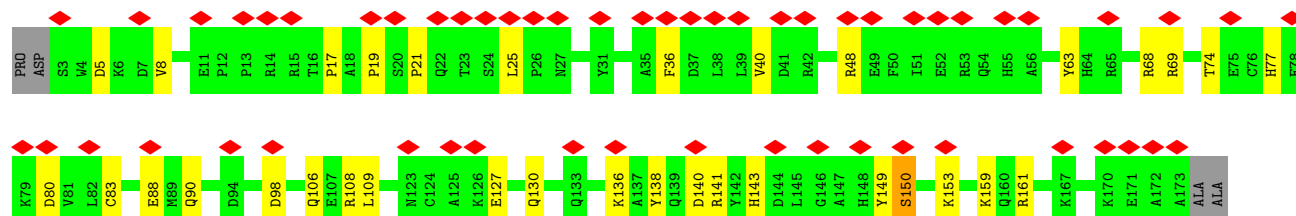
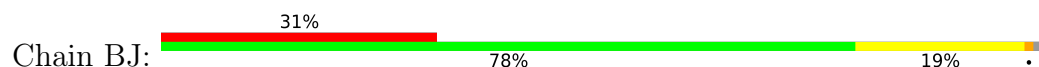


- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

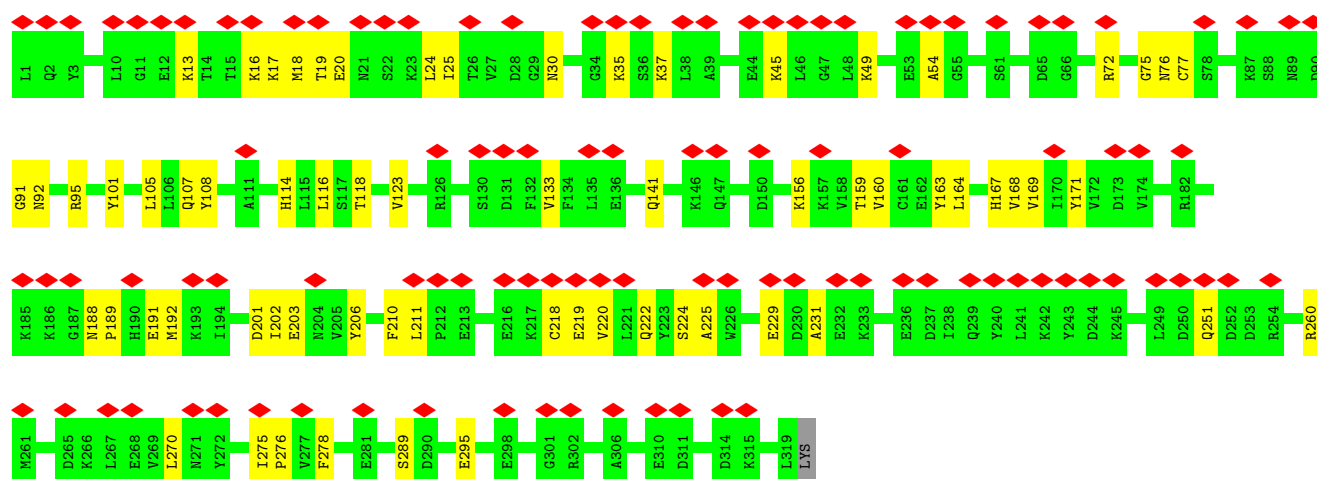
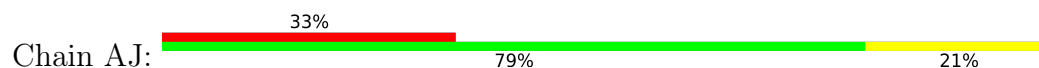




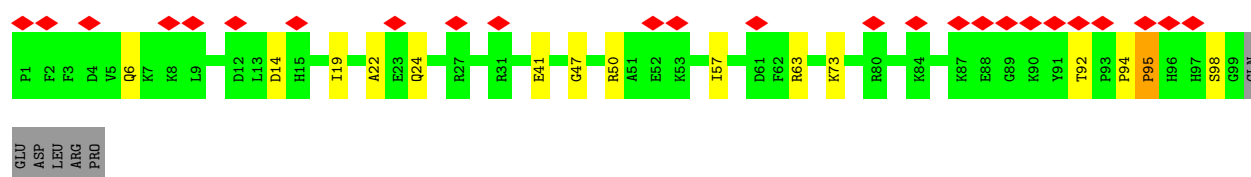
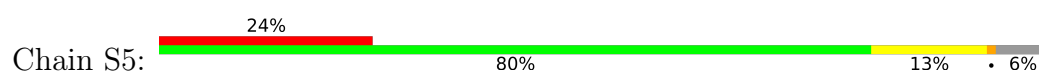
• Molecule 28: NDUFB10



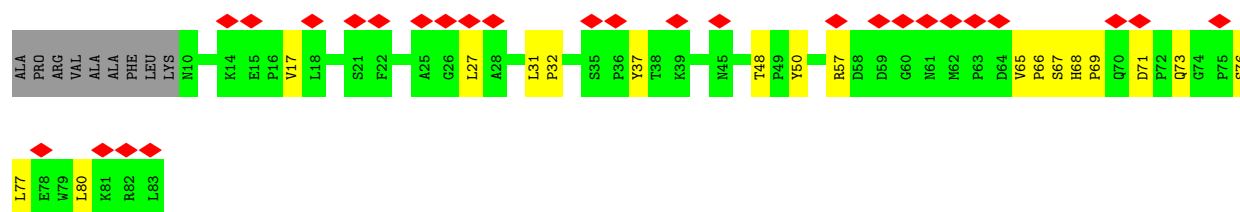
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



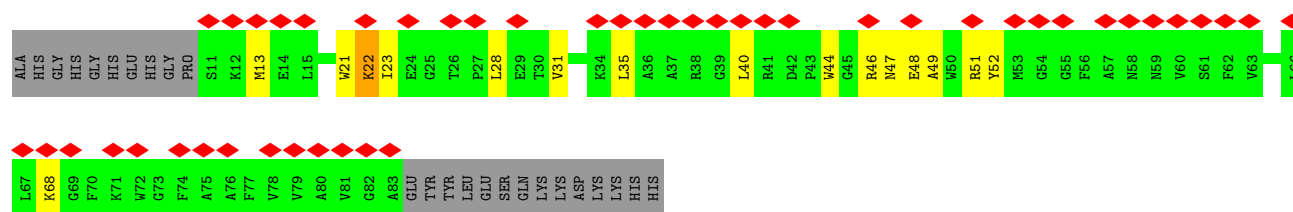
• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



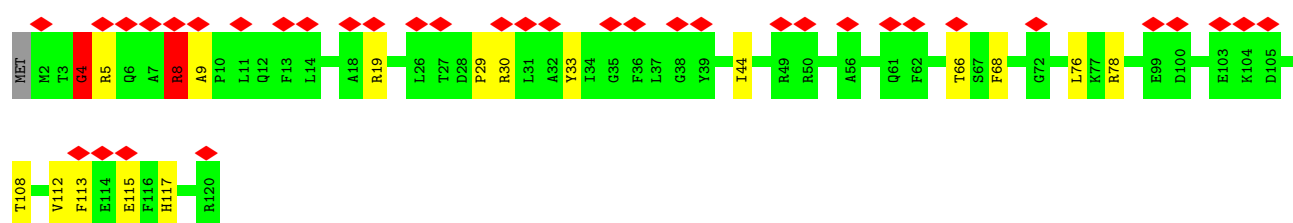
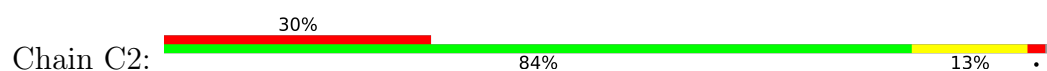
• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3



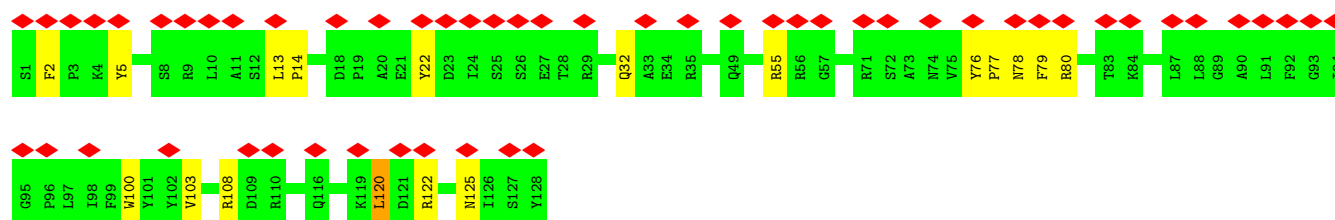
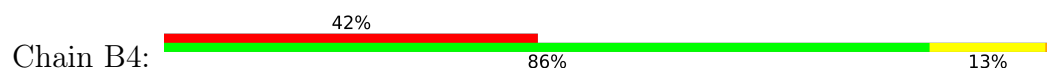
- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3



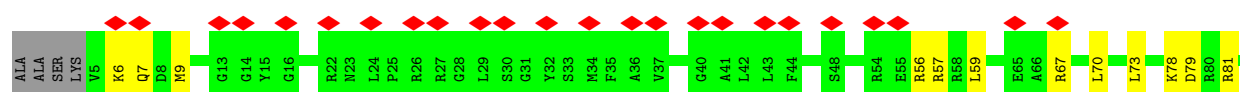
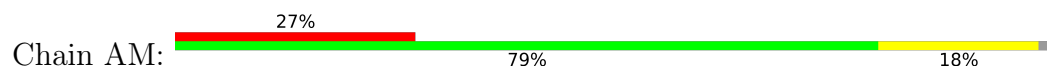
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2



- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

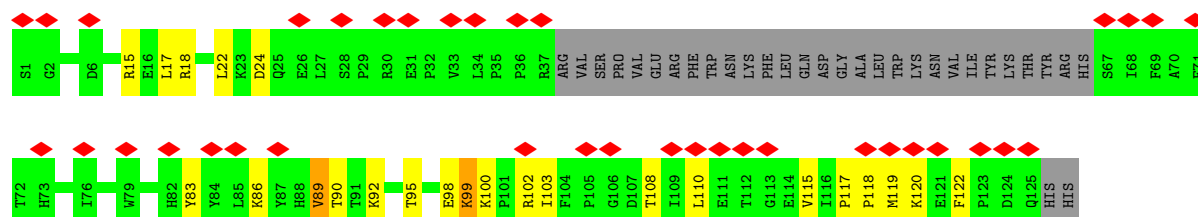


- Molecule 35: NDUFA13

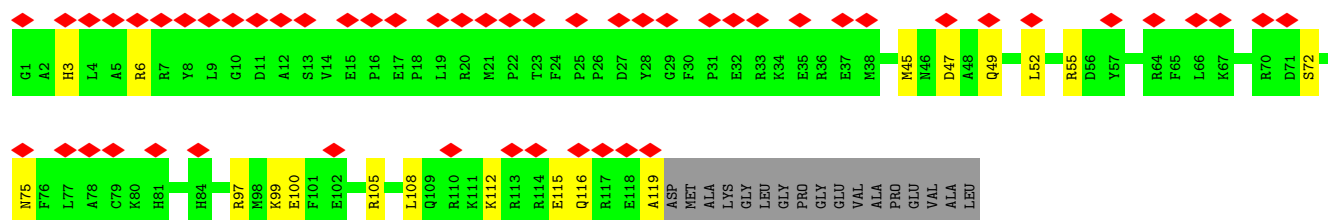
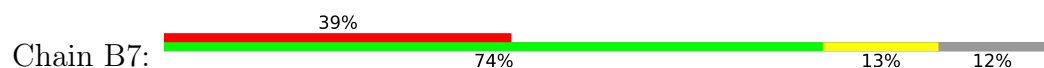




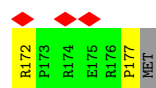
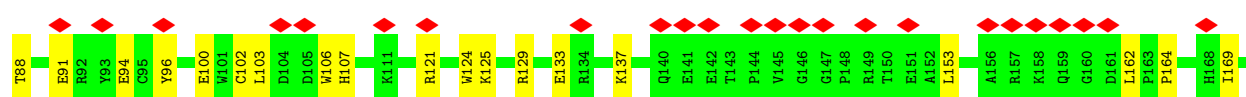
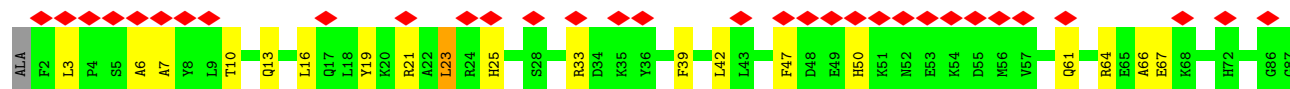
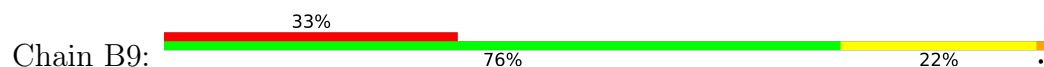
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



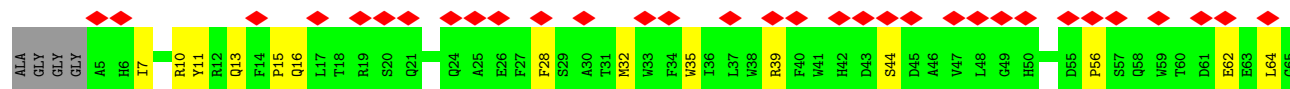
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

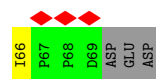


- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

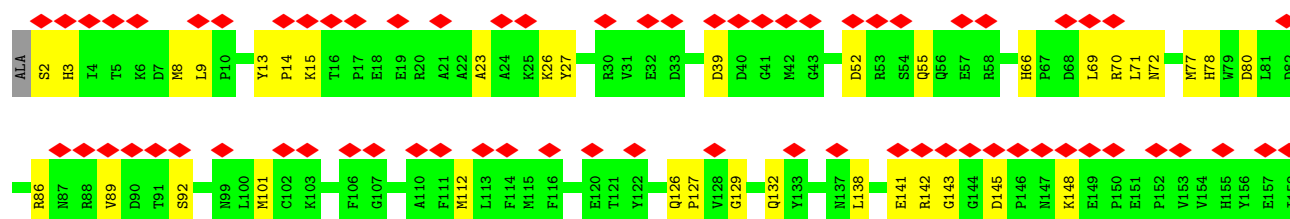
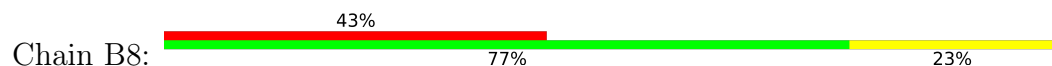


- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

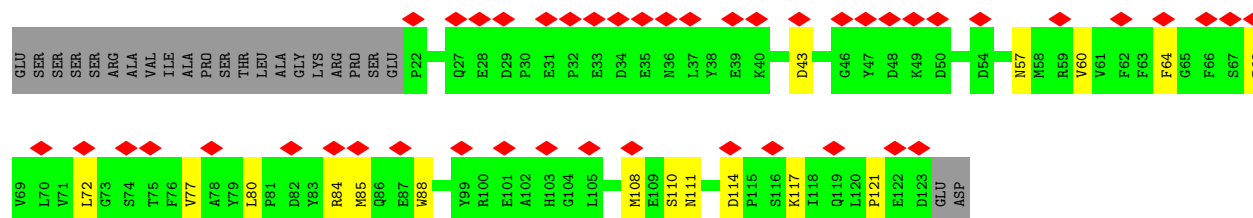




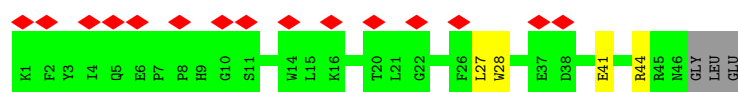
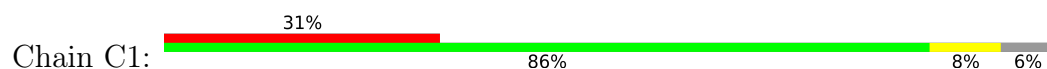
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



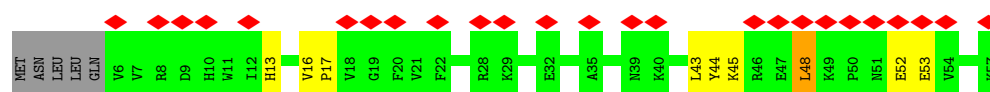
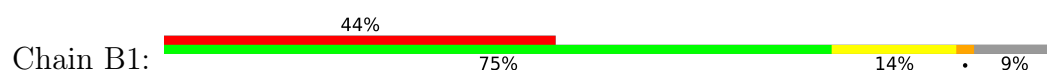
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



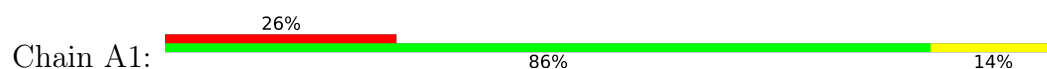
- Molecule 42: NDUFC1



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



- Molecule 44: NDUFA1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	57160	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 ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.169	Depositor
Minimum map value	-0.272	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.14	Depositor
Map size ($\text{\AA}$)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, FMN, FES, SF4, NDP, 3PE, PC1, CDL, ZN

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	0.30	0/3386	0.63	0/4575
2	V2	0.31	0/1687	0.78	1/2295 (0.0%)
3	S1	0.31	0/5362	0.64	0/7266
4	S2	0.35	0/3526	0.65	4/4778 (0.1%)
5	S3	0.31	0/1776	0.66	0/2417
6	S7	0.36	0/1279	0.67	0/1728
7	S8	0.37	0/1446	0.65	0/1956
8	V3	0.28	0/344	0.69	0/465
9	S6	0.27	0/749	0.56	0/1009
10	S4	0.28	0/1048	0.62	2/1415 (0.1%)
11	A9	0.27	0/2373	0.65	1/3207 (0.0%)
12	A2	0.24	0/676	0.62	0/911
13	A5	0.27	0/922	0.66	0/1249
14	A6	0.26	0/994	0.62	2/1336 (0.1%)
15	A7	0.27	0/770	0.63	0/1040
16	AL	0.26	0/1233	0.62	0/1676
17	AA	0.23	0/655	0.63	0/881
17	AB	0.24	0/714	0.58	0/963
18	D3	0.29	0/807	0.61	0/1103
19	D1	0.35	0/2460	0.74	2/3361 (0.1%)
20	D6	0.28	0/1339	0.69	0/1810
21	4L	0.30	0/758	0.67	0/1024
22	D5	0.31	0/4933	0.71	1/6710 (0.0%)
23	D4	0.35	0/3740	0.74	0/5095
24	D2	0.36	0/2788	0.69	2/3795 (0.1%)
25	AK	0.24	0/1046	0.71	4/1419 (0.3%)
26	B5	0.27	0/1189	0.56	0/1607
27	A8	0.29	0/1441	0.72	2/1942 (0.1%)
28	BJ	0.28	0/1475	0.66	3/1989 (0.2%)
29	AJ	0.28	0/2644	0.69	5/3579 (0.1%)
30	S5	0.29	0/843	0.64	0/1128
31	A3	0.26	0/602	0.65	0/828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	B3	0.28	0/595	0.76	0/803
33	C2	0.28	0/1028	0.70	4/1388 (0.3%)
34	B4	0.24	0/1085	0.61	0/1467
35	AM	0.30	0/1172	0.65	0/1579
36	B6	0.29	0/841	0.77	2/1144 (0.2%)
37	B7	0.27	0/1051	0.68	0/1408
38	B9	0.26	0/1568	0.62	0/2123
39	B2	0.30	0/590	0.73	2/810 (0.2%)
40	B8	0.29	0/1379	0.77	4/1884 (0.2%)
41	BK	0.27	0/880	0.64	0/1196
42	C1	0.24	0/404	0.60	0/548
43	B1	0.24	0/462	0.59	0/624
44	A1	0.29	0/592	0.67	0/795
All	All	0.30	0/66652	0.67	41/90326 (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	2
2	V2	0	3
3	S1	0	5
4	S2	0	1
5	S3	0	3
7	S8	0	1
11	A9	0	1
13	A5	0	1
15	A7	0	1
16	AL	0	3
19	D1	0	1
20	D6	0	2
22	D5	0	3
23	D4	0	3
25	AK	0	1
27	A8	0	1
28	BJ	0	1
29	AJ	0	1
30	S5	0	1
32	B3	0	1
33	C2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
34	B4	0	1
36	B6	0	3
39	B2	0	1
40	B8	0	1
43	B1	0	1
All	All	0	45

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	V2	36	LYS	N-CA-C	-8.28	104.04	114.56
28	BJ	21	PRO	CA-C-N	7.87	135.86	121.70
28	BJ	21	PRO	C-N-CA	7.87	135.86	121.70
29	AJ	229	GLU	CA-C-N	7.72	135.60	121.70
29	AJ	229	GLU	C-N-CA	7.72	135.60	121.70
39	B2	44	SER	CA-C-N	7.17	134.60	121.70
39	B2	44	SER	C-N-CA	7.17	134.60	121.70
14	A6	110	GLU	CA-C-N	7.15	134.57	121.70
14	A6	110	GLU	C-N-CA	7.15	134.57	121.70
33	C2	8	ARG	CA-C-N	6.69	133.74	121.70
33	C2	8	ARG	C-N-CA	6.69	133.74	121.70
24	D2	342	ILE	N-CA-C	-6.61	106.03	111.91
25	AK	17	CYS	CA-C-N	6.04	133.07	121.54
25	AK	17	CYS	C-N-CA	6.04	133.07	121.54
4	S2	230	THR	CA-C-N	5.95	132.91	121.54
4	S2	230	THR	C-N-CA	5.95	132.91	121.54
4	S2	73	VAL	CB-CA-C	-5.83	106.26	111.74
27	A8	52	PRO	CA-C-N	5.71	132.45	121.54
27	A8	52	PRO	C-N-CA	5.71	132.45	121.54
11	A9	320	ARG	CA-CB-CG	5.62	125.34	114.10
28	BJ	25	LEU	C-N-CD	-5.60	108.29	120.60
10	S4	10	LEU	CA-C-N	5.57	129.75	120.62
10	S4	10	LEU	C-N-CA	5.57	129.75	120.62
22	D5	69	LEU	CA-CB-CG	5.52	135.61	116.30
33	C2	4	GLY	CA-C-N	5.47	131.54	121.70
33	C2	4	GLY	C-N-CA	5.47	131.54	121.70
29	AJ	275	ILE	C-N-CD	-5.39	108.73	120.60
40	B8	72	ASN	CA-C-N	5.37	131.80	121.54
40	B8	72	ASN	C-N-CA	5.37	131.80	121.54
40	B8	86	ARG	CA-C-N	5.32	135.51	125.66
40	B8	86	ARG	C-N-CA	5.32	135.51	125.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AJ	251	GLN	CA-C-N	5.29	131.22	121.70
29	AJ	251	GLN	C-N-CA	5.29	131.22	121.70
24	D2	255	PRO	N-CA-C	5.21	117.06	110.70
4	S2	165	THR	N-CA-C	5.13	121.16	109.81
19	D1	199	ASP	CA-C-N	5.06	130.81	121.70
19	D1	199	ASP	C-N-CA	5.06	130.81	121.70
36	B6	99	LYS	CA-C-N	5.05	127.84	120.51
36	B6	99	LYS	C-N-CA	5.05	127.84	120.51
25	AK	137	GLU	CA-C-N	5.05	139.11	127.00
25	AK	137	GLU	C-N-CA	5.05	139.11	127.00

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A5	113	TRP	Peptide
15	A7	69	MET	Peptide
27	A8	52	PRO	Peptide
11	A9	310	LEU	Peptide
29	AJ	278	PHE	Peptide
25	AK	46	THR	Peptide
16	AL	102	PRO	Peptide
16	AL	31	ASN	Peptide
16	AL	43	LYS	Peptide
43	B1	52	GLU	Peptide
39	B2	56	PRO	Peptide
32	B3	22	LYS	Peptide
34	B4	76	TYR	Peptide
36	B6	122	PHE	Peptide
36	B6	86	LYS	Peptide
36	B6	98	GLU	Peptide
40	B8	141	GLU	Peptide
28	BJ	150	SER	Peptide
33	C2	4	GLY	Peptide
33	C2	8	ARG	Peptide
19	D1	91	MET	Peptide
23	D4	17	LEU	Peptide
23	D4	52	PHE	Peptide
23	D4	53	SER	Peptide
22	D5	359	MET	Peptide
22	D5	364	LYS	Peptide
22	D5	365	ALA	Peptide

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Mol	Chain	Res	Type	Group
20	D6	115	ILE	Peptide
20	D6	137	SER	Peptide
3	S1	247	VAL	Peptide
3	S1	253	ARG	Peptide
3	S1	341	ASP	Peptide
3	S1	380	VAL	Peptide
3	S1	484	THR	Peptide
4	S2	73	VAL	Peptide
5	S3	76	ALA	Peptide
5	S3	79	THR	Peptide
5	S3	80	ALA	Peptide
30	S5	92	THR	Peptide
7	S8	106	THR	Peptide
1	V1	28	ARG	Peptide
1	V1	331	THR	Peptide
2	V2	13	PRO	Peptide
2	V2	194	GLU	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	3268	70	0
2	V2	1647	0	1660	28	0
3	S1	5275	0	5304	106	0
4	S2	3436	0	3379	60	0
5	S3	1726	0	1676	42	0
6	S7	1248	0	1256	27	0
7	S8	1415	0	1374	33	0
8	V3	335	0	316	13	0
9	S6	737	0	710	12	0
10	S4	1025	0	1023	21	0
11	A9	2321	0	2350	48	0
12	A2	665	0	678	10	0
13	A5	902	0	936	12	0
14	A6	970	0	980	25	0
15	A7	752	0	766	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	AL	1192	0	1164	14	0
17	AA	645	0	649	7	0
17	AB	702	0	692	13	0
18	D3	787	0	832	7	0
19	D1	2390	0	2517	54	0
20	D6	1308	0	1329	27	0
21	4L	748	0	794	18	0
22	D5	4805	0	4950	114	0
23	D4	3646	0	3850	73	0
24	D2	2724	0	2930	57	0
25	AK	1025	0	1033	10	0
26	B5	1156	0	1177	15	0
27	A8	1404	0	1384	30	0
28	BJ	1441	0	1417	26	0
29	AJ	2583	0	2547	38	0
30	S5	822	0	820	13	0
31	A3	582	0	583	16	0
32	B3	578	0	570	15	0
33	C2	997	0	983	17	0
34	B4	1059	0	1062	13	0
35	AM	1143	0	1137	22	0
36	B6	815	0	837	17	0
37	B7	1026	0	995	15	0
38	B9	1515	0	1469	28	0
39	B2	563	0	509	10	0
40	B8	1324	0	1219	25	0
41	BK	853	0	800	15	0
42	C1	391	0	391	5	0
43	B1	449	0	453	9	0
44	A1	577	0	570	10	0
45	S1	16	0	0	1	0
45	S7	8	0	0	0	0
45	S8	16	0	0	0	0
45	V1	8	0	0	2	0
46	V1	31	0	19	1	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	S6	1	0	0	0	0
49	A9	48	0	26	5	0
50	AA	34	0	40	7	0
50	B9	31	0	34	3	0
51	A8	25	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	D1	19	0	12	0	0
51	D4	40	0	54	2	0
51	D5	38	0	50	4	0
52	D5	36	0	16	2	0
53	D4	28	0	30	0	0
All	All	65403	0	65644	1011	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 (1011) 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:S3:38:GLN:O	15:A7:70:SER:HA	1.62	0.98
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.62	0.97
5:S3:38:GLN:HA	15:A7:70:SER:O	1.78	0.82
3:S1:266:LYS:O	3:S1:270:ALA:HB2	1.79	0.81
37:B7:108:LEU:O	37:B7:112:LYS:HB2	1.80	0.81
14:A6:70:ALA:HA	50:AA:101:ZMP:O2	1.82	0.80
37:B7:115:GLU:O	37:B7:119:ALA:HB3	1.84	0.78
14:A6:37:ALA:O	14:A6:41:GLU:HB2	1.86	0.75
38:B9:50:HIS:NE2	50:B9:201:ZMP:H8A	2.02	0.74
12:A2:21:HIS:O	12:A2:62:PRO:HA	1.88	0.73
5:S3:80:ALA:HA	5:S3:91:GLU:O	1.90	0.71
11:A9:108:ASP:O	11:A9:112:LYS:HB3	1.91	0.70
27:A8:146:ARG:HH12	30:S5:41:GLU:HB3	1.56	0.70
15:A7:39:LYS:H	35:AM:7:GLN:HB2	1.58	0.69
14:A6:62:VAL:CG2	50:AA:101:ZMP:H22	2.23	0.69
3:S1:675:ASP:O	3:S1:679:ARG:HB2	1.93	0.68
4:S2:282:GLU:HB2	4:S2:313:GLN:HE22	1.59	0.66
14:A6:66:PHE:HA	50:AA:101:ZMP:O1	1.94	0.66
23:D4:204:MET:HB3	23:D4:209:LEU:HD22	1.77	0.66
23:D4:370:PRO:HA	23:D4:375:LEU:HD13	1.77	0.66
4:S2:105:ARG:NH1	6:S7:149:CYS:SG	2.62	0.66
11:A9:135:LEU:HA	11:A9:167:LYS:HD3	1.76	0.66
14:A6:62:VAL:HG23	50:AA:101:ZMP:H22	1.78	0.66
32:B3:22:LYS:H	32:B3:46:ARG:HH11	1.43	0.66
3:S1:126:ASP:HB2	4:S2:328:ALA:HB3	1.77	0.65
22:D5:597:ILE:HD11	25:AK:34:VAL:HG22	1.78	0.65
4:S2:405:MET:SD	4:S2:421:GLN:NE2	2.70	0.65
14:A6:63:ARG:HB2	17:AA:45:LEU:HD21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:117:GLN:NE2	45:S1:801:SF4:S3	2.70	0.65
23:D4:82:HIS:HB2	23:D4:432:ARG:HH12	1.62	0.65
33:C2:113:PHE:HB2	41:BK:121:PRO:HG2	1.79	0.65
3:S1:318:ILE:HA	3:S1:344:CYS:O	1.96	0.65
7:S8:65:HIS:HE2	7:S8:116:CYS:HG	1.39	0.64
5:S3:48:LEU:HB3	5:S3:105:ILE:HG22	1.80	0.64
5:S3:88:ASN:HD22	5:S3:112:ASP:HB3	1.61	0.64
1:V1:213:VAL:HG13	1:V1:217:GLY:HA2	1.80	0.64
4:S2:19:MET:HG2	24:D2:295:ARG:HH12	1.63	0.63
35:AM:124:TYR:HB3	35:AM:132:ILE:HG22	1.78	0.63
22:D5:267:THR:O	22:D5:274:GLN:NE2	2.32	0.63
22:D5:380:LEU:HD23	22:D5:381:THR:HG23	1.80	0.63
29:AJ:13:LYS:HD2	29:AJ:16:LYS:HG3	1.79	0.63
1:V1:301:GLY:HA2	1:V1:333:ALA:HB3	1.81	0.63
3:S1:286:ASN:O	3:S1:289:GLY:N	2.32	0.63
19:D1:152:SER:HG	19:D1:301:CYS:HG	1.47	0.63
22:D5:288:THR:O	22:D5:292:ALA:HB2	1.98	0.62
22:D5:554:ASP:O	22:D5:558:LEU:HB3	2.00	0.62
3:S1:355:GLY:HA2	3:S1:361:ASN:HD21	1.65	0.62
22:D5:451:ILE:O	22:D5:455:LYS:HB2	1.98	0.62
33:C2:30:ARG:HE	33:C2:76:LEU:HD11	1.64	0.62
11:A9:109:VAL:O	11:A9:113:ILE:HB	1.98	0.62
22:D5:161:ARG:NH1	38:B9:88:THR:O	2.33	0.62
23:D4:231:LEU:O	23:D4:235:LEU:HB2	2.00	0.62
6:S7:165:LYS:NZ	16:AL:78:ASP:OD1	2.33	0.62
26:B5:132:LEU:HD11	30:S5:19:ILE:HD12	1.82	0.61
3:S1:40:PHE:O	3:S1:158:ARG:NH2	2.33	0.61
24:D2:347:GLU:O	33:C2:78:ARG:NH2	2.33	0.61
31:A3:66:PRO:HB3	31:A3:73:GLN:HB2	1.82	0.61
39:B2:7:ILE:HD12	39:B2:16:GLN:HE21	1.66	0.61
20:D6:133:SER:OG	35:AM:67:ARG:NH2	2.33	0.61
22:D5:482:MET:SD	22:D5:487:LYS:NZ	2.72	0.61
29:AJ:77:CYS:O	29:AJ:92:ASN:ND2	2.32	0.61
4:S2:48:THR:HG22	4:S2:67:GLU:HG2	1.82	0.61
24:D2:222:ASN:HD21	24:D2:233:THR:HG22	1.64	0.61
5:S3:78:LEU:HA	5:S3:93:VAL:O	2.00	0.61
6:S7:65:PRO:HB3	19:D1:33:PHE:HB2	1.83	0.61
6:S7:70:ASP:OD2	19:D1:34:ARG:NH1	2.34	0.61
1:V1:366:ARG:NH1	3:S1:155:GLN:OE1	2.34	0.61
16:AL:117:LEU:HD13	16:AL:123:GLN:HA	1.83	0.61
19:D1:310:LEU:HD21	31:A3:32:PRO:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:318:ILE:HG12	3:S1:344:CYS:HB2	1.82	0.61
3:S1:377:VAL:O	3:S1:406:VAL:HA	2.01	0.61
51:D4:501:3PE:H291	24:D2:288:LEU:HD23	1.82	0.61
13:A5:37:ILE:O	13:A5:44:ARG:NH1	2.33	0.61
29:AJ:19:THR:HG23	29:AJ:20:GLU:HG3	1.83	0.61
37:B7:112:LYS:O	37:B7:116:GLN:HB2	2.00	0.61
22:D5:267:THR:OG1	22:D5:274:GLN:NE2	2.34	0.60
22:D5:483:PRO:HD2	22:D5:486:LEU:HD22	1.82	0.60
4:S2:338:MET:SD	4:S2:348:HIS:ND1	2.74	0.60
35:AM:97:MET:HE3	35:AM:100:VAL:HG11	1.83	0.60
3:S1:283:MET:HB2	3:S1:560:ILE:HB	1.84	0.60
23:D4:1:MET:HG2	23:D4:111:THR:HG21	1.84	0.60
29:AJ:101:TYR:HH	29:AJ:159:THR:HG1	1.48	0.60
11:A9:51:CYS:SG	11:A9:52:GLU:N	2.74	0.60
13:A5:34:LEU:O	13:A5:44:ARG:NH1	2.35	0.60
22:D5:22:ILE:HD11	22:D5:119:LYS:HD3	1.83	0.60
18:D3:10:ASN:HD21	19:D1:10:ILE:HG21	1.65	0.60
17:AB:82:ASP:OD1	36:B6:15:ARG:NH2	2.34	0.60
1:V1:126:GLY:HA2	1:V1:131:ALA:HB3	1.84	0.60
11:A9:92:ILE:HG22	11:A9:130:ILE:HB	1.84	0.60
23:D4:269:MET:SD	23:D4:399:ASN:ND2	2.75	0.60
14:A6:62:VAL:HG22	50:AA:101:ZMP:H2	1.84	0.60
22:D5:556:ILE:HD11	34:B4:79:PHE:HB2	1.84	0.59
28:BJ:161:ARG:NH2	41:BK:111:ASN:OD1	2.34	0.59
3:S1:240:VAL:HG12	3:S1:250:ILE:HG22	1.83	0.59
4:S2:72:MET:HG3	4:S2:73:VAL:HG22	1.84	0.59
4:S2:130:PRO:HG2	4:S2:135:GLN:HE21	1.67	0.59
20:D6:169:MET:HE1	20:D6:175:ASN:HD22	1.68	0.59
1:V1:134:ALA:HB3	1:V1:175:VAL:HG12	1.82	0.59
31:A3:27:LEU:O	31:A3:31:LEU:HB2	2.02	0.59
3:S1:227:SER:H	3:S1:253:ARG:HH22	1.49	0.59
7:S8:135:PRO:HG3	7:S8:164:GLU:HG2	1.83	0.59
2:V2:39:PRO:HA	8:V3:65:GLN:HB3	1.84	0.59
27:A8:136:LEU:HB3	31:A3:57:ARG:HH21	1.66	0.59
4:S2:360:PRO:HA	4:S2:380:SER:O	2.02	0.59
29:AJ:202:ILE:O	29:AJ:206:TYR:HB2	2.02	0.59
37:B7:6:ARG:HH12	37:B7:105:ARG:HH21	1.51	0.59
1:V1:27:GLY:H	1:V1:113:HIS:HE1	1.51	0.59
19:D1:22:LEU:HB3	19:D1:48:PRO:HG2	1.84	0.59
20:D6:141:MET:HA	20:D6:144:ALA:HB3	1.84	0.59
23:D4:204:MET:HE2	23:D4:243:MET:HE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:54:PHE:HE1	22:D5:60:GLU:HG2	1.68	0.59
24:D2:235:ASN:HD21	29:AJ:289:SER:HB2	1.68	0.59
7:S8:65:HIS:NE2	7:S8:116:CYS:SG	2.70	0.58
28:BJ:159:LYS:NZ	33:C2:112:VAL:O	2.36	0.58
3:S1:592:LEU:O	3:S1:594:ARG:NH1	2.35	0.58
38:B9:102:CYS:SG	38:B9:103:LEU:N	2.75	0.58
19:D1:131:GLY:HA2	19:D1:134:ARG:HE	1.66	0.58
23:D4:22:MET:O	23:D4:26:ASN:ND2	2.35	0.58
23:D4:221:VAL:HG23	23:D4:222:GLU:HG3	1.84	0.58
1:V1:32:ARG:HG3	1:V1:34:LYS:H	1.66	0.58
3:S1:41:CYS:SG	3:S1:52:CYS:HB3	2.43	0.58
1:V1:297:VAL:HG22	1:V1:336:VAL:HG12	1.86	0.58
21:4L:55:LEU:HD13	30:S5:24:GLN:HA	1.86	0.58
22:D5:83:ASP:O	22:D5:87:MET:HB2	2.04	0.58
38:B9:10:THR:HB	38:B9:13:GLN:H	1.69	0.58
24:D2:130:LEU:O	24:D2:134:GLN:HB2	2.04	0.58
28:BJ:98:ASP:OD2	28:BJ:141:ARG:NH2	2.37	0.58
32:B3:23:ILE:HB	32:B3:46:ARG:HG2	1.85	0.58
1:V1:202:LYS:HB3	1:V1:361:GLN:HE21	1.68	0.57
23:D4:170:THR:HG23	23:D4:171:MET:HG3	1.86	0.57
38:B9:91:GLU:HB3	38:B9:94:GLU:HB2	1.85	0.57
9:S6:68:HIS:HE1	9:S6:87:CYS:SG	2.14	0.57
6:S7:147:PRO:HG2	7:S8:139:PHE:HD2	1.70	0.57
15:A7:45:SER:O	15:A7:46:HIS:ND1	2.37	0.57
34:B4:13:LEU:HD22	34:B4:14:PRO:HD2	1.86	0.57
4:S2:413:ASP:OD2	19:D1:281:ARG:NH1	2.37	0.57
13:A5:10:LEU:HD22	13:A5:13:LEU:HD13	1.86	0.57
1:V1:109:GLU:OE2	1:V1:112:ARG:NH2	2.36	0.57
24:D2:232:HIS:HE1	29:AJ:276:PRO:HG3	1.68	0.57
24:D2:88:LYS:HG3	24:D2:148:SER:HB3	1.86	0.57
40:B8:145:ASP:HB3	40:B8:148:LYS:HB2	1.87	0.57
27:A8:144:ARG:HH12	30:S5:57:ILE:HD13	1.69	0.57
41:BK:114:ASP:HB3	41:BK:117:LYS:HB2	1.86	0.57
1:V1:154:ARG:HD2	8:V3:54:LEU:HD21	1.87	0.57
4:S2:261:ARG:NH2	4:S2:268:ASP:OD1	2.37	0.57
27:A8:9:LEU:HA	27:A8:12:LEU:HB2	1.86	0.57
7:S8:104:ARG:O	7:S8:105:ARG:NH1	2.37	0.57
24:D2:154:ILE:HG23	24:D2:191:THR:HG22	1.87	0.57
29:AJ:72:ARG:NH1	29:AJ:295:GLU:OE1	2.37	0.57
2:V2:98:TYR:H	2:V2:136:LEU:HA	1.70	0.56
20:D6:58:LEU:O	20:D6:62:GLY:CA	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:B6:89:VAL:HG22	36:B6:95:THR:HG21	1.87	0.56
5:S3:150:ARG:NH2	14:A6:91:GLU:OE1	2.38	0.56
28:BJ:8:VAL:O	28:BJ:108:ARG:NH2	2.32	0.56
29:AJ:19:THR:OG1	29:AJ:20:GLU:N	2.38	0.56
1:V1:106:LYS:HD3	1:V1:332:ALA:HB2	1.88	0.56
1:V1:165:ASN:ND2	1:V1:169:SER:O	2.37	0.56
6:S7:62:MET:HG2	6:S7:156:LEU:HD23	1.87	0.56
1:V1:362:CYS:HB3	1:V1:364:PRO:HD2	1.87	0.56
5:S3:94:TYR:HB2	5:S3:107:VAL:HB	1.87	0.56
12:A2:19:ARG:HH21	12:A2:65:TRP:HE3	1.52	0.56
25:AK:68:ILE:HG21	25:AK:99:THR:HG21	1.88	0.56
27:A8:46:ARG:NH1	35:AM:79:ASP:OD2	2.39	0.56
29:AJ:168:VAL:HG12	29:AJ:219:GLU:HB2	1.87	0.56
2:V2:105:THR:OG1	2:V2:106:THR:N	2.38	0.56
4:S2:204:PRO:HD3	7:S8:60:ARG:HH22	1.69	0.56
4:S2:388:ARG:NH1	4:S2:389:CYS:O	2.37	0.56
22:D5:341:MET:HE3	22:D5:454:ILE:HD13	1.87	0.56
24:D2:69:LEU:HD11	24:D2:97:LEU:HD22	1.86	0.56
27:A8:35:CYS:SG	27:A8:36:ASP:N	2.78	0.56
22:D5:547:LYS:O	22:D5:552:LEU:CB	2.53	0.56
27:A8:142:HIS:H	35:AM:114:ARG:HD3	1.70	0.56
3:S1:252:PRO:HB3	3:S1:263:ILE:HB	1.88	0.56
23:D4:363:SER:O	23:D4:367:LEU:HB2	2.06	0.56
31:A3:48:THR:HG21	35:AM:57:ARG:HH21	1.71	0.56
44:A1:1:MET:HG3	44:A1:3:PHE:H	1.71	0.56
9:S6:12:THR:OG1	9:S6:14:THR:O	2.23	0.56
10:S4:12:THR:HG21	14:A6:15:SER:HA	1.88	0.56
22:D5:586:LEU:HD21	25:AK:44:THR:HG23	1.87	0.56
26:B5:43:ILE:HG13	26:B5:71:ILE:HD11	1.87	0.56
1:V1:292:ASP:HA	1:V1:309:LYS:HE3	1.86	0.56
4:S2:35:ASP:O	24:D2:49:ASN:ND2	2.35	0.56
2:V2:40:GLU:HB3	8:V3:67:SER:HB2	1.86	0.55
19:D1:152:SER:OG	19:D1:301:CYS:SG	2.58	0.55
28:BJ:68:ARG:NH1	43:B1:43:LEU:O	2.39	0.55
34:B4:120:LEU:HD12	34:B4:122:ARG:HB3	1.88	0.55
3:S1:453:LEU:HB3	3:S1:492:ILE:HG22	1.89	0.55
23:D4:165:ILE:HD11	24:D2:264:TRP:HE1	1.71	0.55
37:B7:97:ARG:NH2	40:B8:129:GLY:O	2.34	0.55
22:D5:119:LYS:NZ	52:D5:901:CDL:OB7	2.36	0.55
1:V1:309:LYS:NZ	1:V1:313:GLU:OE2	2.40	0.55
4:S2:231:ASN:OD1	4:S2:236:ARG:NH2	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V3:58:LEU:O	8:V3:62:ARG:NH2	2.39	0.55
23:D4:52:PHE:O	23:D4:56:PHE:HB2	2.06	0.55
23:D4:225:ILE:HG13	23:D4:229:MET:HE2	1.87	0.55
9:S6:20:ASP:OD1	9:S6:25:ARG:NH1	2.39	0.55
27:A8:148:GLU:OE1	30:S5:50:ARG:NH1	2.39	0.55
2:V2:98:TYR:HD2	2:V2:136:LEU:HB2	1.71	0.55
3:S1:225:THR:HB	3:S1:240:VAL:HG23	1.88	0.55
3:S1:396:ARG:NH1	3:S1:416:THR:O	2.40	0.55
22:D5:389:PHE:O	22:D5:393:ASP:HB2	2.06	0.55
15:A7:11:ARG:HB3	15:A7:19:LEU:HD13	1.88	0.55
22:D5:3:LEU:HD22	22:D5:53:MET:HE1	1.87	0.55
25:AK:122:ALA:O	25:AK:126:MET:HB2	2.07	0.55
40:B8:55:GLN:O	40:B8:70:ARG:NH2	2.40	0.55
5:S3:85:THR:HG21	10:S4:87:SER:H	1.72	0.55
6:S7:165:LYS:NZ	16:AL:77:VAL:O	2.40	0.55
7:S8:22:ALA:O	7:S8:26:LEU:HB2	2.07	0.55
3:S1:382:THR:HB	3:S1:454:GLY:HA3	1.89	0.55
3:S1:588:MET:HG3	10:S4:63:GLU:HA	1.88	0.55
4:S2:208:MET:H	35:AM:9:MET:HE2	1.71	0.55
23:D4:25:ILE:HG23	41:BK:60:VAL:HG11	1.88	0.55
28:BJ:68:ARG:NH2	43:B1:45:LYS:O	2.39	0.55
5:S3:38:GLN:CA	15:A7:70:SER:O	2.53	0.54
23:D4:389:SER:OG	34:B4:108:ARG:NH2	2.40	0.54
3:S1:163:ALA:O	3:S1:168:GLY:N	2.38	0.54
22:D5:123:LEU:HA	22:D5:126:ILE:HD12	1.89	0.54
4:S2:116:GLN:HG3	4:S2:138:ARG:HD3	1.89	0.54
4:S2:335:ARG:HG2	4:S2:339:LYS:HE2	1.89	0.54
3:S1:8:LEU:HD22	3:S1:19:MET:HB3	1.89	0.54
3:S1:40:PHE:HB2	3:S1:52:CYS:HB2	1.90	0.54
19:D1:165:LEU:HD21	19:D1:241:LEU:HA	1.89	0.54
22:D5:33:PRO:HB3	22:D5:118:PHE:HE2	1.73	0.54
22:D5:342:CYS:HG	22:D5:369:THR:HG1	1.54	0.54
1:V1:362:CYS:N	45:V1:500:SF4:S2	2.75	0.54
11:A9:137:ALA:HA	11:A9:146:LEU:HB3	1.88	0.54
19:D1:102:VAL:HB	19:D1:150:LEU:HD21	1.90	0.54
20:D6:51:PHE:O	20:D6:55:MET:HB2	2.07	0.54
23:D4:459:TYR:O	41:BK:84:ARG:NH1	2.41	0.54
37:B7:52:LEU:HD22	40:B8:138:LEU:HD21	1.89	0.54
22:D5:233:LEU:HG	22:D5:303:ALA:HB1	1.89	0.54
51:A8:301:3PE:H231	33:C2:29:PRO:HB2	1.89	0.54
3:S1:276:ARG:HG2	3:S1:277:GLN:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:38:GLN:O	15:A7:70:SER:CA	2.47	0.54
7:S8:74:GLU:OE2	7:S8:105:ARG:NH2	2.40	0.54
20:D6:137:SER:HB2	20:D6:140:ALA:H	1.73	0.54
20:D6:159:TRP:HE1	24:D2:12:THR:HG22	1.73	0.54
3:S1:229:ASP:HB3	3:S1:235:GLY:HA2	1.90	0.54
22:D5:227:PHE:H	22:D5:284:THR:HG22	1.73	0.54
27:A8:110:VAL:O	27:A8:115:GLY:N	2.37	0.54
1:V1:305:PRO:HG3	1:V1:413:TRP:HB3	1.88	0.54
5:S3:41:GLN:NE2	5:S3:49:GLU:OE1	2.41	0.54
7:S8:79:ALA:HB2	7:S8:106:THR:HG22	1.89	0.54
11:A9:136:ASN:ND2	11:A9:291:ASP:OD1	2.41	0.54
20:D6:163:ILE:HG13	24:D2:12:THR:HG21	1.90	0.54
23:D4:134:THR:O	23:D4:142:ARG:NH1	2.41	0.54
24:D2:292:PHE:HA	24:D2:295:ARG:HG2	1.88	0.54
28:BJ:80:ASP:HB3	28:BJ:83:CYS:HB3	1.89	0.54
3:S1:366:THR:HG21	3:S1:450:MET:HE2	1.90	0.53
17:AB:87:TYR:HB2	36:B6:22:LEU:HD23	1.90	0.53
30:S5:94:PRO:O	30:S5:98:SER:OG	2.26	0.53
1:V1:101:GLU:O	1:V1:104:THR:OG1	2.25	0.53
22:D5:154:LEU:HB3	22:D5:243:VAL:HG13	1.91	0.53
38:B9:153:LEU:HD13	38:B9:164:PRO:HG2	1.90	0.53
24:D2:109:ALA:HB2	24:D2:161:SER:HA	1.90	0.53
1:V1:358:SER:OG	45:V1:500:SF4:S3	2.62	0.53
2:V2:24:THR:HG22	2:V2:26:GLU:H	1.73	0.53
11:A9:19:ILE:O	11:A9:43:SER:OG	2.27	0.53
22:D5:547:LYS:O	22:D5:552:LEU:HB3	2.09	0.53
1:V1:378:ARG:O	1:V1:382:GLY:N	2.42	0.53
4:S2:6:PRO:HG3	24:D2:303:THR:HB	1.91	0.53
6:S7:139:ILE:HG22	6:S7:140:VAL:HG13	1.90	0.53
11:A9:167:LYS:O	11:A9:229:ALA:HA	2.07	0.53
7:S8:3:LYS:HG3	15:A7:110:PRO:HA	1.88	0.53
29:AJ:169:VAL:O	29:AJ:220:VAL:HA	2.08	0.53
37:B7:72:SER:HB2	37:B7:75:ASN:HB2	1.91	0.53
3:S1:378:LEU:HG	3:S1:451:VAL:HG22	1.91	0.53
19:D1:77:LEU:HD11	19:D1:111:LEU:HD12	1.90	0.53
22:D5:294:THR:H	22:D5:425:ARG:HH12	1.56	0.53
25:AK:39:SER:HB2	25:AK:54:ARG:HH22	1.74	0.53
22:D5:149:ILE:HG12	23:D4:364:LEU:HD21	1.90	0.53
23:D4:55:THR:O	23:D4:113:THR:OG1	2.27	0.53
32:B3:28:LEU:HA	32:B3:31:VAL:HG12	1.90	0.53
40:B8:23:ALA:O	40:B8:27:TYR:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V2:27:ASN:OD1	2:V2:30:ARG:NH1	2.42	0.53
5:S3:64:LEU:HD23	5:S3:96:LEU:HD22	1.90	0.53
12:A2:17:GLU:HG2	12:A2:51:PRO:HG2	1.90	0.53
23:D4:364:LEU:HD23	23:D4:367:LEU:HD23	1.89	0.53
40:B8:71:LEU:HD11	40:B8:77:MET:HG2	1.89	0.53
21:4L:73:LEU:HD21	24:D2:41:ILE:HG13	1.91	0.53
28:BJ:69:ARG:NH1	28:BJ:90:GLN:OE1	2.41	0.53
1:V1:33:LEU:HD23	1:V1:155:GLU:HB3	1.90	0.52
4:S2:146:ARG:HH22	4:S2:270:ARG:HD3	1.73	0.52
5:S3:192:GLN:HE21	5:S3:195:ARG:HH12	1.56	0.52
49:A9:401:NDP:N3A	49:A9:401:NDP:O3X	2.42	0.52
29:AJ:30:ASN:ND2	29:AJ:203:GLU:OE2	2.42	0.52
3:S1:312:GLY:N	3:S1:339:ASP:OD2	2.39	0.52
21:4L:58:MET:HB3	21:4L:62:ILE:HD12	1.91	0.52
22:D5:81:LYS:NZ	22:D5:83:ASP:OD2	2.41	0.52
22:D5:130:ILE:HG23	22:D5:139:GLN:HE21	1.74	0.52
23:D4:158:LEU:HD21	24:D2:283:ALA:HB1	1.91	0.52
23:D4:388:TRP:O	34:B4:108:ARG:NH2	2.42	0.52
23:D4:457:PRO:O	41:BK:84:ARG:NH2	2.42	0.52
27:A8:166:LEU:HD23	27:A8:167:PHE:H	1.73	0.52
38:B9:3:LEU:HD11	38:B9:6:ALA:HB3	1.90	0.52
40:B8:69:LEU:HB3	40:B8:71:LEU:HD23	1.90	0.52
1:V1:59:GLU:HG3	1:V1:234:ILE:HG22	1.91	0.52
3:S1:442:VAL:O	3:S1:446:ALA:HB2	2.09	0.52
10:S4:36:ARG:NH2	10:S4:58:GLU:OE1	2.43	0.52
17:AB:21:LEU:HD21	32:B3:47:ASN:HA	1.91	0.52
4:S2:295:ASP:OD1	7:S8:6:ASN:ND2	2.42	0.52
9:S6:51:GLN:HG2	9:S6:92:ARG:HB2	1.90	0.52
22:D5:76:LEU:HB2	22:D5:136:ASN:HD21	1.74	0.52
22:D5:264:TYR:HA	22:D5:267:THR:HG22	1.91	0.52
3:S1:41:CYS:H	3:S1:52:CYS:HB3	1.75	0.52
19:D1:153:VAL:O	19:D1:157:ASN:ND2	2.42	0.52
23:D4:153:THR:O	23:D4:157:SER:HB3	2.09	0.52
3:S1:157:THR:HG23	3:S1:160:ILE:HD12	1.91	0.52
19:D1:55:LEU:HD22	19:D1:221:ALA:HB2	1.91	0.52
24:D2:338:PRO:O	27:A8:169:TRP:NE1	2.42	0.52
28:BJ:68:ARG:HH12	43:B1:45:LYS:H	1.58	0.52
4:S2:46:ASN:HD21	4:S2:74:ARG:HH21	1.58	0.52
20:D6:132:ASP:OD1	35:AM:78:LYS:NZ	2.43	0.52
27:A8:17:VAL:HG21	35:AM:73:LEU:HD21	1.92	0.52
1:V1:36:ALA:HB1	1:V1:41:ASP:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B8:52:ASP:OD1	40:B8:78:HIS:NE2	2.33	0.52
1:V1:28:ARG:HH21	2:V2:199:LEU:HD22	1.75	0.52
22:D5:224:SER:OG	22:D5:226:GLN:NE2	2.43	0.52
3:S1:403:ASP:OD1	10:S4:126:LYS:NZ	2.43	0.52
3:S1:564:ALA:HB3	3:S1:569:LYS:HD3	1.92	0.51
7:S8:25:LEU:HD21	31:A3:17:VAL:HA	1.92	0.51
24:D2:106:LEU:HD11	24:D2:108:MET:HE2	1.92	0.51
29:AJ:116:LEU:O	29:AJ:260:ARG:NH2	2.41	0.51
8:V3:70:ARG:NH2	10:S4:125:ASN:O	2.43	0.51
26:B5:26:ARG:O	26:B5:30:LEU:HB2	2.11	0.51
36:B6:92:LYS:O	36:B6:95:THR:OG1	2.28	0.51
1:V1:368:GLY:HA2	1:V1:395:ILE:HD11	1.93	0.51
3:S1:285:ARG:HH22	16:AL:144:TYR:H	1.59	0.51
19:D1:111:LEU:HD13	19:D1:114:TYR:HD2	1.75	0.51
20:D6:25:SER:HB3	20:D6:28:TYR:HD2	1.76	0.51
24:D2:243:LEU:HD21	33:C2:44:ILE:HD11	1.91	0.51
26:B5:66:TYR:HA	28:BJ:63:TYR:H	1.75	0.51
27:A8:37:LYS:NZ	31:A3:67:SER:O	2.43	0.51
27:A8:77:CYS:HB2	27:A8:113:LYS:HD2	1.92	0.51
36:B6:100:LYS:HB3	37:B7:49:GLN:HE22	1.75	0.51
5:S3:78:LEU:CA	5:S3:93:VAL:O	2.58	0.51
18:D3:67:LEU:HD22	21:4L:65:VAL:HG23	1.92	0.51
20:D6:14:VAL:HG21	21:4L:7:ASN:HB2	1.92	0.51
26:B5:64:TRP:HB2	26:B5:73:ARG:HG3	1.92	0.51
3:S1:159:CYS:HB2	3:S1:199:ILE:HD11	1.92	0.51
3:S1:450:MET:HA	3:S1:489:VAL:O	2.11	0.51
3:S1:544:VAL:HG22	3:S1:559:VAL:HB	1.93	0.51
37:B7:115:GLU:O	37:B7:119:ALA:CB	2.58	0.51
1:V1:343:ILE:HD13	1:V1:422:PHE:HE2	1.75	0.51
4:S2:261:ARG:O	4:S2:288:GLY:N	2.43	0.51
14:A6:43:PRO:HA	14:A6:46:VAL:HG12	1.93	0.51
23:D4:4:TYR:HB3	23:D4:70:MET:HE1	1.90	0.51
33:C2:66:THR:HG22	42:C1:27:LEU:HD23	1.93	0.51
38:B9:133:GLU:O	38:B9:137:LYS:HB2	2.11	0.51
12:A2:78:LEU:HD22	12:A2:86:VAL:HG22	1.92	0.51
19:D1:168:THR:HG22	35:AM:56:ARG:HH12	1.75	0.51
21:4L:40:LEU:HD22	24:D2:75:ILE:HD12	1.93	0.51
4:S2:91:ILE:HG12	4:S2:99:ALA:HB1	1.91	0.51
13:A5:34:LEU:HD11	13:A5:44:ARG:HA	1.92	0.51
22:D5:77:SER:OG	22:D5:79:SER:OG	2.25	0.51
36:B6:24:ASP:OD2	38:B9:124:TRP:NE1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V1:111:ILE:HD11	1:V1:149:LEU:HD22	1.92	0.51
1:V1:300:GLY:HA2	1:V1:329:LEU:HD12	1.93	0.51
3:S1:449:PRO:HG2	3:S1:489:VAL:HG22	1.93	0.51
5:S3:79:THR:O	5:S3:93:VAL:N	2.44	0.51
18:D3:97:LEU:HD21	20:D6:162:LEU:HB2	1.93	0.51
5:S3:74:SER:HB3	5:S3:97:LEU:HB3	1.92	0.51
5:S3:142:PHE:HB2	5:S3:148:LEU:HD11	1.93	0.51
3:S1:222:THR:HG22	3:S1:243:ARG:HB2	1.92	0.50
3:S1:434:SER:O	3:S1:476:LYS:NZ	2.44	0.50
3:S1:568:GLU:HB3	3:S1:589:PRO:HG3	1.91	0.50
16:AL:8:LYS:O	16:AL:12:GLN:NE2	2.44	0.50
19:D1:92:PRO:HG3	19:D1:255:TYR:HD2	1.76	0.50
19:D1:149:ILE:HG21	19:D1:185:TRP:HB2	1.93	0.50
23:D4:123:GLU:HB2	24:D2:255:PRO:HG2	1.93	0.50
26:B5:32:THR:HA	26:B5:35:PRO:HD2	1.93	0.50
1:V1:246:GLY:HA3	1:V1:272:MET:HB3	1.93	0.50
4:S2:50:ASN:HD22	4:S2:65:VAL:HG22	1.77	0.50
5:S3:47:GLU:OE1	5:S3:106:ARG:NH1	2.44	0.50
7:S8:74:GLU:OE1	7:S8:99:ARG:NH1	2.44	0.50
20:D6:64:MET:HE3	21:4L:68:ALA:HB1	1.93	0.50
22:D5:245:ALA:O	22:D5:249:SER:CB	2.60	0.50
22:D5:386:LEU:HD23	22:D5:387:THR:H	1.76	0.50
17:AB:12:LYS:HE3	17:AB:32:VAL:HG11	1.92	0.50
36:B6:17:LEU:HD11	38:B9:162:LEU:HD22	1.92	0.50
1:V1:21:ILE:O	1:V1:117:LYS:NZ	2.44	0.50
3:S1:237:ASN:OD1	3:S1:253:ARG:NH2	2.44	0.50
7:S8:71:PRO:HB3	16:AL:106:ARG:HE	1.76	0.50
11:A9:50:ARG:HG2	49:A9:401:NDP:H2A	1.93	0.50
19:D1:236:ILE:HG23	19:D1:259:PHE:HZ	1.76	0.50
35:AM:93:GLU:HA	35:AM:96:ILE:HG22	1.94	0.50
21:4L:80:MET:HG2	24:D2:45:MET:HE1	1.94	0.50
24:D2:270:MET:HG2	24:D2:279:PRO:HG3	1.92	0.50
29:AJ:189:PRO:HA	29:AJ:192:MET:HB2	1.93	0.50
31:A3:68:HIS:HB3	31:A3:71:ASP:HB2	1.92	0.50
3:S1:114:CYS:SG	3:S1:115:ASP:N	2.85	0.50
4:S2:54:GLN:HE22	6:S7:80:PRO:HG3	1.76	0.50
23:D4:300:ALA:O	23:D4:308:SER:OG	2.29	0.50
31:A3:27:LEU:O	31:A3:31:LEU:CB	2.60	0.50
3:S1:113:GLU:OE2	10:S4:43:ASN:ND2	2.39	0.50
6:S7:46:TRP:N	6:S7:84:ASP:OD2	2.45	0.50
19:D1:154:LEU:HA	19:D1:157:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:521:MET:HG3	3:S1:542:PHE:HD2	1.77	0.50
4:S2:40:LYS:HG2	4:S2:41:ASP:HB2	1.94	0.50
6:S7:109:GLU:O	11:A9:54:TYR:OH	2.27	0.50
19:D1:126:LYS:O	19:D1:129:LEU:N	2.43	0.50
22:D5:200:GLN:OE1	28:BJ:106:GLN:NE2	2.39	0.50
23:D4:254:THR:O	23:D4:258:ALA:CB	2.59	0.50
28:BJ:5:ASP:HB2	28:BJ:8:VAL:HG12	1.93	0.50
30:S5:47:GLY:H	30:S5:50:ARG:HE	1.59	0.50
20:D6:167:VAL:HG22	24:D2:42:PRO:HG2	1.93	0.50
27:A8:129:LYS:HD2	31:A3:65:VAL:HG13	1.93	0.50
28:BJ:88:GLU:OE1	28:BJ:150:SER:OG	2.26	0.50
29:AJ:171:TYR:HD2	29:AJ:222:GLN:HG3	1.77	0.50
37:B7:99:LYS:HB3	39:B2:64:LEU:HD21	1.94	0.50
3:S1:280:THR:HG21	16:AL:136:GLU:HG2	1.94	0.50
6:S7:46:TRP:NE1	6:S7:82:GLN:O	2.45	0.50
19:D1:90:PRO:HG3	19:D1:162:LEU:HG	1.94	0.50
20:D6:4:TYR:HB3	20:D6:7:PHE:HB3	1.92	0.50
27:A8:132:THR:OG1	31:A3:57:ARG:NH1	2.40	0.50
22:D5:246:LEU:O	22:D5:251:THR:OG1	2.30	0.49
1:V1:259:SER:OG	1:V1:260:GLY:N	2.44	0.49
1:V1:295:LEU:HB2	1:V1:339:ARG:HA	1.93	0.49
3:S1:69:CYS:SG	3:S1:70:ALA:N	2.84	0.49
7:S8:93:THR:HB	7:S8:110:ASP:HB2	1.93	0.49
3:S1:11:VAL:HG12	3:S1:77:TRP:HB2	1.94	0.49
4:S2:151:ILE:HD13	4:S2:304:MET:HE1	1.94	0.49
11:A9:166:ILE:HG13	11:A9:228:PHE:HB2	1.93	0.49
19:D1:312:SER:OG	31:A3:37:TYR:O	2.31	0.49
22:D5:341:MET:SD	22:D5:453:SER:OG	2.66	0.49
22:D5:584:ILE:HD11	24:D2:58:LYS:HE2	1.95	0.49
24:D2:199:THR:HG23	24:D2:346:LEU:HD22	1.94	0.49
38:B9:169:ILE:O	38:B9:172:ARG:NH1	2.40	0.49
40:B8:66:HIS:HB3	40:B8:69:LEU:HB2	1.94	0.49
1:V1:100:GLY:HA3	1:V1:184:TYR:HD1	1.78	0.49
24:D2:163:THR:HA	24:D2:285:THR:HG21	1.94	0.49
29:AJ:141:GLN:NE2	29:AJ:201:ASP:OD2	2.41	0.49
3:S1:470:VAL:HG12	3:S1:490:MET:HE1	1.94	0.49
3:S1:569:LYS:NZ	3:S1:596:ASP:OD2	2.39	0.49
9:S6:26:VAL:HB	11:A9:87:HIS:HB2	1.92	0.49
1:V1:184:TYR:CZ	46:V1:501:FMN:H6	2.47	0.49
6:S7:55:CYS:HB3	6:S7:89:ALA:HB1	1.94	0.49
11:A9:29:PHE:N	49:A9:401:NDP:O1N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A9:48:PRO:HB3	11:A9:71:MET:HG3	1.94	0.49
23:D4:385:THR:HG21	23:D4:396:MET:HE3	1.93	0.49
1:V1:233:THR:O	1:V1:237:ARG:HB2	2.12	0.49
11:A9:50:ARG:NE	49:A9:401:NDP:O3X	2.42	0.49
16:AL:46:ASN:ND2	16:AL:48:TYR:OH	2.46	0.49
16:AL:67:GLU:HG2	16:AL:72:ASN:H	1.77	0.49
22:D5:283:MET:HE1	40:B8:112:MET:HG3	1.95	0.49
22:D5:294:THR:H	22:D5:425:ARG:NH1	2.10	0.49
22:D5:538:PRO:HG3	51:D5:902:3PE:H222	1.95	0.49
22:D5:547:LYS:O	22:D5:552:LEU:HB2	2.13	0.49
6:S7:41:ARG:HA	19:D1:54:LYS:HG3	1.94	0.49
11:A9:94:LEU:HG	11:A9:132:ILE:HG12	1.95	0.49
19:D1:195:ARG:NH2	19:D1:228:TYR:OH	2.45	0.49
31:A3:76:SER:OG	31:A3:77:LEU:N	2.45	0.49
38:B9:125:LYS:HE2	38:B9:129:ARG:HH22	1.77	0.49
4:S2:300:ARG:NH2	4:S2:420:THR:O	2.46	0.49
5:S3:65:ARG:NH1	5:S3:123:VAL:O	2.46	0.49
3:S1:52:CYS:SG	3:S1:53:ARG:N	2.85	0.48
12:A2:57:CYS:SG	12:A2:58:SER:N	2.83	0.48
22:D5:71:ILE:HG13	22:D5:72:GLN:H	1.78	0.48
23:D4:178:ILE:O	23:D4:182:TRP:N	2.46	0.48
3:S1:9:ILE:HG23	3:S1:75:LYS:HA	1.93	0.48
4:S2:258:VAL:HA	4:S2:261:ARG:HB2	1.94	0.48
11:A9:48:PRO:HA	11:A9:71:MET:O	2.13	0.48
22:D5:241:THR:HG21	22:D5:344:GLY:HA3	1.95	0.48
22:D5:358:LYS:HE2	22:D5:438:PRO:HD3	1.95	0.48
23:D4:165:ILE:HG21	24:D2:268:GLN:HA	1.95	0.48
39:B2:10:ARG:HD3	39:B2:13:GLN:HB2	1.94	0.48
1:V1:278:GLU:O	1:V1:282:LYS:HB2	2.13	0.48
3:S1:80:LEU:HB3	3:S1:83:SER:HB3	1.95	0.48
3:S1:377:VAL:HA	3:S1:450:MET:O	2.14	0.48
11:A9:215:ILE:HA	11:A9:218:ILE:HG22	1.95	0.48
22:D5:558:LEU:HA	22:D5:561:ILE:HG22	1.96	0.48
24:D2:109:ALA:O	24:D2:112:HIS:ND1	2.42	0.48
28:BJ:17:PRO:HB3	36:B6:103:ILE:HG22	1.94	0.48
33:C2:19:ARG:HB3	42:C1:41:GLU:HG2	1.94	0.48
5:S3:39:GLN:HB3	5:S3:51:CYS:HB2	1.94	0.48
40:B8:138:LEU:O	40:B8:142:ARG:N	2.40	0.48
3:S1:283:MET:HE2	3:S1:291:LEU:HG	1.96	0.48
20:D6:58:LEU:O	20:D6:62:GLY:HA3	2.13	0.48
23:D4:209:LEU:HG	23:D4:211:GLY:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:B8:2:SER:OG	40:B8:3:HIS:N	2.45	0.48
1:V1:103:GLY:N	2:V2:148:CYS:SG	2.86	0.48
28:BJ:77:HIS:HA	33:C2:108:THR:HA	1.96	0.48
32:B3:21:TRP:HB2	32:B3:46:ARG:HD2	1.94	0.48
1:V1:179:ARG:NH1	2:V2:52:ASP:OD2	2.47	0.48
3:S1:237:ASN:HB3	3:S1:253:ARG:HG3	1.96	0.48
13:A5:26:LEU:HA	13:A5:29:LYS:HZ1	1.78	0.48
13:A5:49:GLN:HE22	15:A7:92:LYS:H	1.61	0.48
14:A6:42:VAL:O	14:A6:45:THR:OG1	2.30	0.48
14:A6:115:LYS:HA	14:A6:120:LYS:HE3	1.96	0.48
22:D5:554:ASP:O	22:D5:558:LEU:CB	2.61	0.48
23:D4:350:THR:OG1	23:D4:351:LEU:N	2.47	0.48
1:V1:24:ASN:HA	1:V1:28:ARG:HB2	1.96	0.48
11:A9:56:THR:HA	11:A9:59:LEU:HG	1.96	0.48
18:D3:69:ILE:HD11	19:D1:144:VAL:HG13	1.95	0.48
22:D5:226:GLN:O	22:D5:230:HIS:N	2.47	0.48
22:D5:541:ASN:HD22	51:D5:902:3PE:H361	1.79	0.48
26:B5:99:GLU:OE1	27:A8:162:HIS:NE2	2.38	0.48
38:B9:50:HIS:CE1	50:B9:201:ZMP:H8A	2.49	0.48
1:V1:105:CYS:SG	2:V2:148:CYS:N	2.87	0.48
5:S3:67:HIS:HB2	13:A5:89:LEU:HD21	1.95	0.48
7:S8:7:LEU:HD22	15:A7:112:LEU:HB3	1.96	0.48
22:D5:260:LEU:HD22	22:D5:277:MET:HE1	1.94	0.48
24:D2:233:THR:HA	24:D2:236:LYS:HG2	1.96	0.48
3:S1:531:CYS:SG	3:S1:532:VAL:N	2.85	0.47
20:D6:65:MET:HE1	21:4L:34:GLU:HG2	1.96	0.47
29:AJ:25:ILE:O	29:AJ:123:VAL:HA	2.12	0.47
32:B3:28:LEU:HD11	32:B3:48:GLU:HB2	1.96	0.47
34:B4:100:TRP:HA	34:B4:103:VAL:HG22	1.96	0.47
4:S2:145:THR:HG1	4:S2:181:TYR:HH	1.60	0.47
4:S2:385:ARG:NH2	5:S3:197:PHE:O	2.46	0.47
11:A9:202:LYS:NZ	11:A9:291:ASP:OD2	2.40	0.47
19:D1:149:ILE:HG23	19:D1:181:LEU:HG	1.96	0.47
23:D4:22:MET:HG2	23:D4:26:ASN:HD21	1.79	0.47
23:D4:364:LEU:HB3	23:D4:369:LEU:HD12	1.95	0.47
17:AB:48:VAL:HG21	38:B9:16:LEU:HD11	1.97	0.47
22:D5:371:THR:OG1	32:B3:68:LYS:NZ	2.47	0.47
23:D4:167:ILE:HA	23:D4:170:THR:HG22	1.96	0.47
29:AJ:54:ALA:HB2	29:AJ:107:GLN:HG2	1.96	0.47
36:B6:102:ARG:HG2	37:B7:49:GLN:HB2	1.96	0.47
38:B9:21:ARG:O	38:B9:25:HIS:ND1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V1:370:ASP:OD1	3:S1:179:ASN:ND2	2.48	0.47
3:S1:250:ILE:HD11	3:S1:268:ARG:HA	1.95	0.47
22:D5:605:HIS:HA	24:D2:92:PRO:HB2	1.96	0.47
28:BJ:149:TYR:HA	28:BJ:153:LYS:HD3	1.95	0.47
3:S1:282:PRO:HD2	3:S1:592:LEU:HD12	1.96	0.47
39:B2:62:GLU:H	39:B2:66:ILE:HD11	1.78	0.47
14:A6:29:ARG:HH21	17:AA:65:ILE:HD13	1.79	0.47
19:D1:86:TRP:HE1	19:D1:233:MET:HB2	1.80	0.47
4:S2:17:ALA:HB2	4:S2:30:PRO:HA	1.97	0.47
4:S2:183:ARG:O	7:S8:60:ARG:NH2	2.48	0.47
19:D1:18:ALA:O	19:D1:21:THR:OG1	2.28	0.47
23:D4:76:MET:HB2	23:D4:76:MET:HE3	1.76	0.47
23:D4:187:PRO:O	23:D4:192:ASN:ND2	2.45	0.47
28:BJ:136:LYS:NZ	28:BJ:140:ASP:OD2	2.39	0.47
29:AJ:108:TYR:OH	29:AJ:164:LEU:O	2.29	0.47
4:S2:236:ARG:NH2	4:S2:294:TYR:OH	2.37	0.47
14:A6:70:ALA:HA	50:AA:101:ZMP:C13	2.43	0.47
23:D4:45:PHE:HB2	41:BK:85:MET:HE2	1.96	0.47
23:D4:196:TRP:CE2	23:D4:200:MET:HG3	2.50	0.47
24:D2:200:MET:HE1	24:D2:265:MET:HE3	1.96	0.47
1:V1:43:TYR:O	1:V1:236:ARG:NH1	2.43	0.47
1:V1:298:ILE:HG12	1:V1:337:MET:HE1	1.96	0.47
3:S1:113:GLU:HA	10:S4:46:GLN:HE21	1.78	0.47
3:S1:233:ALA:O	3:S1:576:THR:N	2.48	0.47
12:A2:13:LEU:HB3	12:A2:14:GLY:H	1.58	0.47
21:4L:55:LEU:HB2	30:S5:24:GLN:HG3	1.96	0.47
22:D5:137:LEU:HB3	22:D5:196:TRP:HB2	1.96	0.47
23:D4:114:GLU:OE2	23:D4:173:SER:OG	2.33	0.47
23:D4:234:ILE:O	23:D4:238:LEU:HB2	2.14	0.47
27:A8:70:PHE:HB3	44:A1:69:ILE:HD12	1.97	0.47
30:S5:6:GLN:NE2	30:S5:14:ASP:OD2	2.48	0.47
3:S1:334:LEU:HD12	3:S1:604:SER:HB2	1.96	0.47
6:S7:85:VAL:HG12	6:S7:112:TYR:HB2	1.97	0.47
24:D2:96:MET:HG3	24:D2:153:LEU:HD11	1.96	0.47
17:AB:7:THR:HG23	17:AB:10:GLY:H	1.80	0.47
28:BJ:143:HIS:NE2	34:B4:125:ASN:O	2.48	0.47
29:AJ:91:GLY:O	29:AJ:95:ARG:NH2	2.41	0.47
38:B9:96:TYR:HB2	38:B9:177:PRO:HG3	1.96	0.47
7:S8:34:LEU:HD12	19:D1:272:TRP:CE2	2.50	0.46
11:A9:52:GLU:HG2	11:A9:54:TYR:H	1.81	0.46
16:AL:31:ASN:HD21	19:D1:39:VAL:HG22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D4:254:THR:O	23:D4:258:ALA:HB3	2.14	0.46
37:B7:100:GLU:OE1	40:B8:132:GLN:NE2	2.48	0.46
3:S1:362:TYR:O	3:S1:494:HIS:NE2	2.42	0.46
3:S1:362:TYR:OH	3:S1:504:ASP:OD1	2.29	0.46
11:A9:289:THR:HG22	11:A9:290:THR:HG23	1.97	0.46
22:D5:180:ILE:HD12	23:D4:397:GLY:HA3	1.97	0.46
22:D5:384:PRO:HA	22:D5:385:PHE:HA	1.56	0.46
22:D5:447:ASN:HD21	22:D5:449:PHE:HB2	1.79	0.46
24:D2:59:TYR:HB2	24:D2:118:VAL:HG21	1.96	0.46
27:A8:97:ARG:HB3	35:AM:59:LEU:HD13	1.98	0.46
1:V1:216:PHE:HZ	2:V2:45:ALA:HB2	1.80	0.46
1:V1:247:ARG:HH22	1:V1:321:ALA:HB2	1.80	0.46
3:S1:145:LEU:HB3	3:S1:269:PHE:HE2	1.80	0.46
5:S3:189:GLU:OE1	11:A9:15:SER:OG	2.32	0.46
19:D1:36:GLY:HA2	19:D1:37:PRO:HA	1.78	0.46
19:D1:169:GLN:NE2	19:D1:240:THR:O	2.40	0.46
22:D5:293:LEU:O	22:D5:523:SER:OG	2.32	0.46
25:AK:36:SER:HB2	25:AK:55:THR:HG22	1.96	0.46
29:AJ:210:PHE:HD2	29:AJ:211:LEU:HD22	1.79	0.46
3:S1:675:ASP:O	3:S1:679:ARG:CB	2.62	0.46
19:D1:85:MET:HE1	19:D1:105:MET:HA	1.97	0.46
22:D5:170:GLN:NE2	51:D5:902:3PE:O11	2.48	0.46
22:D5:418:PHE:HA	22:D5:421:ILE:HG12	1.98	0.46
14:A6:26:GLU:HG3	14:A6:29:ARG:HH12	1.81	0.46
23:D4:197:LEU:O	23:D4:201:MET:CB	2.63	0.46
33:C2:8:ARG:H	33:C2:9:ALA:HB3	1.80	0.46
33:C2:115:GLU:OE1	33:C2:117:HIS:NE2	2.43	0.46
7:S8:153:LYS:O	7:S8:157:ASN:HB2	2.16	0.46
13:A5:37:ILE:HD11	13:A5:94:ILE:HG13	1.97	0.46
22:D5:209:SER:O	22:D5:270:ASN:ND2	2.45	0.46
22:D5:400:ASN:O	40:B8:126:GLN:NE2	2.49	0.46
25:AK:98:LEU:HG	25:AK:114:CYS:HB2	1.98	0.46
26:B5:132:LEU:HD13	30:S5:22:ALA:HB2	1.97	0.46
29:AJ:49:LYS:HD2	29:AJ:114:HIS:CE1	2.50	0.46
29:AJ:202:ILE:O	29:AJ:206:TYR:CB	2.64	0.46
32:B3:49:ALA:HA	32:B3:52:TYR:HB2	1.98	0.46
3:S1:321:GLY:O	3:S1:498:SER:OG	2.30	0.46
5:S3:80:ALA:CA	5:S3:91:GLU:O	2.62	0.46
6:S7:116:MET:HA	6:S7:146:VAL:HG23	1.97	0.46
19:D1:81:LEU:HD11	19:D1:111:LEU:HB3	1.97	0.46
44:A1:25:ARG:O	44:A1:29:PHE:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S2:221:ARG:HD3	4:S2:221:ARG:HA	1.73	0.46
11:A9:168:PRO:HA	11:A9:230:PHE:HB2	1.98	0.46
21:4L:73:LEU:HD22	24:D2:38:LEU:HD23	1.98	0.46
22:D5:245:ALA:O	22:D5:249:SER:HB3	2.15	0.46
22:D5:332:HIS:CE1	22:D5:336:LYS:HD2	2.51	0.46
33:C2:66:THR:OG1	42:C1:28:TRP:NE1	2.48	0.46
37:B7:3:HIS:CE1	40:B8:127:PRO:HD3	2.51	0.46
4:S2:112:MET:HE1	4:S2:193:TYR:HD2	1.81	0.46
11:A9:134:HIS:ND1	11:A9:135:LEU:O	2.44	0.46
11:A9:185:ILE:HD11	11:A9:195:SER:HB3	1.98	0.46
13:A5:35:GLY:HA2	13:A5:44:ARG:HH22	1.81	0.46
13:A5:39:LYS:HA	13:A5:44:ARG:HD3	1.97	0.46
22:D5:82:MET:HB2	22:D5:87:MET:HE2	1.96	0.46
5:S3:77:ASP:O	5:S3:93:VAL:O	2.34	0.45
22:D5:397:GLU:HB3	22:D5:482:MET:HE2	1.98	0.45
38:B9:100:GLU:O	38:B9:121:ARG:NH2	2.49	0.45
42:C1:41:GLU:OE2	42:C1:44:ARG:NH2	2.39	0.45
1:V1:237:ARG:NH2	2:V2:212:GLY:O	2.48	0.45
1:V1:365:CYS:SG	1:V1:366:ARG:N	2.88	0.45
3:S1:296:TRP:HE1	3:S1:592:LEU:HB3	1.82	0.45
3:S1:575:ASN:OD1	3:S1:579:ARG:N	2.46	0.45
7:S8:96:ALA:HA	7:S8:106:THR:HA	1.97	0.45
19:D1:199:ASP:HB2	19:D1:279:ARG:HD2	1.98	0.45
23:D4:197:LEU:O	23:D4:201:MET:HB2	2.17	0.45
34:B4:2:PHE:HE2	34:B4:5:TYR:HB2	1.81	0.45
40:B8:138:LEU:HB3	40:B8:142:ARG:HG2	1.98	0.45
5:S3:79:THR:O	5:S3:91:GLU:O	2.35	0.45
5:S3:135:TRP:HH2	14:A6:80:LEU:HD11	1.81	0.45
21:4L:48:ILE:HG23	21:4L:53:PHE:HB3	1.98	0.45
22:D5:553:LEU:HD12	23:D4:271:MET:HE2	1.97	0.45
24:D2:335:MET:O	33:C2:33:TYR:OH	2.29	0.45
4:S2:287:ILE:HB	7:S8:4:TYR:HB3	1.97	0.45
11:A9:130:ILE:HG12	11:A9:164:THR:HB	1.97	0.45
22:D5:374:ILE:O	22:D5:378:LEU:HB2	2.17	0.45
1:V1:91:LYS:HB2	1:V1:131:ALA:HA	1.97	0.45
16:AL:44:TYR:OH	16:AL:112:ASN:O	2.29	0.45
17:AA:32:VAL:HB	17:AA:74:GLN:HB2	1.99	0.45
1:V1:189:GLU:OE1	1:V1:206:LYS:NZ	2.49	0.45
3:S1:13:VAL:HG11	3:S1:33:VAL:HG21	1.99	0.45
5:S3:182:ARG:NH2	14:A6:52:ASP:OD2	2.49	0.45
23:D4:305:THR:HG22	23:D4:307:TRP:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AB:70:LEU:HD23	17:AB:76:ILE:HG12	1.98	0.45
29:AJ:45:LYS:HG3	29:AJ:231:ALA:HB1	1.98	0.45
38:B9:19:TYR:HB2	38:B9:47:PHE:HE2	1.81	0.45
1:V1:214:GLY:HA3	1:V1:220:THR:HG22	1.99	0.45
4:S2:195:ARG:HG2	4:S2:200:HIS:HB2	1.99	0.45
9:S6:59:CYS:O	9:S6:70:ARG:HA	2.17	0.45
22:D5:172:ILE:HG21	23:D4:408:LEU:HD22	1.99	0.45
17:AB:14:ARG:HE	39:B2:11:TYR:HE1	1.65	0.45
35:AM:81:ARG:HH12	44:A1:46:TYR:HE1	1.63	0.45
3:S1:91:GLU:OE2	15:A7:54:CYS:N	2.50	0.45
4:S2:237:ASN:O	19:D1:284:GLN:NE2	2.49	0.45
9:S6:57:ILE:O	9:S6:72:TYR:HA	2.17	0.45
12:A2:64:LEU:HB3	12:A2:76:VAL:HG23	1.99	0.45
22:D5:40:ILE:HG13	22:D5:101:MET:HE3	1.99	0.45
23:D4:403:THR:HA	23:D4:406:TYR:CE1	2.52	0.45
29:AJ:169:VAL:HG23	29:AJ:218:CYS:HB3	1.98	0.45
32:B3:51:ARG:HH12	38:B9:33:ARG:HE	1.64	0.45
3:S1:428:ILE:O	3:S1:432:ILE:HB	2.17	0.45
4:S2:366:ALA:HA	4:S2:374:PHE:O	2.17	0.45
15:A7:3:ALA:HB1	15:A7:7:ILE:HD11	1.99	0.45
20:D6:37:GLY:HA3	20:D6:61:LEU:HD11	1.98	0.45
22:D5:535:ARG:HH21	40:B8:92:SER:HB2	1.81	0.45
24:D2:328:THR:HG23	33:C2:68:PHE:HZ	1.82	0.45
26:B5:104:ARG:NH2	27:A8:166:LEU:O	2.50	0.45
5:S3:82:ASP:OD1	5:S3:82:ASP:N	2.49	0.45
22:D5:532:ILE:HD11	40:B8:101:MET:HB3	1.98	0.45
26:B5:112:ARG:HG3	26:B5:113:LEU:HD12	1.99	0.45
39:B2:35:TRP:O	39:B2:39:ARG:HB2	2.16	0.45
11:A9:245:VAL:HA	11:A9:248:VAL:HG12	1.99	0.44
22:D5:7:LEU:HA	22:D5:10:VAL:HG22	1.99	0.44
22:D5:234:PRO:HB3	22:D5:300:LYS:HG2	1.98	0.44
23:D4:26:ASN:OD1	43:B1:13:HIS:NE2	2.50	0.44
17:AB:21:LEU:HD11	32:B3:46:ARG:HB2	1.99	0.44
43:B1:48:LEU:HB2	43:B1:53:GLU:HA	1.98	0.44
11:A9:55:ASP:O	11:A9:58:HIS:ND1	2.51	0.44
22:D5:15:LEU:HB3	22:D5:126:ILE:HG12	1.98	0.44
27:A8:142:HIS:ND1	35:AM:113:THR:O	2.48	0.44
36:B6:103:ILE:HD11	37:B7:47:ASP:HB3	1.98	0.44
1:V1:250:ASN:OD1	1:V1:250:ASN:N	2.50	0.44
24:D2:309:ASN:HD21	29:AJ:95:ARG:HG3	1.82	0.44
29:AJ:24:LEU:HB2	29:AJ:167:HIS:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:AM:139:PHE:HB2	44:A1:45:TRP:CD1	2.52	0.44
38:B9:66:ALA:HB1	50:B9:201:ZMP:H6	2.00	0.44
44:A1:25:ARG:O	44:A1:29:PHE:CB	2.65	0.44
1:V1:289:GLY:HA3	1:V1:293:ASN:HD22	1.82	0.44
2:V2:47:VAL:O	2:V2:51:LEU:HB2	2.17	0.44
2:V2:113:SER:HA	2:V2:152:PRO:HG3	1.99	0.44
3:S1:41:CYS:SG	3:S1:52:CYS:N	2.91	0.44
3:S1:237:ASN:HB3	3:S1:253:ARG:O	2.17	0.44
8:V3:57:ASP:O	8:V3:60:LYS:NZ	2.47	0.44
15:A7:111:TYR:HA	15:A7:112:LEU:HA	1.77	0.44
22:D5:451:ILE:O	22:D5:455:LYS:CB	2.64	0.44
1:V1:208:PRO:HG3	10:S4:118:TYR:HD2	1.83	0.44
3:S1:242:THR:HG21	3:S1:586:ALA:HB1	2.00	0.44
19:D1:142:TYR:CE2	19:D1:191:ALA:HB1	2.53	0.44
21:4L:62:ILE:HA	21:4L:65:VAL:HG12	1.98	0.44
22:D5:224:SER:HB2	22:D5:310:LEU:HD23	2.00	0.44
23:D4:102:LEU:HD21	23:D4:230:VAL:HG11	2.00	0.44
24:D2:202:LEU:HB3	24:D2:346:LEU:HD11	1.99	0.44
19:D1:197:PRO:HA	19:D1:279:ARG:HG2	1.98	0.44
22:D5:279:CYS:SG	22:D5:405:ASN:ND2	2.90	0.44
35:AM:110:PHE:HE2	35:AM:116:VAL:HG21	1.83	0.44
2:V2:156:ILE:HD11	2:V2:159:ASN:HD22	1.83	0.44
3:S1:226:GLU:HA	3:S1:253:ARG:HH12	1.83	0.44
4:S2:224:GLU:OE1	7:S8:40:TYR:OH	2.30	0.44
6:S7:69:MET:HE1	6:S7:76:PHE:HB3	1.98	0.44
7:S8:45:PRO:HB2	7:S8:47:THR:HG23	1.99	0.44
9:S6:12:THR:HG22	9:S6:35:VAL:HG23	1.99	0.44
11:A9:95:VAL:O	49:A9:401:NDP:O3D	2.29	0.44
21:4L:19:LEU:HD13	21:4L:33:LEU:HB2	2.00	0.44
27:A8:90:TYR:HB3	44:A1:34:ARG:HH11	1.82	0.44
3:S1:357:ASP:OD2	12:A2:40:TYR:OH	2.35	0.44
4:S2:202:ASP:HB3	4:S2:323:ILE:HG23	1.99	0.44
7:S8:30:LEU:O	19:D1:277:TYR:OH	2.34	0.44
22:D5:198:LEU:HA	22:D5:201:ILE:HB	1.99	0.44
41:BK:68:ILE:HA	41:BK:72:LEU:HD13	2.00	0.44
23:D4:424:ASN:OD1	34:B4:55:ARG:NH1	2.51	0.44
34:B4:22:TYR:OH	38:B9:67:GLU:OE1	2.34	0.44
4:S2:379:VAL:HG12	4:S2:387:TYR:HB3	1.99	0.43
22:D5:441:ILE:HB	22:D5:443:ILE:HG13	1.98	0.43
23:D4:277:LEU:HD12	23:D4:402:ILE:HG23	1.98	0.43
27:A8:82:THR:HA	27:A8:85:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B4:77:PRO:HA	34:B4:78:ASN:HA	1.75	0.43
43:B1:16:VAL:HG23	43:B1:17:PRO:HD3	2.00	0.43
1:V1:140:GLY:O	1:V1:179:ARG:NH2	2.52	0.43
4:S2:284:ASP:OD1	4:S2:284:ASP:N	2.51	0.43
14:A6:28:LYS:HB3	14:A6:32:ARG:HH21	1.83	0.43
19:D1:1:MET:HA	19:D1:4:ILE:HD12	2.00	0.43
20:D6:20:PHE:HE2	21:4L:32:CYS:HA	1.83	0.43
24:D2:314:LYS:NZ	29:AJ:270:LEU:O	2.50	0.43
28:BJ:138:TYR:HA	41:BK:108:MET:HE1	1.99	0.43
3:S1:332:LYS:HD3	3:S1:507:TYR:HE1	1.84	0.43
17:AA:64:ASP:O	17:AA:68:GLU:HB2	2.17	0.43
34:B4:32:GLN:HB3	38:B9:7:ALA:HB1	1.99	0.43
41:BK:77:VAL:HA	41:BK:80:LEU:HD23	2.01	0.43
1:V1:30:ASP:OD1	1:V1:30:ASP:N	2.48	0.43
1:V1:109:GLU:HG3	1:V1:113:HIS:HD2	1.83	0.43
11:A9:81:ILE:HG21	11:A9:117:ILE:HG22	1.98	0.43
29:AJ:133:VAL:HG11	29:AJ:206:TYR:HD1	1.84	0.43
3:S1:11:VAL:O	3:S1:17:SER:HA	2.18	0.43
3:S1:522:LEU:O	3:S1:543:ILE:HA	2.18	0.43
12:A2:21:HIS:HB2	12:A2:63:LYS:H	1.83	0.43
17:AA:16:LEU:HD23	17:AA:30:LEU:HD12	2.00	0.43
22:D5:375:ILE:HD12	39:B2:32:MET:HG3	2.00	0.43
23:D4:282:LEU:HD12	23:D4:285:LEU:HD12	2.00	0.43
31:A3:77:LEU:HB2	31:A3:80:LEU:HD23	2.00	0.43
39:B2:10:ARG:HD2	39:B2:15:PRO:HA	2.01	0.43
6:S7:137:ASP:OD2	7:S8:144:HIS:ND1	2.51	0.43
14:A6:28:LYS:HA	14:A6:31:VAL:HG12	2.01	0.43
22:D5:83:ASP:O	22:D5:87:MET:CB	2.66	0.43
3:S1:316:ALA:O	3:S1:522:LEU:HA	2.19	0.43
9:S6:24:ARG:HA	9:S6:27:ARG:HG2	2.01	0.43
11:A9:144:LYS:O	11:A9:148:ASN:ND2	2.51	0.43
23:D4:106:LEU:HD13	23:D4:234:ILE:HG21	2.01	0.43
25:AK:46:THR:HA	25:AK:47:SER:HA	1.71	0.43
27:A8:82:THR:HA	27:A8:85:TRP:NE1	2.34	0.43
3:S1:73:VAL:HA	3:S1:77:TRP:HE1	1.83	0.43
11:A9:53:PRO:O	11:A9:57:MET:HB2	2.18	0.43
14:A6:62:VAL:HG22	50:AA:101:ZMP:C2	2.49	0.43
22:D5:391:SER:OG	22:D5:392:LYS:N	2.52	0.43
22:D5:431:LEU:HB2	22:D5:432:LEU:HD12	2.00	0.43
22:D5:581:LYS:NZ	25:AK:43:LYS:O	2.45	0.43
33:C2:4:GLY:HA2	33:C2:5:ARG:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BK:85:MET:HB3	41:BK:88:TRP:HB3	2.01	0.43
1:V1:25:LEU:O	1:V1:113:HIS:NE2	2.51	0.43
3:S1:226:GLU:HA	3:S1:253:ARG:NH1	2.33	0.43
10:S4:130:VAL:HG22	10:S4:132:THR:HG22	2.00	0.43
23:D4:41:LEU:HD22	23:D4:63:THR:HG23	2.01	0.43
24:D2:135:LYS:HD2	24:D2:187:MET:HE2	2.00	0.43
32:B3:13:MET:HE2	39:B2:11:TYR:HB2	2.00	0.43
35:AM:94:ALA:HA	35:AM:103:TRP:HH2	1.82	0.43
40:B8:8:MET:O	40:B8:26:LYS:NZ	2.46	0.43
3:S1:324:ASP:HA	3:S1:573:TYR:HE1	1.83	0.43
3:S1:357:ASP:N	3:S1:357:ASP:OD1	2.45	0.43
7:S8:175:TYR:CZ	15:A7:38:PRO:HG3	2.54	0.43
9:S6:19:ASP:OD2	11:A9:2:HIS:ND1	2.52	0.43
10:S4:17:LEU:HB2	10:S4:98:LYS:HG3	2.01	0.43
11:A9:91:VAL:O	11:A9:129:PHE:HA	2.19	0.43
22:D5:298:ILE:HA	22:D5:301:ILE:HD12	1.99	0.43
17:AB:49:GLU:HB3	32:B3:44:TRP:HZ3	1.84	0.43
29:AJ:75:GLY:HA3	29:AJ:76:ASN:HA	1.72	0.43
8:V3:47:SER:OG	8:V3:48:THR:N	2.52	0.42
23:D4:47:ASP:OD1	23:D4:47:ASP:N	2.52	0.42
24:D2:90:PHE:HB3	30:S5:63:ARG:HH22	1.83	0.42
28:BJ:48:ARG:HD2	36:B6:83:TYR:HE1	1.83	0.42
2:V2:17:PRO:HA	2:V2:19:THR:H	1.83	0.42
4:S2:68:LEU:HA	4:S2:74:ARG:N	2.34	0.42
5:S3:150:ARG:HE	5:S3:155:TYR:HA	1.84	0.42
5:S3:204:GLU:H	10:S4:50:ASN:HD22	1.67	0.42
8:V3:41:LEU:HG	8:V3:44:HIS:HB2	2.01	0.42
15:A7:41:PRO:HB3	35:AM:6:LYS:HD2	2.01	0.42
22:D5:54:PHE:O	22:D5:58:GLY:N	2.42	0.42
22:D5:338:MET:HE3	22:D5:458:LEU:HB3	2.00	0.42
23:D4:207:MET:HG3	23:D4:298:ILE:HD11	2.02	0.42
24:D2:102:LEU:HD22	24:D2:138:PRO:HB3	2.00	0.42
24:D2:243:LEU:HD23	24:D2:243:LEU:HA	1.80	0.42
28:BJ:36:PHE:O	28:BJ:40:VAL:HB	2.18	0.42
29:AJ:35:LYS:HG3	29:AJ:37:LYS:HG2	2.00	0.42
3:S1:314:ASP:HA	3:S1:519:PRO:HA	2.01	0.42
22:D5:439:THR:HG23	17:AB:14:ARG:HH21	1.84	0.42
23:D4:298:ILE:HD13	23:D4:298:ILE:HA	1.74	0.42
1:V1:157:TYR:HD2	8:V3:58:LEU:HD12	1.84	0.42
20:D6:127:ILE:H	20:D6:127:ILE:HG13	1.69	0.42
22:D5:89:PHE:HE2	22:D5:132:VAL:HG11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A8:85:TRP:O	27:A8:89:ASP:HB2	2.20	0.42
28:BJ:74:THR:O	33:C2:108:THR:OG1	2.29	0.42
3:S1:125:SER:OG	3:S1:126:ASP:N	2.52	0.42
21:4L:47:MET:HB3	21:4L:47:MET:HE2	1.74	0.42
22:D5:281:GLY:O	22:D5:284:THR:OG1	2.32	0.42
23:D4:169:ASN:ND2	24:D2:271:THR:O	2.51	0.42
23:D4:229:MET:SD	23:D4:324:SER:OG	2.71	0.42
40:B8:13:TYR:HE1	40:B8:39:ASP:H	1.67	0.42
41:BK:57:ASN:HA	41:BK:60:VAL:HG12	2.01	0.42
44:A1:1:MET:HE3	44:A1:3:PHE:HB2	2.02	0.42
4:S2:251:LEU:HD13	5:S3:73:LYS:HG3	2.02	0.42
15:A7:63:MET:HE3	15:A7:64:PRO:HD2	2.01	0.42
18:D3:87:MET:HE3	18:D3:87:MET:HB2	1.87	0.42
19:D1:2:PHE:HA	19:D1:5:ASN:HD22	1.84	0.42
22:D5:60:GLU:HB2	36:B6:99:LYS:HB3	2.02	0.42
22:D5:384:PRO:HG3	22:D5:491:LEU:HD13	2.00	0.42
23:D4:270:ILE:HG13	23:D4:395:LEU:HD22	2.00	0.42
29:AJ:18:MET:HB3	29:AJ:19:THR:HB	2.02	0.42
3:S1:424:ASP:OD1	3:S1:424:ASP:N	2.53	0.42
6:S7:39:TRP:HA	6:S7:42:ARG:HG2	2.01	0.42
11:A9:290:THR:HB	11:A9:292:ARG:HH11	1.84	0.42
19:D1:28:LEU:HG	19:D1:271:LEU:HD11	2.00	0.42
19:D1:310:LEU:HD23	19:D1:310:LEU:HA	1.86	0.42
22:D5:203:MET:HG2	28:BJ:109:LEU:HD11	2.02	0.42
23:D4:19:LYS:NZ	23:D4:22:MET:SD	2.91	0.42
24:D2:142:LEU:HB3	24:D2:194:LEU:HD21	2.01	0.42
26:B5:84:GLU:HG2	43:B1:44:TYR:CG	2.55	0.42
17:AB:52:MET:HG2	38:B9:23:LEU:HD12	2.01	0.42
29:AJ:188:ASN:HB3	29:AJ:191:GLU:HB2	2.01	0.42
1:V1:298:ILE:HG22	1:V1:306:LEU:HA	2.02	0.42
14:A6:46:VAL:HA	14:A6:51:LEU:HD12	2.02	0.42
24:D2:207:ILE:HD13	24:D2:262:PRO:HD3	2.00	0.42
27:A8:77:CYS:HA	27:A8:78:ALA:HA	1.68	0.42
32:B3:35:LEU:HG	32:B3:40:LEU:HB2	2.01	0.42
36:B6:108:THR:HB	36:B6:115:VAL:HG12	2.02	0.42
40:B8:14:PRO:HA	40:B8:15:LYS:HA	1.76	0.42
43:B1:48:LEU:HD13	43:B1:53:GLU:HG2	2.02	0.42
1:V1:69:GLY:H	1:V1:331:THR:HG21	1.85	0.42
2:V2:79:ARG:NE	10:S4:131:SER:O	2.52	0.42
4:S2:84:HIS:CD2	5:S3:152:LEU:HB3	2.54	0.42
4:S2:174:ARG:HD3	6:S7:61:HIS:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S8:52:PHE:HZ	16:AL:29:ARG:HG2	1.85	0.42
8:V3:60:LYS:H	8:V3:60:LYS:HD2	1.85	0.42
10:S4:57:MET:HB3	10:S4:84:LEU:HB2	2.02	0.42
22:D5:398:SER:O	22:D5:402:SER:OG	2.37	0.42
24:D2:98:MET:HE1	24:D2:145:ILE:HG21	2.02	0.42
29:AJ:188:ASN:O	29:AJ:192:MET:N	2.50	0.42
1:V1:138:ILE:HD13	1:V1:146:ALA:HB2	2.01	0.42
1:V1:200:GLN:NE2	3:S1:174:THR:OG1	2.43	0.42
2:V2:9:HIS:CD2	2:V2:11:ASP:HA	2.54	0.42
2:V2:120:ILE:HD13	2:V2:173:ILE:HD11	2.01	0.42
2:V2:120:ILE:O	2:V2:124:LEU:HB3	2.20	0.42
3:S1:360:SER:O	3:S1:365:ASN:ND2	2.42	0.42
3:S1:437:HIS:HD2	3:S1:439:PHE:HB3	1.83	0.42
3:S1:511:VAL:HG11	3:S1:531:CYS:HB2	2.01	0.42
4:S2:110:SER:OG	4:S2:114:ASN:OD1	2.31	0.42
10:S4:10:LEU:HB3	14:A6:18:PRO:HD3	2.01	0.42
36:B6:18:ARG:HE	38:B9:172:ARG:CZ	2.32	0.42
2:V2:108:CYS:HB3	2:V2:152:PRO:HB3	2.02	0.41
3:S1:101:HIS:O	3:S1:134:LYS:NZ	2.53	0.41
4:S2:227:GLU:OE1	15:A7:17:ARG:NH2	2.45	0.41
16:AL:78:ASP:HB2	16:AL:81:MET:HE3	2.02	0.41
22:D5:172:ILE:O	22:D5:176:ARG:HG2	2.20	0.41
22:D5:297:ASP:HB2	22:D5:300:LYS:HD3	2.02	0.41
22:D5:548:SER:HA	22:D5:552:LEU:HB3	2.02	0.41
23:D4:436:LEU:O	23:D4:440:HIS:ND1	2.49	0.41
31:A3:68:HIS:HD2	31:A3:69:PRO:HD2	1.85	0.41
34:B4:80:ARG:NH2	40:B8:39:ASP:O	2.44	0.41
3:S1:585:VAL:O	10:S4:61:THR:OG1	2.31	0.41
6:S7:124:GLY:HA2	7:S8:115:LYS:HA	2.01	0.41
8:V3:38:TYR:CZ	8:V3:40:ASN:HB2	2.54	0.41
11:A9:318:LEU:HD13	11:A9:318:LEU:HA	1.90	0.41
16:AL:42:ASP:OD1	16:AL:43:LYS:N	2.53	0.41
22:D5:95:PHE:HZ	22:D5:456:ARG:HG2	1.85	0.41
23:D4:203:PHE:O	23:D4:207:MET:HG2	2.20	0.41
27:A8:70:PHE:HA	27:A8:73:ILE:HG22	2.02	0.41
28:BJ:19:PRO:HD3	36:B6:110:LEU:HD12	2.02	0.41
33:C2:19:ARG:HH21	42:C1:41:GLU:HB2	1.85	0.41
36:B6:117:PRO:HA	36:B6:118:PRO:HD3	1.84	0.41
36:B6:119:MET:SD	36:B6:120:LYS:N	2.93	0.41
3:S1:44:GLU:O	3:S1:45:ARG:NH1	2.48	0.41
4:S2:63:ARG:NH1	14:A6:96:TRP:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:56:GLY:O	5:S3:60:VAL:HB	2.21	0.41
5:S3:92:ILE:HB	5:S3:109:THR:HG23	2.02	0.41
15:A7:26:ARG:HG3	15:A7:30:ILE:HD11	2.02	0.41
20:D6:163:ILE:HA	20:D6:166:VAL:HG12	2.02	0.41
22:D5:366:MET:HG3	22:D5:445:GLU:HB2	2.02	0.41
5:S3:61:LEU:HD22	5:S3:124:TYR:HE2	1.85	0.41
9:S6:5:SER:OG	9:S6:9:GLU:N	2.46	0.41
11:A9:48:PRO:HB2	11:A9:73:TRP:CD1	2.55	0.41
11:A9:108:ASP:HA	11:A9:111:VAL:HB	2.02	0.41
14:A6:46:VAL:HG11	14:A6:55:VAL:HG22	2.02	0.41
19:D1:318:THR:O	44:A1:41:TYR:OH	2.32	0.41
20:D6:13:PHE:HD1	20:D6:39:VAL:HG23	1.85	0.41
20:D6:169:MET:O	20:D6:174:GLY:N	2.54	0.41
25:AK:89:TYR:HD2	25:AK:125:LYS:HB2	1.85	0.41
27:A8:94:GLN:HE22	44:A1:37:ARG:CZ	2.33	0.41
1:V1:379:PHE:CZ	1:V1:389:ILE:HG22	2.56	0.41
2:V2:76:PRO:HA	2:V2:77:PRO:HD3	1.89	0.41
4:S2:273:GLN:OE1	5:S3:104:ARG:NH1	2.45	0.41
4:S2:422:ASP:OD1	4:S2:422:ASP:N	2.52	0.41
17:AA:62:ILE:HG22	17:AA:67:ALA:HB2	2.02	0.41
19:D1:85:MET:HB3	19:D1:233:MET:SD	2.60	0.41
22:D5:265:PRO:HA	22:D5:268:GLU:HG3	2.03	0.41
24:D2:131:LEU:HD23	24:D2:131:LEU:HA	1.92	0.41
32:B3:23:ILE:HD13	32:B3:46:ARG:HA	2.02	0.41
1:V1:236:ARG:HG3	1:V1:237:ARG:HG3	2.02	0.41
11:A9:26:ALA:HA	11:A9:31:GLY:HA3	2.03	0.41
19:D1:288:LEU:O	19:D1:292:ASN:HB2	2.20	0.41
24:D2:235:ASN:ND2	24:D2:307:SER:OG	2.49	0.41
26:B5:13:PRO:O	38:B9:106:TRP:NE1	2.45	0.41
17:AB:73:PRO:HA	17:AB:76:ILE:HD12	2.03	0.41
4:S2:22:THR:H	4:S2:25:THR:HG22	1.85	0.41
5:S3:167:PRO:HA	10:S4:82:LEU:HD21	2.03	0.41
6:S7:39:TRP:CZ2	19:D1:46:LEU:HD13	2.56	0.41
22:D5:293:LEU:HA	22:D5:425:ARG:HH22	1.85	0.41
52:D5:901:CDL:HA31	26:B5:22:LEU:HD21	2.03	0.41
24:D2:254:LEU:HA	24:D2:255:PRO:HD3	1.94	0.41
1:V1:312:CYS:HA	1:V1:315:VAL:HB	2.02	0.41
3:S1:278:ARG:HA	3:S1:549:HIS:HB3	2.02	0.41
4:S2:423:ILE:H	4:S2:423:ILE:HG13	1.65	0.41
9:S6:53:GLY:HA2	9:S6:94:GLN:H	1.86	0.41
11:A9:72:ASP:O	11:A9:80:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:D1:271:LEU:HD23	19:D1:274:ARG:HH21	1.85	0.41
20:D6:112:GLU:OE1	30:S5:73:LYS:NZ	2.54	0.41
21:4L:27:MET:HE2	21:4L:78:LEU:HD22	2.02	0.41
21:4L:66:PHE:HB3	24:D2:34:GLU:OE1	2.20	0.41
22:D5:405:ASN:HB3	22:D5:408:ALA:H	1.86	0.41
22:D5:567:SER:OG	51:D4:501:3PE:O22	2.34	0.41
23:D4:205:VAL:HG22	23:D4:212:LEU:HD11	2.03	0.41
23:D4:278:ARG:NH2	40:B8:80:ASP:OD1	2.53	0.41
24:D2:115:VAL:HG12	24:D2:180:ALA:HB1	2.03	0.41
26:B5:64:TRP:CD1	26:B5:65:GLU:HG3	2.56	0.41
2:V2:30:ARG:NH2	8:V3:53:ASP:OD1	2.45	0.41
2:V2:53:LEU:HD12	8:V3:52:LEU:HD13	2.03	0.41
3:S1:101:HIS:HD2	4:S2:342:MET:HE2	1.86	0.41
3:S1:323:VAL:HG11	3:S1:525:LEU:HB3	2.03	0.41
3:S1:409:ILE:HG12	3:S1:422:LEU:HB2	2.02	0.41
4:S2:19:MET:SD	24:D2:295:ARG:NH2	2.73	0.41
5:S3:72:PHE:HB3	5:S3:96:LEU:HD23	2.03	0.41
5:S3:202:PRO:HA	10:S4:50:ASN:HB3	2.03	0.41
6:S7:125:TYR:CG	7:S8:117:ILE:HD12	2.56	0.41
11:A9:45:VAL:HB	11:A9:68:ILE:HG22	2.03	0.41
18:D3:80:GLN:OE1	31:A3:50:TYR:OH	2.37	0.41
19:D1:243:LEU:HD13	19:D1:262:LYS:HD3	2.03	0.41
20:D6:174:GLY:HA2	20:D6:175:ASN:HA	1.78	0.41
22:D5:455:LYS:HG3	39:B2:28:PHE:HZ	1.86	0.41
22:D5:548:SER:O	22:D5:553:LEU:N	2.53	0.41
27:A8:24:LEU:HG	35:AM:70:LEU:HD11	2.02	0.41
29:AJ:156:LYS:HG2	29:AJ:160:VAL:HG21	2.02	0.41
41:BK:64:PHE:HA	41:BK:68:ILE:HG22	2.02	0.41
1:V1:202:LYS:HB3	1:V1:361:GLN:NE2	2.34	0.41
4:S2:169:TRP:CE2	7:S8:40:TYR:HD2	2.38	0.41
5:S3:66:ASP:HB2	13:A5:89:LEU:HD23	2.03	0.41
30:S5:95:PRO:HB3	35:AM:126:LEU:HD13	2.02	0.41
1:V1:258:ILE:HG22	1:V1:262:VAL:HG21	2.02	0.40
2:V2:55:GLN:NE2	2:V2:91:ASN:OD1	2.46	0.40
3:S1:112:GLY:O	10:S4:46:GLN:NE2	2.54	0.40
3:S1:584:LYS:HG3	10:S4:36:ARG:HH11	1.86	0.40
11:A9:165:ILE:O	11:A9:227:THR:HA	2.21	0.40
11:A9:203:GLN:HB3	11:A9:235:ARG:HA	2.03	0.40
19:D1:92:PRO:HG2	19:D1:252:PRO:HB2	2.03	0.40
22:D5:142:ILE:HA	23:D4:370:PRO:HB2	2.02	0.40
22:D5:280:LEU:O	22:D5:284:THR:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:538:PRO:HB2	40:B8:89:VAL:HG22	2.03	0.40
23:D4:272:THR:HA	23:D4:275:ILE:HG22	2.02	0.40
28:BJ:68:ARG:NH1	43:B1:45:LYS:H	2.19	0.40
29:AJ:105:LEU:HD11	29:AJ:163:TYR:HE2	1.86	0.40
1:V1:42:TRP:N	1:V1:120:GLU:OE2	2.51	0.40
11:A9:40:ARG:HH12	14:A6:109:THR:HB	1.86	0.40
13:A5:55:LEU:HD11	13:A5:59:LYS:HE3	2.02	0.40
18:D3:98:LEU:HD22	19:D1:298:LEU:HD21	2.03	0.40
22:D5:82:MET:SD	22:D5:82:MET:N	2.93	0.40
22:D5:173:LEU:HD22	51:D5:902:3PE:H241	2.02	0.40
29:AJ:17:LYS:HG2	29:AJ:118:THR:HA	2.03	0.40
37:B7:45:MET:HG2	37:B7:55:ARG:HH11	1.86	0.40
6:S7:154:GLU:HG3	7:S8:50:TYR:HE1	1.85	0.40
15:A7:32:LYS:O	15:A7:35:GLN:NE2	2.54	0.40
20:D6:55:MET:HB2	20:D6:55:MET:HE2	1.82	0.40
23:D4:96:ILE:O	23:D4:100:ILE:HG12	2.22	0.40
26:B5:31:LEU:HD23	26:B5:32:THR:HG23	2.03	0.40
27:A8:121:LEU:HA	27:A8:122:GLY:HA2	1.81	0.40
29:AJ:224:SER:OG	29:AJ:225:ALA:N	2.55	0.40
38:B9:107:HIS:NE2	41:BK:43:ASP:OD1	2.53	0.40
2:V2:126:ILE:HG21	2:V2:132:THR:HA	2.02	0.40
6:S7:127:HIS:CG	7:S8:115:LYS:HE3	2.56	0.40
7:S8:95:GLU:O	7:S8:107:THR:N	2.42	0.40
17:AA:11:ILE:HA	17:AA:14:ARG:HG2	2.03	0.40
28:BJ:127:GLU:HA	28:BJ:130:GLN:HG2	2.04	0.40
38:B9:39:PHE:HA	38:B9:42:LEU:HB2	2.02	0.40
38:B9:61:GLN:HG3	38:B9:64:ARG:NH2	2.36	0.40
41:BK:110:SER:OG	41:BK:111:ASN:N	2.54	0.40
1:V1:352:GLU:HG2	1:V1:373:ASN:HD21	1.87	0.40
2:V2:91:ASN:OD1	2:V2:91:ASN:N	2.55	0.40
3:S1:51:ASN:HD21	10:S4:133:LYS:NZ	2.19	0.40
6:S7:39:TRP:HH2	19:D1:46:LEU:HB2	1.86	0.40
6:S7:179:ARG:HG3	11:A9:50:ARG:HH22	1.85	0.40
11:A9:171:ILE:HD13	11:A9:207:ILE:HD13	2.04	0.40
12:A2:22:LEU:HD23	12:A2:22:LEU:HA	1.88	0.40
19:D1:316:PRO:HG3	35:AM:56:ARG:HG2	2.02	0.40
20:D6:71:THR:HG22	20:D6:74:MET:HE2	2.03	0.40
22:D5:401:THR:HA	40:B8:126:GLN:HE22	1.85	0.40
23:D4:44:GLN:HB2	23:D4:50:LEU:HD23	2.03	0.40
32:B3:28:LEU:HA	32:B3:28:LEU:HD23	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	380 (89%)	48 (11%)	0	100	100
2	V2	210/217 (97%)	166 (79%)	44 (21%)	0	100	100
3	S1	686/704 (97%)	619 (90%)	66 (10%)	1 (0%)	48	81
4	S2	423/430 (98%)	373 (88%)	50 (12%)	0	100	100
5	S3	206/228 (90%)	174 (84%)	32 (16%)	0	100	100
6	S7	154/179 (86%)	135 (88%)	19 (12%)	0	100	100
7	S8	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
8	V3	38/75 (51%)	29 (76%)	9 (24%)	0	100	100
9	S6	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
10	S4	124/133 (93%)	105 (85%)	19 (15%)	0	100	100
11	A9	284/338 (84%)	253 (89%)	31 (11%)	0	100	100
12	A2	80/98 (82%)	69 (86%)	11 (14%)	0	100	100
13	A5	109/115 (95%)	95 (87%)	14 (13%)	0	100	100
14	A6	112/127 (88%)	102 (91%)	10 (9%)	0	100	100
15	A7	90/112 (80%)	80 (89%)	10 (11%)	0	100	100
16	AL	141/145 (97%)	112 (79%)	29 (21%)	0	100	100
17	AA	78/88 (89%)	66 (85%)	12 (15%)	0	100	100
17	AB	85/88 (97%)	75 (88%)	10 (12%)	0	100	100
18	D3	93/115 (81%)	84 (90%)	9 (10%)	0	100	100
19	D1	293/318 (92%)	264 (90%)	29 (10%)	0	100	100
20	D6	167/175 (95%)	141 (84%)	25 (15%)	1 (1%)	21	58
21	4L	96/98 (98%)	89 (93%)	6 (6%)	1 (1%)	12	46
22	D5	604/606 (100%)	537 (89%)	67 (11%)	0	100	100
23	D4	457/459 (100%)	418 (92%)	38 (8%)	1 (0%)	43	76
24	D2	345/347 (99%)	320 (93%)	25 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	AK	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
26	B5	137/143 (96%)	125 (91%)	12 (9%)	0	100	100
27	A8	169/171 (99%)	139 (82%)	30 (18%)	0	100	100
28	BJ	169/175 (97%)	153 (90%)	16 (10%)	0	100	100
29	AJ	317/320 (99%)	279 (88%)	38 (12%)	0	100	100
30	S5	97/105 (92%)	79 (81%)	18 (19%)	0	100	100
31	A3	72/83 (87%)	63 (88%)	9 (12%)	0	100	100
32	B3	71/97 (73%)	60 (84%)	11 (16%)	0	100	100
33	C2	117/120 (98%)	105 (90%)	12 (10%)	0	100	100
34	B4	126/128 (98%)	108 (86%)	18 (14%)	0	100	100
35	AM	137/143 (96%)	122 (89%)	15 (11%)	0	100	100
36	B6	92/127 (72%)	80 (87%)	12 (13%)	0	100	100
37	B7	117/136 (86%)	97 (83%)	20 (17%)	0	100	100
38	B9	174/178 (98%)	142 (82%)	32 (18%)	0	100	100
39	B2	63/72 (88%)	55 (87%)	8 (13%)	0	100	100
40	B8	155/158 (98%)	127 (82%)	27 (17%)	1 (1%)	21	58
41	BK	100/125 (80%)	88 (88%)	12 (12%)	0	100	100
42	C1	44/49 (90%)	38 (86%)	6 (14%)	0	100	100
43	B1	50/57 (88%)	43 (86%)	7 (14%)	0	100	100
44	A1	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
All	All	7983/8509 (94%)	7022 (88%)	956 (12%)	5 (0%)	49	81

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	D4	53	SER
20	D6	137	SER
21	4L	3	LEU
3	S1	359	ARG
40	B8	143	GLY

5.3.2 Protein sidechains ⓘ

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%)	343 (100%)	1 (0%)	86	85
2	V2	182/183 (100%)	181 (100%)	1 (0%)	81	82
3	S1	578/588 (98%)	576 (100%)	2 (0%)	86	85
4	S2	370/371 (100%)	367 (99%)	3 (1%)	73	77
5	S3	189/204 (93%)	188 (100%)	1 (0%)	81	82
6	S7	132/150 (88%)	131 (99%)	1 (1%)	73	77
7	S8	151/151 (100%)	151 (100%)	0	100	100
8	V3	39/68 (57%)	38 (97%)	1 (3%)	40	61
9	S6	79/80 (99%)	78 (99%)	1 (1%)	61	72
10	S4	113/119 (95%)	113 (100%)	0	100	100
11	A9	249/292 (85%)	249 (100%)	0	100	100
12	A2	73/81 (90%)	73 (100%)	0	100	100
13	A5	99/101 (98%)	98 (99%)	1 (1%)	68	76
14	A6	107/113 (95%)	107 (100%)	0	100	100
15	A7	82/94 (87%)	82 (100%)	0	100	100
16	AL	129/131 (98%)	128 (99%)	1 (1%)	73	77
17	AA	74/81 (91%)	73 (99%)	1 (1%)	59	71
17	AB	80/81 (99%)	79 (99%)	1 (1%)	61	72
18	D3	88/103 (85%)	87 (99%)	1 (1%)	65	74
19	D1	263/278 (95%)	261 (99%)	2 (1%)	73	77
20	D6	140/144 (97%)	138 (99%)	2 (1%)	59	71
21	4L	87/87 (100%)	87 (100%)	0	100	100
22	D5	539/539 (100%)	538 (100%)	1 (0%)	87	87
23	D4	412/412 (100%)	409 (99%)	3 (1%)	76	79
24	D2	315/315 (100%)	315 (100%)	0	100	100
25	AK	101/101 (100%)	101 (100%)	0	100	100
26	B5	122/125 (98%)	122 (100%)	0	100	100
27	A8	154/154 (100%)	154 (100%)	0	100	100
28	BJ	155/157 (99%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	AJ	283/284 (100%)	283 (100%)	0	100	100
30	S5	88/94 (94%)	87 (99%)	1 (1%)	65	74
31	A3	65/71 (92%)	65 (100%)	0	100	100
32	B3	55/75 (73%)	55 (100%)	0	100	100
33	C2	106/107 (99%)	106 (100%)	0	100	100
34	B4	114/114 (100%)	113 (99%)	1 (1%)	70	76
35	AM	119/121 (98%)	119 (100%)	0	100	100
36	B6	92/121 (76%)	90 (98%)	2 (2%)	45	64
37	B7	108/119 (91%)	108 (100%)	0	100	100
38	B9	159/160 (99%)	158 (99%)	1 (1%)	78	80
39	B2	59/62 (95%)	59 (100%)	0	100	100
40	B8	142/142 (100%)	141 (99%)	1 (1%)	76	79
41	BK	93/112 (83%)	93 (100%)	0	100	100
42	C1	42/44 (96%)	42 (100%)	0	100	100
43	B1	48/53 (91%)	47 (98%)	1 (2%)	47	65
44	A1	59/59 (100%)	59 (100%)	0	100	100
All	All	7078/7395 (96%)	7047 (100%)	31 (0%)	81	83

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

Mol	Chain	Res	Type
1	V1	365	CYS
2	V2	51	LEU
3	S1	484	THR
3	S1	543	ILE
4	S2	402	LEU
4	S2	418	ILE
4	S2	423	ILE
5	S3	85	THR
6	S7	54	CYS
8	V3	54	LEU
9	S6	26	VAL
13	A5	94	ILE
16	AL	117	LEU
17	AA	80	ILE
18	D3	73	LEU

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Mol	Chain	Res	Type
19	D1	103	LEU
19	D1	129	LEU
20	D6	12	ILE
20	D6	54	LEU
22	D5	350	LEU
23	D4	54	LEU
23	D4	150	LEU
23	D4	216	LEU
17	AB	80	ILE
30	S5	95	PRO
34	B4	120	LEU
36	B6	89	VAL
36	B6	90	THR
38	B9	23	LEU
40	B8	9	LEU
43	B1	48	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (141) such sidechains are listed below:

Mol	Chain	Res	Type
1	V1	29	HIS
1	V1	283	HIS
1	V1	361	GLN
1	V1	373	ASN
2	V2	9	HIS
2	V2	42	HIS
2	V2	101	GLN
2	V2	150	ASN
2	V2	157	ASN
2	V2	159	ASN
3	S1	51	ASN
3	S1	117	GLN
3	S1	336	ASN
3	S1	437	HIS
3	S1	535	GLN
3	S1	548	HIS
3	S1	621	ASN
4	S2	34	ASN
4	S2	46	ASN
4	S2	50	ASN
4	S2	54	GLN
4	S2	135	GLN

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Mol	Chain	Res	Type
4	S2	201	GLN
5	S3	38	GLN
5	S3	39	GLN
5	S3	88	ASN
5	S3	192	GLN
6	S7	106	GLN
7	S8	168	ASN
8	V3	40	ASN
8	V3	65	GLN
9	S6	94	GLN
10	S4	46	GLN
11	A9	3	HIS
11	A9	36	ASN
11	A9	89	ASN
11	A9	148	ASN
11	A9	288	HIS
11	A9	306	GLN
12	A2	24	GLN
12	A2	47	ASN
13	A5	49	GLN
13	A5	82	GLN
14	A6	94	ASN
14	A6	125	HIS
15	A7	20	GLN
16	AL	12	GLN
16	AL	31	ASN
16	AL	72	ASN
18	D3	10	ASN
19	D1	5	ASN
19	D1	157	ASN
19	D1	194	ASN
19	D1	287	HIS
20	D6	175	ASN
21	4L	25	HIS
21	4L	83	ASN
22	D5	113	ASN
22	D5	116	GLN
22	D5	136	ASN
22	D5	139	GLN
22	D5	194	ASN
22	D5	199	GLN
22	D5	200	GLN

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Mol	Chain	Res	Type
22	D5	226	GLN
22	D5	274	GLN
22	D5	323	HIS
22	D5	405	ASN
22	D5	434	GLN
22	D5	446	ASN
22	D5	447	ASN
22	D5	541	ASN
22	D5	580	GLN
23	D4	26	ASN
23	D4	30	HIS
23	D4	83	HIS
23	D4	138	ASN
23	D4	220	HIS
23	D4	319	HIS
23	D4	399	ASN
23	D4	425	ASN
23	D4	450	ASN
24	D2	36	ASN
24	D2	63	GLN
24	D2	204	ASN
24	D2	222	ASN
24	D2	235	ASN
24	D2	316	GLN
26	B5	86	ASN
26	B5	95	GLN
26	B5	124	GLN
17	AB	33	ASN
17	AB	47	GLN
17	AB	74	GLN
27	A8	63	ASN
27	A8	76	HIS
27	A8	150	ASN
28	BJ	55	HIS
28	BJ	103	ASN
28	BJ	106	GLN
28	BJ	113	GLN
28	BJ	114	GLN
28	BJ	122	GLN
29	AJ	21	ASN
29	AJ	92	ASN
29	AJ	151	HIS

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Mol	Chain	Res	Type
29	AJ	200	GLN
29	AJ	204	ASN
29	AJ	251	GLN
29	AJ	271	ASN
30	S5	44	HIS
31	A3	68	HIS
31	A3	70	GLN
32	B3	47	ASN
33	C2	59	HIS
34	B4	47	GLN
34	B4	74	ASN
35	AM	60	GLN
35	AM	89	ASN
36	B6	13	GLN
36	B6	88	HIS
37	B7	43	GLN
37	B7	83	GLN
37	B7	91	HIS
38	B9	12	GLN
38	B9	50	HIS
38	B9	140	GLN
38	B9	168	HIS
39	B2	16	GLN
40	B8	3	HIS
40	B8	66	HIS
40	B8	104	HIS
40	B8	126	GLN
40	B8	136	ASN
40	B8	137	ASN
40	B8	155	HIS
41	BK	36	ASN
41	BK	45	HIS
41	BK	57	ASN
42	C1	34	GLN
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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	$\# Z > 2$
47	FES	S1	803	3	0,4,4	-	-	-		
47	FES	V2	300	2	0,4,4	-	-	-		
50	ZMP	B9	201	17	25,30,36	0.67	0	29,37,45	1.02	2 (6%)
51	3PE	D4	501	-	39,39,50	0.34	0	42,44,55	0.32	0
51	3PE	D5	902	-	37,37,50	0.36	0	40,42,55	0.35	0
45	SF4	S7	300	6	0,12,12	-	-	-		
52	CDL	D5	901	-	35,35,99	0.44	0	41,47,111	0.75	2 (4%)
45	SF4	S1	802	3	0,12,12	-	-	-		
51	3PE	D1	501	-	18,18,50	0.43	0	21,23,55	0.44	0
51	3PE	A8	301	-	24,24,50	0.44	0	27,29,55	0.37	0
45	SF4	V1	500	1	0,12,12	-	-	-		
53	PC1	D4	502	-	27,27,53	0.39	0	33,35,61	0.41	0
50	ZMP	AA	101	17	28,33,36	0.69	1 (3%)	32,40,45	0.96	1 (3%)
45	SF4	S1	801	3	0,12,12	-	-	-		
46	FMN	V1	501	-	33,33,33	0.35	0	48,50,50	0.37	0
49	NDP	A9	401	-	51,52,52	0.43	0	71,80,80	0.54	1 (1%)
45	SF4	S8	201	7	0,12,12	-	-	-		
45	SF4	S8	202	7	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
47	FES	S1	803	3	-	-	0/1/1/1
47	FES	V2	300	2	-	-	0/1/1/1
50	ZMP	B9	201	17	-	12/35/37/43	-
51	3PE	D4	501	-	-	7/43/43/54	-
45	SF4	S8	202	7	-	-	0/6/5/5
45	SF4	S7	300	6	-	-	0/6/5/5
52	CDL	D5	901	-	-	16/42/42/110	-
45	SF4	S8	201	7	-	-	0/6/5/5
45	SF4	S1	802	3	-	-	0/6/5/5
51	3PE	D1	501	-	-	10/20/20/54	-
51	3PE	A8	301	-	-	4/28/28/54	-
45	SF4	V1	500	1	-	-	0/6/5/5
53	PC1	D4	502	-	-	7/31/31/57	-
46	FMN	V1	501	-	-	10/18/18/18	0/3/3/3
45	SF4	S1	801	3	-	-	0/6/5/5
49	NDP	A9	401	-	-	13/34/77/77	0/5/5/5
51	3PE	D5	902	-	-	9/41/41/54	-
50	ZMP	AA	101	17	-	13/38/40/43	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	AA	101	ZMP	C9-C10	2.47	1.53	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	D5	901	CDL	CB4-OB6-CB5	3.03	123.19	117.85
49	A9	401	NDP	P2B-O2B-C2B	2.51	130.15	123.43
50	B9	201	ZMP	O1-C10-C9	-2.47	121.13	123.98
50	B9	201	ZMP	C11-C12-N1	-2.36	107.50	112.41
50	AA	101	ZMP	O1-C10-C9	-2.34	121.28	123.98
52	D5	901	CDL	OB6-CB4-CB3	2.12	115.96	108.34

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	N10-C1'-C2'-O2'
46	V1	501	FMN	C1'-C2'-C3'-O3'
46	V1	501	FMN	C1'-C2'-C3'-C4'
46	V1	501	FMN	C5'-O5'-P-O1P
46	V1	501	FMN	C5'-O5'-P-O2P
46	V1	501	FMN	C5'-O5'-P-O3P
49	A9	401	NDP	C5B-O5B-PA-O1A
49	A9	401	NDP	C5B-O5B-PA-O2A
49	A9	401	NDP	C5B-O5B-PA-O3
49	A9	401	NDP	C1B-C2B-O2B-P2B
49	A9	401	NDP	C5D-O5D-PN-O2N
49	A9	401	NDP	C2N-C3N-C7N-N7N
50	AA	101	ZMP	C19-C18-C21-O5
50	AA	101	ZMP	C20-C18-C21-O5
50	AA	101	ZMP	C17-C18-C21-O5
50	AA	101	ZMP	N2-C16-C17-O4
50	B9	201	ZMP	C12-C11-S1-C10
50	B9	201	ZMP	O1-C10-S1-C11
50	B9	201	ZMP	C9-C10-S1-C11
51	D1	501	3PE	C1-O11-P-O12
51	D1	501	3PE	C1-O11-P-O13
51	D1	501	3PE	C1-O11-P-O14
51	D1	501	3PE	C11-O13-P-O14
51	D5	902	3PE	C11-O13-P-O11
51	D5	902	3PE	C11-O13-P-O12
51	D5	902	3PE	C11-O13-P-O14
51	D5	902	3PE	O13-C11-C12-N
51	D5	902	3PE	O21-C2-C3-O31
51	D4	501	3PE	C11-O13-P-O11
51	D4	501	3PE	C11-O13-P-O12
51	A8	301	3PE	C11-O13-P-O11
51	A8	301	3PE	C11-O13-P-O14
52	D5	901	CDL	CA2-OA2-PA1-OA3
52	D5	901	CDL	CA2-OA2-PA1-OA5
52	D5	901	CDL	CA3-OA5-PA1-OA2
52	D5	901	CDL	CA3-OA5-PA1-OA3
52	D5	901	CDL	CB2-OB2-PB2-OB4
52	D5	901	CDL	CB2-OB2-PB2-OB5
52	D5	901	CDL	CB3-OB5-PB2-OB2
52	D5	901	CDL	CB3-OB5-PB2-OB3
52	D5	901	CDL	CB3-OB5-PB2-OB4
53	D4	502	PC1	C1-O11-P-O12
53	D4	502	PC1	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
50	AA	101	ZMP	C14-C13-N1-C12
50	B9	201	ZMP	C14-C13-N1-C12
50	AA	101	ZMP	O2-C13-N1-C12
50	B9	201	ZMP	O2-C13-N1-C12
52	D5	901	CDL	OB5-CB3-CB4-OB6
51	D5	902	3PE	C21-C22-C23-C24
51	D5	902	3PE	C1-C2-C3-O31
51	D1	501	3PE	O21-C2-C3-O31
51	D1	501	3PE	C1-C2-C3-O31
50	AA	101	ZMP	C2-C3-C4-C5
46	V1	501	FMN	O2'-C2'-C3'-O3'
49	A9	401	NDP	PN-O3-PA-O5B
46	V1	501	FMN	O2'-C2'-C3'-C4'
52	D5	901	CDL	OB5-CB3-CB4-CB6
53	D4	502	PC1	O11-C1-C2-C3
50	AA	101	ZMP	C16-C17-C18-C19
53	D4	502	PC1	O13-C11-C12-N
50	AA	101	ZMP	O3-C16-C17-O4
50	B9	201	ZMP	O3-C16-C17-O4
46	V1	501	FMN	N10-C1'-C2'-C3'
50	AA	101	ZMP	C16-C17-C18-C21
53	D4	502	PC1	O11-C1-C2-O21
49	A9	401	NDP	C2N-C3N-C7N-O7N
49	A9	401	NDP	C5D-O5D-PN-O3
49	A9	401	NDP	C5D-O5D-PN-O1N
51	D1	501	3PE	C11-O13-P-O11
51	D1	501	3PE	C11-O13-P-O12
51	D4	501	3PE	C11-O13-P-O14
51	A8	301	3PE	C11-O13-P-O12
52	D5	901	CDL	CA2-OA2-PA1-OA4
52	D5	901	CDL	CA3-OA5-PA1-OA4
50	B9	201	ZMP	C6-C7-C8-C9
46	V1	501	FMN	C4'-C5'-O5'-P
52	D5	901	CDL	C1-CA2-OA2-PA1
50	AA	101	ZMP	O4-C17-C18-C20
50	B9	201	ZMP	O4-C17-C18-C20
51	D5	902	3PE	C26-C27-C28-C29
49	A9	401	NDP	O4D-C1D-N1N-C6N
52	D5	901	CDL	CB6-CB4-OB6-CB5
51	D1	501	3PE	C2-C1-O11-P
51	D4	501	3PE	C36-C37-C38-C39
51	D5	902	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
50	AA	101	ZMP	C7-C8-C9-C10
49	A9	401	NDP	C4B-C5B-O5B-PA
51	D4	501	3PE	C2-C1-O11-P
51	D4	501	3PE	C34-C35-C36-C37
51	A8	301	3PE	C2-C1-O11-P
52	D5	901	CDL	C1-CB2-OB2-PB2
50	AA	101	ZMP	C16-C17-C18-C20
50	B9	201	ZMP	C16-C17-C18-C19
50	B9	201	ZMP	C16-C17-C18-C20
51	D1	501	3PE	C12-C11-O13-P
53	D4	502	PC1	O31-C31-C32-C33
51	D4	501	3PE	C38-C39-C3A-C3B
49	A9	401	NDP	C2B-O2B-P2B-O3X
50	B9	201	ZMP	C16-C17-C18-C21
53	D4	502	PC1	O32-C31-C32-C33
50	B9	201	ZMP	N2-C16-C17-O4

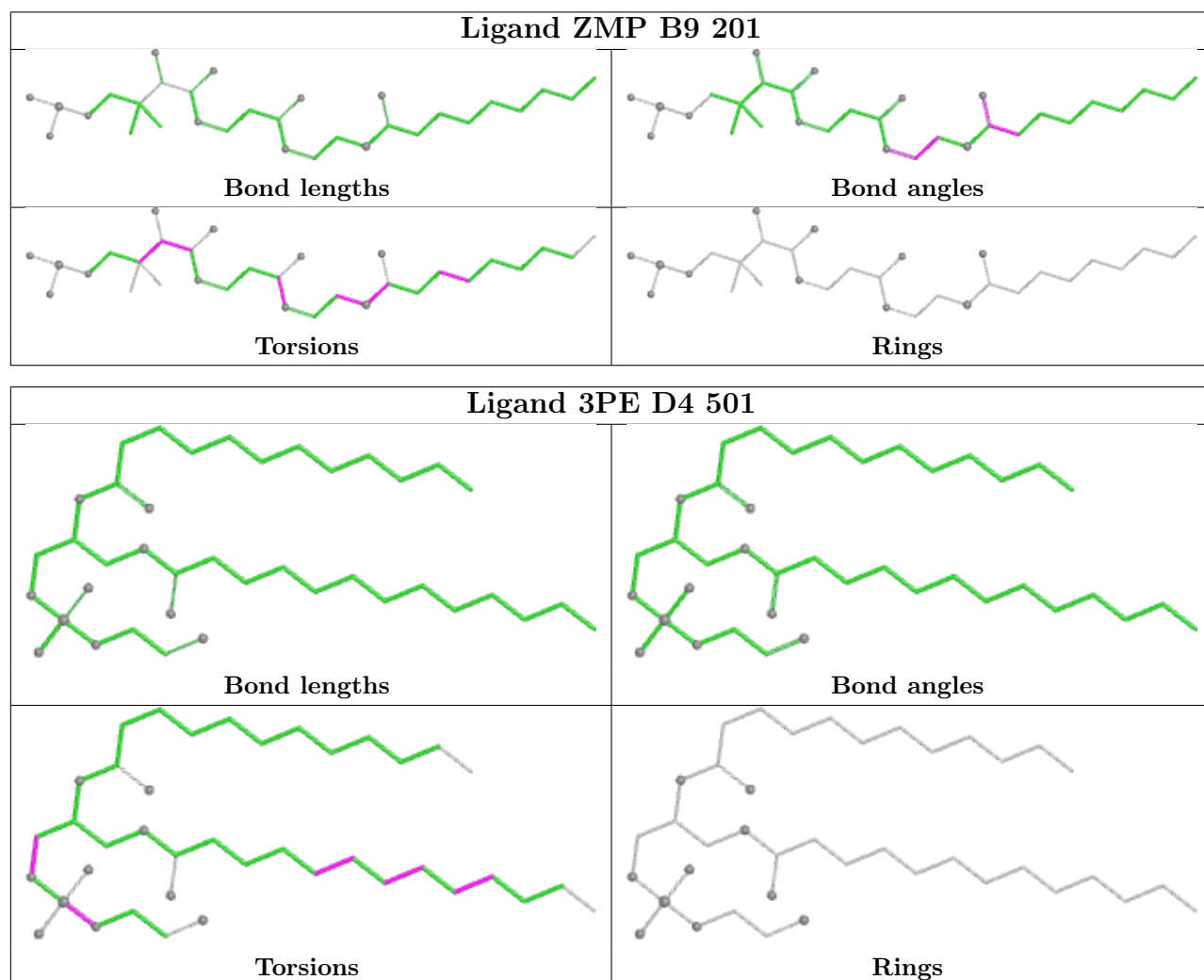
There are no ring outliers.

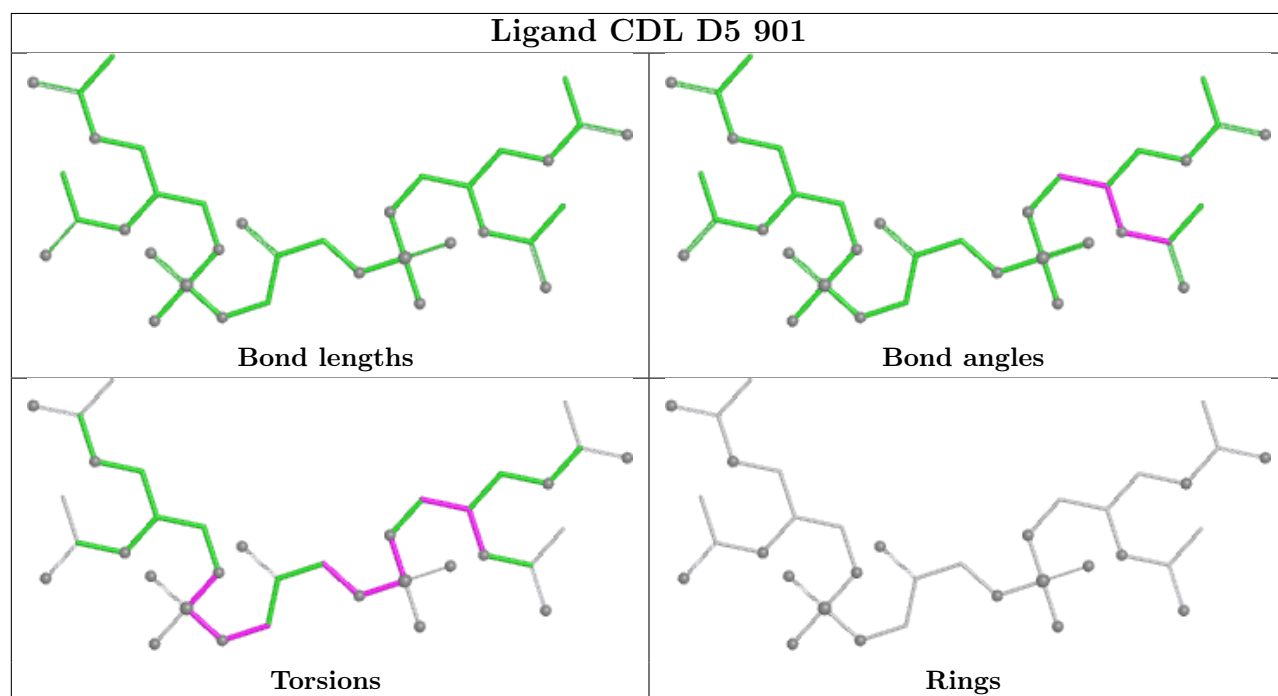
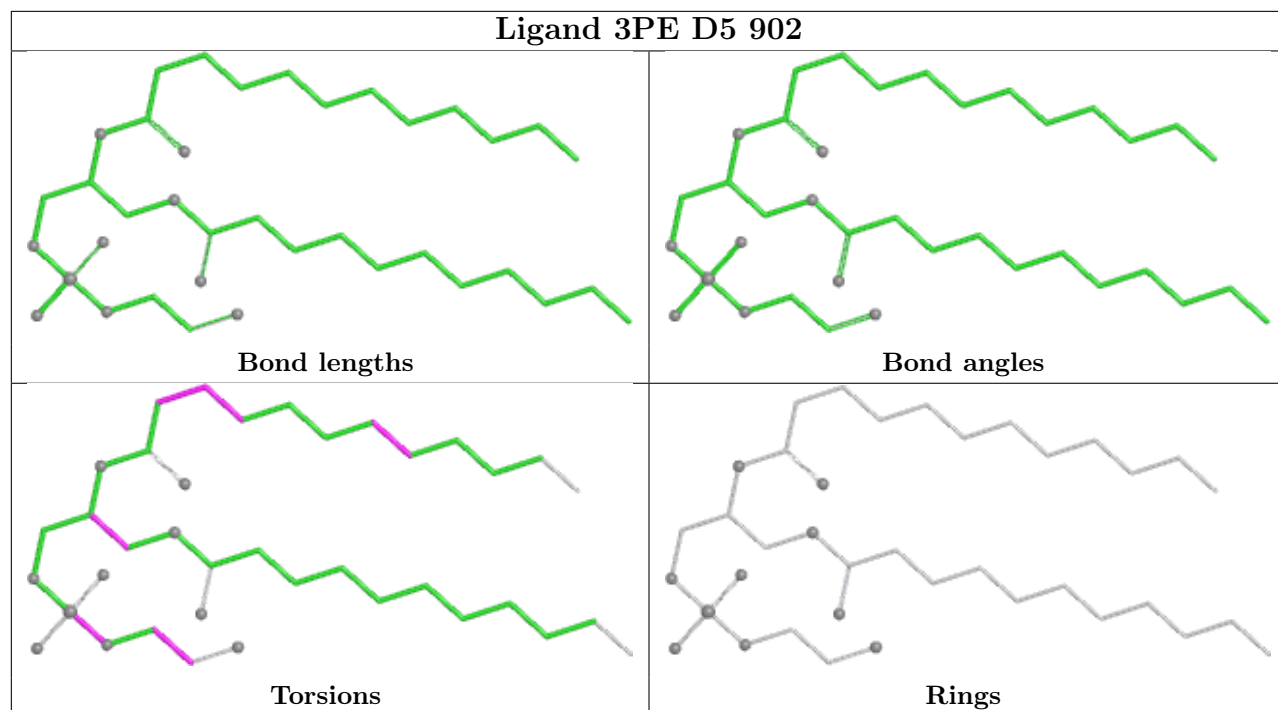
10 monomers are involved in 28 short contacts:

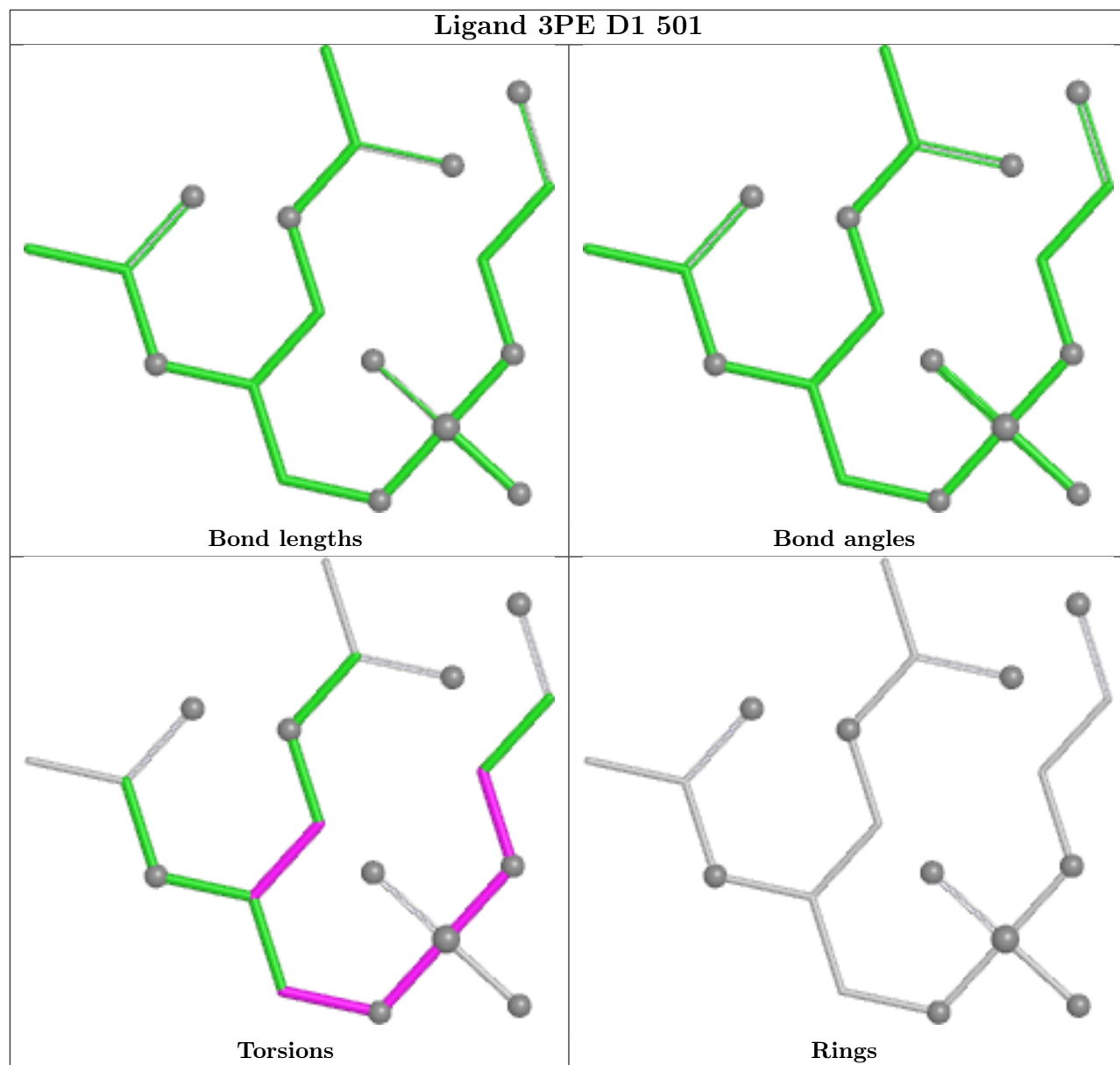
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	B9	201	ZMP	3	0
51	D4	501	3PE	2	0
51	D5	902	3PE	4	0
52	D5	901	CDL	2	0
51	A8	301	3PE	1	0
45	V1	500	SF4	2	0
50	AA	101	ZMP	7	0
45	S1	801	SF4	1	0
46	V1	501	FMN	1	0
49	A9	401	NDP	5	0

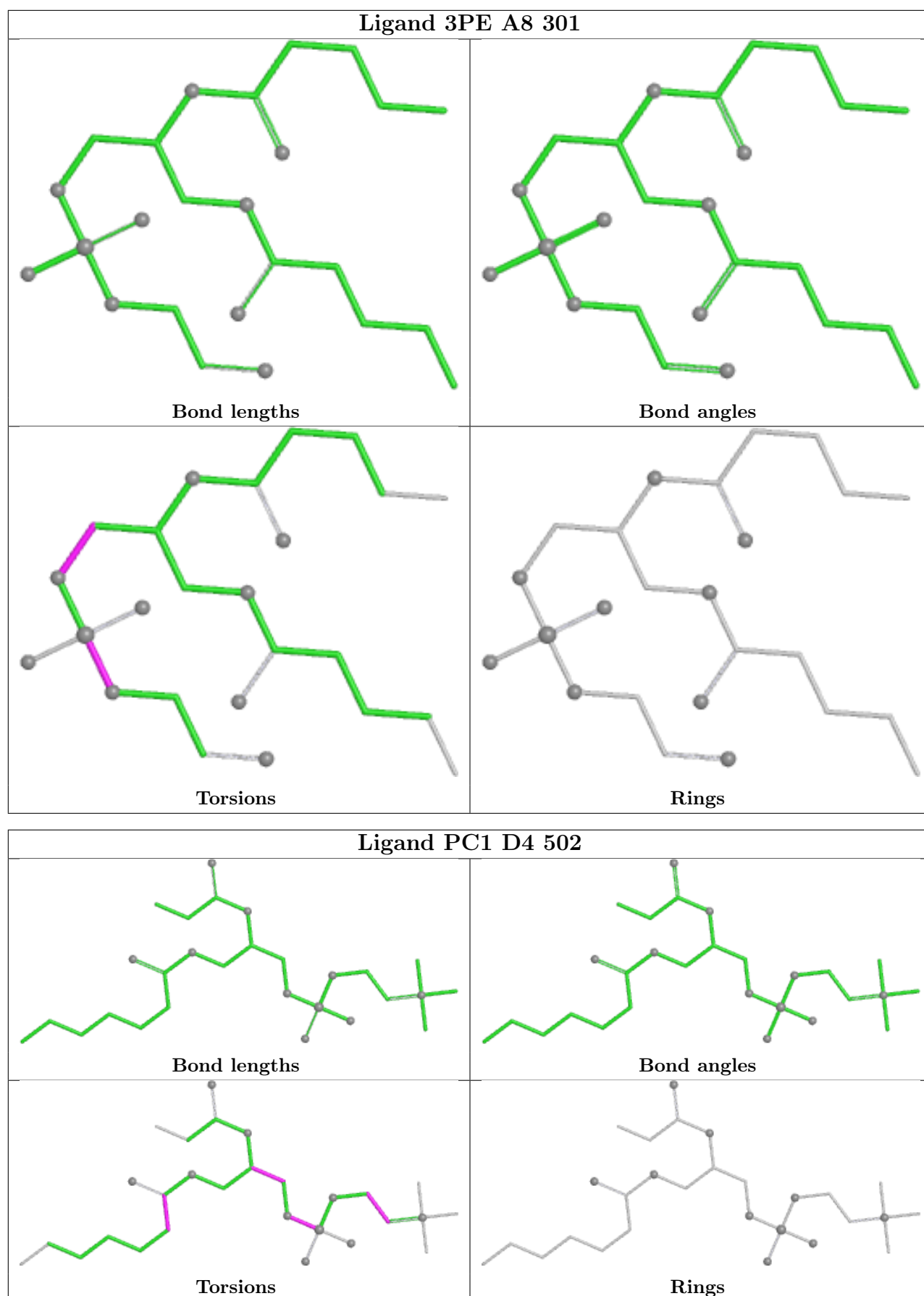
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

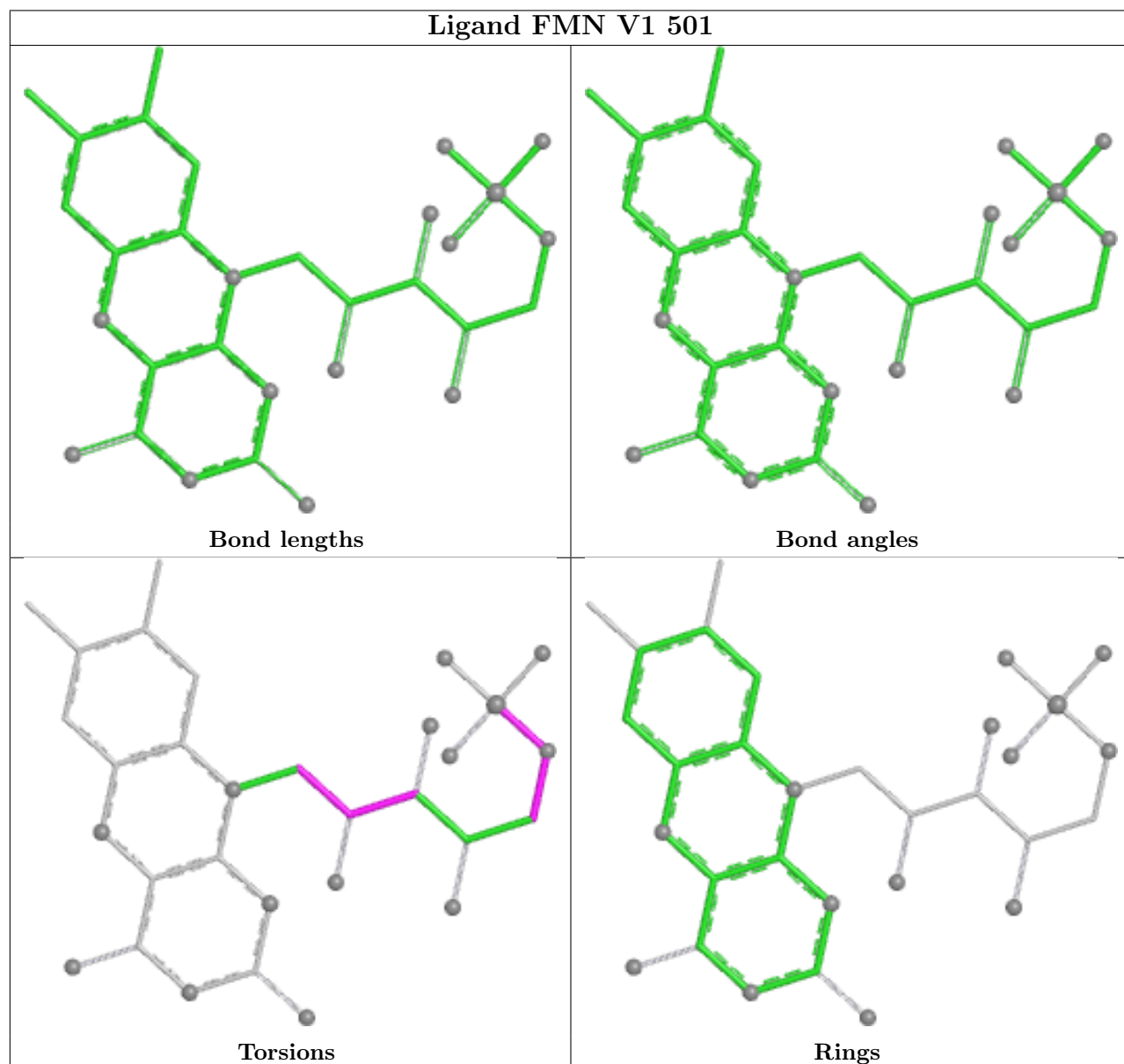
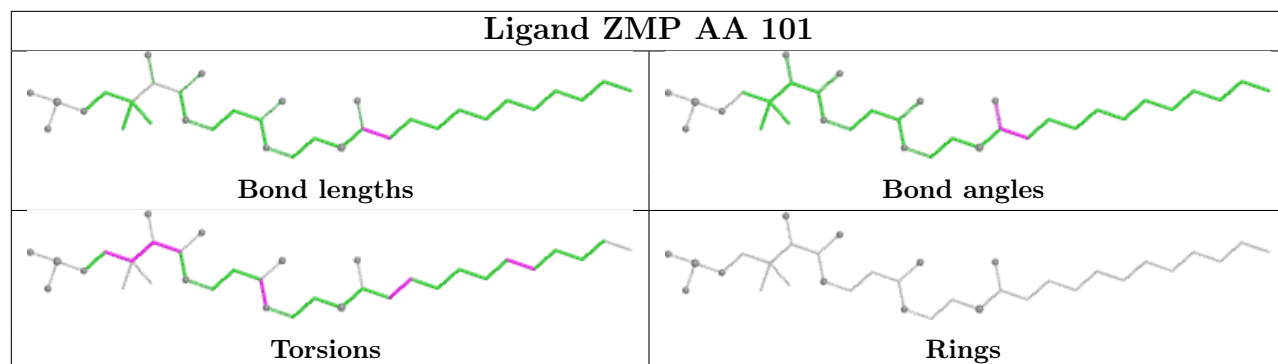
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

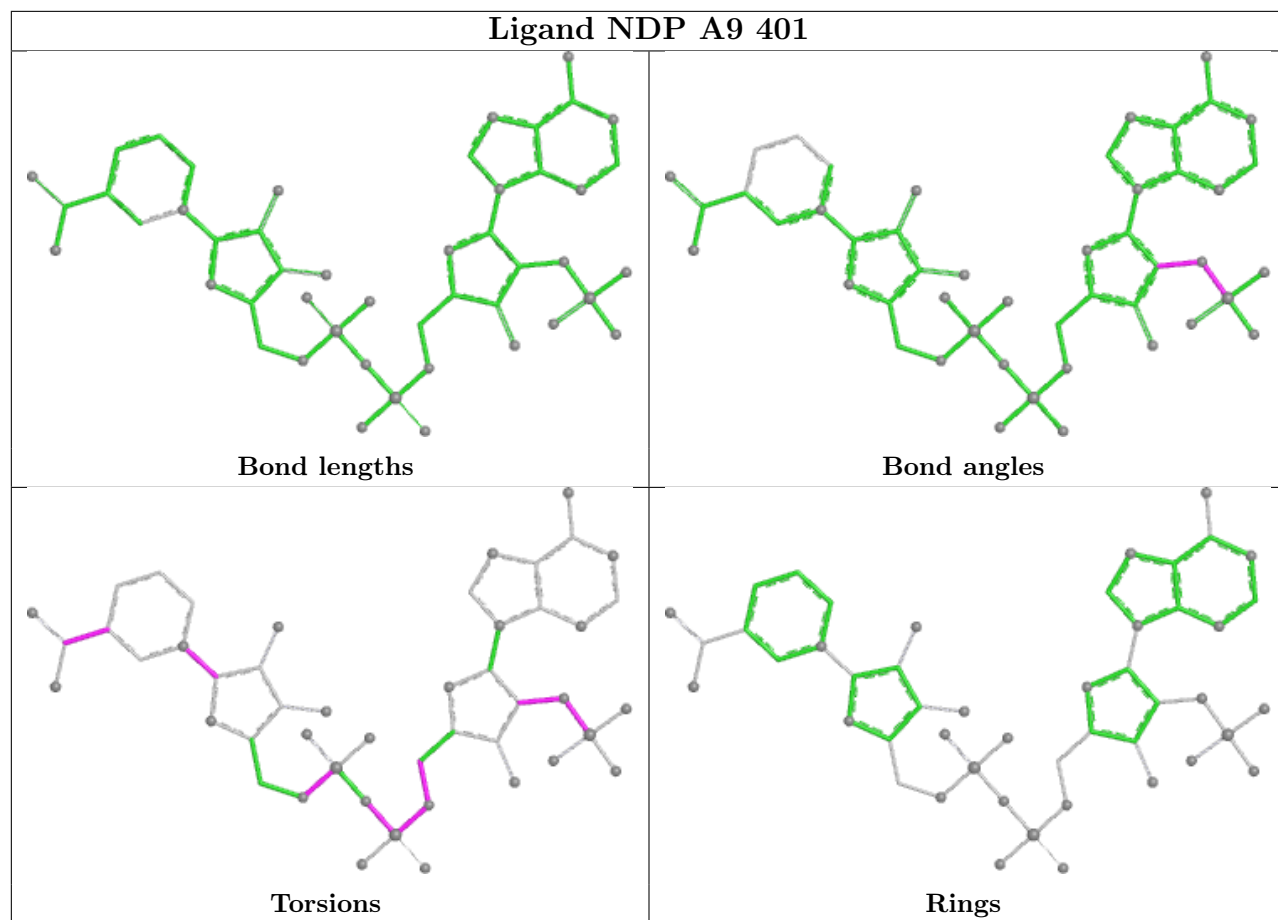












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

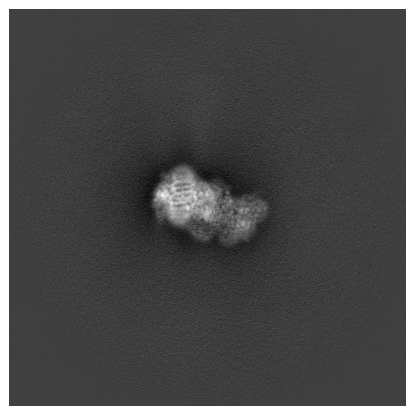
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4482. These allow visual inspection of the internal detail of the map and identification of artifacts.

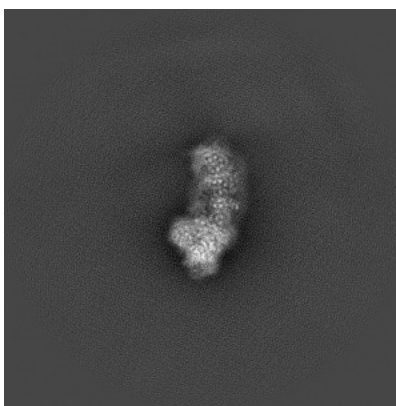
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

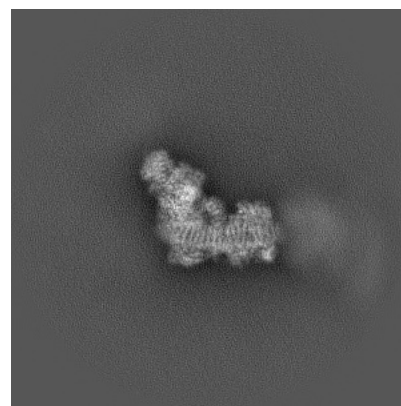
6.1.1 Primary map



X

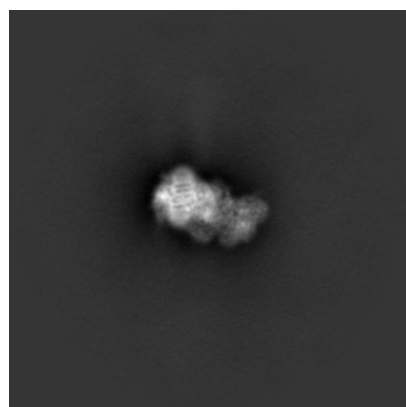


Y

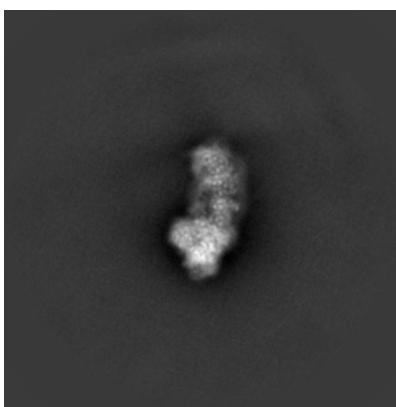


Z

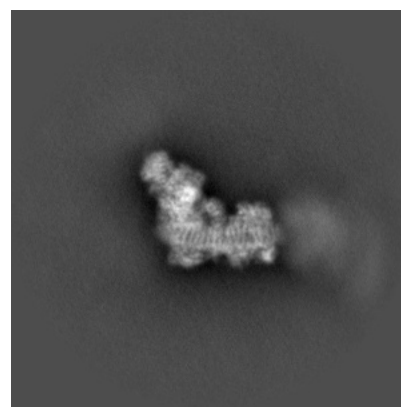
6.1.2 Raw map



X



Y

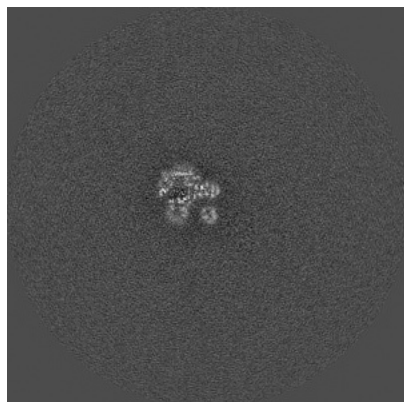


Z

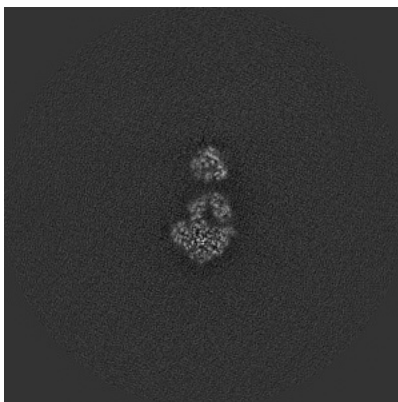
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

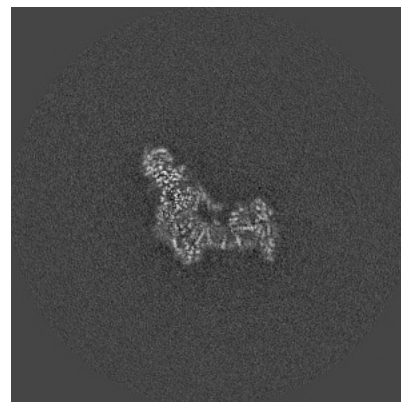
6.2.1 Primary map



X Index: 256

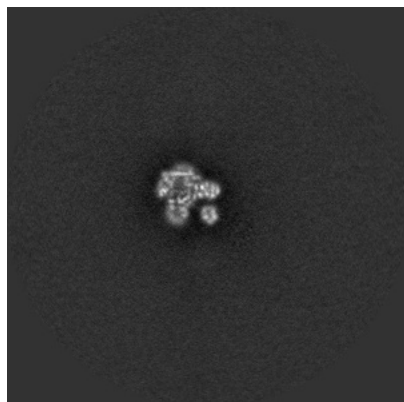


Y Index: 256

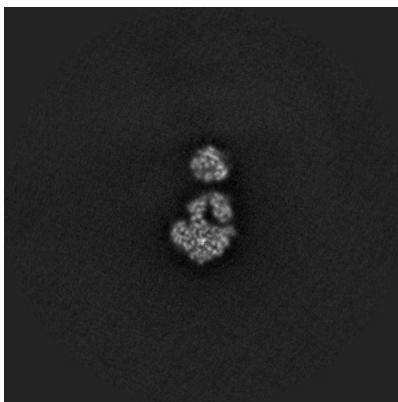


Z Index: 256

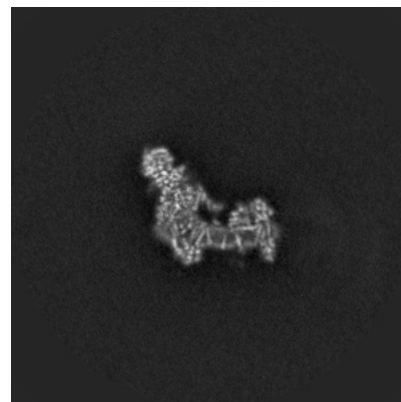
6.2.2 Raw map



X Index: 256



Y Index: 256

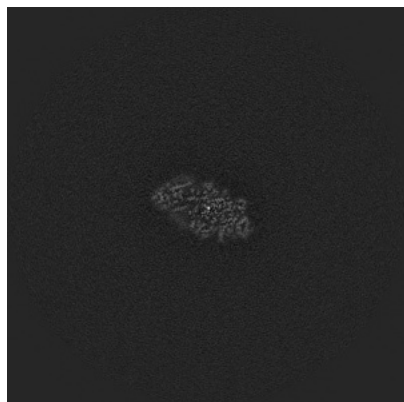


Z Index: 256

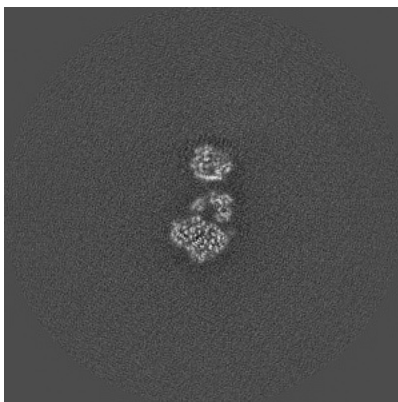
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

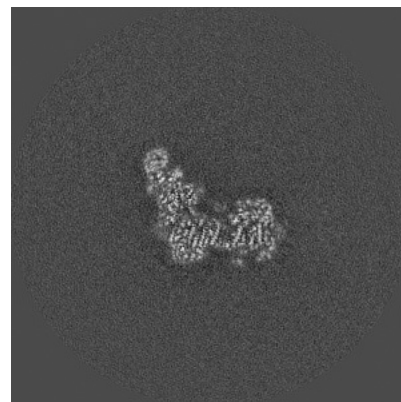
6.3.1 Primary map



X Index: 212

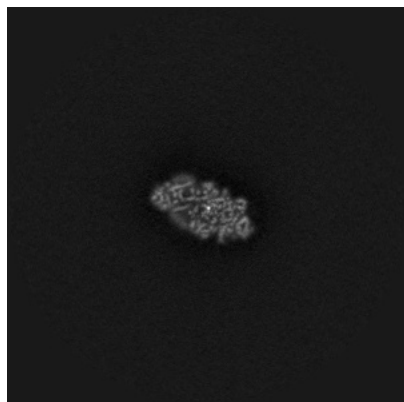


Y Index: 252

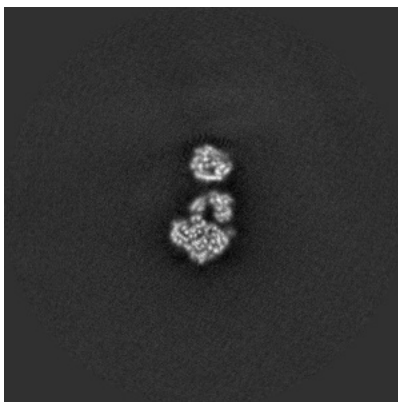


Z Index: 263

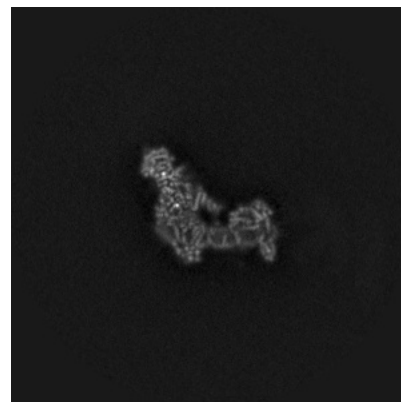
6.3.2 Raw map



X Index: 212



Y Index: 253

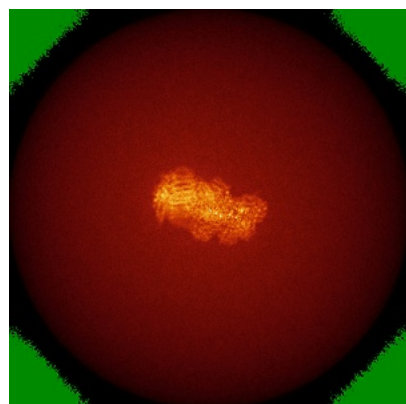


Z Index: 254

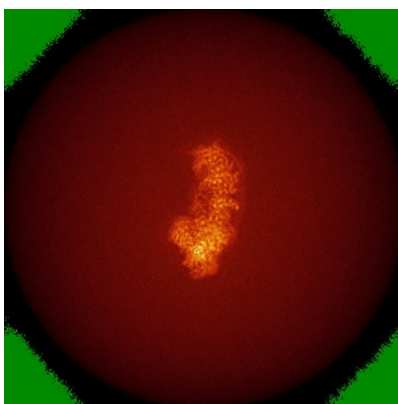
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

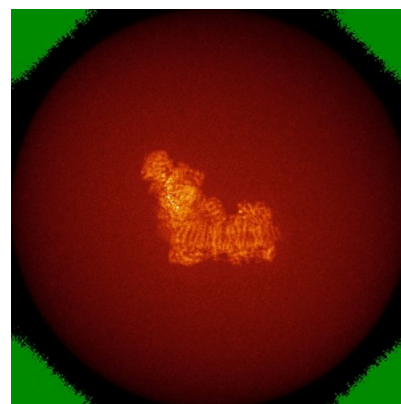
6.4.1 Primary map



X

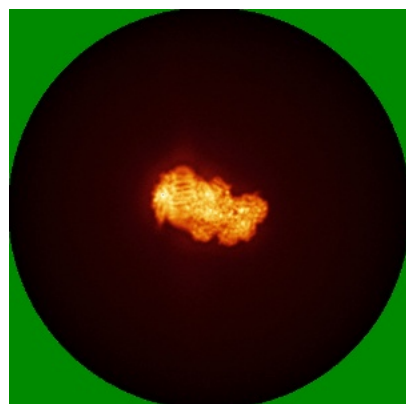


Y



Z

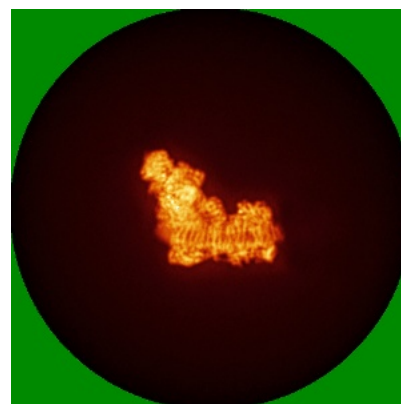
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



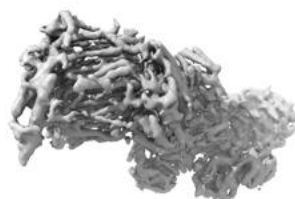
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

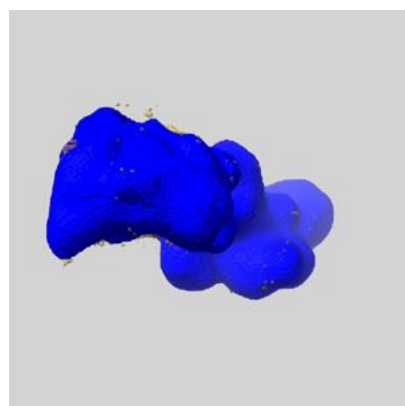
6.6 Mask visualisation [i](#)

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

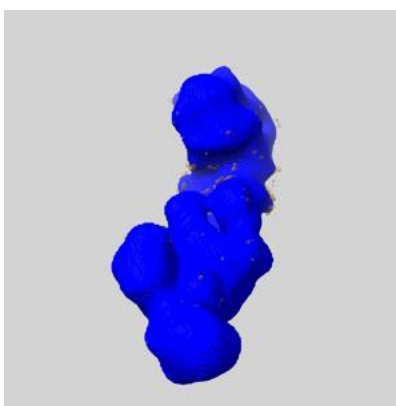
A mask typically either:

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

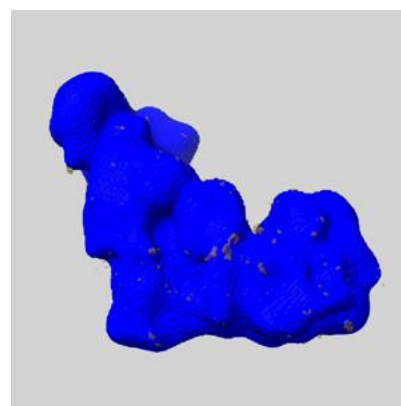
6.6.1 emd_4482_msk_1.map [i](#)



X



Y

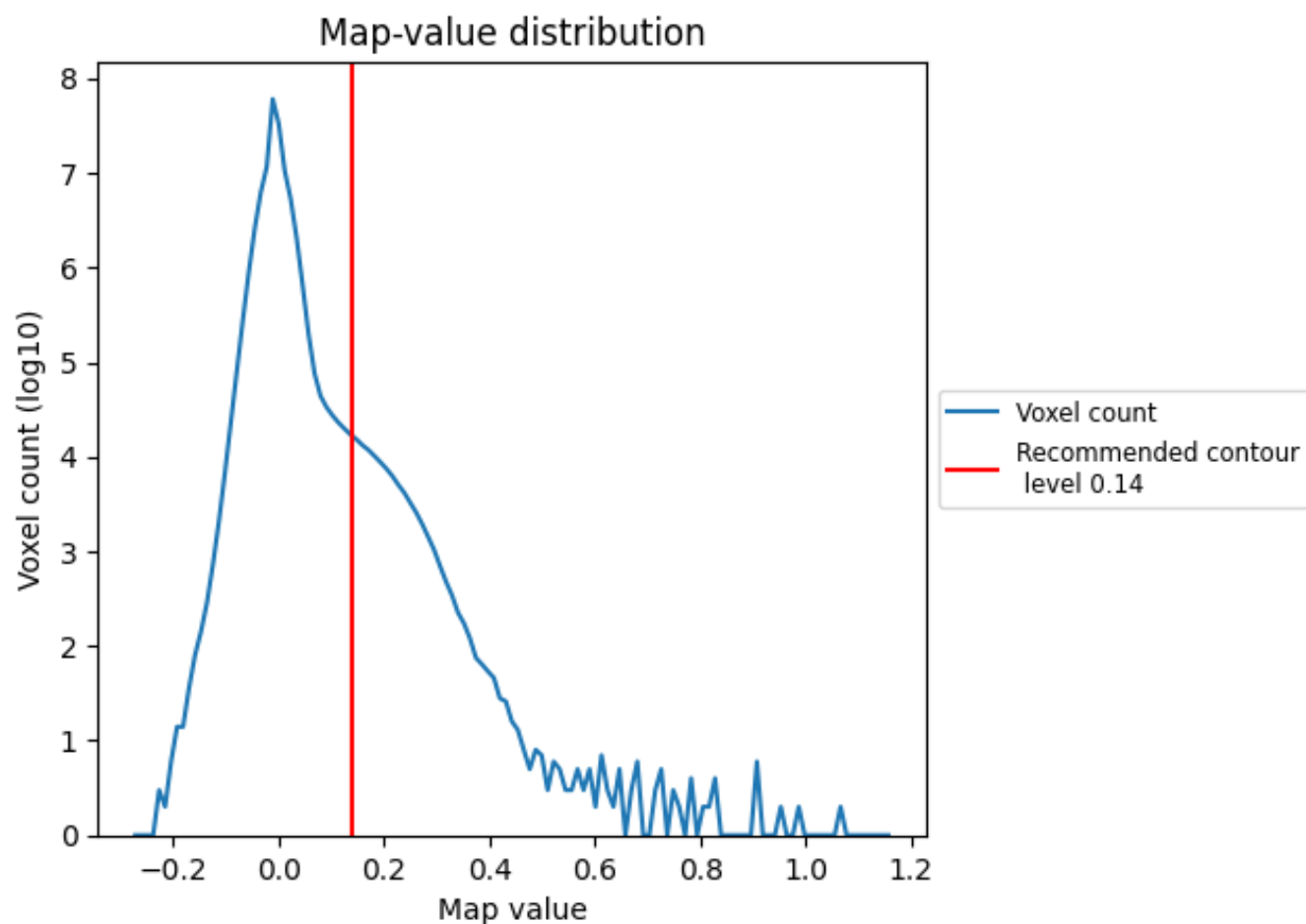


Z

7 Map analysis [i](#)

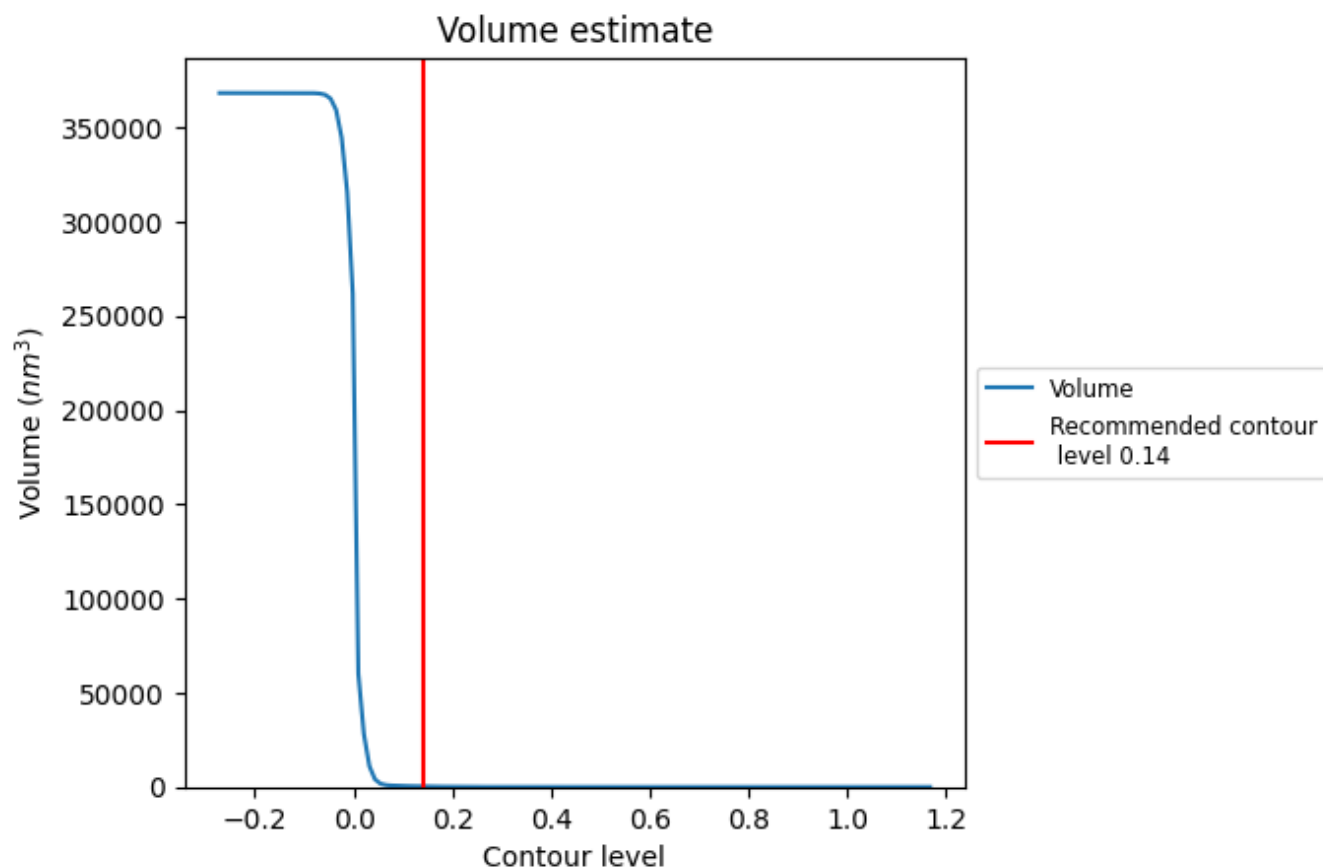
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

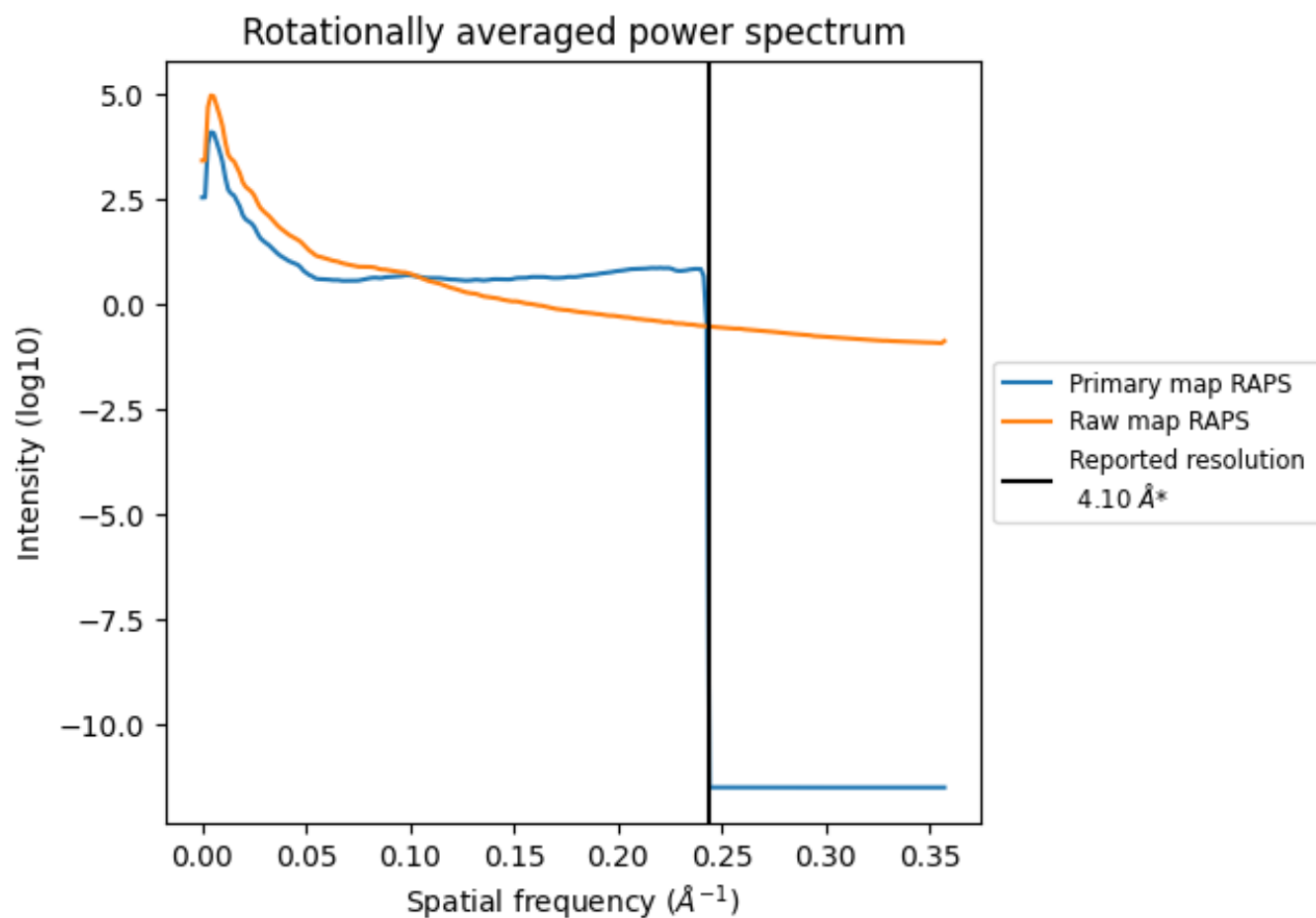
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 294 nm^3 ; this corresponds to an approximate mass of 266 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 ⓘ

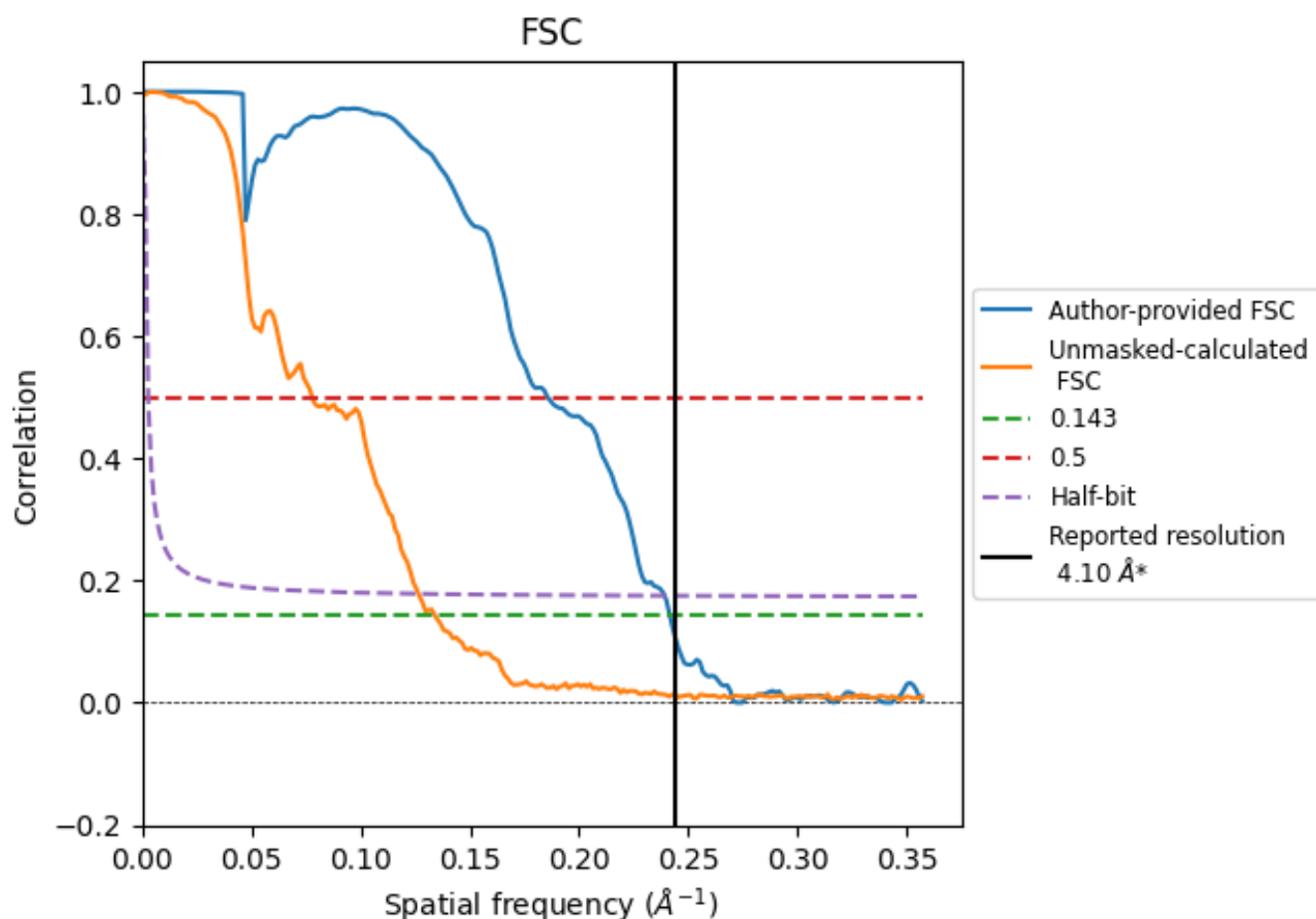


*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of $0.244 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

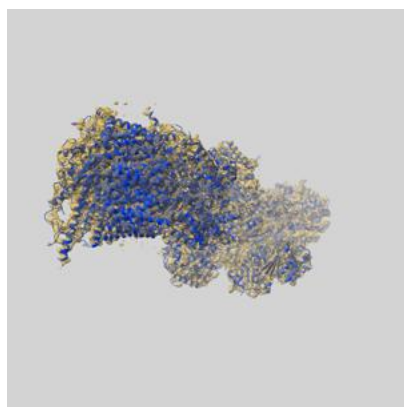
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	5.39	4.18
Unmasked-calculated*	7.47	12.85	7.91

*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 7.47 differs from the reported value 4.1 by more than 10 %

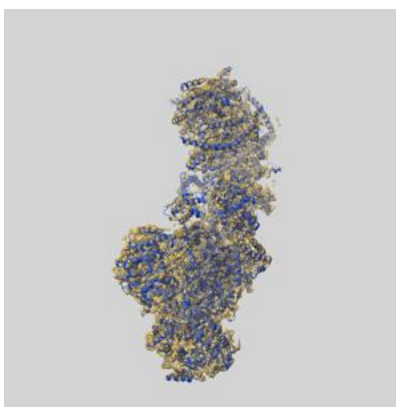
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4482 and PDB model 6QA9. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

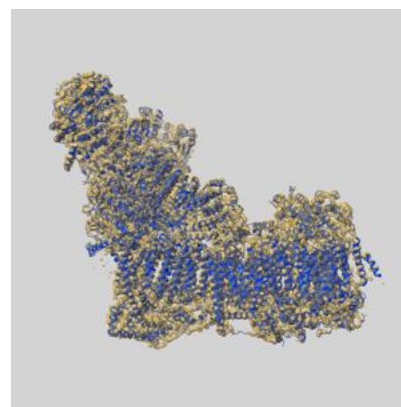
9.1 Map-model overlay [i](#)



X



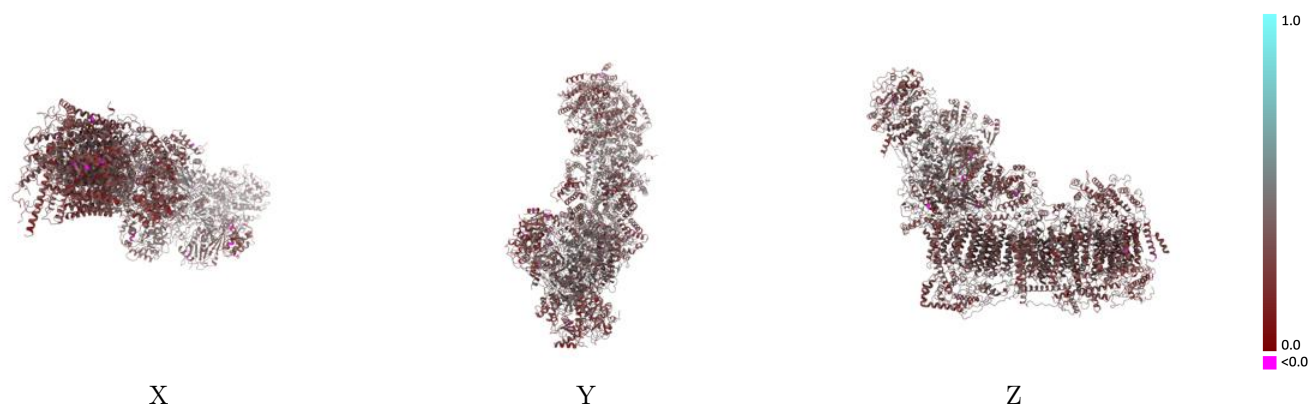
Y



Z

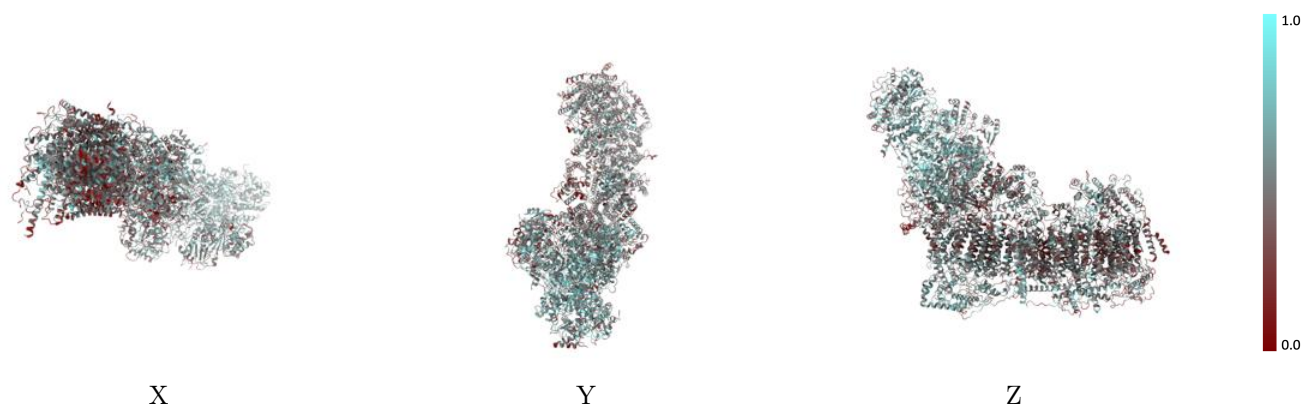
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



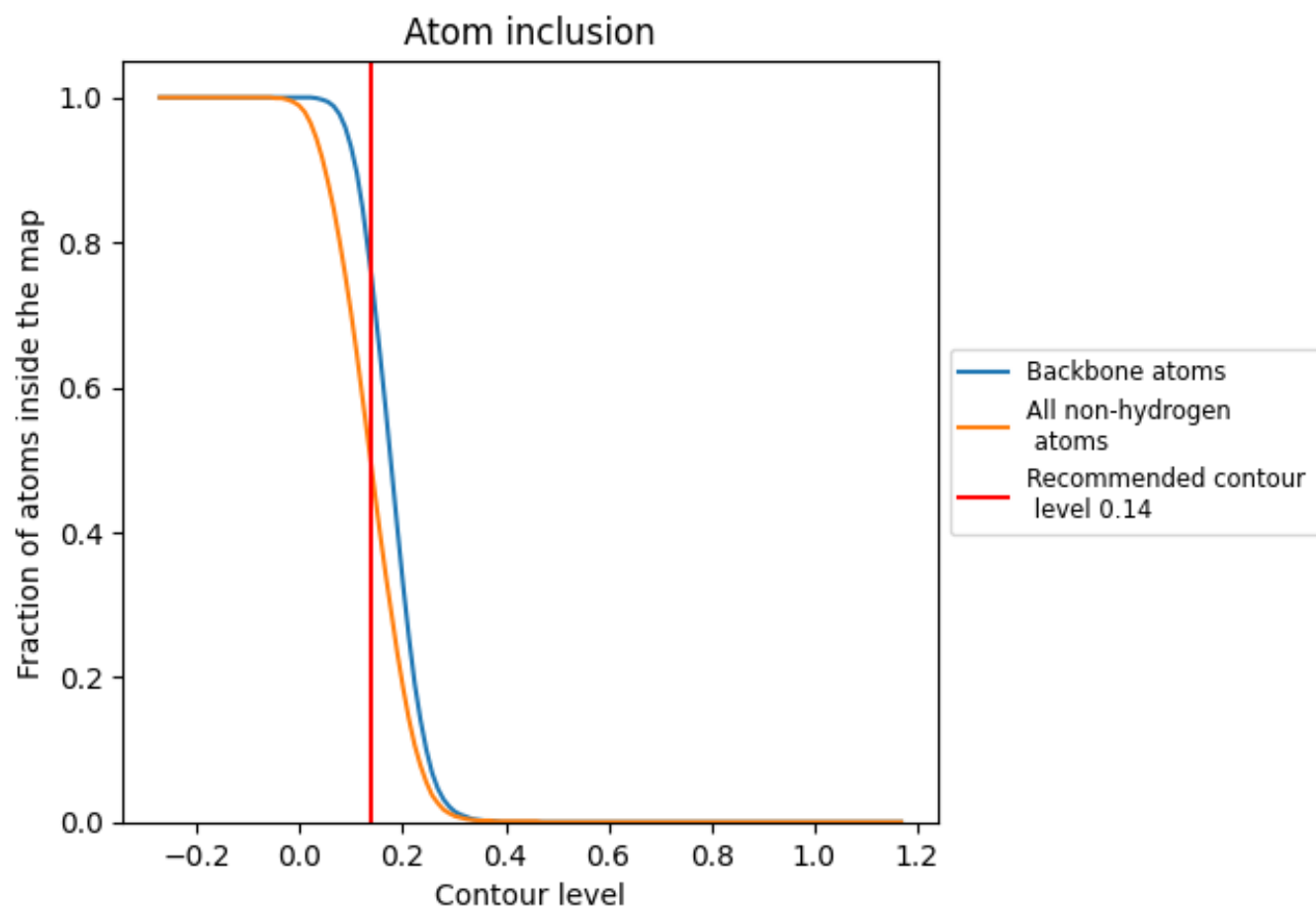
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.14).

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 49% 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 (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4870	 0.3370
4L	 0.4330	 0.3330
A1	 0.5540	 0.3400
A2	 0.4890	 0.2930
A3	 0.4980	 0.3470
A5	 0.5120	 0.3270
A6	 0.4690	 0.3290
A7	 0.4300	 0.3650
A8	 0.5420	 0.3340
A9	 0.4630	 0.3220
AA	 0.2730	 0.2560
AB	 0.4250	 0.2950
AJ	 0.4670	 0.3350
AK	 0.3350	 0.3040
AL	 0.3600	 0.3630
AM	 0.5170	 0.3260
B1	 0.3900	 0.3110
B2	 0.3850	 0.2960
B3	 0.3470	 0.2840
B4	 0.4470	 0.3120
B5	 0.5190	 0.3560
B6	 0.4250	 0.3000
B7	 0.4240	 0.2790
B8	 0.4490	 0.3290
B9	 0.4920	 0.3100
BJ	 0.5000	 0.3190
BK	 0.4130	 0.3130
C1	 0.4710	 0.3390
C2	 0.4860	 0.3340
D1	 0.4880	 0.3460
D2	 0.5070	 0.3630
D3	 0.3850	 0.3360
D4	 0.4720	 0.3590
D5	 0.4170	 0.3160
D6	 0.3840	 0.3110



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S1	 0.5570	 0.3520
S2	 0.5260	 0.3680
S3	 0.5750	 0.3850
S4	 0.5300	 0.3790
S5	 0.5270	 0.3420
S6	 0.5560	 0.3780
S7	 0.5630	 0.3860
S8	 0.6080	 0.3900
V1	 0.5730	 0.3220
V2	 0.5440	 0.3160
V3	 0.5640	 0.3150