



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:31 AM UTC

PDB ID : 6QC6 / pdb_00006qc6
EMDB ID : EMD-4498
Title : Ovine respiratory complex I FRC open class 1
Authors : Letts, J.A.; Sazanov, L.A.
Deposited on : 2018-12-27
Resolution : 4.10 Å(reported)
Based on initial model : 5LNK

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

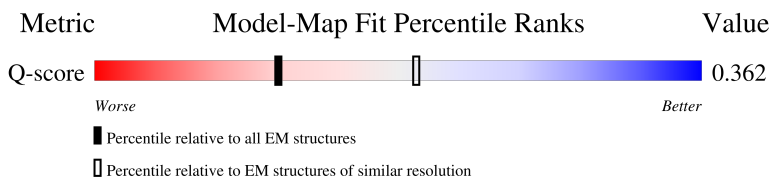
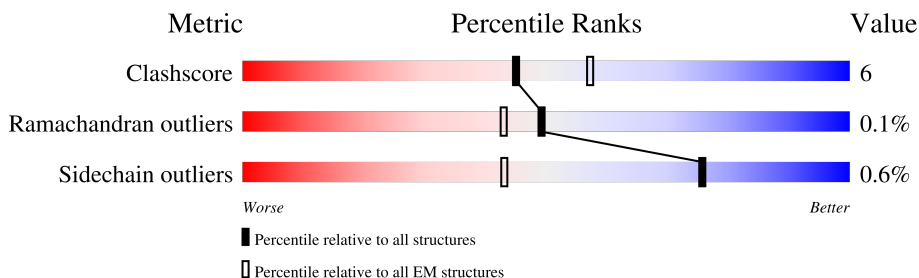
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

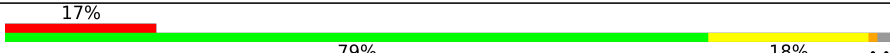
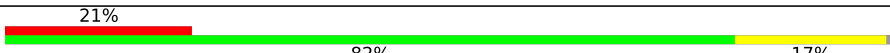
The reported resolution of this entry is 4.10 Å.

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	
2	V2	217	
3	S1	704	
4	S2	430	

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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	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 65344 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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	S2	424	Total	C	N	O	S	0	0
			3414	2180	584	625	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 NADH:ubiquinone oxidoreductase core subunit S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S7	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

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

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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
			1024	646	182	193	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A9	287	Total	C	N	O	S	0	0
			2293	1464	419	405	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 sub-

unit 5.

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

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

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

- Molecule 15 is a protein called NADH:ubiquinone oxidoreductase subunit A7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	144	Total	C	N	O	S	0	0
			1201	773	215	209	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	90	Total	C	N	O	S	0	0
			728	500	103	120	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D1	303	Total	C	N	O	S	0	0
			2415	1633	368	395	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 NADH:ubiquinone oxidoreductase subunit B10.

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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

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 NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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		

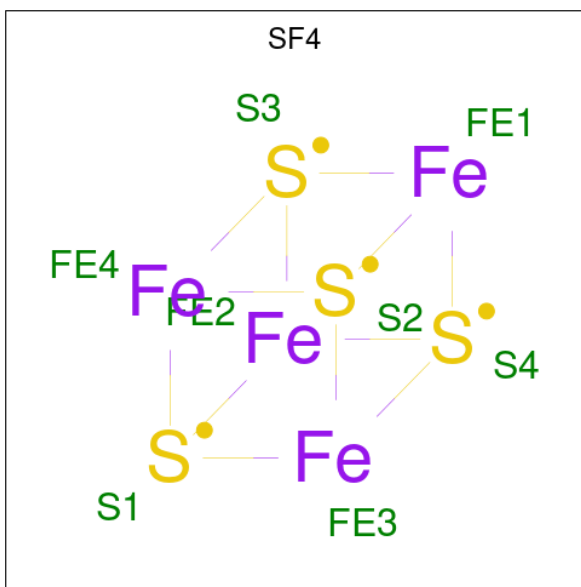
There are 3 discrepancies between the modelled and reference sequences:

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 NADH dehydrogenase 1 alpha subcomplex.

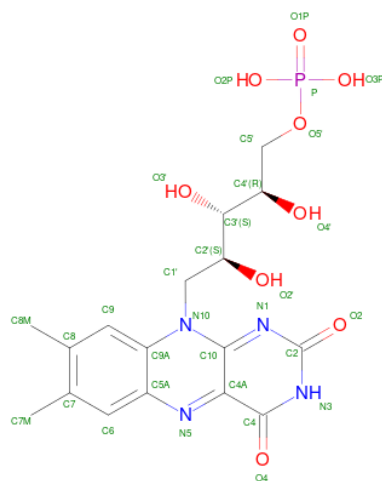
Mol	Chain	Residues	Atoms					AltConf	Trace
44	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

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



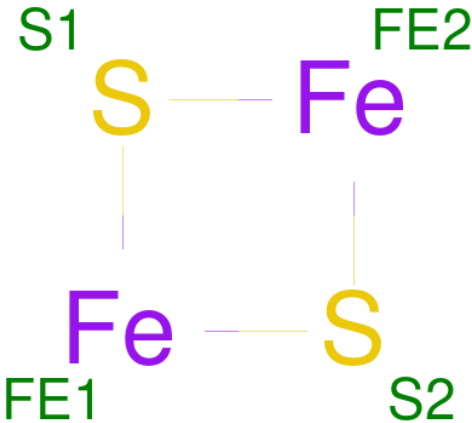
Mol	Chain	Residues	Atoms			AltConf
45	V1	1	Total	Fe	S	0
			8	4	4	
45	S1	1	Total	Fe	S	0
			8	4	4	
45	S1	1	Total	Fe	S	0
			8	4	4	
45	S7	1	Total	Fe	S	0
			8	4	4	
45	S8	1	Total	Fe	S	0
			8	4	4	
45	S8	1	Total	Fe	S	0
			8	4	4	

- 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).

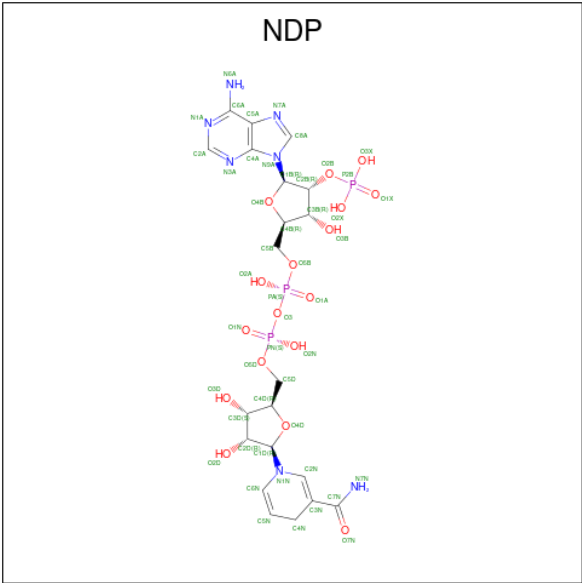


Mol	Chain	Residues	Atoms			AltConf
47	V2	1	Total 4	Fe 2	S 2	0
47	S1	1	Total 4	Fe 2	S 2	0

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

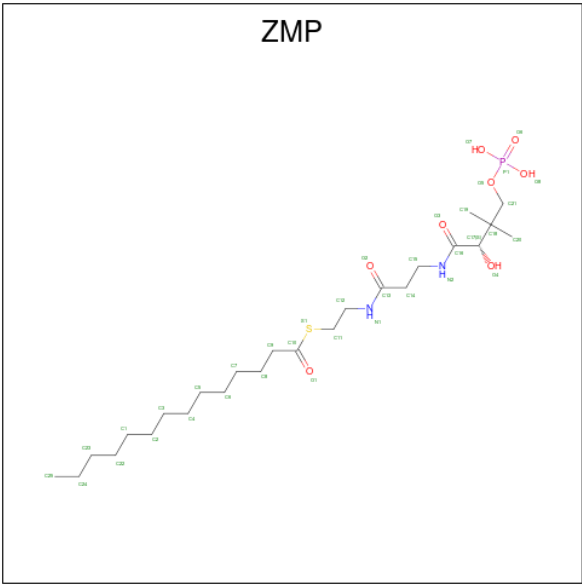
Mol	Chain	Residues	Atoms		AltConf
48	S6	1	Total	Zn	0
			1	1	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



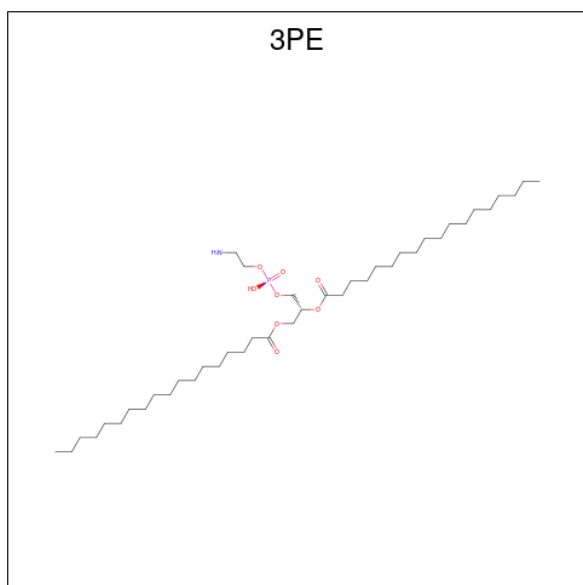
Mol	Chain	Residues	Atoms					AltConf
49	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



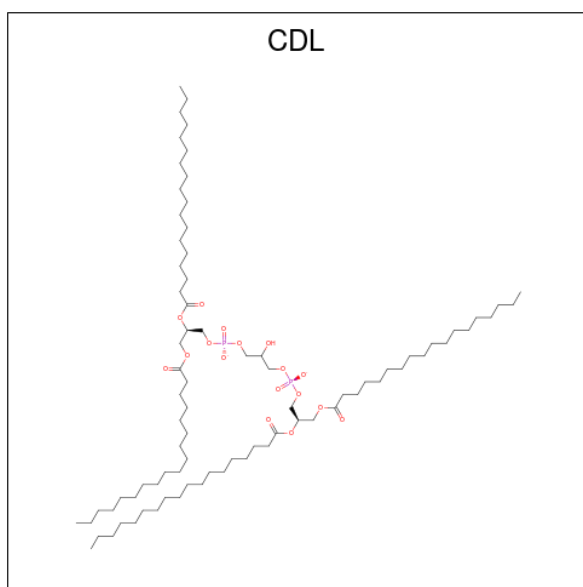
Mol	Chain	Residues	Atoms						AltConf
50	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
50	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

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



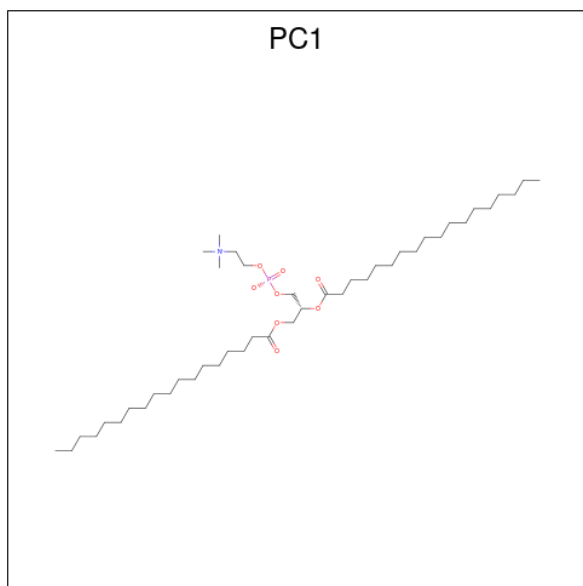
Mol	Chain	Residues	Atoms					AltConf
51	D1	1	Total	C	N	O	P	0
			26	16	1	8	1	
51	D4	1	Total	C	N	O	P	0
			40	30	1	8	1	
51	B8	1	Total	C	N	O	P	0
			38	28	1	8	1	

- 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	60	41	17	2	0

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

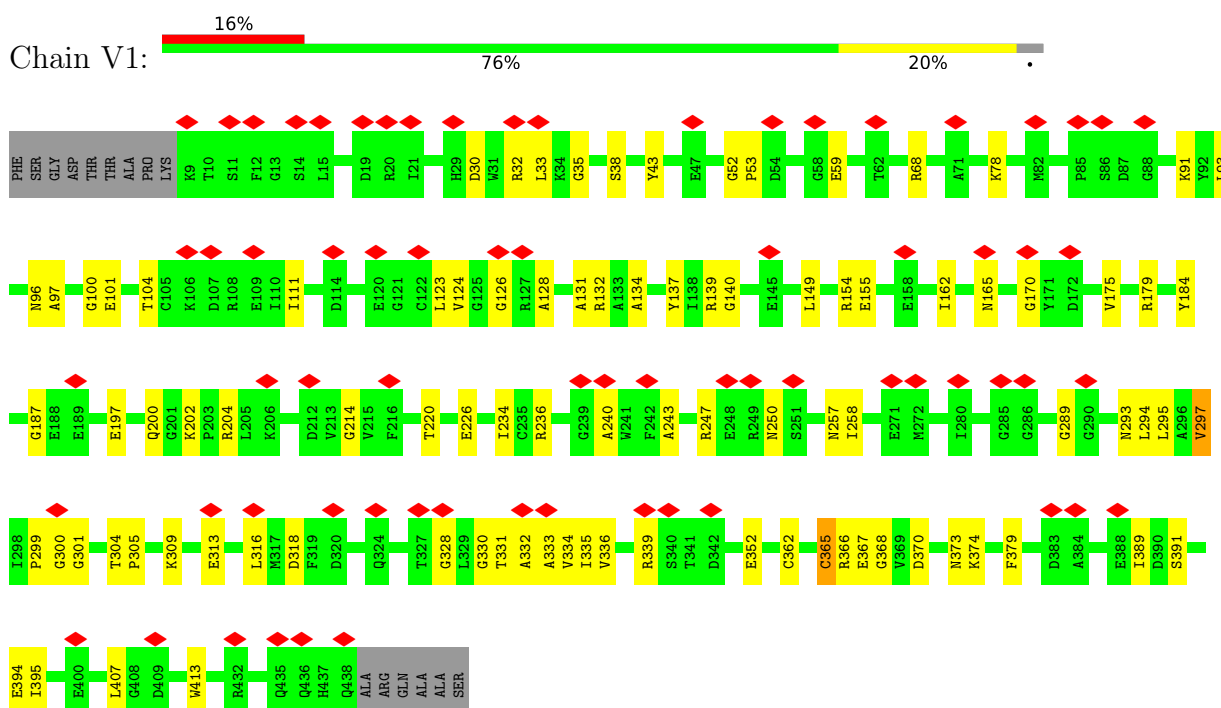


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
53	D4	1	28	18	1	8	1	0

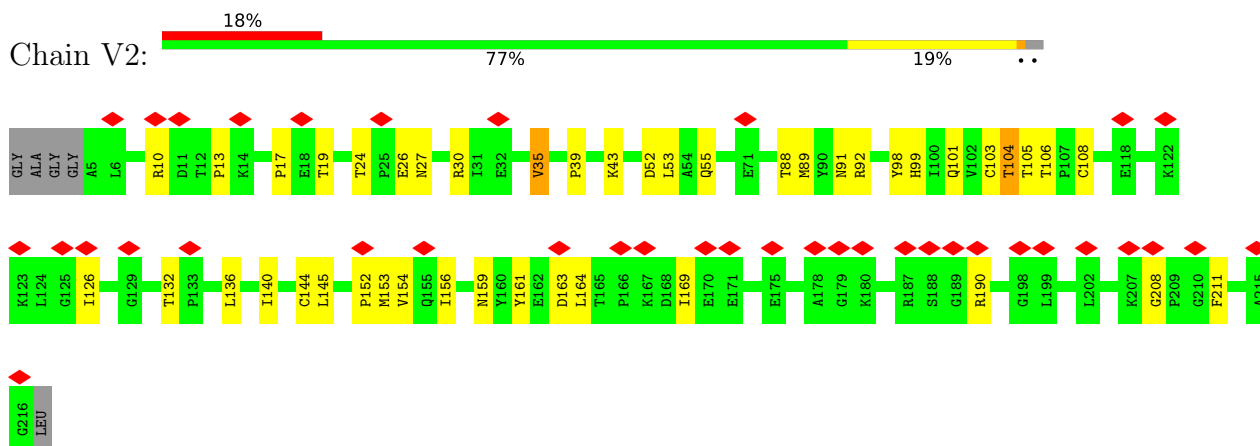
3 Residue-property plots

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.

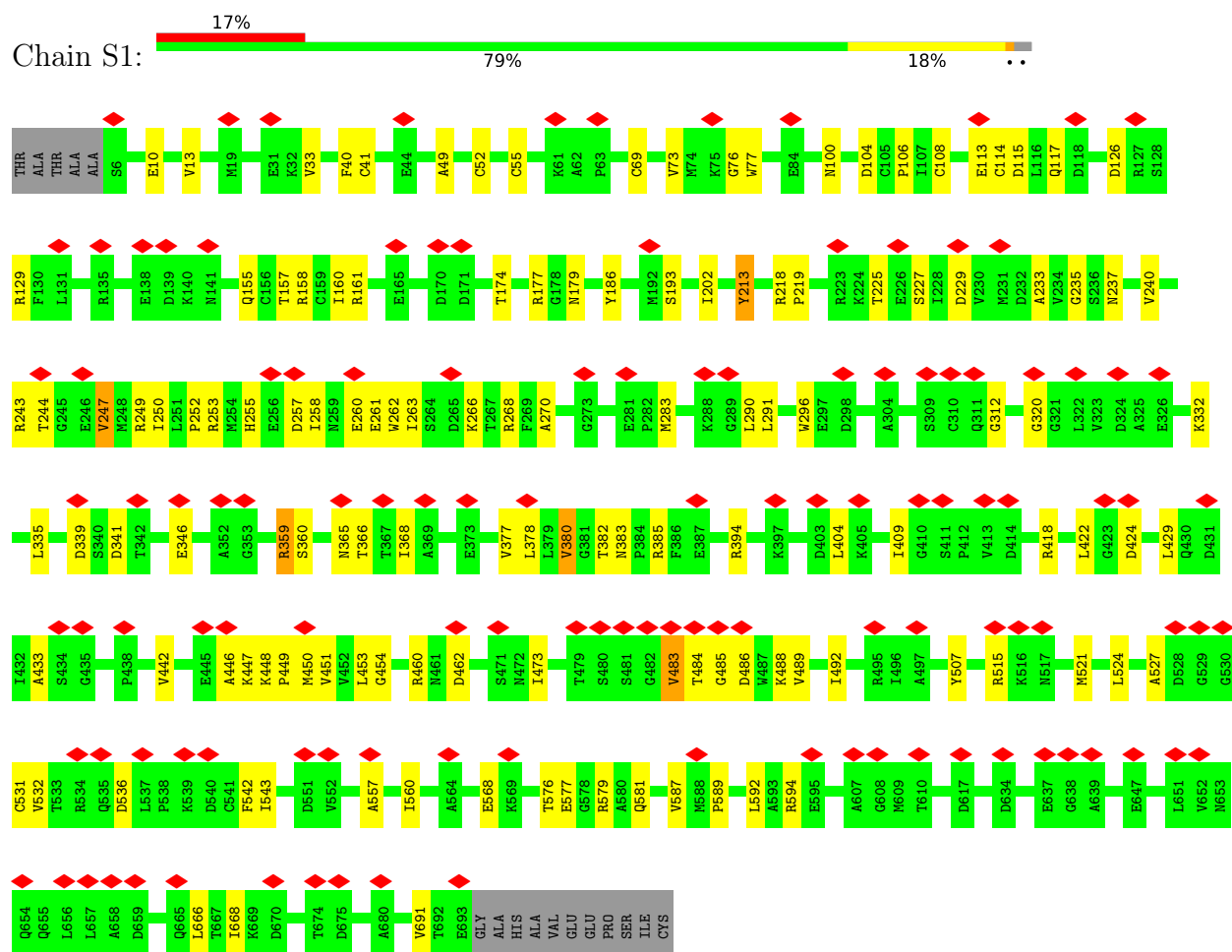
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



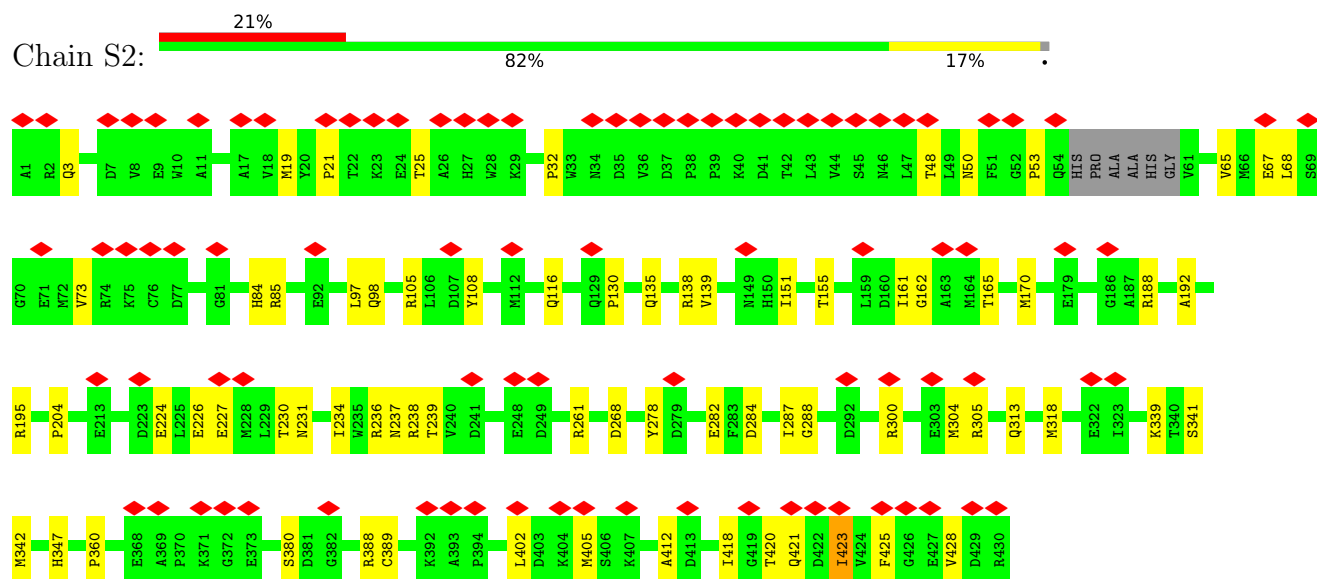
- Molecule 2: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



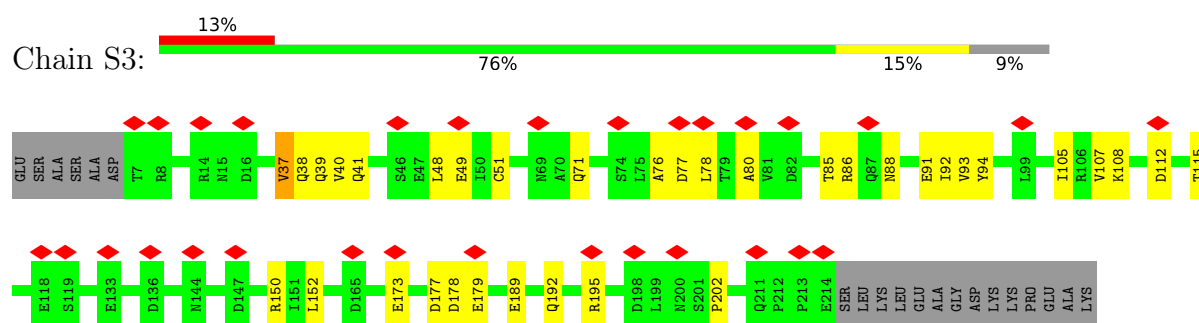
- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1



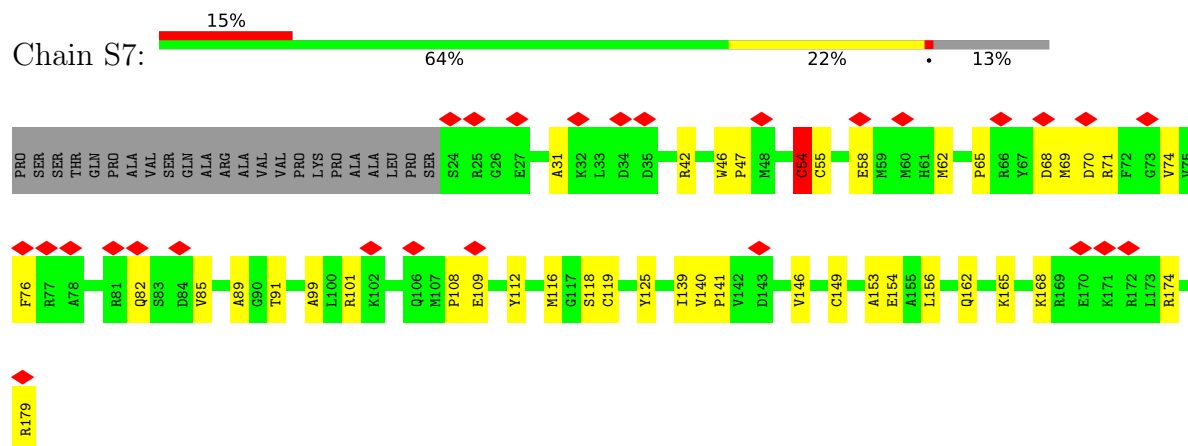
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



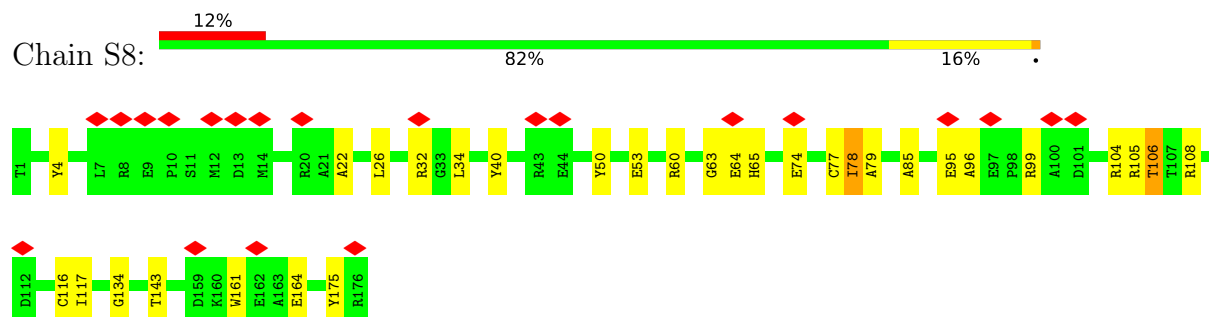
- Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3



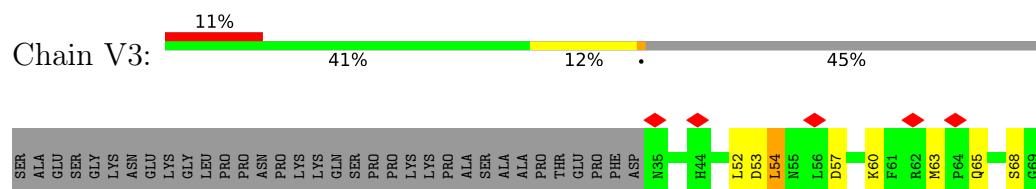
- Molecule 6: NADH:ubiquinone oxidoreductase core subunit S7



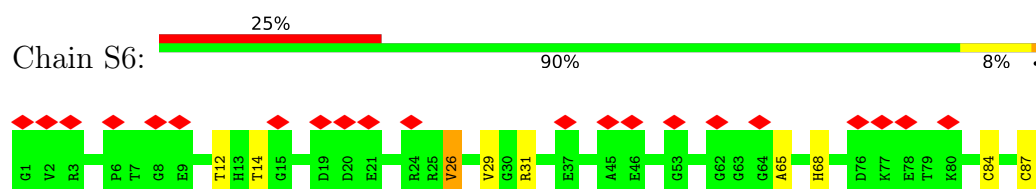
- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



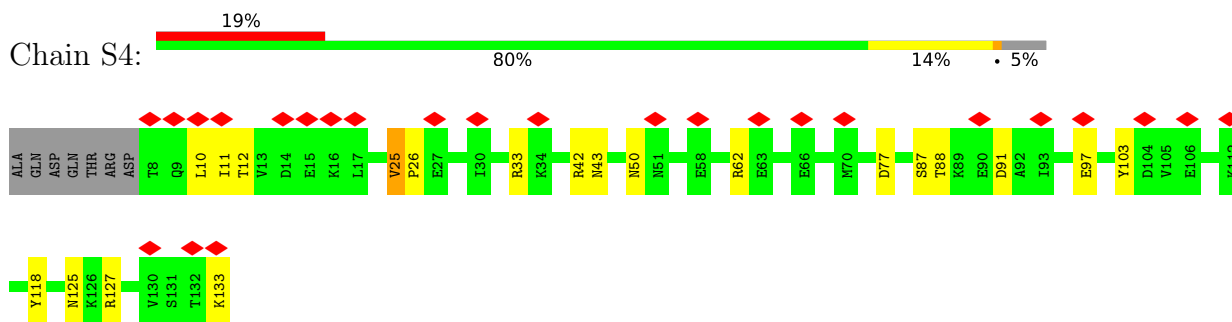
- Molecule 8: NADH:ubiquinone oxidoreductase subunit V3



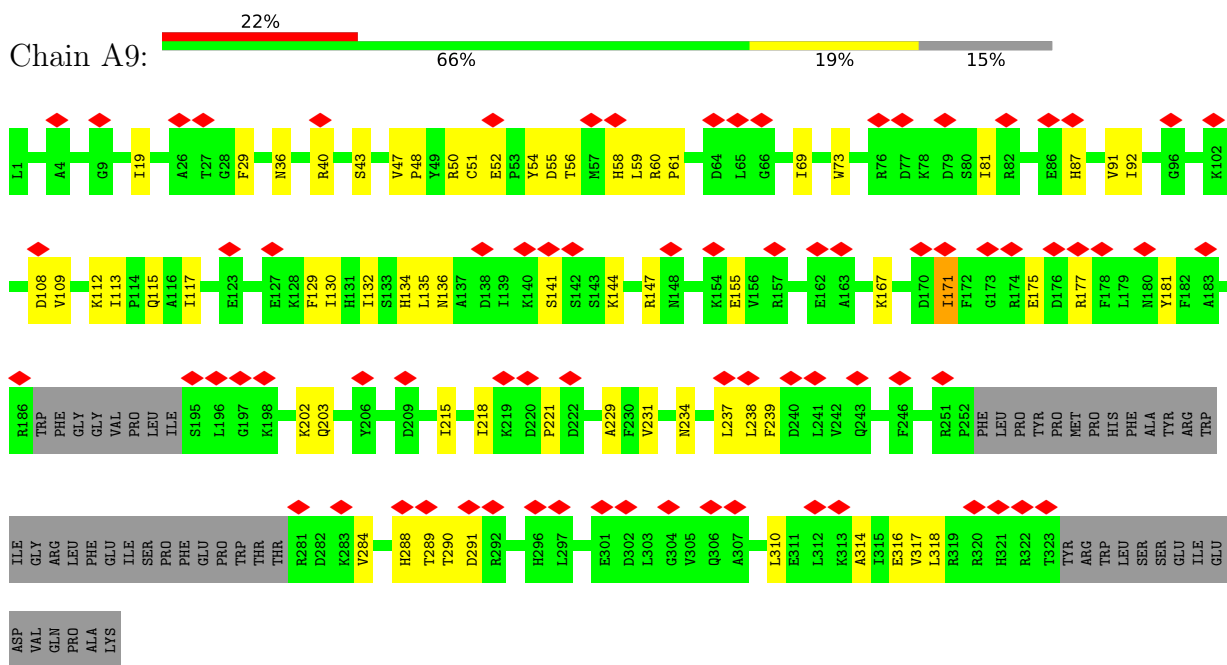
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



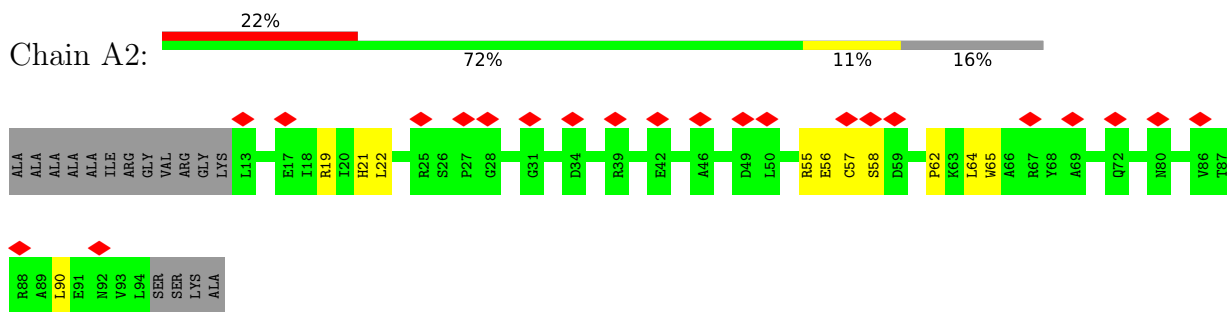
- Molecule 10: NADH:ubiquinone oxidoreductase subunit S4



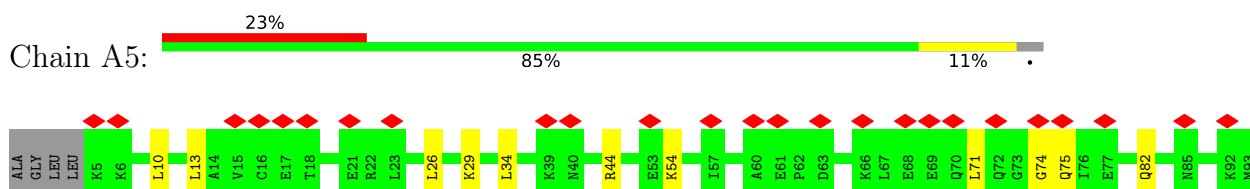
- Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

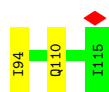


- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

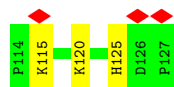
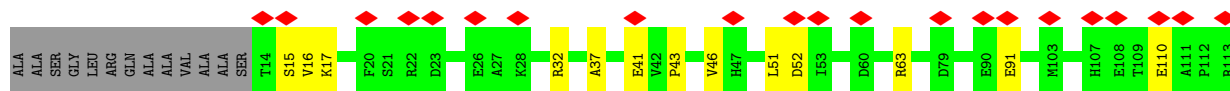
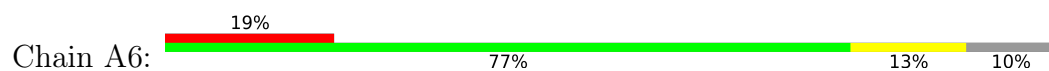


- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

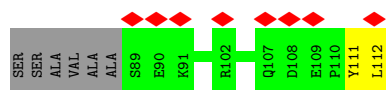
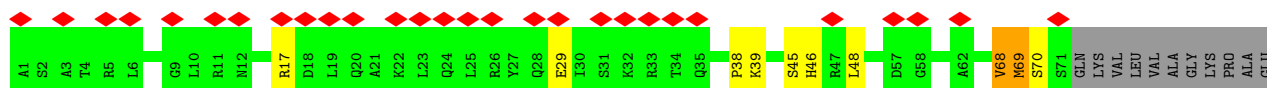
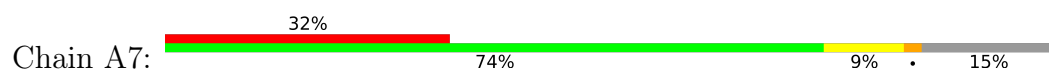




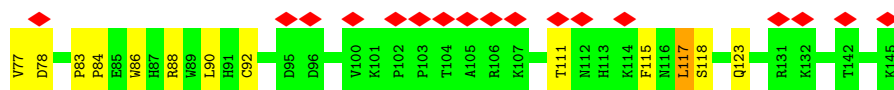
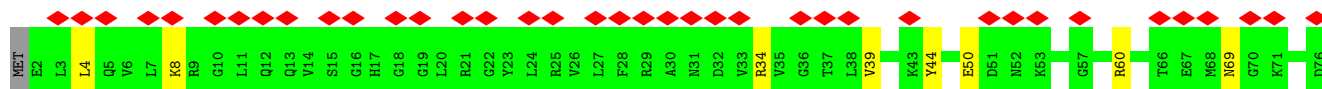
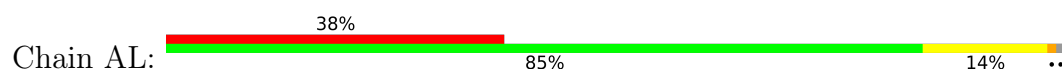
- Molecule 14: NADH:ubiquinone oxidoreductase subunit A6



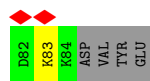
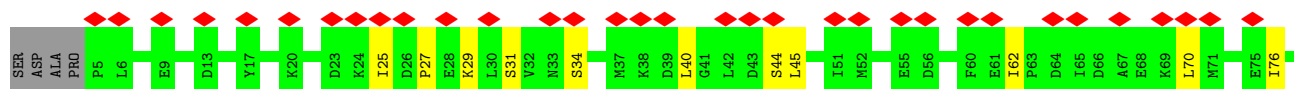
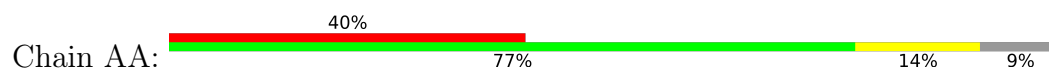
- Molecule 15: NADH:ubiquinone oxidoreductase subunit A7



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

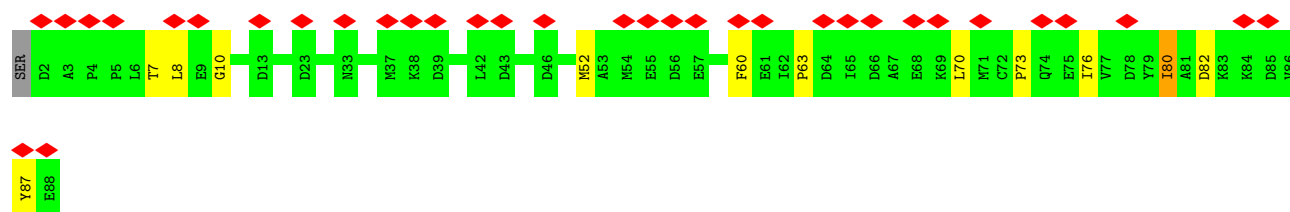


- Molecule 17: Acyl carrier protein



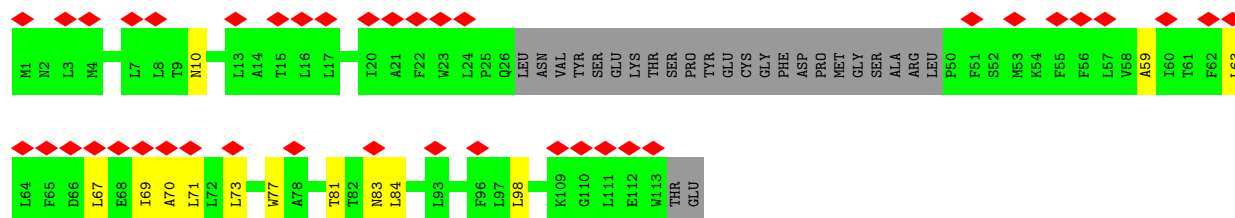
- Molecule 17: Acyl carrier protein

Chain AB: 



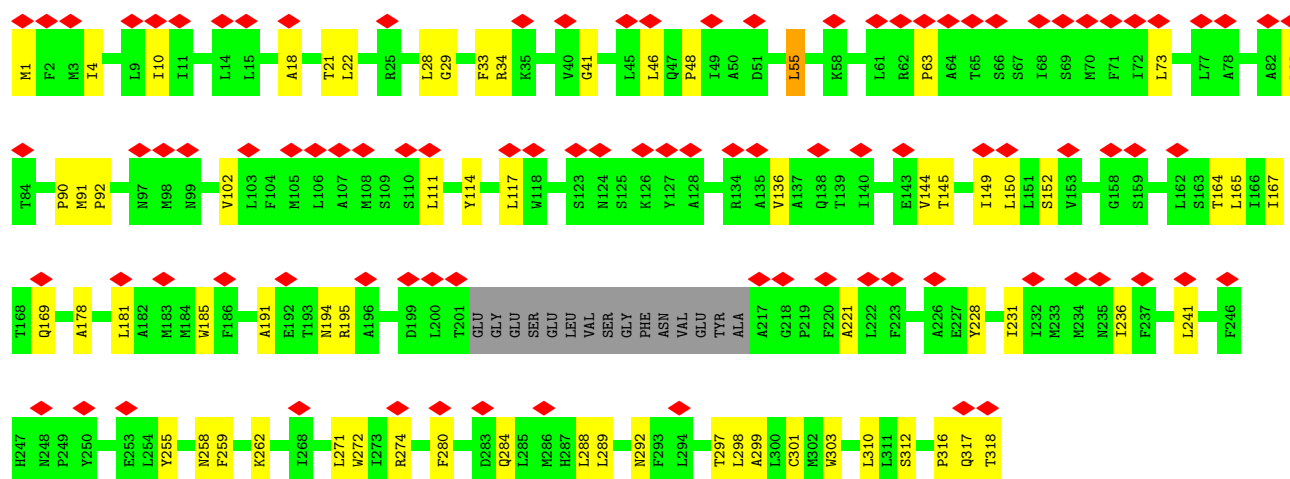
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain D3: 



• Molecule 19: NADH-ubiquinone oxidoreductase chain 1

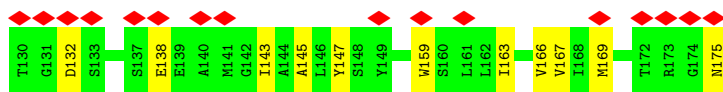
Chain D1: 



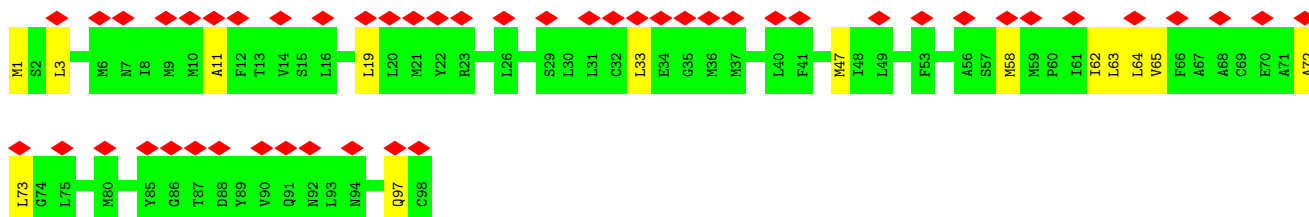
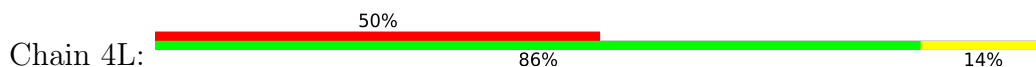
• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

Chain D6: 

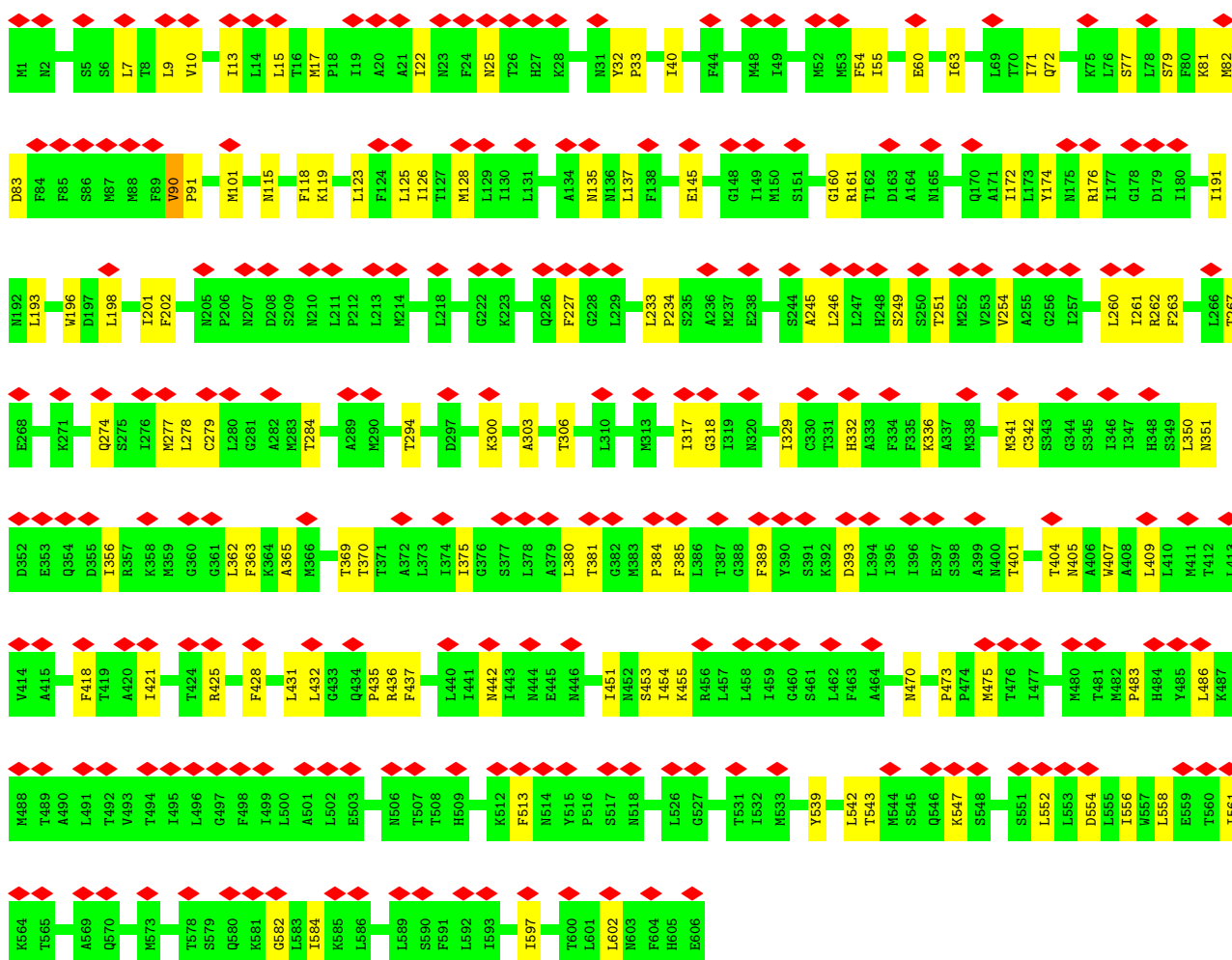
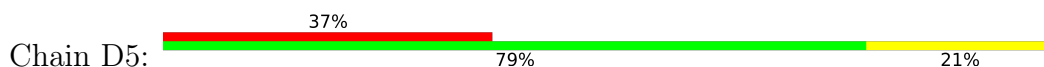




- Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

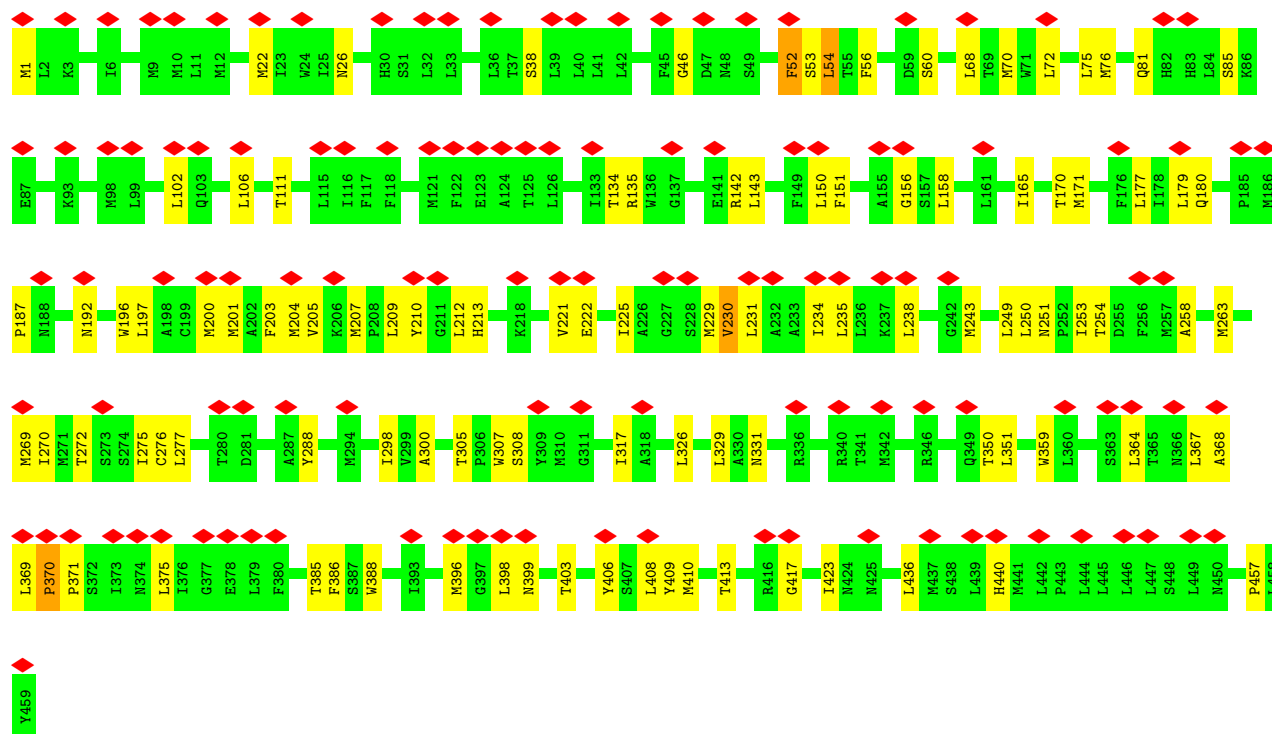


- Molecule 22: NADH-ubiquinone oxidoreductase chain 5



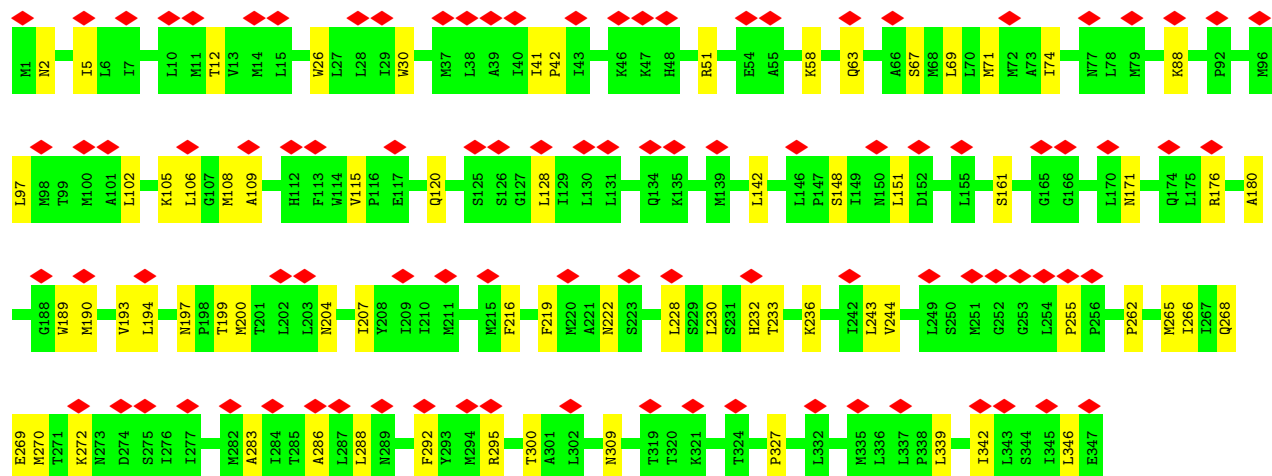
- Molecule 23: NADH-ubiquinone oxidoreductase chain 4

Chain D4: 



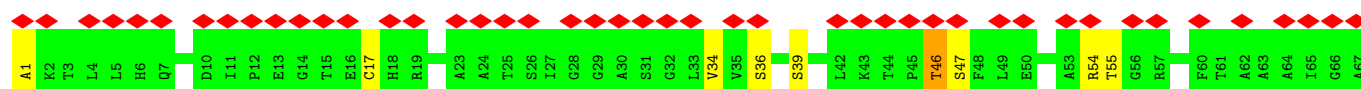
• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

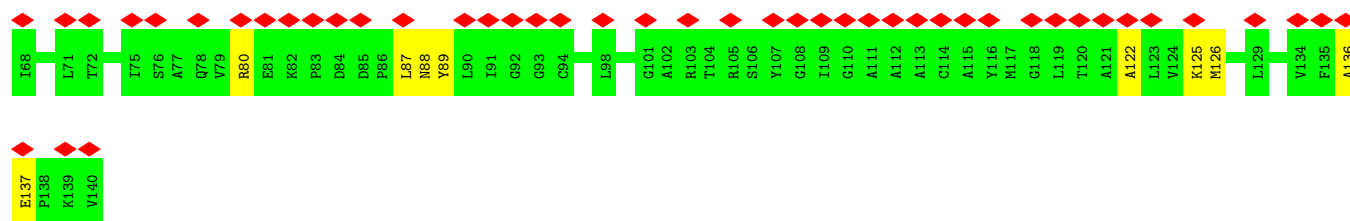
Chain D2: 



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

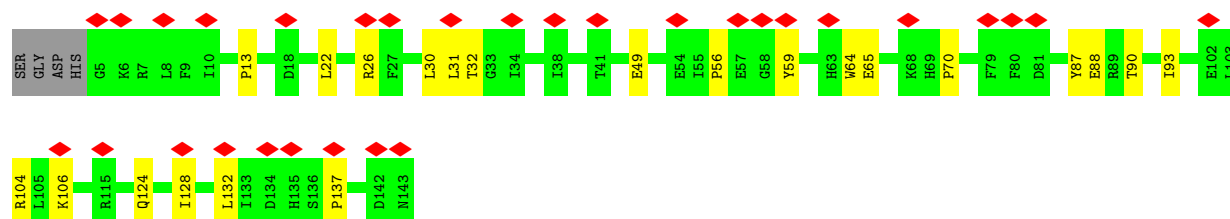
Chain AK: 





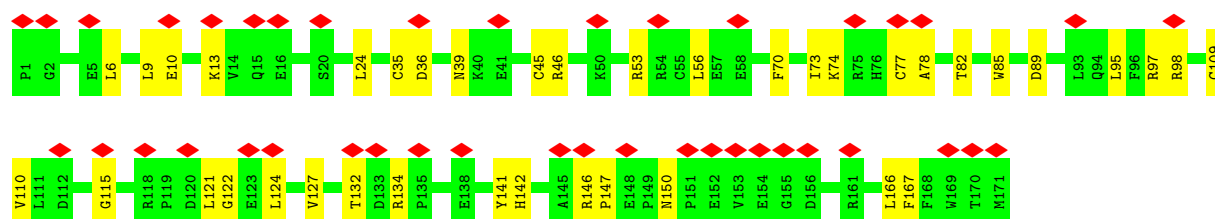
- Molecule 26: NADH:ubiquinone oxidoreductase subunit B5

Chain B5: 21% 82% 15%



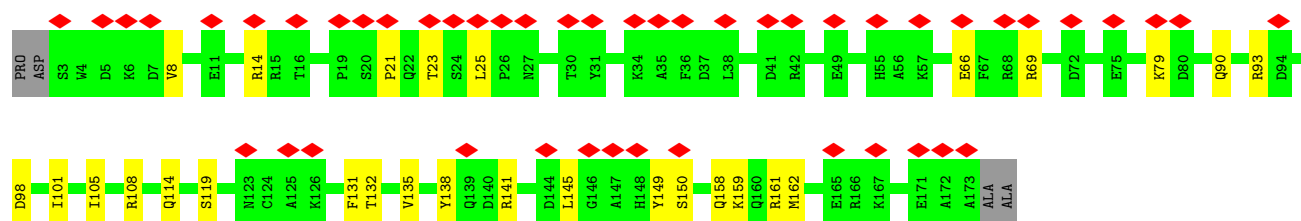
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain A8: 24% 77% 23%



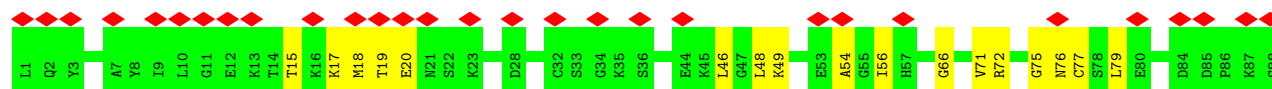
- Molecule 28: NADH:ubiquinone oxidoreductase subunit B10

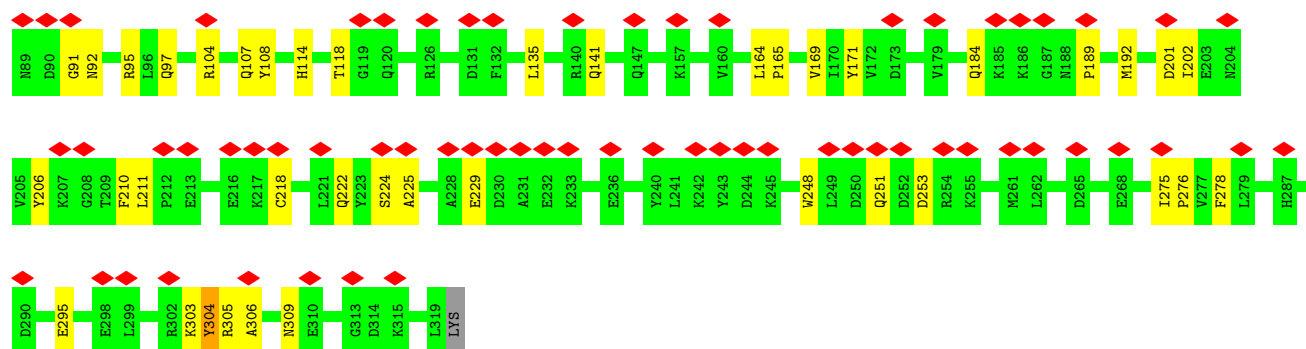
Chain BJ: 27% 82% 16%



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

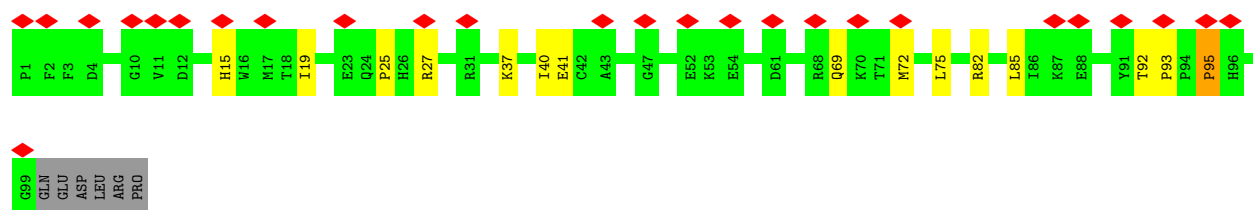
Chain AJ: 29% 82% 18%





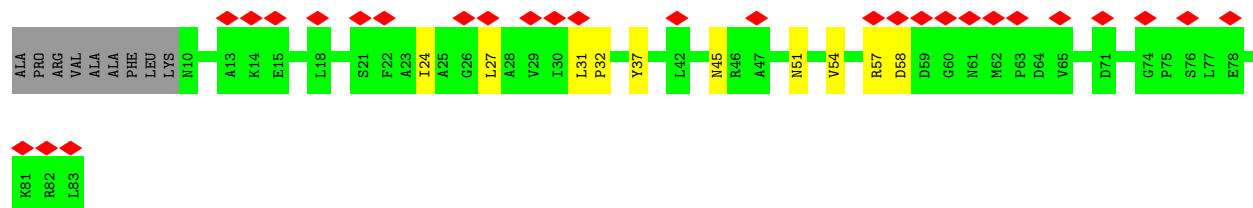
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5

Chain S5: 25% 80% 13% 6%



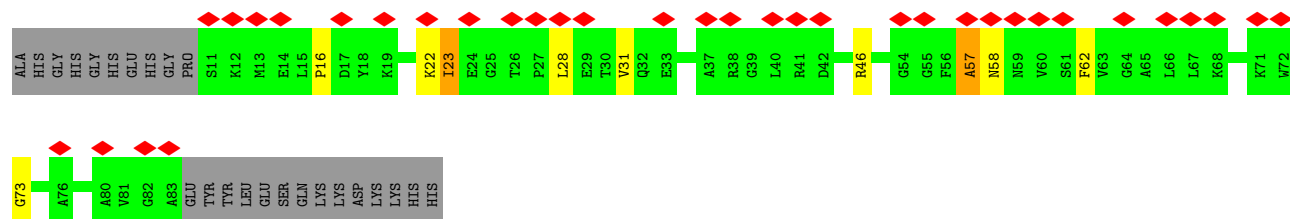
- Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

Chain A3: 34% 77% 12% 11%



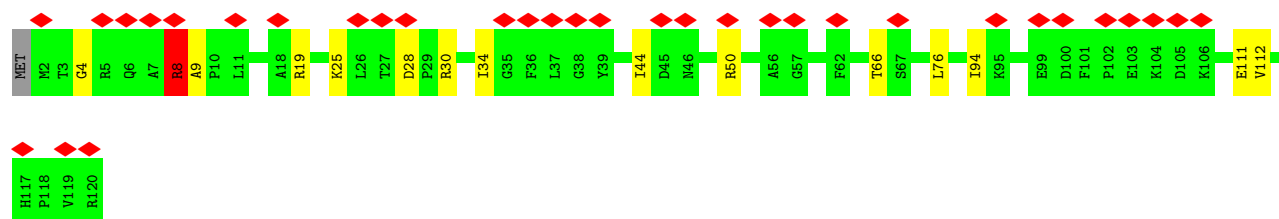
- Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

Chain B3: 36% 65% 8% 25%

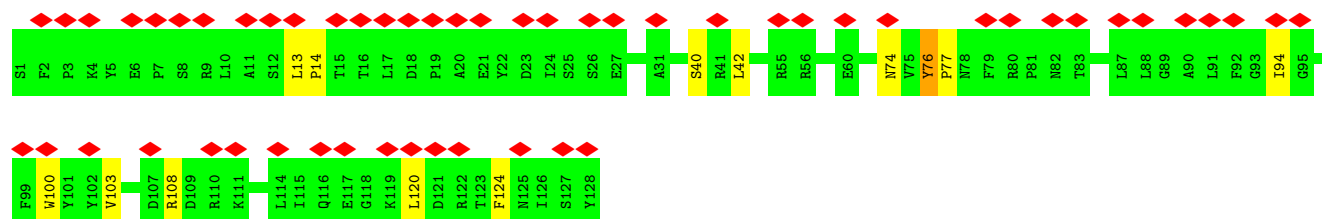
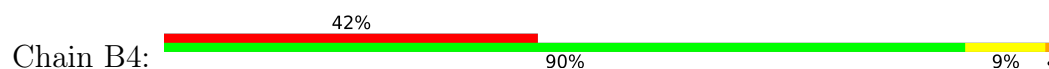


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

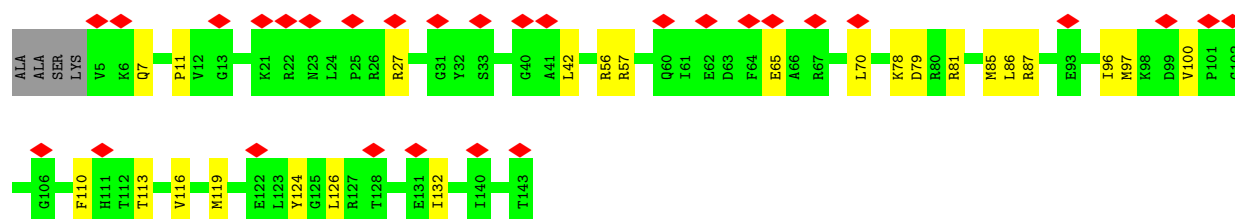
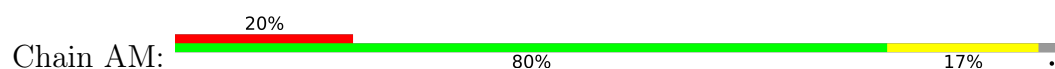
Chain C2: 28% 87% 12% 2%



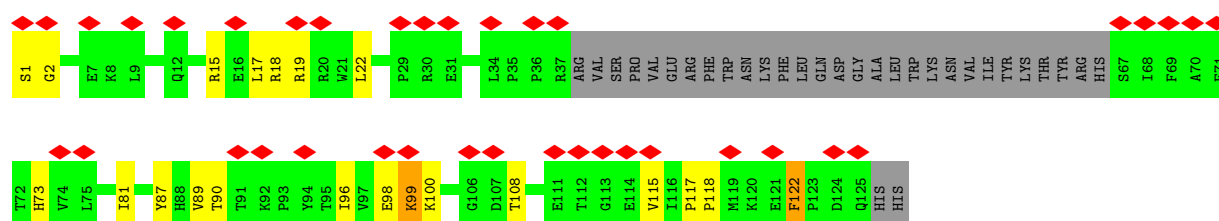
- Molecule 34: NADH:ubiquinone oxidoreductase subunit B4



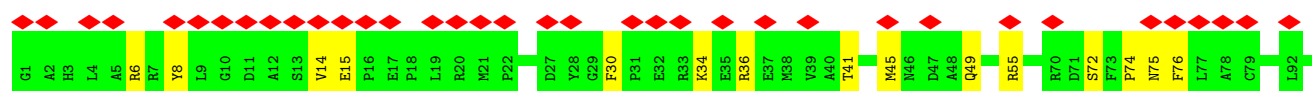
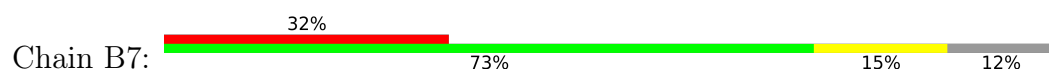
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

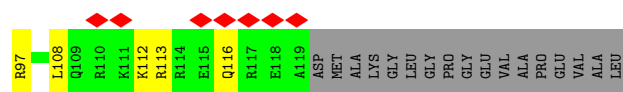


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

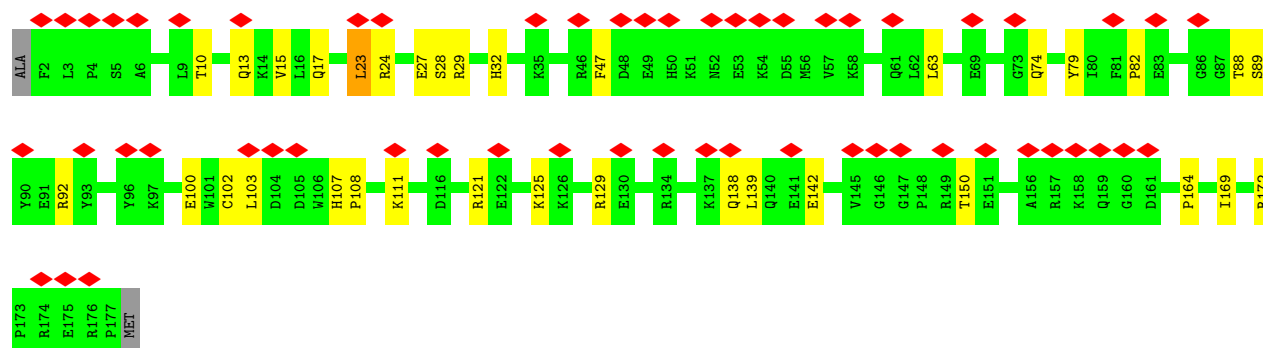
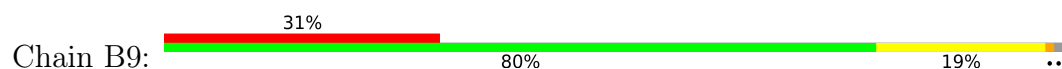


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

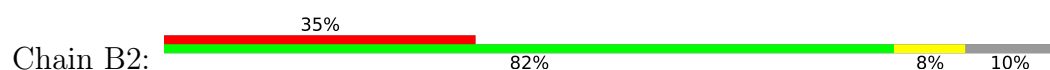




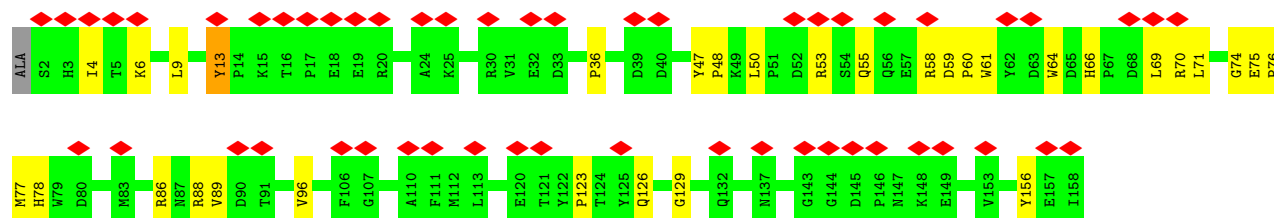
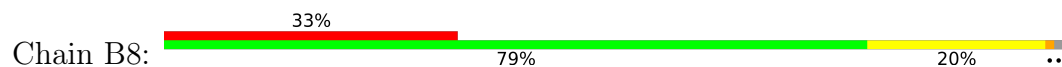
- Molecule 38: NADH:ubiquinone oxidoreductase subunit B9



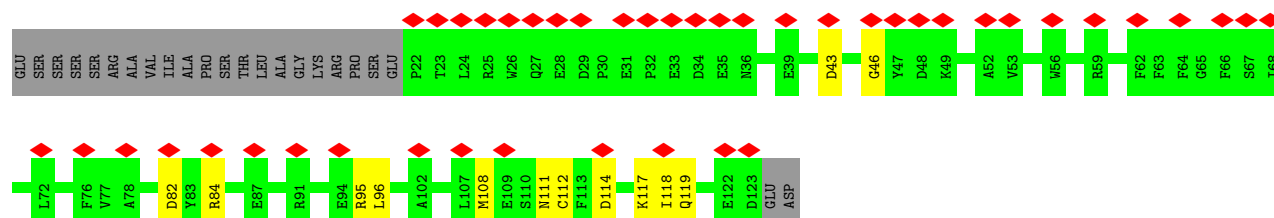
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2



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

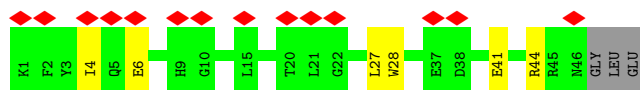


- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



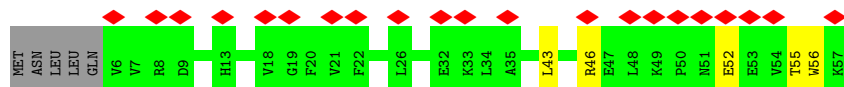
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain C1: 

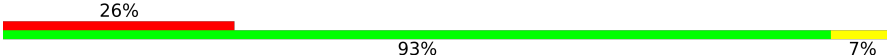


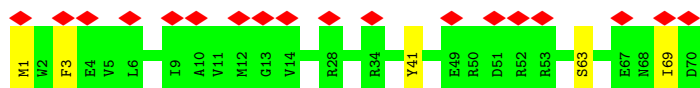
- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain B1: 



- Molecule 44: NADH dehydrogenase 1 alpha subcomplex

Chain A1: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26978	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)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.343	Depositor
Minimum map value	-0.394	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.27	0/3386	0.66	4/4575 (0.1%)
2	V2	0.28	0/1687	0.75	0/2295
3	S1	0.25	0/5362	0.61	0/7266
4	S2	0.28	0/3502	0.62	3/4744 (0.1%)
5	S3	0.28	0/1776	0.78	2/2417 (0.1%)
6	S7	0.28	0/1278	0.62	2/1728 (0.1%)
7	S8	0.30	0/1445	0.62	0/1956
8	V3	0.25	0/355	0.66	0/480
9	S6	0.21	0/749	0.52	0/1009
10	S4	0.22	0/1047	0.57	0/1415
11	A9	0.24	0/2343	0.66	4/3164 (0.1%)
12	A2	0.22	0/676	0.59	0/911
13	A5	0.24	0/921	0.64	0/1249
14	A6	0.24	0/993	0.59	2/1336 (0.1%)
15	A7	0.25	0/775	0.63	0/1048
16	AL	0.24	0/1242	0.62	0/1688
17	AA	0.21	0/655	0.64	0/881
17	AB	0.21	0/714	0.55	0/963
18	D3	0.26	0/747	0.60	0/1022
19	D1	0.32	0/2487	0.72	2/3401 (0.1%)
20	D6	0.25	0/1339	0.66	0/1810
21	4L	0.28	0/758	0.68	0/1024
22	D5	0.29	0/4933	0.71	1/6710 (0.0%)
23	D4	0.31	0/3740	0.72	3/5095 (0.1%)
24	D2	0.30	0/2788	0.65	1/3795 (0.0%)
25	AK	0.25	0/1046	0.71	5/1419 (0.4%)
26	B5	0.23	0/1189	0.55	0/1607
27	A8	0.26	0/1441	0.66	0/1942
28	BJ	0.25	0/1475	0.65	3/1989 (0.2%)
29	AJ	0.25	0/2644	0.66	6/3579 (0.2%)
30	S5	0.24	0/843	0.63	0/1128
31	A3	0.26	0/602	0.66	0/828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	B3	0.27	0/595	0.78	2/803 (0.2%)
33	C2	0.26	0/1028	0.66	4/1388 (0.3%)
34	B4	0.21	0/1085	0.60	1/1467 (0.1%)
35	AM	0.25	0/1172	0.59	0/1579
36	B6	0.26	0/841	0.74	1/1144 (0.1%)
37	B7	0.24	0/1051	0.67	0/1408
38	B9	0.24	0/1568	0.63	0/2123
39	B2	0.26	0/590	0.69	2/810 (0.2%)
40	B8	0.26	0/1379	0.73	1/1884 (0.1%)
41	BK	0.22	0/880	0.67	1/1196 (0.1%)
42	C1	0.21	0/404	0.56	0/548
43	B1	0.21	0/462	0.59	0/624
44	A1	0.25	0/592	0.65	0/795
All	All	0.26	0/66585	0.66	50/90243 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	V2	0	4
3	S1	0	4
4	S2	0	4
5	S3	0	1
7	S8	0	2
15	A7	0	2
19	D1	0	2
20	D6	0	1
22	D5	0	1
23	D4	0	2
25	AK	0	1
27	A8	0	1
28	BJ	0	2
29	AJ	0	1
30	S5	0	1
32	B3	0	4
33	C2	0	1
34	B4	0	1
36	B6	0	2
37	B7	0	1
39	B2	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
40	B8	0	2
42	C1	0	1
43	B1	0	1
44	A1	0	1
All	All	0	44

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S3	37	VAL	CA-C-N	13.95	147.57	122.46
5	S3	37	VAL	C-N-CA	13.95	147.57	122.46
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	7.59	135.37	121.70
29	AJ	229	GLU	C-N-CA	7.59	135.37	121.70
19	D1	63	PRO	CA-C-N	7.42	135.05	121.70
19	D1	63	PRO	C-N-CA	7.42	135.05	121.70
41	BK	46	GLY	N-CA-C	6.88	120.97	112.64
14	A6	110	GLU	CA-C-N	6.70	133.76	121.70
14	A6	110	GLU	C-N-CA	6.70	133.76	121.70
39	B2	44	SER	CA-C-N	6.67	133.72	121.70
39	B2	44	SER	C-N-CA	6.67	133.72	121.70
33	C2	8	ARG	CA-C-N	6.55	133.49	121.70
33	C2	8	ARG	C-N-CA	6.55	133.49	121.70
4	S2	230	THR	CA-C-N	6.40	133.76	121.54
4	S2	230	THR	C-N-CA	6.40	133.76	121.54
25	AK	17	CYS	CA-C-N	6.17	133.33	121.54
25	AK	17	CYS	C-N-CA	6.17	133.33	121.54
34	B4	94	ILE	N-CA-C	-5.89	107.76	113.53
33	C2	4	GLY	CA-C-N	5.76	132.06	121.70
33	C2	4	GLY	C-N-CA	5.76	132.06	121.70
32	B3	57	ALA	CA-C-N	5.73	132.49	121.54
32	B3	57	ALA	C-N-CA	5.73	132.49	121.54
22	D5	407	TRP	N-CA-C	-5.66	108.17	114.62
28	BJ	25	LEU	C-N-CD	-5.64	108.20	120.60
1	V1	331	THR	CA-C-N	5.62	132.27	121.54
1	V1	331	THR	C-N-CA	5.62	132.27	121.54
1	V1	297	VAL	CA-C-N	-5.55	117.33	123.43
1	V1	297	VAL	C-N-CA	-5.55	117.33	123.43
24	D2	255	PRO	N-CA-C	5.49	117.39	110.70
4	S2	165	THR	N-CA-C	5.38	121.69	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D4	370	PRO	N-CA-C	5.29	117.15	110.70
29	AJ	304	TYR	CA-CB-CG	5.28	123.41	113.90
40	B8	13	TYR	N-CA-C	5.18	121.26	109.81
36	B6	122	PHE	N-CA-C	5.15	121.18	109.81
11	A9	221	PRO	CA-C-N	5.14	131.36	121.54
11	A9	221	PRO	C-N-CA	5.14	131.36	121.54
25	AK	137	GLU	CA-C-N	5.14	139.34	127.00
25	AK	137	GLU	C-N-CA	5.14	139.34	127.00
25	AK	137	GLU	C-N-CD	-5.04	109.50	120.60
29	AJ	251	GLN	CA-C-N	5.04	130.78	121.70
29	AJ	251	GLN	C-N-CA	5.04	130.78	121.70
29	AJ	275	ILE	C-N-CD	-5.02	109.56	120.60
11	A9	289	THR	CA-C-N	5.01	131.12	121.54
11	A9	289	THR	C-N-CA	5.01	131.12	121.54
23	D4	423	ILE	CA-C-N	5.01	131.12	121.54
23	D4	423	ILE	C-N-CA	5.01	131.12	121.54
6	S7	108	PRO	CA-C-N	5.01	126.02	120.06
6	S7	108	PRO	C-N-CA	5.01	126.02	120.06

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	A1	63	SER	Peptide
15	A7	29	GLU	Peptide
15	A7	68	VAL	Peptide
27	A8	127	VAL	Peptide
29	AJ	278	PHE	Peptide
25	AK	46	THR	Peptide
43	B1	52	GLU	Peptide
39	B2	56	PRO	Peptide
32	B3	16	PRO	Peptide
32	B3	22	LYS	Peptide
32	B3	57	ALA	Peptide
32	B3	58	ASN	Peptide
34	B4	76	TYR	Peptide
36	B6	122	PHE	Peptide
36	B6	99	LYS	Peptide
37	B7	30	PHE	Peptide
40	B8	53	ARG	Peptide
40	B8	86	ARG	Peptide
28	BJ	150	SER	Peptide

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Mol	Chain	Res	Type	Group
28	BJ	79	LYS	Peptide
42	C1	6	GLU	Peptide
33	C2	8	ARG	Peptide
19	D1	90	PRO	Peptide
19	D1	91	MET	Peptide
23	D4	52	PHE	Peptide
23	D4	53	SER	Peptide
22	D5	365	ALA	Peptide
20	D6	115	ILE	Peptide
3	S1	213	TYR	Peptide
3	S1	247	VAL	Peptide
3	S1	341	ASP	Peptide
3	S1	380	VAL	Peptide
4	S2	162	GLY	Peptide
4	S2	192	ALA	Peptide
4	S2	68	LEU	Peptide
4	S2	73	VAL	Peptide
5	S3	76	ALA	Peptide
30	S5	92	THR	Peptide
7	S8	106	THR	Peptide
7	S8	63	GLY	Peptide
2	V2	10	ARG	Peptide
2	V2	13	PRO	Peptide
2	V2	152	PRO	Peptide
2	V2	35	VAL	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	V1	3312	0	3266	59	0
2	V2	1647	0	1657	28	0
3	S1	5275	0	5300	86	0
4	S2	3414	0	3360	46	0
5	S3	1726	0	1676	30	0
6	S7	1247	0	1256	30	0
7	S8	1414	0	1371	22	0
8	V3	345	0	323	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	S6	737	0	710	7	0
10	S4	1024	0	1023	17	0
11	A9	2293	0	2326	43	0
12	A2	665	0	678	6	0
13	A5	901	0	936	8	0
14	A6	969	0	980	12	0
15	A7	757	0	771	10	0
16	AL	1201	0	1170	14	0
17	AA	645	0	649	7	0
17	AB	702	0	692	10	0
18	D3	728	0	773	14	0
19	D1	2415	0	2542	42	0
20	D6	1308	0	1329	24	0
21	4L	748	0	794	14	0
22	D5	4805	0	4950	87	0
23	D4	3646	0	3850	71	0
24	D2	2724	0	2930	49	0
25	AK	1025	0	1033	10	0
26	B5	1156	0	1177	17	0
27	A8	1404	0	1384	28	0
28	BJ	1441	0	1417	19	0
29	AJ	2583	0	2547	34	0
30	S5	822	0	820	14	0
31	A3	582	0	583	11	0
32	B3	578	0	570	4	0
33	C2	997	0	983	13	0
34	B4	1059	0	1062	9	0
35	AM	1143	0	1137	20	0
36	B6	815	0	837	18	0
37	B7	1026	0	995	14	0
38	B9	1515	0	1469	24	0
39	B2	563	0	509	3	0
40	B8	1324	0	1219	20	0
41	BK	853	0	800	13	0
42	C1	391	0	391	5	0
43	B1	449	0	453	4	0
44	A1	577	0	570	4	0
45	S1	16	0	0	1	0
45	S7	8	0	0	1	0
45	S8	16	0	0	0	0
45	V1	8	0	0	1	0
46	V1	31	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
50	AA	34	0	40	0	0
50	AB	31	0	34	1	0
51	B8	38	0	50	1	0
51	D1	26	0	26	0	0
51	D4	40	0	54	2	0
52	D5	60	0	64	4	0
53	D4	28	0	30	0	0
All	All	65344	0	65611	819	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 6.

All (819) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:80:ALA:HA	5:S3:91:GLU:O	1.12	1.27
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.51	1.08
5:S3:80:ALA:CA	5:S3:91:GLU:O	2.08	1.01
5:S3:38:GLN:HA	15:A7:70:SER:O	1.69	0.92
23:D4:52:PHE:O	23:D4:56:PHE:HB2	1.74	0.88
12:A2:21:HIS:O	12:A2:62:PRO:HA	1.75	0.87
38:B9:138:GLN:O	38:B9:142:GLU:HB2	1.83	0.78
22:D5:81:LYS:HZ2	22:D5:83:ASP:HB2	1.51	0.74
26:B5:26:ARG:O	26:B5:30:LEU:HB2	1.89	0.73
22:D5:547:LYS:O	22:D5:552:LEU:HB2	1.90	0.71
22:D5:294:THR:H	22:D5:425:ARG:HH12	1.39	0.71
5:S3:88:ASN:HD22	5:S3:112:ASP:HB3	1.56	0.70
4:S2:105:ARG:NH1	6:S7:149:CYS:SG	2.66	0.69
5:S3:78:LEU:HA	5:S3:93:VAL:O	1.94	0.68
17:AB:70:LEU:HD23	17:AB:76:ILE:HG12	1.76	0.68
23:D4:204:MET:HB3	23:D4:209:LEU:HD22	1.75	0.67
3:S1:227:SER:H	3:S1:253:ARG:HH22	1.42	0.66
1:V1:257:ASN:HB2	1:V1:332:ALA:HA	1.78	0.66
23:D4:22:MET:HG2	23:D4:26:ASN:HD21	1.61	0.66
22:D5:22:ILE:HA	22:D5:25:ASN:HB2	1.76	0.66
3:S1:450:MET:HA	3:S1:489:VAL:O	1.96	0.66
9:S6:68:HIS:HE1	9:S6:87:CYS:SG	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BJ:23:THR:HG21	37:B7:74:PRO:HD2	1.79	0.65
14:A6:115:LYS:HA	14:A6:120:LYS:HE3	1.79	0.65
29:AJ:306:ALA:HA	29:AJ:309:ASN:HB2	1.78	0.65
15:A7:39:LYS:H	35:AM:7:GLN:HB2	1.62	0.64
11:A9:92:ILE:HG22	11:A9:130:ILE:HB	1.80	0.64
33:C2:30:ARG:HE	33:C2:76:LEU:HD11	1.62	0.64
17:AA:27:PRO:HG2	17:AA:29:LYS:HB2	1.78	0.64
20:D6:58:LEU:O	20:D6:62:GLY:HA3	1.97	0.64
20:D6:167:VAL:HG22	24:D2:42:PRO:HG2	1.80	0.64
3:S1:243:ARG:HG2	3:S1:244:THR:HG23	1.79	0.64
11:A9:51:CYS:SG	11:A9:52:GLU:N	2.71	0.64
3:S1:266:LYS:O	3:S1:270:ALA:HB2	1.98	0.64
13:A5:26:LEU:HA	13:A5:29:LYS:HZ1	1.63	0.63
23:D4:234:ILE:O	23:D4:238:LEU:HB2	1.98	0.63
23:D4:102:LEU:HD21	23:D4:230:VAL:HG11	1.81	0.63
23:D4:177:LEU:O	23:D4:180:GLN:C	2.41	0.63
4:S2:388:ARG:NH1	4:S2:389:CYS:O	2.32	0.63
22:D5:597:ILE:HD11	25:AK:34:VAL:HG22	1.81	0.63
21:4L:58:MET:HB3	21:4L:62:ILE:HD12	1.80	0.62
3:S1:229:ASP:HB3	3:S1:235:GLY:HA2	1.80	0.62
3:S1:449:PRO:HG2	3:S1:489:VAL:HG22	1.80	0.62
23:D4:156:GLY:HA3	23:D4:205:VAL:HG21	1.81	0.62
1:V1:134:ALA:HB3	1:V1:175:VAL:HG12	1.82	0.62
11:A9:316:GLU:HG2	14:A6:52:ASP:HB3	1.81	0.62
19:D1:41:GLY:HA3	19:D1:46:LEU:HD21	1.82	0.62
17:AB:82:ASP:OD1	36:B6:15:ARG:NH2	2.32	0.62
1:V1:33:LEU:HD23	1:V1:155:GLU:HB3	1.82	0.62
19:D1:310:LEU:HD21	31:A3:32:PRO:HA	1.82	0.62
20:D6:132:ASP:OD1	35:AM:78:LYS:NZ	2.33	0.61
9:S6:31:ARG:HH22	11:A9:69:ILE:HD11	1.66	0.61
1:V1:289:GLY:HA3	1:V1:293:ASN:HD22	1.64	0.61
11:A9:109:VAL:O	11:A9:113:ILE:HB	2.01	0.61
3:S1:377:VAL:HG22	3:S1:450:MET:HB3	1.83	0.61
23:D4:221:VAL:HG23	23:D4:222:GLU:HG3	1.82	0.61
5:S3:48:LEU:HB3	5:S3:105:ILE:HG22	1.83	0.61
7:S8:79:ALA:HB2	7:S8:106:THR:HG22	1.83	0.61
22:D5:380:LEU:HD23	22:D5:381:THR:HG23	1.82	0.60
38:B9:10:THR:HG23	38:B9:13:GLN:H	1.64	0.60
13:A5:34:LEU:HD11	13:A5:44:ARG:HA	1.82	0.60
23:D4:38:SER:OG	23:D4:70:MET:SD	2.55	0.60
15:A7:45:SER:O	15:A7:46:HIS:ND1	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:404:LEU:H	10:S4:127:ARG:HH22	1.48	0.60
22:D5:451:ILE:O	22:D5:455:LYS:HB2	2.01	0.60
38:B9:139:LEU:HD22	38:B9:164:PRO:HG3	1.83	0.60
1:V1:97:ALA:HB3	1:V1:137:TYR:O	2.02	0.60
22:D5:54:PHE:HE1	22:D5:60:GLU:HG2	1.67	0.60
28:BJ:145:LEU:HD13	28:BJ:149:TYR:HB3	1.84	0.60
29:AJ:202:ILE:O	29:AJ:206:TYR:HB2	2.00	0.60
38:B9:100:GLU:O	38:B9:121:ARG:NH2	2.34	0.60
3:S1:252:PRO:HB3	3:S1:263:ILE:HB	1.84	0.60
20:D6:14:VAL:HG22	21:4L:11:ALA:HB2	1.83	0.60
28:BJ:161:ARG:NH2	41:BK:111:ASN:OD1	2.33	0.60
24:D2:88:LYS:HG3	24:D2:148:SER:HB3	1.84	0.60
1:V1:297:VAL:HG22	1:V1:336:VAL:HG12	1.84	0.60
3:S1:114:CYS:SG	3:S1:115:ASP:N	2.75	0.60
9:S6:26:VAL:HB	11:A9:87:HIS:HB2	1.84	0.60
1:V1:258:ILE:HG23	1:V1:335:ILE:HG22	1.83	0.59
22:D5:198:LEU:HD21	22:D5:262:ARG:HD2	1.82	0.59
27:A8:45:CYS:SG	27:A8:134:ARG:NH2	2.74	0.59
6:S7:70:ASP:OD2	19:D1:34:ARG:NH1	2.35	0.59
7:S8:77:CYS:SG	7:S8:78:ILE:N	2.75	0.59
3:S1:255:HIS:HD2	3:S1:258:ILE:H	1.50	0.59
6:S7:62:MET:HG2	6:S7:156:LEU:HD23	1.83	0.59
8:V3:57:ASP:O	8:V3:60:LYS:NZ	2.34	0.59
23:D4:231:LEU:O	23:D4:235:LEU:HB2	2.03	0.59
24:D2:233:THR:HA	24:D2:236:LYS:HG2	1.84	0.59
2:V2:39:PRO:HA	8:V3:65:GLN:HB3	1.85	0.58
32:B3:23:ILE:HB	32:B3:46:ARG:HG2	1.85	0.58
6:S7:154:GLU:HG3	7:S8:50:TYR:HE1	1.68	0.58
19:D1:102:VAL:HB	19:D1:150:LEU:HD21	1.84	0.58
23:D4:46:GLY:H	41:BK:84:ARG:HA	1.69	0.58
10:S4:118:TYR:OH	10:S4:133:LYS:NZ	2.36	0.58
37:B7:72:SER:HB2	37:B7:75:ASN:HB2	1.84	0.58
3:S1:312:GLY:N	3:S1:339:ASP:OD2	2.36	0.58
3:S1:442:VAL:O	3:S1:446:ALA:HB2	2.04	0.58
3:S1:568:GLU:HB3	3:S1:589:PRO:HG3	1.86	0.58
6:S7:85:VAL:HG12	6:S7:112:TYR:HB2	1.85	0.58
25:AK:36:SER:HB2	25:AK:55:THR:HG22	1.86	0.58
29:AJ:19:THR:HG23	29:AJ:20:GLU:HG3	1.86	0.58
5:S3:39:GLN:HB3	5:S3:51:CYS:HB2	1.85	0.58
11:A9:177:ARG:O	11:A9:181:TYR:HB2	2.02	0.58
19:D1:22:LEU:HB3	19:D1:48:PRO:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:240:VAL:HG12	3:S1:250:ILE:HG22	1.85	0.58
6:S7:165:LYS:NZ	16:AL:78:ASP:OD1	2.33	0.58
22:D5:341:MET:HE3	22:D5:454:ILE:HD13	1.85	0.58
19:D1:111:LEU:HA	19:D1:114:TYR:HD2	1.69	0.58
22:D5:172:ILE:HG21	23:D4:408:LEU:HD23	1.85	0.58
37:B7:113:ARG:NH2	37:B7:116:GLN:OE1	2.37	0.57
3:S1:260:GLU:HG3	3:S1:394:ARG:HH22	1.68	0.57
6:S7:42:ARG:HH12	6:S7:168:LYS:HD2	1.68	0.57
51:D4:501:3PE:H291	24:D2:288:LEU:HD23	1.86	0.57
7:S8:104:ARG:O	7:S8:105:ARG:NH1	2.38	0.57
38:B9:125:LYS:HE2	38:B9:129:ARG:HH22	1.70	0.57
3:S1:453:LEU:HB3	3:S1:492:ILE:HG22	1.87	0.57
5:S3:37:VAL:HG12	15:A7:69:MET:HG2	1.86	0.57
6:S7:65:PRO:HB3	19:D1:33:PHE:HB2	1.85	0.57
22:D5:267:THR:O	22:D5:274:GLN:NE2	2.37	0.57
22:D5:432:LEU:HD23	32:B3:62:PHE:HA	1.87	0.57
5:S3:85:THR:HG21	10:S4:87:SER:H	1.70	0.57
24:D2:30:TRP:NE1	24:D2:67:SER:OG	2.37	0.57
2:V2:92:ARG:NH1	3:S1:186:TYR:OH	2.37	0.57
3:S1:126:ASP:HA	4:S2:347:HIS:HE1	1.69	0.57
27:A8:141:TYR:HE2	30:S5:37:LYS:HD3	1.69	0.57
38:B9:102:CYS:SG	38:B9:103:LEU:N	2.77	0.57
22:D5:278:LEU:HB3	22:D5:318:GLY:HA3	1.86	0.57
3:S1:589:PRO:HD2	14:A6:125:HIS:HE1	1.70	0.57
18:D3:67:LEU:HB3	21:4L:65:VAL:HG23	1.87	0.57
22:D5:17:MET:HG2	36:B6:73:HIS:HE1	1.70	0.57
35:AM:124:TYR:HB3	35:AM:132:ILE:HG22	1.87	0.57
3:S1:117:GLN:NE2	45:S1:801:SF4:S3	2.78	0.56
23:D4:351:LEU:HD23	26:B5:13:PRO:HB3	1.85	0.56
18:D3:84:LEU:HD11	31:A3:45:ASN:HD22	1.70	0.56
20:D6:118:LYS:HB2	30:S5:69:GLN:HE21	1.70	0.56
23:D4:225:ILE:HG13	23:D4:229:MET:HE2	1.88	0.56
27:A8:24:LEU:HG	35:AM:70:LEU:HD11	1.86	0.56
1:V1:391:SER:HB2	15:A7:48:LEU:HD23	1.87	0.56
3:S1:233:ALA:HB1	3:S1:576:THR:HB	1.87	0.56
23:D4:81:GLN:HB2	23:D4:85:SER:HB3	1.88	0.56
40:B8:88:ARG:HG3	40:B8:89:VAL:HG23	1.86	0.56
2:V2:105:THR:OG1	2:V2:106:THR:N	2.36	0.56
22:D5:542:LEU:HD21	23:D4:277:LEU:HD22	1.88	0.56
6:S7:101:ARG:NH1	6:S7:139:ILE:O	2.39	0.56
26:B5:124:GLN:NE2	27:A8:150:ASN:OD1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:341:MET:SD	22:D5:453:SER:OG	2.63	0.56
24:D2:230:LEU:HB3	24:D2:300:THR:HG22	1.88	0.56
29:AJ:19:THR:OG1	29:AJ:20:GLU:N	2.39	0.56
38:B9:29:ARG:NH2	38:B9:74:GLN:O	2.38	0.56
4:S2:231:ASN:OD1	4:S2:236:ARG:NH2	2.37	0.56
22:D5:279:CYS:SG	22:D5:405:ASN:ND2	2.72	0.56
7:S8:74:GLU:OE1	7:S8:99:ARG:NH2	2.35	0.55
40:B8:55:GLN:O	40:B8:70:ARG:NH2	2.39	0.55
3:S1:237:ASN:HB3	3:S1:253:ARG:HG3	1.87	0.55
4:S2:161:ILE:HD11	4:S2:238:ARG:HE	1.71	0.55
23:D4:388:TRP:O	34:B4:108:ARG:NH2	2.39	0.55
24:D2:339:LEU:HD21	33:C2:34:ILE:HD11	1.87	0.55
1:V1:200:GLN:HE21	1:V1:202:LYS:HE3	1.72	0.55
23:D4:457:PRO:O	41:BK:84:ARG:NH1	2.39	0.55
17:AB:52:MET:SD	38:B9:24:ARG:NH2	2.80	0.55
17:AA:31:SER:HB2	17:AA:34:SER:HB2	1.88	0.55
37:B7:6:ARG:NH1	37:B7:15:GLU:OE2	2.40	0.55
1:V1:179:ARG:NH1	2:V2:52:ASP:OD2	2.39	0.55
1:V1:304:THR:HG23	1:V1:328:GLY:H	1.71	0.55
5:S3:94:TYR:HB2	5:S3:107:VAL:HB	1.88	0.55
23:D4:187:PRO:O	23:D4:192:ASN:ND2	2.40	0.55
25:AK:39:SER:HB2	25:AK:54:ARG:HH22	1.72	0.55
1:V1:126:GLY:HA2	1:V1:131:ALA:HB3	1.87	0.55
3:S1:73:VAL:HA	3:S1:77:TRP:HE1	1.72	0.55
3:S1:447:LYS:HG3	3:S1:448:LYS:HG3	1.88	0.55
23:D4:72:LEU:HD12	23:D4:75:LEU:HD23	1.88	0.55
27:A8:70:PHE:HB3	44:A1:69:ILE:HD12	1.88	0.55
1:V1:111:ILE:HD11	1:V1:149:LEU:HD22	1.88	0.55
3:S1:543:ILE:HD11	3:S1:557:ALA:HA	1.89	0.55
5:S3:93:VAL:HG22	5:S3:108:LYS:HG2	1.88	0.55
23:D4:326:LEU:HD21	23:D4:410:MET:HE1	1.89	0.55
28:BJ:159:LYS:NZ	33:C2:112:VAL:O	2.39	0.55
18:D3:10:ASN:HD21	19:D1:10:ILE:HG21	1.71	0.55
26:B5:88:GLU:OE1	43:B1:56:TRP:NE1	2.40	0.55
29:AJ:72:ARG:NH1	29:AJ:295:GLU:OE1	2.40	0.55
3:S1:106:PRO:O	3:S1:218:ARG:NH2	2.40	0.54
18:D3:77:TRP:HA	19:D1:317:GLN:HE22	1.72	0.54
4:S2:237:ASN:O	19:D1:284:GLN:NE2	2.41	0.54
4:S2:339:LYS:HG3	9:S6:65:ALA:HA	1.89	0.54
43:B1:46:ARG:NH2	43:B1:55:THR:OG1	2.41	0.54
22:D5:15:LEU:HD21	22:D5:125:LEU:HD22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A8:146:ARG:NH2	30:S5:41:GLU:OE1	2.38	0.54
19:D1:164:THR:HG22	35:AM:56:ARG:HH22	1.72	0.54
3:S1:13:VAL:HG11	3:S1:33:VAL:HG21	1.87	0.54
19:D1:55:LEU:HD12	19:D1:221:ALA:HB2	1.90	0.54
52:D5:901:CDL:H711	52:D5:901:CDL:H542	1.90	0.54
4:S2:405:MET:SD	4:S2:421:GLN:NE2	2.81	0.54
19:D1:169:GLN:NE2	19:D1:241:LEU:O	2.37	0.54
20:D6:159:TRP:HE1	24:D2:12:THR:HG22	1.72	0.54
4:S2:19:MET:HG2	24:D2:295:ARG:HH12	1.72	0.54
4:S2:226:GLU:OE2	4:S2:305:ARG:NH2	2.41	0.54
11:A9:19:ILE:O	11:A9:43:SER:OG	2.25	0.54
11:A9:132:ILE:HD13	49:A9:401:NDP:H1D	1.90	0.54
1:V1:123:LEU:HD22	1:V1:162:ILE:HG22	1.90	0.54
3:S1:577:GLU:OE2	3:S1:579:ARG:NH1	2.41	0.54
28:BJ:8:VAL:O	28:BJ:108:ARG:NH2	2.35	0.54
6:S7:165:LYS:NZ	16:AL:77:VAL:O	2.41	0.53
22:D5:547:LYS:O	22:D5:552:LEU:CB	2.57	0.53
23:D4:205:VAL:HG22	23:D4:212:LEU:HD13	1.88	0.53
23:D4:300:ALA:O	23:D4:308:SER:OG	2.27	0.53
29:AJ:108:TYR:OH	29:AJ:164:LEU:O	2.26	0.53
5:S3:86:ARG:NH1	5:S3:91:GLU:OE2	2.40	0.53
28:BJ:66:GLU:OE2	41:BK:95:ARG:NH1	2.41	0.53
3:S1:521:MET:HG3	3:S1:542:PHE:HD2	1.74	0.53
18:D3:69:ILE:HD11	19:D1:144:VAL:HG13	1.89	0.53
18:D3:73:LEU:HD21	20:D6:55:MET:HE1	1.90	0.53
23:D4:134:THR:O	23:D4:142:ARG:NH1	2.41	0.53
4:S2:227:GLU:OE1	15:A7:17:ARG:NH2	2.42	0.53
7:S8:32:ARG:NH2	35:AM:27:ARG:O	2.42	0.53
23:D4:76:MET:HE1	23:D4:230:VAL:HG23	1.91	0.53
23:D4:436:LEU:O	23:D4:440:HIS:ND1	2.41	0.53
3:S1:378:LEU:HG	3:S1:451:VAL:HG22	1.91	0.53
4:S2:261:ARG:NH2	4:S2:268:ASP:OD1	2.42	0.53
14:A6:46:VAL:HG23	14:A6:51:LEU:HB2	1.89	0.53
23:D4:170:THR:HG23	23:D4:171:MET:HG3	1.89	0.53
3:S1:592:LEU:O	3:S1:594:ARG:NH1	2.41	0.53
9:S6:12:THR:OG1	9:S6:14:THR:O	2.26	0.53
20:D6:59:ILE:HG13	21:4L:64:LEU:HD21	1.89	0.53
22:D5:15:LEU:HB3	22:D5:126:ILE:HG12	1.91	0.53
22:D5:81:LYS:HG2	22:D5:135:ASN:HB3	1.91	0.53
22:D5:160:GLY:H	23:D4:417:GLY:HA2	1.73	0.53
23:D4:1:MET:HG2	23:D4:111:THR:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:366:THR:HG21	3:S1:450:MET:HE2	1.91	0.53
3:S1:515:ARG:HH12	3:S1:536:ASP:HB3	1.73	0.53
5:S3:71:GLN:HG3	13:A5:82:GLN:HE22	1.74	0.53
37:B7:97:ARG:NH2	40:B8:129:GLY:O	2.39	0.53
6:S7:139:ILE:HG22	6:S7:140:VAL:HG13	1.91	0.53
34:B4:13:LEU:HD22	34:B4:14:PRO:HD2	1.91	0.53
29:AJ:77:CYS:O	29:AJ:92:ASN:ND2	2.40	0.52
11:A9:237:LEU:HG	11:A9:239:PHE:H	1.73	0.52
22:D5:161:ARG:NH1	38:B9:88:THR:O	2.42	0.52
29:AJ:184:GLN:HG2	29:AJ:192:MET:HE1	1.90	0.52
11:A9:81:ILE:HG21	11:A9:117:ILE:HG22	1.91	0.52
23:D4:68:LEU:HD22	23:D4:317:ILE:HG23	1.91	0.52
27:A8:142:HIS:ND1	35:AM:113:THR:O	2.40	0.52
1:V1:132:ARG:NH2	8:V3:63:MET:SD	2.83	0.52
4:S2:116:GLN:HG3	4:S2:138:ARG:HD3	1.91	0.52
14:A6:43:PRO:HA	14:A6:46:VAL:HG12	1.92	0.52
38:B9:15:VAL:HG22	38:B9:63:LEU:HD13	1.90	0.52
3:S1:225:THR:HB	3:S1:240:VAL:HG23	1.92	0.52
3:S1:377:VAL:HA	3:S1:450:MET:O	2.09	0.52
5:S3:178:ASP:H	11:A9:36:ASN:HD21	1.57	0.52
24:D2:109:ALA:HB2	24:D2:161:SER:HA	1.91	0.52
3:S1:360:SER:HA	3:S1:365:ASN:HD21	1.75	0.52
4:S2:98:GLN:NE2	7:S8:85:ALA:O	2.43	0.52
23:D4:385:THR:HG21	23:D4:396:MET:HE3	1.91	0.52
4:S2:50:ASN:HD22	4:S2:65:VAL:HG22	1.73	0.52
19:D1:18:ALA:O	19:D1:21:THR:OG1	2.26	0.52
28:BJ:141:ARG:HD2	41:BK:112:CYS:H	1.75	0.52
38:B9:108:PRO:HA	38:B9:111:LYS:HB2	1.92	0.52
10:S4:33:ARG:NH2	10:S4:77:ASP:OD1	2.43	0.51
22:D5:363:PHE:HA	22:D5:370:THR:HG21	1.92	0.51
6:S7:109:GLU:O	11:A9:54:TYR:OH	2.28	0.51
27:A8:10:GLU:HA	27:A8:13:LYS:HE2	1.91	0.51
29:AJ:17:LYS:HG2	29:AJ:118:THR:HA	1.93	0.51
1:V1:91:LYS:HB2	1:V1:131:ALA:HA	1.91	0.51
5:S3:41:GLN:NE2	5:S3:49:GLU:OE1	2.43	0.51
10:S4:12:THR:HG21	14:A6:15:SER:HA	1.91	0.51
18:D3:71:LEU:O	20:D6:147:TYR:OH	2.27	0.51
17:AB:7:THR:HG23	17:AB:10:GLY:H	1.75	0.51
29:AJ:141:GLN:NE2	29:AJ:201:ASP:OD2	2.43	0.51
34:B4:40:SER:OG	38:B9:150:THR:O	2.28	0.51
3:S1:668:ILE:HG21	3:S1:691:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A9:167:LYS:O	11:A9:229:ALA:HA	2.10	0.51
26:B5:56:PRO:HG2	26:B5:59:TYR:HB3	1.93	0.51
28:BJ:69:ARG:NH1	28:BJ:90:GLN:OE1	2.43	0.51
2:V2:126:ILE:HG21	2:V2:132:THR:HA	1.93	0.51
3:S1:247:VAL:HG22	3:S1:587:VAL:HG21	1.93	0.51
6:S7:46:TRP:NE1	6:S7:82:GLN:O	2.39	0.51
1:V1:32:ARG:HB3	1:V1:35:GLY:H	1.75	0.51
1:V1:68:ARG:NH1	1:V1:226:GLU:OE1	2.41	0.51
5:S3:80:ALA:HB2	5:S3:92:ILE:HD13	1.93	0.51
1:V1:93:LEU:O	1:V1:134:ALA:HA	2.11	0.51
22:D5:128:MET:HE3	22:D5:251:THR:HA	1.92	0.51
23:D4:76:MET:HE2	23:D4:229:MET:HB2	1.92	0.51
23:D4:250:LEU:HB3	23:D4:253:ILE:HD11	1.92	0.51
11:A9:108:ASP:O	11:A9:112:LYS:HB3	2.11	0.51
12:A2:64:LEU:HD21	12:A2:90:LEU:HD23	1.93	0.51
18:D3:63:LEU:HD22	21:4L:72:ALA:HB2	1.94	0.50
22:D5:145:GLU:HB2	23:D4:370:PRO:HG3	1.92	0.50
22:D5:435:PRO:HB2	22:D5:437:PHE:HE1	1.75	0.50
34:B4:42:LEU:HD13	40:B8:74:GLY:HA3	1.91	0.50
44:A1:1:MET:HG3	44:A1:3:PHE:H	1.75	0.50
1:V1:184:TYR:HE2	1:V1:407:LEU:HD13	1.75	0.50
3:S1:157:THR:O	3:S1:161:ARG:NE	2.44	0.50
3:S1:460:ARG:HG3	3:S1:462:ASP:H	1.75	0.50
11:A9:135:LEU:HA	11:A9:167:LYS:HD3	1.93	0.50
24:D2:200:MET:HE1	24:D2:265:MET:HE3	1.93	0.50
1:V1:30:ASP:OD2	1:V1:38:SER:OG	2.29	0.50
6:S7:162:GLN:HE22	16:AL:118:SER:HB3	1.75	0.50
8:V3:70:ARG:NH2	10:S4:125:ASN:O	2.45	0.50
16:AL:83:PRO:HG2	16:AL:86:TRP:HD1	1.76	0.50
40:B8:47:TYR:OH	40:B8:76:PRO:O	2.29	0.50
4:S2:360:PRO:HA	4:S2:380:SER:O	2.12	0.50
19:D1:258:ASN:OD1	19:D1:262:LYS:NZ	2.42	0.50
22:D5:260:LEU:HD22	22:D5:277:MET:HE1	1.94	0.50
27:A8:35:CYS:SG	27:A8:36:ASP:N	2.83	0.50
38:B9:89:SER:HA	38:B9:92:ARG:HB2	1.93	0.50
23:D4:254:THR:O	23:D4:258:ALA:CB	2.59	0.50
23:D4:254:THR:O	23:D4:258:ALA:HB3	2.12	0.50
27:A8:53:ARG:HA	27:A8:56:LEU:HD23	1.94	0.50
2:V2:55:GLN:NE2	2:V2:89:MET:O	2.40	0.50
3:S1:382:THR:HB	3:S1:454:GLY:HA3	1.93	0.50
7:S8:64:GLU:HB3	7:S8:134:GLY:HA3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:D1:178:ALA:HB1	19:D1:181:LEU:HB3	1.93	0.50
22:D5:40:ILE:HG13	22:D5:101:MET:HE3	1.93	0.50
23:D4:165:ILE:HG21	24:D2:268:GLN:HA	1.92	0.50
24:D2:26:TRP:HB3	24:D2:74:ILE:HD13	1.94	0.50
26:B5:87:TYR:O	26:B5:90:THR:OG1	2.30	0.50
22:D5:7:LEU:HA	22:D5:10:VAL:HG22	1.93	0.50
38:B9:24:ARG:NH1	38:B9:27:GLU:OE1	2.43	0.50
1:V1:197:GLU:OE2	1:V1:204:ARG:NH2	2.46	0.49
1:V1:295:LEU:HB2	1:V1:339:ARG:HA	1.94	0.49
3:S1:261:GLU:OE2	10:S4:42:ARG:NH2	2.44	0.49
22:D5:513:PHE:HE1	38:B9:29:ARG:HG2	1.76	0.49
20:D6:58:LEU:O	20:D6:62:GLY:CA	2.59	0.49
20:D6:163:ILE:HG13	24:D2:12:THR:HG21	1.95	0.49
22:D5:584:ILE:HD11	24:D2:58:LYS:HE2	1.94	0.49
37:B7:14:VAL:HA	37:B7:108:LEU:HD22	1.94	0.49
39:B2:39:ARG:NH2	39:B2:43:ASP:OD2	2.46	0.49
2:V2:91:ASN:OD1	2:V2:91:ASN:N	2.46	0.49
19:D1:303:TRP:HH2	35:AM:42:LEU:HD11	1.78	0.49
20:D6:17:PHE:HD2	21:4L:11:ALA:HB1	1.76	0.49
24:D2:243:LEU:HD21	33:C2:44:ILE:HD11	1.95	0.49
30:S5:27:ARG:H	31:A3:51:ASN:HD21	1.59	0.49
1:V1:250:ASN:HD21	1:V1:318:ASP:HB3	1.78	0.49
11:A9:91:VAL:HG13	11:A9:129:PHE:HD1	1.77	0.49
22:D5:33:PRO:HB3	22:D5:118:PHE:HE2	1.78	0.49
23:D4:369:LEU:HD23	23:D4:371:PRO:HD2	1.94	0.49
26:B5:49:GLU:HA	26:B5:70:PRO:HD3	1.93	0.49
6:S7:69:MET:HE1	6:S7:76:PHE:HB3	1.94	0.49
37:B7:36:ARG:NH2	40:B8:156:TYR:O	2.45	0.49
40:B8:47:TYR:OH	40:B8:77:MET:O	2.30	0.49
19:D1:228:TYR:HA	19:D1:231:ILE:HD12	1.94	0.49
34:B4:74:ASN:ND2	34:B4:77:PRO:O	2.45	0.49
11:A9:55:ASP:O	11:A9:58:HIS:ND1	2.46	0.49
20:D6:25:SER:HB3	20:D6:28:TYR:HD2	1.77	0.49
7:S8:95:GLU:OE1	7:S8:108:ARG:NH1	2.46	0.49
12:A2:22:LEU:HB2	12:A2:56:GLU:HG2	1.95	0.49
14:A6:37:ALA:O	14:A6:41:GLU:HB2	2.13	0.49
18:D3:98:LEU:HD22	19:D1:298:LEU:HD21	1.94	0.49
19:D1:149:ILE:HG21	19:D1:185:TRP:HB2	1.95	0.49
29:AJ:71:VAL:O	29:AJ:76:ASN:ND2	2.46	0.49
29:AJ:305:ARG:HB2	33:C2:50:ARG:HB2	1.95	0.49
3:S1:193:SER:OG	3:S1:385:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S7:55:CYS:HB3	6:S7:89:ALA:HB1	1.95	0.48
13:A5:54:LYS:HE2	13:A5:71:LEU:HD11	1.95	0.48
7:S8:53:GLU:OE2	16:AL:34:ARG:NH2	2.46	0.48
22:D5:10:VAL:HA	22:D5:13:ILE:HG22	1.94	0.48
22:D5:473:PRO:HB2	22:D5:475:MET:HE2	1.95	0.48
29:AJ:56:ILE:HD11	29:AJ:79:LEU:HB2	1.94	0.48
29:AJ:18:MET:HB3	29:AJ:19:THR:HB	1.96	0.48
36:B6:89:VAL:HG21	36:B6:96:ILE:HG12	1.95	0.48
36:B6:100:LYS:HB3	37:B7:49:GLN:HE22	1.78	0.48
22:D5:554:ASP:O	22:D5:558:LEU:HB3	2.13	0.48
24:D2:292:PHE:HA	24:D2:295:ARG:HG2	1.95	0.48
17:AB:63:PRO:HB3	40:B8:61:TRP:HB3	1.94	0.48
27:A8:46:ARG:NH1	35:AM:79:ASP:OD2	2.46	0.48
27:A8:132:THR:OG1	31:A3:57:ARG:NH1	2.47	0.48
29:AJ:189:PRO:HA	29:AJ:192:MET:HB2	1.95	0.48
1:V1:247:ARG:HH21	1:V1:316:LEU:HD11	1.78	0.48
22:D5:245:ALA:O	22:D5:249:SER:HB3	2.13	0.48
23:D4:409:TYR:O	23:D4:413:THR:OG1	2.29	0.48
24:D2:128:LEU:HD13	24:D2:216:PHE:HB2	1.95	0.48
3:S1:531:CYS:SG	3:S1:532:VAL:N	2.87	0.48
22:D5:60:GLU:HB2	36:B6:99:LYS:HB3	1.95	0.48
23:D4:177:LEU:O	23:D4:180:GLN:O	2.30	0.48
27:A8:95:LEU:HB2	27:A8:98:ARG:HG2	1.96	0.48
4:S2:238:ARG:HG3	4:S2:239:THR:HG23	1.96	0.48
19:D1:316:PRO:HB3	35:AM:57:ARG:HD2	1.93	0.48
22:D5:351:ASN:OD1	22:D5:442:ASN:ND2	2.42	0.48
22:D5:451:ILE:O	22:D5:455:LYS:CB	2.62	0.48
24:D2:327:PRO:HB3	33:C2:44:ILE:HG23	1.95	0.48
26:B5:132:LEU:HD11	30:S5:19:ILE:HD12	1.96	0.48
40:B8:58:ARG:NH1	40:B8:75:GLU:OE2	2.47	0.48
33:C2:66:THR:HG22	42:C1:27:LEU:HD23	1.96	0.48
2:V2:27:ASN:OD1	2:V2:30:ARG:NH1	2.47	0.48
19:D1:145:THR:HG23	19:D1:297:THR:HG21	1.95	0.48
24:D2:228:LEU:O	24:D2:232:HIS:ND1	2.42	0.48
19:D1:236:ILE:HG23	19:D1:259:PHE:HZ	1.79	0.47
28:BJ:132:THR:HA	28:BJ:135:VAL:HG12	1.95	0.47
3:S1:365:ASN:HB3	3:S1:488:LYS:HD3	1.95	0.47
19:D1:152:SER:HG	19:D1:301:CYS:HG	1.60	0.47
52:D5:901:CDL:HA31	26:B5:22:LEU:HD21	1.95	0.47
27:A8:77:CYS:HA	27:A8:78:ALA:HA	1.71	0.47
28:BJ:119:SER:HB3	37:B7:55:ARG:HH22	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AJ:54:ALA:HB2	29:AJ:107:GLN:HG2	1.96	0.47
1:V1:101:GLU:O	1:V1:104:THR:OG1	2.32	0.47
1:V1:366:ARG:NH1	3:S1:155:GLN:OE1	2.48	0.47
4:S2:287:ILE:HB	7:S8:4:TYR:HB3	1.95	0.47
20:D6:121:GLY:HA2	21:4L:3:LEU:HD22	1.96	0.47
24:D2:199:THR:HG23	24:D2:346:LEU:HD22	1.95	0.47
37:B7:108:LEU:O	37:B7:112:LYS:HB2	2.14	0.47
4:S2:19:MET:SD	24:D2:295:ARG:NH2	2.75	0.47
4:S2:97:LEU:HD11	4:S2:195:ARG:HD2	1.96	0.47
35:AM:110:PHE:HE2	35:AM:116:VAL:HG21	1.79	0.47
2:V2:156:ILE:HG12	2:V2:161:TYR:HE2	1.79	0.47
3:S1:40:PHE:O	3:S1:158:ARG:NH2	2.48	0.47
6:S7:116:MET:HA	6:S7:146:VAL:HG23	1.97	0.47
11:A9:29:PHE:HE1	11:A9:175:GLU:H	1.61	0.47
16:AL:39:VAL:HG21	16:AL:50:GLU:HB3	1.97	0.47
20:D6:71:THR:HA	20:D6:74:MET:HG3	1.96	0.47
22:D5:342:CYS:SG	22:D5:369:THR:OG1	2.70	0.47
1:V1:100:GLY:HA3	1:V1:184:TYR:CD1	2.50	0.47
2:V2:35:VAL:HG11	2:V2:43:LYS:HG3	1.95	0.47
4:S2:204:PRO:HD3	7:S8:60:ARG:HH22	1.78	0.47
16:AL:117:LEU:HD13	16:AL:123:GLN:HA	1.95	0.47
19:D1:1:MET:HA	19:D1:4:ILE:HD12	1.97	0.47
23:D4:60:SER:OG	41:BK:84:ARG:NH2	2.47	0.47
3:S1:202:ILE:HD11	3:S1:262:TRP:HH2	1.80	0.47
4:S2:282:GLU:HB2	4:S2:313:GLN:HE22	1.79	0.47
7:S8:22:ALA:O	7:S8:26:LEU:HB2	2.14	0.47
7:S8:65:HIS:NE2	7:S8:116:CYS:SG	2.88	0.47
10:S4:88:THR:HG23	10:S4:91:ASP:H	1.79	0.47
11:A9:136:ASN:HD21	11:A9:291:ASP:HA	1.80	0.47
22:D5:9:LEU:HB3	36:B6:81:ILE:HD13	1.96	0.47
23:D4:204:MET:HE2	23:D4:243:MET:HE1	1.96	0.47
26:B5:31:LEU:HD23	26:B5:32:THR:HG23	1.96	0.47
28:BJ:98:ASP:OD2	28:BJ:141:ARG:NH2	2.48	0.47
3:S1:250:ILE:HD11	3:S1:268:ARG:HA	1.95	0.47
3:S1:283:MET:HE2	3:S1:291:LEU:HG	1.96	0.47
4:S2:3:GLN:NE2	23:D4:135:ARG:O	2.48	0.47
19:D1:152:SER:OG	19:D1:301:CYS:SG	2.62	0.47
22:D5:418:PHE:HA	22:D5:421:ILE:HG12	1.96	0.47
22:D5:554:ASP:O	22:D5:558:LEU:CB	2.63	0.47
2:V2:24:THR:HG22	2:V2:26:GLU:H	1.79	0.47
12:A2:57:CYS:SG	12:A2:58:SER:N	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:246:LEU:O	22:D5:251:THR:OG1	2.33	0.47
50:AB:101:ZMP:H6A	38:B9:47:PHE:HE1	1.79	0.47
38:B9:107:HIS:NE2	41:BK:43:ASP:OD1	2.44	0.47
1:V1:59:GLU:HG3	1:V1:234:ILE:HG22	1.97	0.47
2:V2:88:THR:HG22	3:S1:177:ARG:HH22	1.79	0.47
6:S7:141:PRO:HB3	11:A9:61:PRO:HD3	1.97	0.47
10:S4:12:THR:HG21	14:A6:16:VAL:H	1.80	0.47
21:4L:73:LEU:HD21	24:D2:41:ILE:HG13	1.97	0.47
22:D5:137:LEU:HB3	22:D5:196:TRP:HB2	1.97	0.47
24:D2:108:MET:SD	24:D2:161:SER:OG	2.67	0.47
26:B5:104:ARG:NH2	27:A8:166:LEU:O	2.48	0.47
11:A9:48:PRO:HB2	11:A9:73:TRP:CD1	2.51	0.46
19:D1:167:ILE:HD12	27:A8:97:ARG:HH22	1.81	0.46
1:V1:165:ASN:HD22	1:V1:170:GLY:HA2	1.80	0.46
4:S2:21:PRO:HA	4:S2:25:THR:HG21	1.97	0.46
4:S2:300:ARG:NH2	4:S2:420:THR:O	2.38	0.46
6:S7:179:ARG:HG3	11:A9:50:ARG:HH12	1.79	0.46
23:D4:106:LEU:HD13	23:D4:234:ILE:HG21	1.97	0.46
23:D4:210:TYR:O	23:D4:213:HIS:ND1	2.39	0.46
27:A8:6:LEU:HD13	35:AM:86:LEU:HB3	1.97	0.46
33:C2:8:ARG:H	33:C2:9:ALA:HB3	1.80	0.46
1:V1:367:GLU:OE1	3:S1:100:ASN:ND2	2.48	0.46
5:S3:115:THR:HG23	14:A6:17:LYS:HB2	1.98	0.46
16:AL:4:LEU:O	16:AL:8:LYS:N	2.48	0.46
19:D1:92:PRO:HG3	19:D1:255:TYR:HD2	1.81	0.46
27:A8:36:ASP:OD1	27:A8:39:ASN:ND2	2.49	0.46
27:A8:85:TRP:O	27:A8:89:ASP:HB2	2.16	0.46
28:BJ:14:ARG:NH1	36:B6:98:GLU:OE2	2.43	0.46
1:V1:96:ASN:ND2	1:V1:187:GLY:O	2.47	0.46
1:V1:124:VAL:O	1:V1:128:ALA:HB3	2.14	0.46
1:V1:309:LYS:NZ	1:V1:313:GLU:OE2	2.46	0.46
2:V2:55:GLN:NE2	2:V2:91:ASN:OD1	2.48	0.46
3:S1:320:GLY:HA3	3:S1:346:GLU:HB2	1.97	0.46
3:S1:409:ILE:HG12	3:S1:422:LEU:HB2	1.98	0.46
7:S8:34:LEU:HD12	19:D1:272:TRP:CE2	2.50	0.46
3:S1:332:LYS:HD3	3:S1:507:TYR:HE1	1.79	0.46
4:S2:224:GLU:OE1	7:S8:40:TYR:OH	2.25	0.46
27:A8:166:LEU:HD23	27:A8:167:PHE:H	1.80	0.46
1:V1:370:ASP:OD1	1:V1:374:LYS:NZ	2.45	0.46
2:V2:53:LEU:HD12	8:V3:52:LEU:HD13	1.98	0.46
4:S2:284:ASP:OD1	4:S2:284:ASP:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:40:VAL:HB	15:A7:68:VAL:O	2.16	0.46
12:A2:19:ARG:HH21	12:A2:65:TRP:HE3	1.63	0.46
17:AA:70:LEU:HD13	17:AA:76:ILE:HG12	1.97	0.46
22:D5:90:VAL:HG13	22:D5:91:PRO:HD3	1.98	0.46
23:D4:158:LEU:HD21	24:D2:283:ALA:HB1	1.97	0.46
24:D2:142:LEU:HB3	24:D2:194:LEU:HD21	1.97	0.46
24:D2:269:GLU:HA	24:D2:272:LYS:HG2	1.98	0.46
29:AJ:202:ILE:O	29:AJ:206:TYR:CB	2.64	0.46
16:AL:60:ARG:NH1	16:AL:92:CYS:SG	2.88	0.46
18:D3:70:ALA:HB2	20:D6:59:ILE:HD11	1.97	0.46
23:D4:368:ALA:HB1	23:D4:375:LEU:HB2	1.98	0.46
26:B5:64:TRP:CD1	26:B5:65:GLU:HG3	2.51	0.46
4:S2:48:THR:HG22	4:S2:67:GLU:HG2	1.98	0.46
16:AL:44:TYR:OH	16:AL:111:THR:O	2.34	0.46
22:D5:470:ASN:ND2	37:B7:76:PHE:O	2.45	0.46
25:AK:46:THR:HA	25:AK:47:SER:HA	1.71	0.46
28:BJ:101:ILE:HD11	41:BK:96:LEU:HD22	1.97	0.46
29:AJ:66:GLY:HA2	42:C1:4:ILE:HD11	1.97	0.46
37:B7:34:LYS:HE3	37:B7:36:ARG:HB2	1.97	0.46
1:V1:100:GLY:O	1:V1:104:THR:OG1	2.30	0.46
1:V1:362:CYS:N	45:V1:500:SF4:S2	2.82	0.46
3:S1:296:TRP:HE1	3:S1:592:LEU:HB3	1.81	0.46
3:S1:433:ALA:HA	3:S1:473:ILE:HD11	1.98	0.46
19:D1:117:LEU:HD12	19:D1:136:VAL:HG11	1.97	0.46
22:D5:332:HIS:CE1	22:D5:336:LYS:HD2	2.51	0.46
17:AB:87:TYR:HE2	36:B6:19:ARG:HG2	1.80	0.46
33:C2:25:LYS:N	33:C2:28:ASP:OD2	2.49	0.46
40:B8:50:LEU:HB2	40:B8:78:HIS:CD2	2.51	0.46
40:B8:66:HIS:HB3	40:B8:69:LEU:HB2	1.97	0.46
23:D4:270:ILE:HD12	23:D4:398:LEU:HD22	1.98	0.45
40:B8:4:ILE:HG22	40:B8:6:LYS:H	1.81	0.45
40:B8:13:TYR:HB3	40:B8:36:PRO:HG3	1.98	0.45
2:V2:103:CYS:HB3	2:V2:153:MET:HG2	1.98	0.45
2:V2:104:THR:HA	2:V2:108:CYS:HB2	1.97	0.45
4:S2:234:ILE:HG12	19:D1:280:PHE:CE1	2.51	0.45
5:S3:177:ASP:OD2	11:A9:40:ARG:NH2	2.47	0.45
26:B5:106:LYS:HD3	33:C2:94:ILE:HG13	1.96	0.45
28:BJ:114:GLN:HE21	36:B6:99:LYS:HB2	1.82	0.45
31:A3:58:ASP:OD1	31:A3:58:ASP:N	2.49	0.45
1:V1:394:GLU:OE1	3:S1:129:ARG:NH1	2.49	0.45
2:V2:30:ARG:NH2	8:V3:53:ASP:OD1	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:258:ILE:HG22	3:S1:368:ILE:HB	1.99	0.45
11:A9:234:ASN:HD21	11:A9:310:LEU:H	1.64	0.45
11:A9:310:LEU:O	11:A9:314:ALA:CB	2.64	0.45
20:D6:145:ALA:HB2	30:S5:25:PRO:HG3	1.98	0.45
23:D4:403:THR:HA	23:D4:406:TYR:CE1	2.51	0.45
27:A8:110:VAL:O	27:A8:115:GLY:N	2.48	0.45
5:S3:77:ASP:O	5:S3:93:VAL:O	2.34	0.45
8:V3:68:SER:HB3	10:S4:125:ASN:HB3	1.99	0.45
11:A9:141:SER:HA	11:A9:147:ARG:HH21	1.82	0.45
18:D3:81:THR:H	31:A3:45:ASN:HD21	1.63	0.45
19:D1:195:ARG:HE	19:D1:274:ARG:HD2	1.80	0.45
23:D4:179:LEU:HD21	23:D4:249:LEU:HD23	1.98	0.45
27:A8:70:PHE:HA	27:A8:73:ILE:HG22	1.98	0.45
31:A3:27:LEU:O	31:A3:31:LEU:CB	2.65	0.45
4:S2:139:VAL:HG13	4:S2:278:TYR:HE1	1.80	0.45
20:D6:122:MET:HE3	20:D6:126:VAL:HG21	1.98	0.45
24:D2:232:HIS:HE1	29:AJ:276:PRO:HG3	1.81	0.45
24:D2:244:VAL:HG11	24:D2:300:THR:HG21	1.98	0.45
28:BJ:159:LYS:HG2	41:BK:118:ILE:HD11	1.98	0.45
29:AJ:171:TYR:HD2	29:AJ:222:GLN:HG3	1.80	0.45
37:B7:8:TYR:OH	40:B8:123:PRO:O	2.27	0.45
3:S1:73:VAL:HG13	3:S1:77:TRP:CD1	2.51	0.45
23:D4:203:PHE:O	23:D4:207:MET:HG2	2.17	0.45
24:D2:222:ASN:OD1	24:D2:222:ASN:N	2.48	0.45
29:AJ:97:GLN:HG2	29:AJ:135:LEU:HD22	1.99	0.45
6:S7:68:ASP:HB2	6:S7:71:ARG:HE	1.81	0.45
11:A9:56:THR:HA	11:A9:59:LEU:HG	1.98	0.45
23:D4:76:MET:HB2	23:D4:76:MET:HE3	1.69	0.45
24:D2:120:GLN:O	24:D2:176:ARG:NH2	2.49	0.45
32:B3:28:LEU:HA	32:B3:31:VAL:HG12	1.99	0.45
1:V1:139:ARG:NH2	2:V2:144:CYS:O	2.49	0.45
14:A6:32:ARG:HH12	17:AA:44:SER:HB2	1.81	0.45
22:D5:77:SER:OG	22:D5:79:SER:OG	2.32	0.45
22:D5:401:THR:HG22	40:B8:126:GLN:HE22	1.82	0.45
1:V1:124:VAL:O	1:V1:128:ALA:CB	2.65	0.45
2:V2:164:LEU:HD23	2:V2:169:ILE:HD11	1.98	0.45
22:D5:362:LEU:H	22:D5:431:LEU:HA	1.81	0.45
22:D5:558:LEU:HA	22:D5:561:ILE:HG22	1.99	0.45
23:D4:197:LEU:O	23:D4:201:MET:CB	2.64	0.45
25:AK:89:TYR:CD2	25:AK:125:LYS:HB2	2.52	0.45
27:A8:124:LEU:HD12	35:AM:65:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:218:ARG:HA	3:S1:219:PRO:HD3	1.83	0.45
5:S3:202:PRO:HA	10:S4:50:ASN:HB3	1.98	0.45
22:D5:71:ILE:HG13	22:D5:72:GLN:H	1.82	0.45
22:D5:404:THR:HG21	22:D5:409:LEU:HB2	1.98	0.45
17:AB:52:MET:HG2	38:B9:23:LEU:HD12	1.99	0.45
32:B3:73:GLY:HA3	39:B2:33:TRP:HD1	1.82	0.45
2:V2:99:HIS:CE1	2:V2:101:GLN:HE21	2.35	0.44
4:S2:261:ARG:O	4:S2:288:GLY:N	2.45	0.44
5:S3:86:ARG:HD3	13:A5:110:GLN:HG3	1.99	0.44
6:S7:31:ALA:HA	6:S7:174:ARG:HD2	1.98	0.44
23:D4:207:MET:HE3	23:D4:298:ILE:HD11	1.99	0.44
38:B9:138:GLN:O	38:B9:142:GLU:CB	2.61	0.44
2:V2:156:ILE:HD11	2:V2:159:ASN:HD22	1.82	0.44
7:S8:143:THR:HA	11:A9:60:ARG:HH22	1.82	0.44
21:4L:47:MET:HE2	21:4L:47:MET:HB3	1.70	0.44
23:D4:305:THR:HG22	23:D4:307:TRP:H	1.82	0.44
3:S1:424:ASP:OD1	3:S1:424:ASP:N	2.51	0.44
4:S2:155:THR:HG21	4:S2:170:MET:HB2	1.99	0.44
15:A7:111:TYR:HA	15:A7:112:LEU:HA	1.76	0.44
23:D4:263:MET:HE1	34:B4:100:TRP:HB2	1.99	0.44
24:D2:151:LEU:HD22	25:AK:136:ALA:HB2	1.99	0.44
28:BJ:138:TYR:HA	41:BK:108:MET:HE1	1.99	0.44
38:B9:82:PRO:O	38:B9:89:SER:OG	2.33	0.44
4:S2:341:SER:OG	4:S2:342:MET:N	2.50	0.44
22:D5:119:LYS:HZ3	52:D5:901:CDL:HB32	1.83	0.44
24:D2:2:ASN:HB2	24:D2:5:ILE:HD12	1.99	0.44
26:B5:137:PRO:HB2	31:A3:54:VAL:HG11	1.99	0.44
17:AB:60:PHE:HZ	17:AB:80:ILE:HG13	1.82	0.44
33:C2:19:ARG:HB3	42:C1:41:GLU:HG2	1.99	0.44
22:D5:306:THR:OG1	22:D5:332:HIS:NE2	2.47	0.44
23:D4:151:PHE:HD2	51:D4:501:3PE:H331	1.82	0.44
11:A9:115:GLN:HE21	11:A9:155:GLU:HG2	1.82	0.44
22:D5:227:PHE:H	22:D5:284:THR:HG22	1.81	0.44
24:D2:69:LEU:HD11	24:D2:97:LEU:HD22	1.99	0.44
24:D2:115:VAL:HG12	24:D2:180:ALA:HB1	1.98	0.44
29:AJ:169:VAL:HG23	29:AJ:218:CYS:HB3	2.00	0.44
4:S2:32:PRO:HD2	24:D2:51:ARG:HH22	1.82	0.44
4:S2:238:ARG:HH22	4:S2:412:ALA:HB1	1.82	0.44
5:S3:77:ASP:N	5:S3:77:ASP:OD1	2.50	0.44
14:A6:63:ARG:HB2	17:AA:45:LEU:HD21	1.98	0.44
16:AL:86:TRP:O	16:AL:90:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:384:PRO:HA	22:D5:385:PHE:HA	1.54	0.44
22:D5:389:PHE:O	22:D5:393:ASP:HB2	2.18	0.44
23:D4:350:THR:OG1	23:D4:351:LEU:N	2.51	0.44
28:BJ:158:GLN:HG3	28:BJ:162:MET:HE3	2.00	0.44
29:AJ:75:GLY:HA3	29:AJ:76:ASN:HA	1.70	0.44
31:A3:27:LEU:O	31:A3:31:LEU:HB3	2.17	0.44
38:B9:169:ILE:O	38:B9:172:ARG:NH1	2.49	0.44
1:V1:78:LYS:NZ	46:V1:501:FMN:O2P	2.42	0.44
2:V2:17:PRO:HA	2:V2:19:THR:H	1.83	0.44
10:S4:33:ARG:HG2	10:S4:62:ARG:HE	1.83	0.44
11:A9:56:THR:O	11:A9:60:ARG:HB2	2.18	0.44
20:D6:127:ILE:H	20:D6:127:ILE:HG13	1.69	0.44
22:D5:375:ILE:HD12	39:B2:32:MET:HG3	1.99	0.44
22:D5:539:TYR:O	22:D5:543:THR:OG1	2.32	0.44
24:D2:309:ASN:HD21	29:AJ:95:ARG:HG3	1.83	0.44
27:A8:121:LEU:HA	27:A8:122:GLY:HA2	1.72	0.44
30:S5:95:PRO:HB3	35:AM:126:LEU:HD13	1.99	0.44
37:B7:41:THR:O	37:B7:45:MET:N	2.47	0.44
1:V1:305:PRO:HG3	1:V1:413:TRP:HB3	1.99	0.43
3:S1:55:CYS:SG	3:S1:69:CYS:N	2.90	0.43
5:S3:150:ARG:NH2	14:A6:91:GLU:OE1	2.51	0.43
5:S3:179:GLU:OE1	11:A9:40:ARG:NH2	2.51	0.43
19:D1:288:LEU:O	19:D1:292:ASN:HB2	2.18	0.43
35:AM:81:ARG:HG2	35:AM:85:MET:HE1	1.99	0.43
35:AM:97:MET:HE3	35:AM:100:VAL:HG11	1.99	0.43
36:B6:18:ARG:HH12	36:B6:22:LEU:HB2	1.83	0.43
1:V1:370:ASP:OD1	3:S1:179:ASN:ND2	2.51	0.43
4:S2:151:ILE:HD13	4:S2:304:MET:HE1	1.99	0.43
21:4L:1:MET:N	30:S5:72:MET:SD	2.91	0.43
22:D5:483:PRO:HD2	22:D5:486:LEU:HD22	2.00	0.43
20:D6:163:ILE:HA	20:D6:166:VAL:HG12	2.01	0.43
22:D5:261:ILE:HG12	22:D5:317:ILE:HD11	2.00	0.43
29:AJ:210:PHE:HD2	29:AJ:211:LEU:HD22	1.84	0.43
33:C2:111:GLU:HB3	41:BK:119:GLN:HB2	2.00	0.43
2:V2:101:GLN:HA	2:V2:140:ILE:O	2.18	0.43
5:S3:173:GLU:OE1	5:S3:189:GLU:N	2.45	0.43
19:D1:165:LEU:HD21	19:D1:241:LEU:HA	2.01	0.43
19:D1:191:ALA:O	19:D1:194:ASN:ND2	2.51	0.43
20:D6:122:MET:HE1	30:S5:75:LEU:HD12	2.00	0.43
23:D4:364:LEU:HD22	23:D4:367:LEU:HD22	2.01	0.43
24:D2:189:TRP:HZ2	24:D2:286:ALA:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:AB:8:LEU:HD11	36:B6:19:ARG:HH12	1.82	0.43
30:S5:93:PRO:HB2	30:S5:95:PRO:HD2	1.99	0.43
3:S1:283:MET:HB2	3:S1:560:ILE:HB	2.01	0.43
15:A7:69:MET:HG3	15:A7:70:SER:H	1.84	0.43
22:D5:254:VAL:HG11	22:D5:329:ILE:HG23	2.00	0.43
23:D4:269:MET:SD	23:D4:399:ASN:ND2	2.92	0.43
40:B8:66:HIS:HB2	40:B8:71:LEU:HB2	2.00	0.43
46:V1:501:FMN:O5'	46:V1:501:FMN:O3'	2.32	0.43
22:D5:245:ALA:O	22:D5:249:SER:CB	2.66	0.43
1:V1:52:GLY:HA2	1:V1:53:PRO:HD3	1.89	0.43
3:S1:483:VAL:HA	3:S1:484:THR:HA	1.55	0.43
4:S2:84:HIS:CD2	5:S3:152:LEU:HB3	2.53	0.43
5:S3:192:GLN:HE21	5:S3:195:ARG:HH12	1.66	0.43
19:D1:312:SER:OG	31:A3:37:TYR:O	2.37	0.43
24:D2:232:HIS:CE1	29:AJ:276:PRO:HG3	2.54	0.43
40:B8:47:TYR:HA	40:B8:48:PRO:HD3	1.90	0.43
41:BK:114:ASP:HB3	41:BK:117:LYS:HB2	2.00	0.43
4:S2:425:PHE:HA	4:S2:428:VAL:HB	2.01	0.43
7:S8:161:TRP:HB3	16:AL:84:PRO:HG2	2.00	0.43
11:A9:202:LYS:HA	11:A9:291:ASP:HB2	2.01	0.43
11:A9:215:ILE:HA	11:A9:218:ILE:HG22	2.00	0.43
13:A5:74:GLY:HA2	13:A5:75:GLN:HA	1.73	0.43
25:AK:88:ASN:OD1	25:AK:89:TYR:N	2.51	0.43
27:A8:82:THR:HA	27:A8:85:TRP:CD1	2.54	0.43
3:S1:10:GLU:O	3:S1:76:GLY:HA2	2.19	0.43
11:A9:134:HIS:ND1	11:A9:135:LEU:O	2.39	0.43
22:D5:191:ILE:HD12	23:D4:386:PHE:HD2	1.83	0.43
22:D5:356:ILE:HD13	22:D5:356:ILE:HA	1.84	0.43
19:D1:299:ALA:HB1	31:A3:24:ILE:HG23	2.01	0.43
23:D4:75:LEU:HD12	23:D4:436:LEU:HG	2.01	0.43
24:D2:63:GLN:HE22	24:D2:105:LYS:HE2	1.83	0.43
25:AK:80:ARG:HH12	25:AK:87:LEU:HB3	1.84	0.43
5:S3:78:LEU:CA	5:S3:93:VAL:O	2.63	0.42
6:S7:125:TYR:CG	7:S8:117:ILE:HD12	2.54	0.42
7:S8:96:ALA:HA	7:S8:106:THR:HA	2.01	0.42
18:D3:81:THR:HG23	18:D3:83:ASN:H	1.84	0.42
24:D2:219:PHE:HE1	24:D2:230:LEU:HD21	1.84	0.42
4:S2:108:TYR:HB2	6:S7:54:CYS:HB3	2.00	0.42
10:S4:10:LEU:HB3	10:S4:11:ILE:H	1.74	0.42
22:D5:172:ILE:O	22:D5:176:ARG:HG2	2.19	0.42
19:D1:318:THR:HG22	44:A1:41:TYR:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:233:LEU:HG	22:D5:303:ALA:HB1	2.02	0.42
23:D4:272:THR:HA	23:D4:275:ILE:HG22	2.00	0.42
3:S1:41:CYS:HB3	3:S1:52:CYS:HB3	2.01	0.42
3:S1:524:LEU:HD22	3:S1:527:ALA:HB2	2.01	0.42
21:4L:62:ILE:HA	21:4L:65:VAL:HG12	2.01	0.42
22:D5:123:LEU:HD21	52:D5:901:CDL:H731	2.02	0.42
22:D5:556:ILE:HG13	34:B4:76:TYR:HD1	1.84	0.42
1:V1:294:LEU:HD22	1:V1:336:VAL:HG11	2.01	0.42
2:V2:98:TYR:H	2:V2:136:LEU:HA	1.84	0.42
11:A9:50:ARG:NE	49:A9:401:NDP:O3X	2.52	0.42
22:D5:32:TYR:HD2	22:D5:115:ASN:HD22	1.68	0.42
23:D4:197:LEU:O	23:D4:201:MET:HB2	2.20	0.42
1:V1:154:ARG:HD2	8:V3:54:LEU:HD21	2.01	0.42
2:V2:103:CYS:HB2	2:V2:145:LEU:HG	2.01	0.42
3:S1:380:VAL:HG23	3:S1:453:LEU:HA	1.99	0.42
4:S2:318:MET:HB3	35:AM:11:PRO:HD3	2.01	0.42
17:AA:62:ILE:H	17:AA:83:LYS:HZ3	1.68	0.42
23:D4:263:MET:HE3	23:D4:263:MET:HB3	1.87	0.42
24:D2:207:ILE:HD13	24:D2:262:PRO:HD3	2.01	0.42
26:B5:132:LEU:HD22	30:S5:15:HIS:HB3	2.00	0.42
30:S5:82:ARG:HH12	30:S5:95:PRO:HG2	1.85	0.42
33:C2:66:THR:OG1	42:C1:28:TRP:NE1	2.52	0.42
7:S8:164:GLU:OE1	16:AL:88:ARG:HB2	2.20	0.42
21:4L:97:GLN:HG2	22:D5:582:GLY:H	1.84	0.42
22:D5:602:LEU:HD23	25:AK:1:ALA:HA	2.01	0.42
23:D4:196:TRP:CE2	23:D4:200:MET:HG3	2.54	0.42
17:AB:73:PRO:HA	17:AB:76:ILE:HD12	2.02	0.42
36:B6:108:THR:HA	36:B6:115:VAL:HA	2.02	0.42
2:V2:208:GLY:H	2:V2:211:PHE:HE1	1.67	0.42
6:S7:47:PRO:HD3	6:S7:74:VAL:HG13	2.02	0.42
11:A9:171:ILE:H	11:A9:171:ILE:HG13	1.72	0.42
22:D5:234:PRO:HB3	22:D5:300:LYS:HG2	2.01	0.42
22:D5:278:LEU:HD11	22:D5:405:ASN:HB2	2.02	0.42
25:AK:122:ALA:O	25:AK:126:MET:HB2	2.19	0.42
1:V1:43:TYR:O	1:V1:236:ARG:NH1	2.53	0.42
1:V1:299:PRO:HA	1:V1:334:VAL:HG12	2.01	0.42
3:S1:213:TYR:CZ	3:S1:249:ARG:HD3	2.54	0.42
13:A5:10:LEU:HD22	13:A5:13:LEU:HD13	2.01	0.42
23:D4:276:CYS:HB3	23:D4:288:TYR:HB2	2.02	0.42
24:D2:102:LEU:O	24:D2:106:LEU:HB2	2.20	0.42
29:AJ:54:ALA:HB3	29:AJ:104:ARG:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:BK:82:ASP:OD1	41:BK:82:ASP:N	2.53	0.42
1:V1:365:CYS:SG	1:V1:366:ARG:N	2.92	0.41
3:S1:49:ALA:H	3:S1:161:ARG:NH1	2.18	0.41
22:D5:428:PHE:HA	22:D5:432:LEU:HB2	2.01	0.41
1:V1:301:GLY:HA2	1:V1:333:ALA:HB3	2.02	0.41
36:B6:1:SER:OG	36:B6:2:GLY:N	2.49	0.41
36:B6:87:TYR:HA	36:B6:90:THR:HG22	2.00	0.41
1:V1:202:LYS:HD3	10:S4:133:LYS:HG2	2.01	0.41
3:S1:383:ASN:HD22	3:S1:666:LEU:HA	1.85	0.41
22:D5:193:LEU:HD22	22:D5:201:ILE:HG12	2.02	0.41
24:D2:197:ASN:ND2	24:D2:269:GLU:OE1	2.52	0.41
38:B9:13:GLN:HE21	38:B9:17:GLN:HE21	1.67	0.41
40:B8:59:ASP:HA	40:B8:60:PRO:HD3	1.83	0.41
4:S2:188:ARG:NH1	6:S7:58:GLU:OE2	2.53	0.41
4:S2:423:ILE:H	4:S2:423:ILE:HG13	1.60	0.41
13:A5:34:LEU:O	13:A5:44:ARG:NH1	2.53	0.41
36:B6:17:LEU:HD23	36:B6:17:LEU:HA	1.85	0.41
2:V2:154:VAL:HB	2:V2:161:TYR:HB2	2.01	0.41
2:V2:163:ASP:OD2	2:V2:190:ARG:NE	2.48	0.41
18:D3:59:ALA:HB1	20:D6:67:VAL:HG13	2.03	0.41
22:D5:60:GLU:O	36:B6:99:LYS:CB	2.68	0.41
36:B6:117:PRO:HA	36:B6:118:PRO:HD3	1.88	0.41
3:S1:442:VAL:O	3:S1:446:ALA:CB	2.67	0.41
4:S2:85:ARG:HG2	6:S7:91:THR:HG21	2.03	0.41
11:A9:317:VAL:HG13	11:A9:318:LEU:HD22	2.03	0.41
19:D1:29:GLY:HA2	19:D1:34:ARG:HE	1.85	0.41
20:D6:169:MET:HE1	20:D6:175:ASN:HD22	1.85	0.41
23:D4:329:LEU:HD23	23:D4:359:TRP:CD2	2.56	0.41
1:V1:214:GLY:HA3	1:V1:220:THR:HG22	2.02	0.41
3:S1:258:ILE:HD11	3:S1:581:GLN:HE22	1.85	0.41
20:D6:127:ILE:HG22	35:AM:119:MET:HB2	2.02	0.41
29:AJ:224:SER:OG	29:AJ:225:ALA:N	2.54	0.41
43:B1:55:THR:HG23	43:B1:56:TRP:HD1	1.84	0.41
1:V1:379:PHE:CZ	1:V1:389:ILE:HG22	2.55	0.41
3:S1:157:THR:HG23	3:S1:160:ILE:HD12	2.02	0.41
6:S7:118:SER:N	45:S7:300:SF4:S4	2.94	0.41
24:D2:339:LEU:HD23	24:D2:342:ILE:HG13	2.02	0.41
28:BJ:93:ARG:HH22	43:B1:43:LEU:HD11	1.86	0.41
38:B9:28:SER:HB3	38:B9:79:TYR:H	1.85	0.41
1:V1:368:GLY:HA2	1:V1:395:ILE:HD11	2.02	0.41
3:S1:104:ASP:O	3:S1:108:CYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:113:GLU:OE2	10:S4:43:ASN:ND2	2.48	0.41
3:S1:359:ARG:HD3	12:A2:55:ARG:HD3	2.03	0.41
4:S2:19:MET:HB3	24:D2:171:ASN:HA	2.03	0.41
4:S2:53:PRO:HG2	6:S7:99:ALA:HB1	2.01	0.41
6:S7:91:THR:OG1	6:S7:119:CYS:SG	2.77	0.41
10:S4:25:VAL:HA	10:S4:26:PRO:HD3	1.93	0.41
11:A9:202:LYS:HD2	11:A9:238:LEU:HD23	2.03	0.41
22:D5:17:MET:HG2	36:B6:73:HIS:CE1	2.53	0.41
23:D4:54:LEU:HA	26:B5:93:ILE:HD12	2.03	0.41
24:D2:266:ILE:O	24:D2:270:MET:HB2	2.21	0.41
27:A8:9:LEU:HG	35:AM:87:ARG:HG2	2.03	0.41
27:A8:146:ARG:HA	27:A8:147:PRO:HD3	1.94	0.41
29:AJ:91:GLY:O	29:AJ:95:ARG:NH2	2.53	0.41
29:AJ:303:LYS:HG2	29:AJ:304:TYR:HD1	1.86	0.41
30:S5:85:LEU:HD21	35:AM:96:ILE:HG12	2.02	0.41
4:S2:130:PRO:HG2	4:S2:135:GLN:HE21	1.86	0.41
22:D5:202:PHE:HZ	22:D5:263:PHE:HA	1.85	0.41
23:D4:75:LEU:HD21	23:D4:440:HIS:CD2	2.56	0.41
29:AJ:15:THR:OG1	29:AJ:253:ASP:OD1	2.36	0.41
29:AJ:49:LYS:HD2	29:AJ:114:HIS:CE1	2.56	0.41
1:V1:200:GLN:NE2	3:S1:174:THR:OG1	2.45	0.40
1:V1:240:ALA:HA	1:V1:243:ALA:HB3	2.02	0.40
22:D5:193:LEU:HA	34:B4:124:PHE:HE2	1.86	0.40
23:D4:225:ILE:HD13	23:D4:331:ASN:HB2	2.02	0.40
26:B5:128:ILE:HG21	30:S5:40:ILE:HG12	2.01	0.40
27:A8:74:LYS:HD2	44:A1:69:ILE:HG13	2.01	0.40
28:BJ:105:ILE:HG22	28:BJ:131:PHE:HD1	1.86	0.40
34:B4:100:TRP:HA	34:B4:103:VAL:HG22	2.02	0.40
1:V1:352:GLU:HG2	1:V1:373:ASN:HD21	1.85	0.40
3:S1:485:GLY:HA2	3:S1:486:ASP:HA	1.90	0.40
7:S8:175:TYR:CZ	15:A7:38:PRO:HG3	2.57	0.40
9:S6:84:CYS:HB3	9:S6:87:CYS:HB2	2.03	0.40
11:A9:144:LYS:HA	11:A9:147:ARG:HG2	2.04	0.40
11:A9:203:GLN:HE22	11:A9:231:VAL:HG13	1.85	0.40
11:A9:284:VAL:HG22	11:A9:288:HIS:HD2	1.85	0.40
18:D3:10:ASN:ND2	19:D1:83:LEU:HB3	2.35	0.40
19:D1:28:LEU:HG	19:D1:271:LEU:HD11	2.03	0.40
21:4L:19:LEU:HD13	21:4L:33:LEU:HB2	2.03	0.40
29:AJ:165:PRO:O	29:AJ:248:TRP:NE1	2.33	0.40
42:C1:41:GLU:OE2	42:C1:44:ARG:NH2	2.54	0.40
1:V1:140:GLY:O	1:V1:179:ARG:NH2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V1:300:GLY:HA2	1:V1:330:GLY:N	2.35	0.40
10:S4:97:GLU:OE2	10:S4:103:TYR:OH	2.37	0.40
16:AL:69:ASN:HD22	16:AL:115:PHE:HE1	1.69	0.40
22:D5:436:ARG:HH21	38:B9:32:HIS:HA	1.86	0.40
40:B8:64:TRP:NE1	40:B8:66:HIS:O	2.48	0.40
40:B8:69:LEU:HB3	40:B8:71:LEU:HD23	2.03	0.40
5:S3:179:GLU:HG3	11:A9:36:ASN:ND2	2.35	0.40
6:S7:62:MET:HB3	6:S7:153:ALA:HB1	2.03	0.40
17:AA:25:ILE:HD11	17:AA:40:LEU:HD23	2.03	0.40
21:4L:63:LEU:HD23	24:D2:71:MET:HE3	2.03	0.40
3:S1:257:ASP:O	3:S1:394:ARG:NH2	2.55	0.40
3:S1:335:LEU:HD12	3:S1:335:LEU:HA	1.90	0.40
3:S1:418:ARG:HG2	8:V3:75:HIS:CD2	2.56	0.40
9:S6:26:VAL:HA	9:S6:29:VAL:HG23	2.04	0.40
22:D5:63:ILE:HG12	22:D5:82:MET:HE1	2.03	0.40
22:D5:174:TYR:HE1	51:B8:201:3PE:H281	1.87	0.40
24:D2:190:MET:HG2	24:D2:204:ASN:HB3	2.02	0.40
29:AJ:46:LEU:HD23	29:AJ:48:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V1	428/445 (96%)	385 (90%)	43 (10%)	0	100	100
2	V2	210/217 (97%)	173 (82%)	37 (18%)	0	100	100
3	S1	686/704 (97%)	620 (90%)	65 (10%)	1 (0%)	48	81
4	S2	420/430 (98%)	379 (90%)	41 (10%)	0	100	100
5	S3	206/228 (90%)	182 (88%)	24 (12%)	0	100	100
6	S7	154/179 (86%)	139 (90%)	14 (9%)	1 (1%)	21	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	S8	174/176 (99%)	159 (91%)	15 (9%)	0	100	100
8	V3	39/75 (52%)	31 (80%)	8 (20%)	0	100	100
9	S6	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
10	S4	124/133 (93%)	116 (94%)	8 (6%)	0	100	100
11	A9	281/338 (83%)	249 (89%)	32 (11%)	0	100	100
12	A2	80/98 (82%)	69 (86%)	11 (14%)	0	100	100
13	A5	109/115 (95%)	97 (89%)	12 (11%)	0	100	100
14	A6	112/127 (88%)	103 (92%)	9 (8%)	0	100	100
15	A7	91/112 (81%)	75 (82%)	15 (16%)	1 (1%)	11	44
16	AL	142/145 (98%)	122 (86%)	20 (14%)	0	100	100
17	AA	78/88 (89%)	68 (87%)	10 (13%)	0	100	100
17	AB	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
18	D3	86/115 (75%)	82 (95%)	4 (5%)	0	100	100
19	D1	299/318 (94%)	276 (92%)	23 (8%)	0	100	100
20	D6	167/175 (95%)	146 (87%)	20 (12%)	1 (1%)	21	58
21	4L	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
22	D5	604/606 (100%)	543 (90%)	61 (10%)	0	100	100
23	D4	457/459 (100%)	422 (92%)	34 (7%)	1 (0%)	43	76
24	D2	345/347 (99%)	324 (94%)	21 (6%)	0	100	100
25	AK	138/140 (99%)	126 (91%)	12 (9%)	0	100	100
26	B5	137/143 (96%)	126 (92%)	11 (8%)	0	100	100
27	A8	169/171 (99%)	146 (86%)	23 (14%)	0	100	100
28	BJ	169/175 (97%)	157 (93%)	12 (7%)	0	100	100
29	AJ	317/320 (99%)	283 (89%)	34 (11%)	0	100	100
30	S5	97/105 (92%)	81 (84%)	16 (16%)	0	100	100
31	A3	72/83 (87%)	59 (82%)	13 (18%)	0	100	100
32	B3	71/97 (73%)	56 (79%)	14 (20%)	1 (1%)	9	39
33	C2	117/120 (98%)	105 (90%)	12 (10%)	0	100	100
34	B4	126/128 (98%)	112 (89%)	14 (11%)	0	100	100
35	AM	137/143 (96%)	127 (93%)	10 (7%)	0	100	100
36	B6	92/127 (72%)	85 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	B7	117/136 (86%)	99 (85%)	18 (15%)	0	100	100
38	B9	174/178 (98%)	154 (88%)	20 (12%)	0	100	100
39	B2	63/72 (88%)	58 (92%)	5 (8%)	0	100	100
40	B8	155/158 (98%)	125 (81%)	30 (19%)	0	100	100
41	BK	100/125 (80%)	89 (89%)	11 (11%)	0	100	100
42	C1	44/49 (90%)	39 (89%)	5 (11%)	0	100	100
43	B1	50/57 (88%)	44 (88%)	6 (12%)	0	100	100
44	A1	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
All	All	7979/8509 (94%)	7152 (90%)	821 (10%)	6 (0%)	49	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S1	359	ARG
23	D4	54	LEU
6	S7	54	CYS
20	D6	138	GLU
15	A7	69	MET
32	B3	23	ILE

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%)	575 (100%)	3 (0%)	81	82
4	S2	368/371 (99%)	365 (99%)	3 (1%)	73	77
5	S3	189/204 (93%)	189 (100%)	0	100	100
6	S7	132/150 (88%)	131 (99%)	1 (1%)	73	77
7	S8	151/151 (100%)	150 (99%)	1 (1%)	76	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	V3	40/68 (59%)	39 (98%)	1 (2%)	42	62
9	S6	79/80 (99%)	78 (99%)	1 (1%)	61	72
10	S4	113/119 (95%)	112 (99%)	1 (1%)	70	76
11	A9	246/292 (84%)	243 (99%)	3 (1%)	63	73
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	83/94 (88%)	83 (100%)	0	100	100
16	AL	130/131 (99%)	129 (99%)	1 (1%)	73	77
17	AA	74/81 (91%)	74 (100%)	0	100	100
17	AB	80/81 (99%)	79 (99%)	1 (1%)	61	72
18	D3	81/103 (79%)	81 (100%)	0	100	100
19	D1	266/278 (96%)	263 (99%)	3 (1%)	65	74
20	D6	140/144 (97%)	137 (98%)	3 (2%)	47	65
21	4L	87/87 (100%)	87 (100%)	0	100	100
22	D5	539/539 (100%)	536 (99%)	3 (1%)	78	80
23	D4	412/412 (100%)	408 (99%)	4 (1%)	68	76
24	D2	315/315 (100%)	314 (100%)	1 (0%)	86	85
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%)	153 (99%)	1 (1%)	78	80
28	BJ	155/157 (99%)	155 (100%)	0	100	100
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%)	92 (100%)	0	100	100
37	B7	108/119 (91%)	108 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	140 (99%)	2 (1%)	59	71
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%)	48 (100%)	0	100	100
44	A1	59/59 (100%)	59 (100%)	0	100	100
All	All	7072/7395 (96%)	7033 (99%)	39 (1%)	76	80

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V1	365	CYS
2	V2	104	THR
3	S1	290	LEU
3	S1	429	LEU
3	S1	483	VAL
4	S2	402	LEU
4	S2	418	ILE
4	S2	423	ILE
6	S7	54	CYS
7	S8	78	ILE
8	V3	54	LEU
9	S6	26	VAL
10	S4	25	VAL
11	A9	47	VAL
11	A9	171	ILE
11	A9	290	THR
13	A5	94	ILE
16	AL	117	LEU
19	D1	55	LEU
19	D1	73	LEU
19	D1	289	LEU
20	D6	12	ILE
20	D6	54	LEU
20	D6	143	ILE
22	D5	55	ILE
22	D5	90	VAL
22	D5	350	LEU
23	D4	143	LEU

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Mol	Chain	Res	Type
23	D4	150	LEU
23	D4	230	VAL
23	D4	251	ASN
24	D2	193	VAL
17	AB	80	ILE
27	A8	109	CYS
30	S5	95	PRO
34	B4	120	LEU
38	B9	23	LEU
40	B8	9	LEU
40	B8	96	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
1	V1	29	HIS
1	V1	116	HIS
1	V1	165	ASN
1	V1	200	GLN
1	V1	257	ASN
1	V1	293	ASN
1	V1	373	ASN
2	V2	42	HIS
2	V2	101	GLN
2	V2	157	ASN
2	V2	159	ASN
3	S1	28	GLN
3	S1	255	HIS
3	S1	308	GLN
3	S1	336	ASN
3	S1	365	ASN
3	S1	383	ASN
3	S1	494	HIS
4	S2	3	GLN
4	S2	34	ASN
4	S2	46	ASN
4	S2	50	ASN
4	S2	79	HIS
4	S2	84	HIS
4	S2	135	GLN
4	S2	149	ASN
4	S2	157	HIS

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Mol	Chain	Res	Type
4	S2	316	ASN
4	S2	347	HIS
4	S2	409	HIS
5	S3	19	HIS
5	S3	38	GLN
5	S3	88	ASN
5	S3	192	GLN
6	S7	61	HIS
6	S7	127	HIS
6	S7	162	GLN
7	S8	49	ASN
7	S8	157	ASN
7	S8	168	ASN
8	V3	44	HIS
8	V3	75	HIS
10	S4	46	GLN
11	A9	3	HIS
11	A9	8	HIS
11	A9	36	ASN
11	A9	115	GLN
11	A9	203	GLN
11	A9	216	ASN
11	A9	234	ASN
11	A9	306	GLN
12	A2	24	GLN
12	A2	61	GLN
13	A5	70	GLN
13	A5	82	GLN
16	AL	31	ASN
16	AL	72	ASN
17	AA	74	GLN
18	D3	10	ASN
19	D1	194	ASN
19	D1	317	GLN
20	D6	175	ASN
21	4L	83	ASN
22	D5	59	GLN
22	D5	67	HIS
22	D5	113	ASN
22	D5	115	ASN
22	D5	139	GLN
22	D5	309	GLN

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Mol	Chain	Res	Type
22	D5	323	HIS
22	D5	348	HIS
22	D5	434	GLN
22	D5	580	GLN
23	D4	26	ASN
23	D4	43	ASN
23	D4	138	ASN
23	D4	304	GLN
23	D4	319	HIS
24	D2	63	GLN
24	D2	120	GLN
24	D2	204	ASN
24	D2	309	ASN
24	D2	316	GLN
25	AK	6	HIS
25	AK	7	GLN
26	B5	95	GLN
26	B5	124	GLN
26	B5	143	ASN
17	AB	33	ASN
17	AB	47	GLN
17	AB	74	GLN
27	A8	29	HIS
27	A8	30	HIS
27	A8	63	ASN
27	A8	94	GLN
27	A8	150	ASN
28	BJ	114	GLN
28	BJ	122	GLN
29	AJ	92	ASN
29	AJ	114	HIS
29	AJ	200	GLN
29	AJ	239	GLN
29	AJ	251	GLN
30	S5	44	HIS
30	S5	69	GLN
31	A3	45	ASN
31	A3	68	HIS
32	B3	47	ASN
32	B3	58	ASN
33	C2	59	HIS
34	B4	47	GLN

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Mol	Chain	Res	Type
35	AM	53	ASN
35	AM	75	GLN
35	AM	89	ASN
36	B6	73	HIS
36	B6	82	HIS
37	B7	43	GLN
37	B7	49	GLN
37	B7	83	GLN
37	B7	91	HIS
38	B9	13	GLN
38	B9	168	HIS
40	B8	104	HIS
40	B8	126	GLN
40	B8	155	HIS
44	A1	58	ASN
44	A1	68	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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
50	ZMP	AA	101	17	28,33,36	0.68	1 (3%)	32,40,45	1.10	3 (9%)
45	SF4	S8	201	7	0,12,12	-	-	-		
45	SF4	S8	202	7	0,12,12	-	-	-		
50	ZMP	AB	101	17	25,30,36	0.80	1 (4%)	29,37,45	0.96	1 (3%)
47	FES	S1	803	3	0,4,4	-	-	-		
51	3PE	B8	201	-	37,37,50	0.35	0	40,42,55	0.34	0
45	SF4	V1	500	1	0,12,12	-	-	-		
52	CDL	D5	901	-	59,59,99	0.39	0	65,71,111	0.55	1 (1%)
46	FMN	V1	501	-	33,33,33	0.28	0	48,50,50	0.40	0
45	SF4	S1	802	3	0,12,12	-	-	-		
49	NDP	A9	401	-	51,52,52	0.41	0	71,80,80	0.53	1 (1%)
51	3PE	D1	501	-	25,25,50	0.39	0	28,30,55	0.38	0
53	PC1	D4	502	-	27,27,53	0.39	0	33,35,61	0.40	0
45	SF4	S1	801	3	0,12,12	-	-	-		
45	SF4	S7	300	6	0,12,12	-	-	-		
47	FES	V2	300	2	0,4,4	-	-	-		
51	3PE	D4	501	-	39,39,50	0.33	0	42,44,55	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	ZMP	AA	101	17	-	6/38/40/43	-
45	SF4	S8	201	7	-	-	0/6/5/5
51	3PE	B8	201	-	-	10/41/41/54	-
50	ZMP	AB	101	17	-	9/35/37/43	-
45	SF4	S8	202	7	-	-	0/6/5/5
47	FES	S1	803	3	-	-	0/1/1/1
52	CDL	D5	901	-	-	18/70/70/110	-
45	SF4	V1	500	1	-	-	0/6/5/5
46	FMN	V1	501	-	-	7/18/18/18	0/3/3/3
45	SF4	S1	802	3	-	-	0/6/5/5
49	NDP	A9	401	-	-	16/34/77/77	0/5/5/5
51	3PE	D1	501	-	-	4/28/28/54	-
53	PC1	D4	502	-	-	12/31/31/57	-
45	SF4	S1	801	3	-	-	0/6/5/5
45	SF4	S7	300	6	-	-	0/6/5/5
47	FES	V2	300	2	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	3PE	D4	501	-	-	7/43/43/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	AB	101	ZMP	C9-C10	2.88	1.53	1.50
50	AA	101	ZMP	C9-C10	2.39	1.53	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	AB	101	ZMP	O1-C10-C9	-2.64	120.93	123.98
50	AA	101	ZMP	C11-C12-N1	-2.44	107.33	112.41
50	AA	101	ZMP	O1-C10-C9	-2.43	121.18	123.98
52	D5	901	CDL	CB4-OB6-CB5	2.41	123.55	117.80
49	A9	401	NDP	P2B-O2B-C2B	2.38	129.80	123.43
50	AA	101	ZMP	C15-C14-C13	-2.03	109.01	112.39

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	C2'-C3'-C4'-O4'
46	V1	501	FMN	O3'-C3'-C4'-O4'
46	V1	501	FMN	O3'-C3'-C4'-C5'
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-O2A
49	A9	401	NDP	C5B-O5B-PA-O3
49	A9	401	NDP	C1B-C2B-O2B-P2B
49	A9	401	NDP	C5D-O5D-PN-O3
49	A9	401	NDP	C5D-O5D-PN-O1N
49	A9	401	NDP	C5D-O5D-PN-O2N
50	AA	101	ZMP	C7-C8-C9-C10
50	AB	101	ZMP	C12-C11-S1-C10
50	AB	101	ZMP	O1-C10-S1-C11
50	AB	101	ZMP	C9-C10-S1-C11
51	D1	501	3PE	C1-O11-P-O12
51	D1	501	3PE	O13-C11-C12-N
51	D4	501	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
51	D4	501	3PE	C11-O13-P-O12
51	B8	201	3PE	C1-O11-P-O12
51	B8	201	3PE	C1-O11-P-O13
51	B8	201	3PE	C1-O11-P-O14
51	B8	201	3PE	C11-O13-P-O11
51	B8	201	3PE	C11-O13-P-O12
51	B8	201	3PE	C11-O13-P-O14
51	B8	201	3PE	O13-C11-C12-N
51	B8	201	3PE	O21-C2-C3-O31
52	D5	901	CDL	CA2-OA2-PA1-OA4
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-OB4
53	D4	502	PC1	C11-O13-P-O14
53	D4	502	PC1	C11-O13-P-O11
53	D4	502	PC1	O13-C11-C12-N
50	AA	101	ZMP	C14-C13-N1-C12
50	AB	101	ZMP	C14-C13-N1-C12
46	V1	501	FMN	C2'-C3'-C4'-C5'
50	AA	101	ZMP	O2-C13-N1-C12
50	AB	101	ZMP	O2-C13-N1-C12
50	AB	101	ZMP	C5-C6-C7-C8
51	B8	201	3PE	C1-C2-C3-O31
52	D5	901	CDL	CA3-CA4-CA6-OA8
50	AA	101	ZMP	C2-C1-C22-C23
52	D5	901	CDL	OB5-CB3-CB4-CB6
52	D5	901	CDL	OA6-CA4-CA6-OA8
50	AA	101	ZMP	C2-C3-C4-C5
49	A9	401	NDP	C2N-C3N-C7N-N7N
49	A9	401	NDP	C2B-C1B-N9A-C8A
53	D4	502	PC1	O11-C1-C2-C3
52	D5	901	CDL	OB6-CB4-CB6-OB8
52	D5	901	CDL	C52-C53-C54-C55
50	AB	101	ZMP	O3-C16-C17-O4
53	D4	502	PC1	O11-C1-C2-O21
49	A9	401	NDP	C2N-C3N-C7N-O7N
53	D4	502	PC1	O22-C21-C22-C23
49	A9	401	NDP	O4D-C1D-N1N-C6N
51	B8	201	3PE	C21-C22-C23-C24
51	D1	501	3PE	C1-O11-P-O13
51	D1	501	3PE	C1-O11-P-O14

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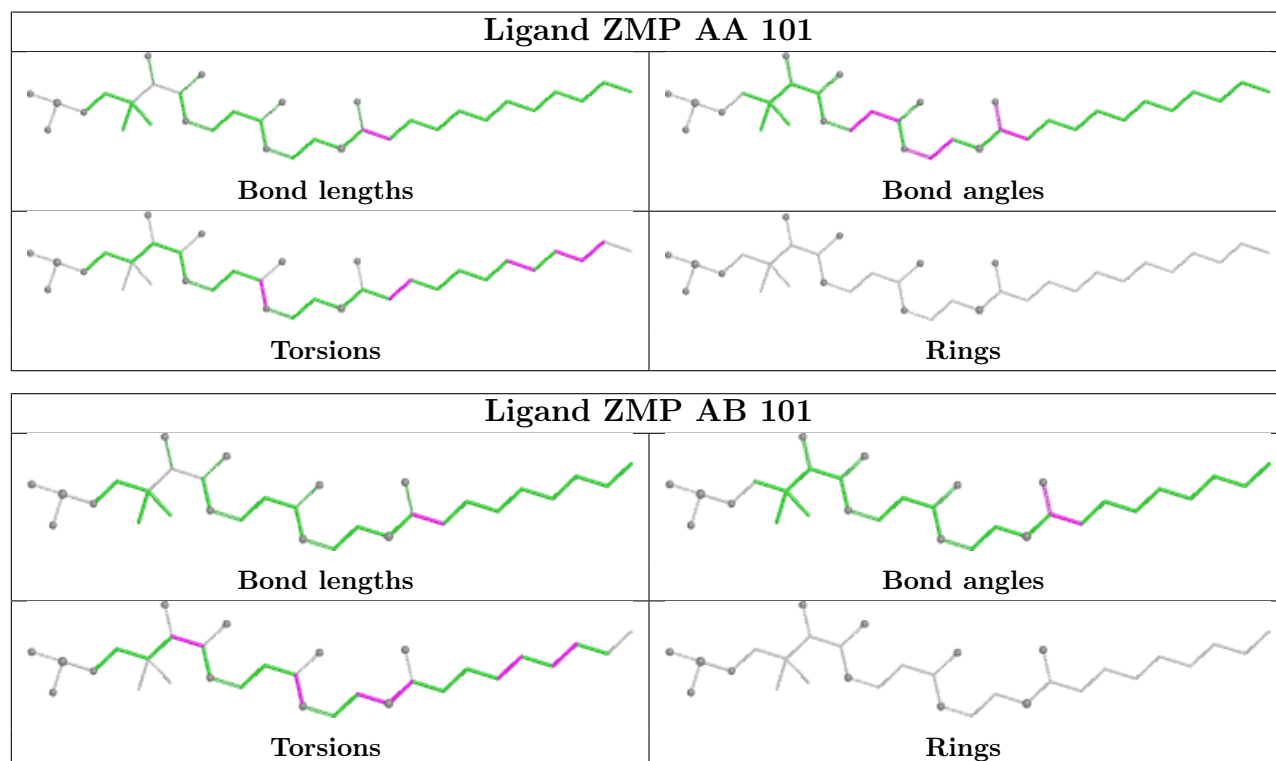
Mol	Chain	Res	Type	Atoms
51	D4	501	3PE	C1-O11-P-O12
51	D4	501	3PE	C1-O11-P-O13
51	D4	501	3PE	C1-O11-P-O14
51	D4	501	3PE	C11-O13-P-O14
52	D5	901	CDL	CA2-OA2-PA1-OA3
52	D5	901	CDL	CA2-OA2-PA1-OA5
53	D4	502	PC1	C11-O13-P-O12
53	D4	502	PC1	O21-C21-C22-C23
51	D4	501	3PE	C34-C35-C36-C37
52	D5	901	CDL	O1-C1-CA2-OA2
49	A9	401	NDP	PA-O3-PN-O1N
49	A9	401	NDP	C2B-C1B-N9A-C4A
49	A9	401	NDP	C2B-O2B-P2B-O3X
50	AB	101	ZMP	C3-C4-C5-C6
52	D5	901	CDL	CB6-CB4-OB6-CB5
52	D5	901	CDL	CA7-C31-C32-C33
52	D5	901	CDL	CB5-C51-C52-C53
53	D4	502	PC1	C2-C1-O11-P
53	D4	502	PC1	C32-C33-C34-C35
49	A9	401	NDP	O4B-C1B-N9A-C8A
52	D5	901	CDL	C12-C11-CA5-OA6
49	A9	401	NDP	PN-O3-PA-O2A
49	A9	401	NDP	PA-O3-PN-O2N
53	D4	502	PC1	O31-C31-C32-C33
53	D4	502	PC1	O32-C31-C32-C33
52	D5	901	CDL	C12-C11-CA5-OA7
50	AB	101	ZMP	N2-C16-C17-O4
50	AA	101	ZMP	C22-C1-C2-C3

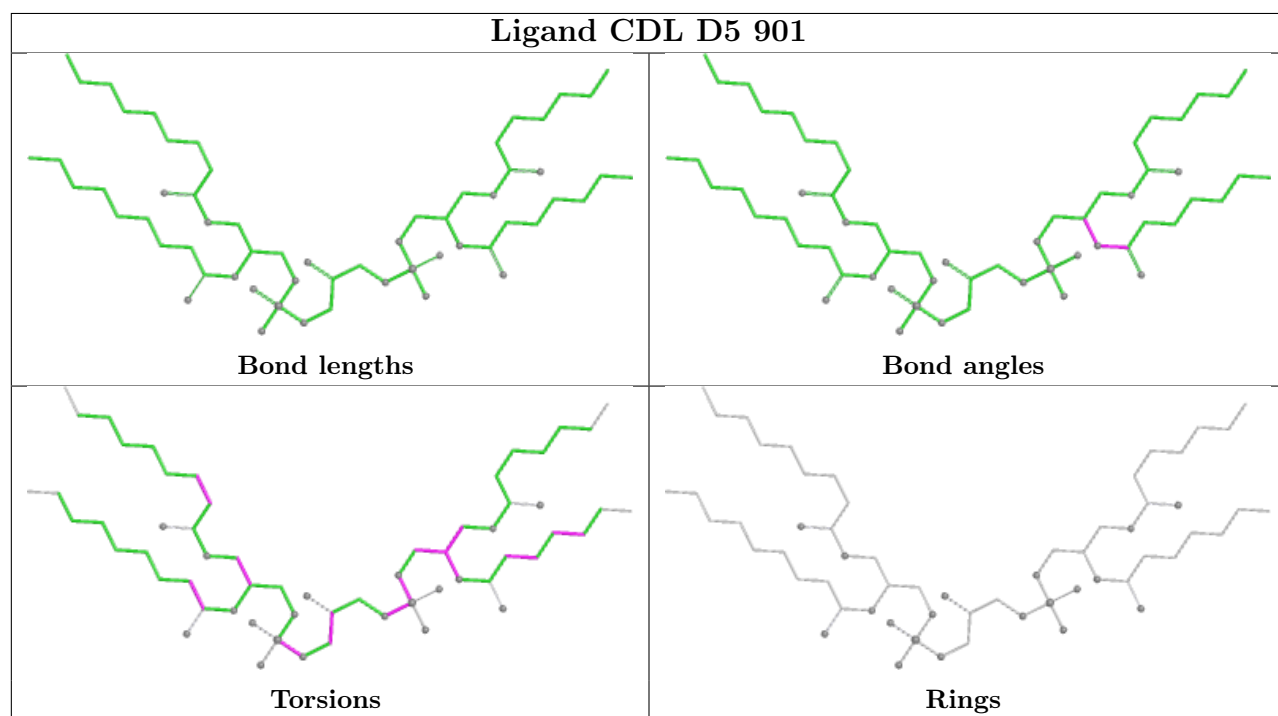
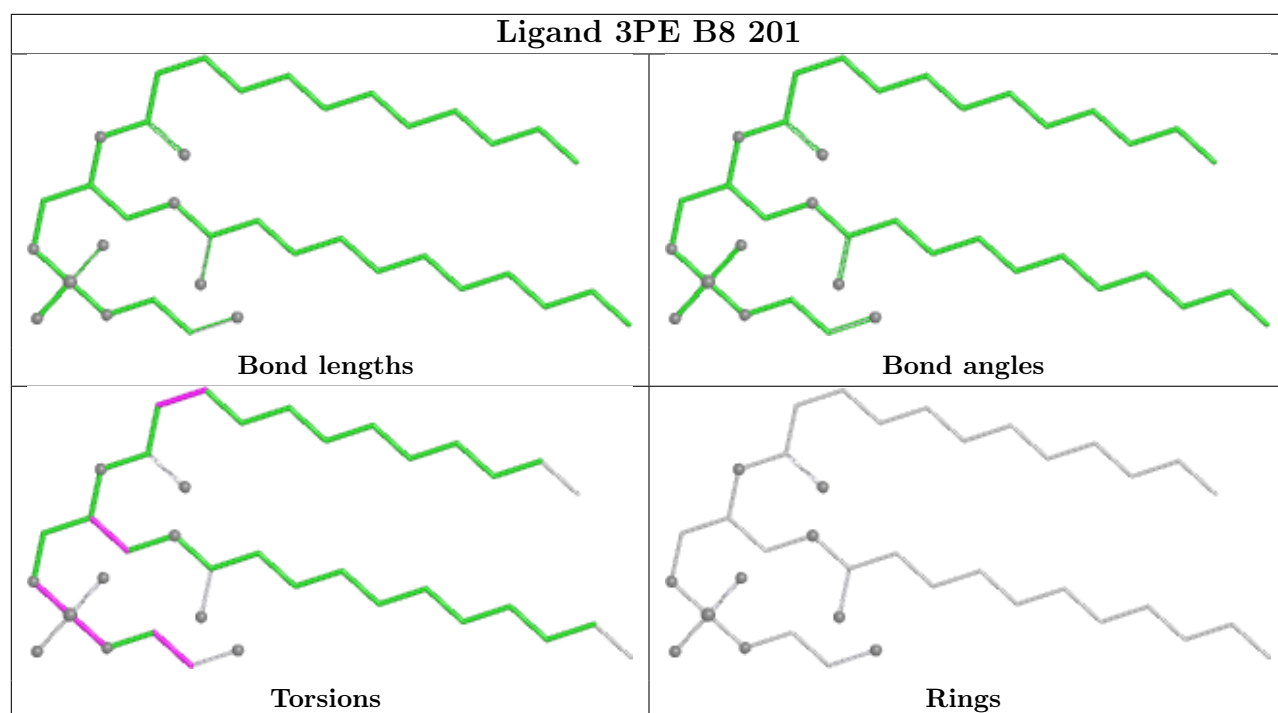
There are no ring outliers.

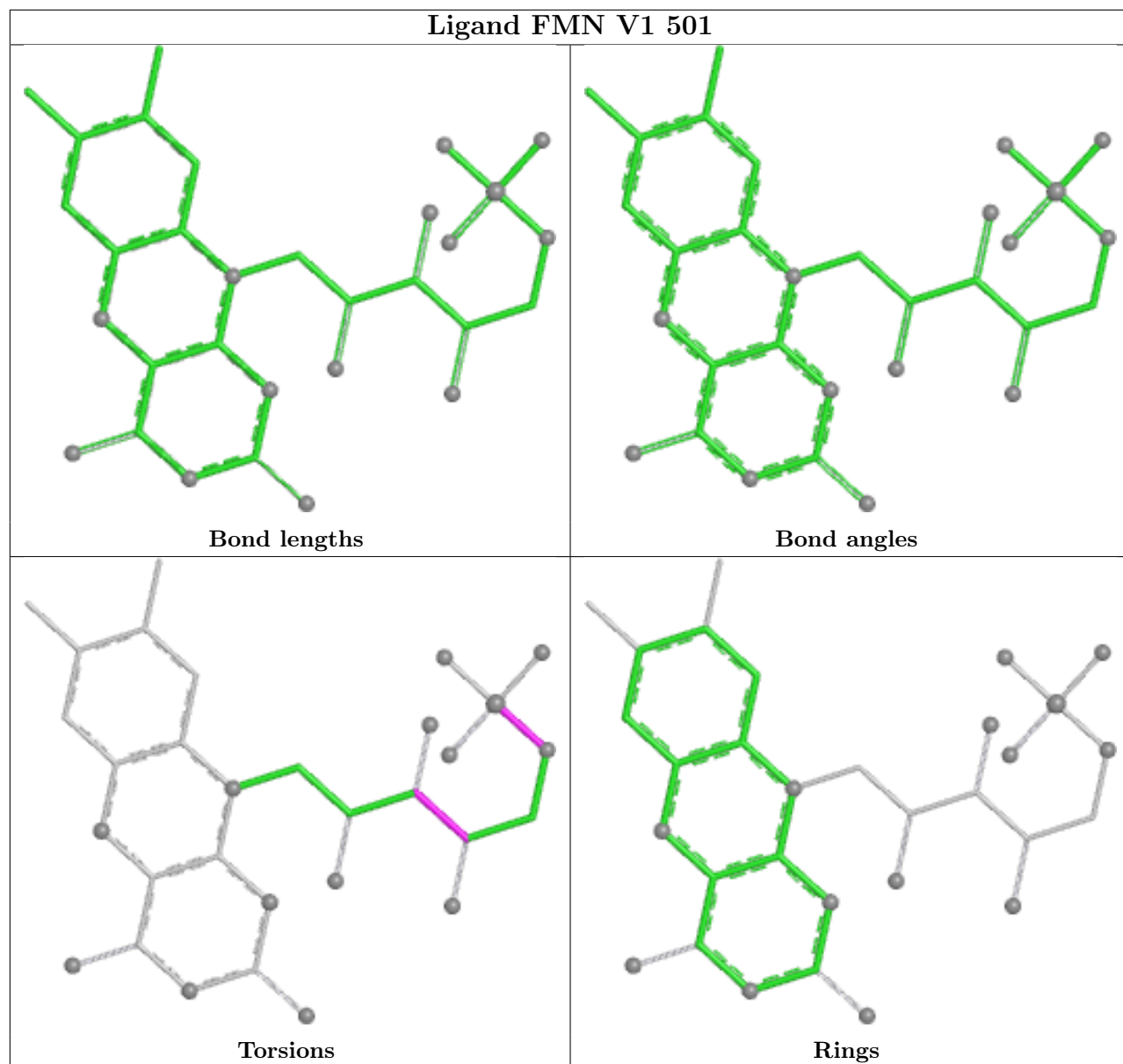
9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	AB	101	ZMP	1	0
51	B8	201	3PE	1	0
45	V1	500	SF4	1	0
52	D5	901	CDL	4	0
46	V1	501	FMN	2	0
49	A9	401	NDP	2	0
45	S1	801	SF4	1	0
45	S7	300	SF4	1	0
51	D4	501	3PE	2	0

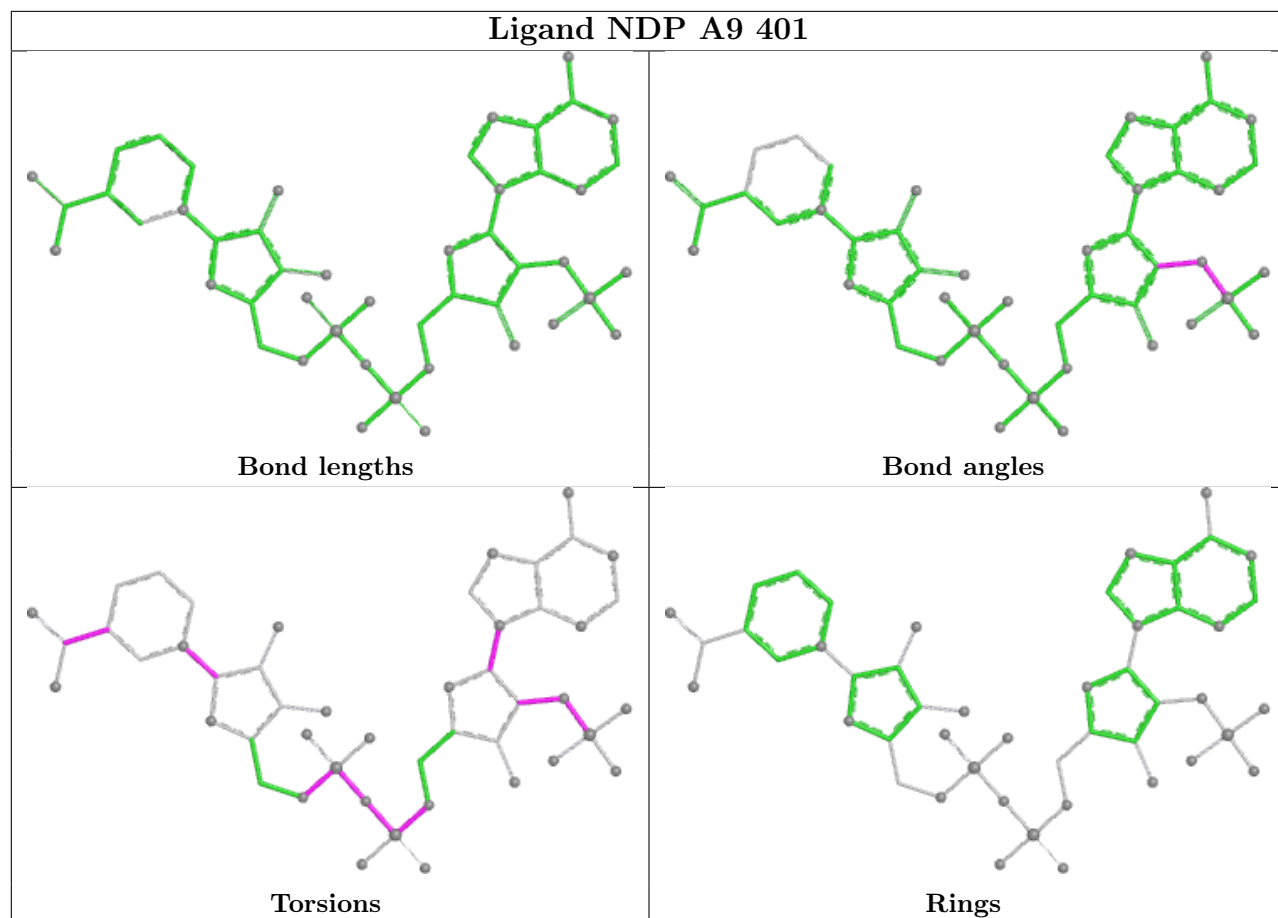
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



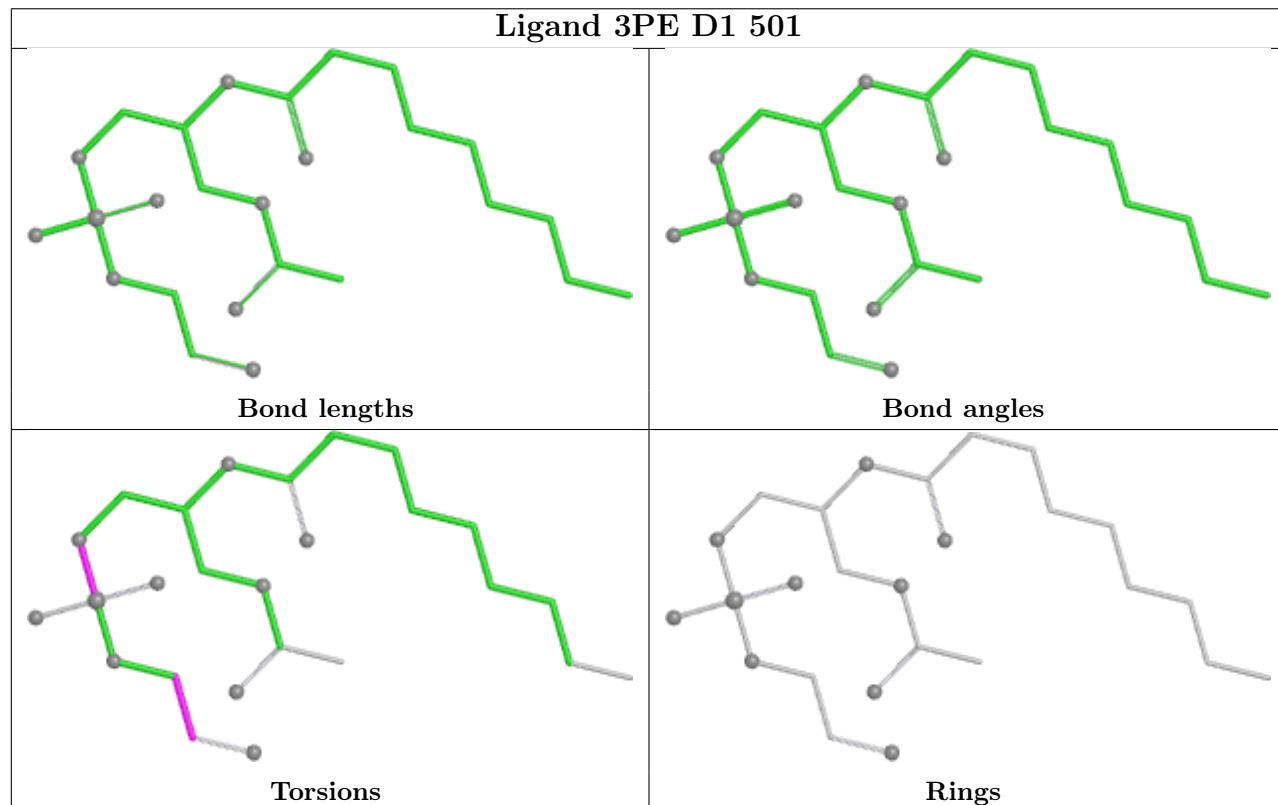


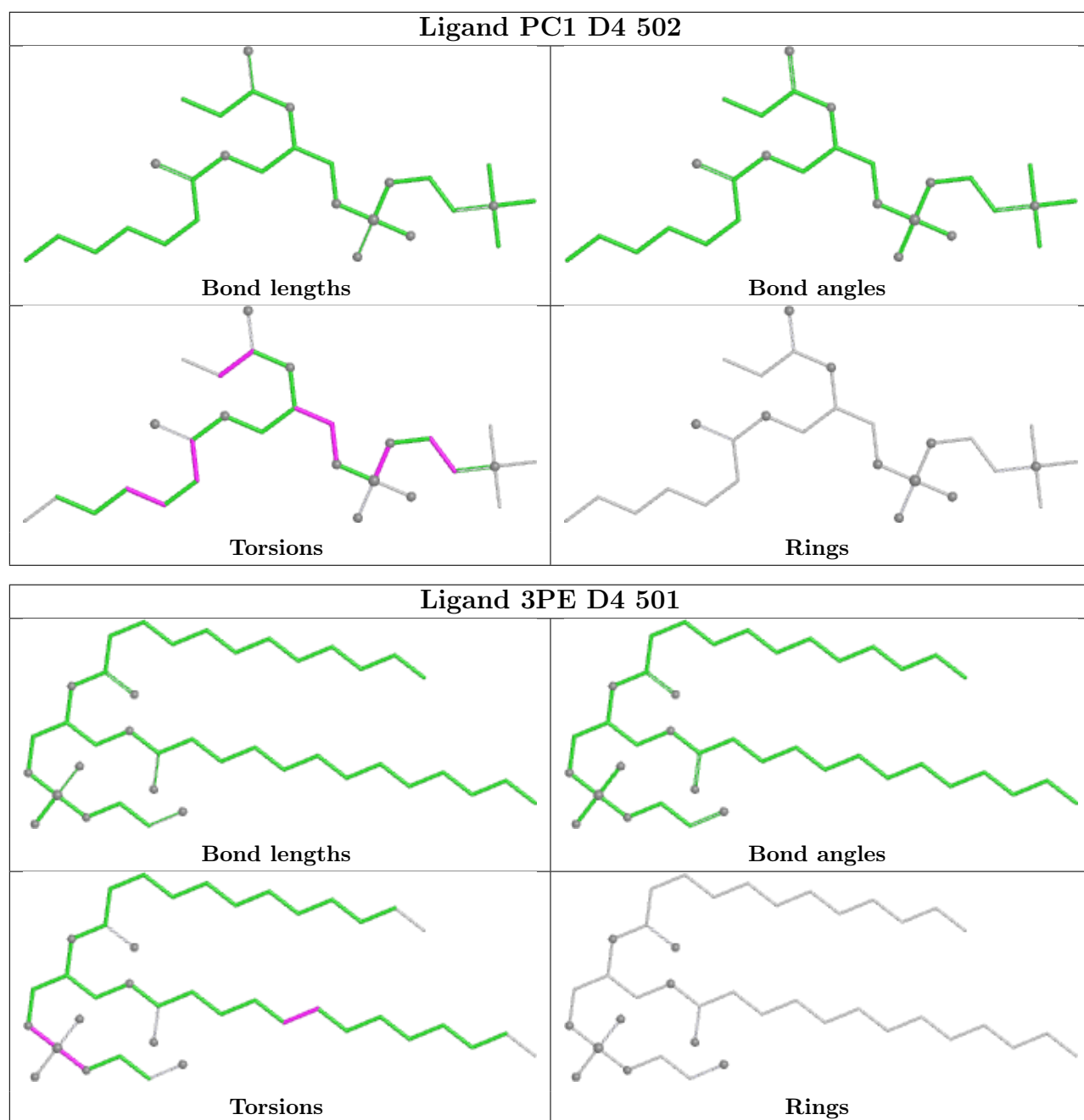


Ligand NDP A9 401



Ligand 3PE D1 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

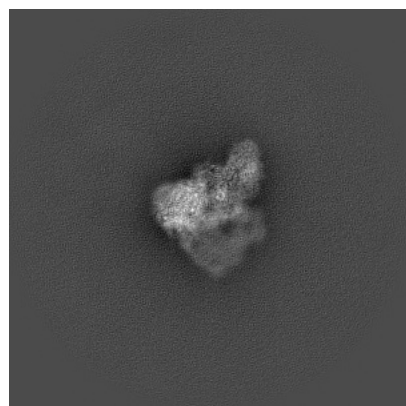
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4498. These allow visual inspection of the internal detail of the map and identification of artifacts.

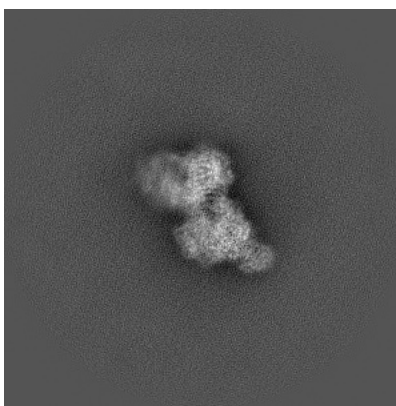
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

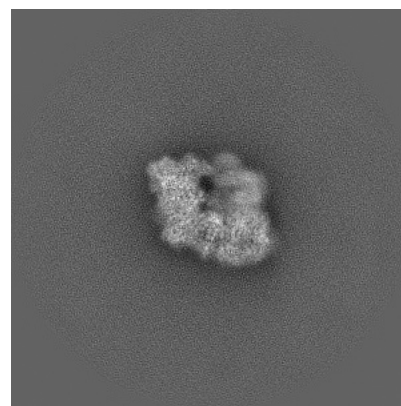
6.1.1 Primary map



X

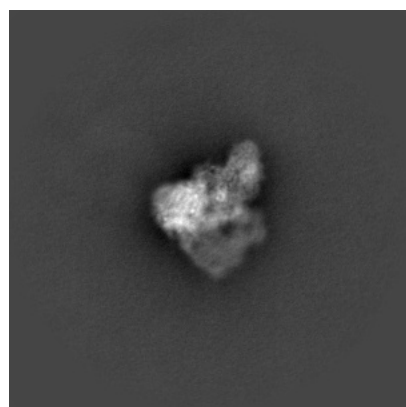


Y

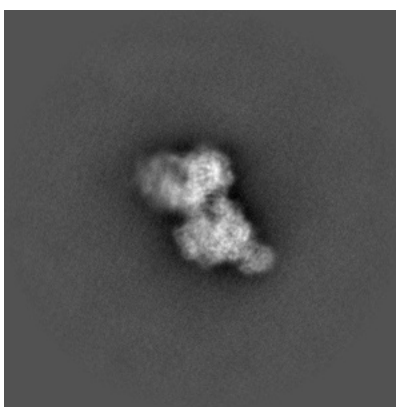


Z

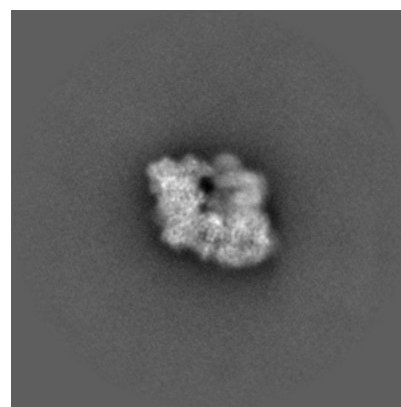
6.1.2 Raw map



X



Y

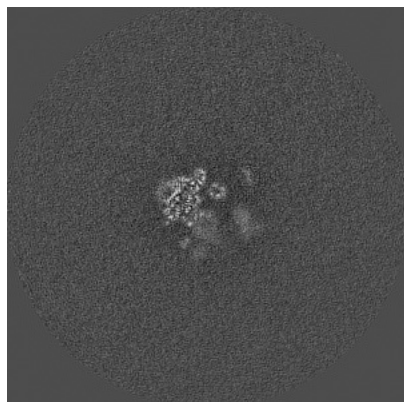


Z

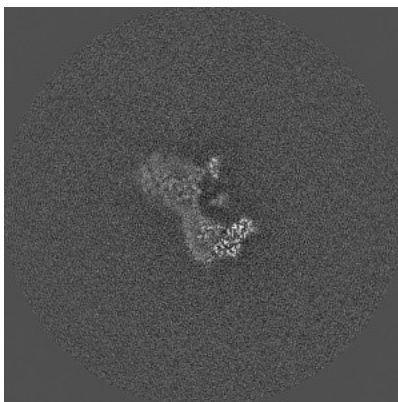
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

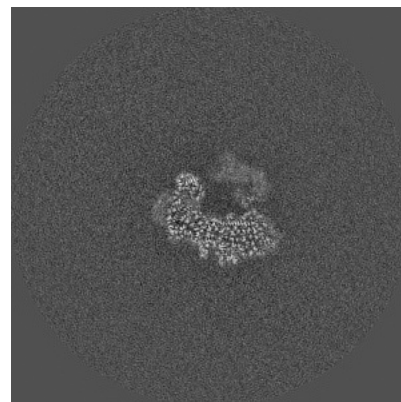
6.2.1 Primary map



X Index: 256

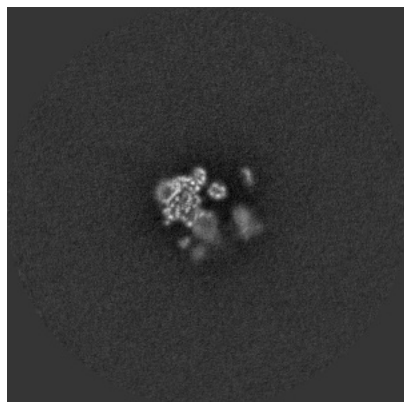


Y Index: 256

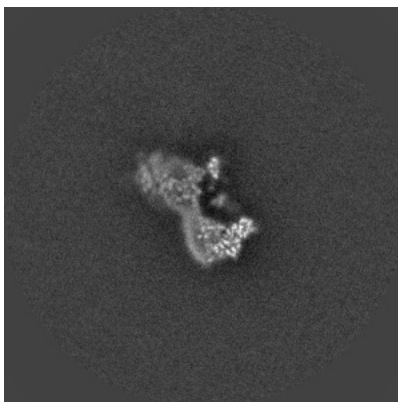


Z Index: 256

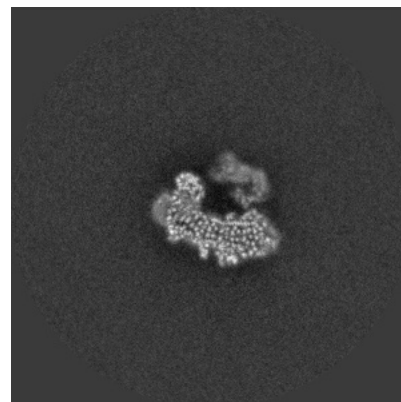
6.2.2 Raw map



X Index: 256



Y Index: 256

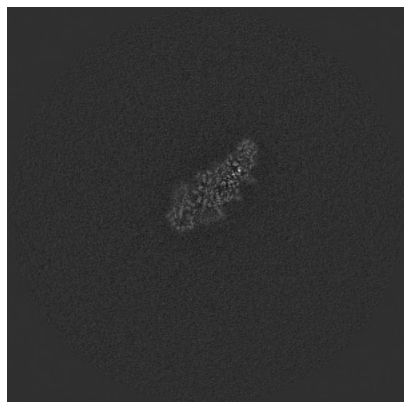


Z Index: 256

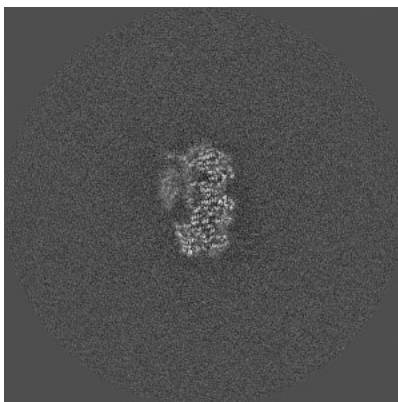
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

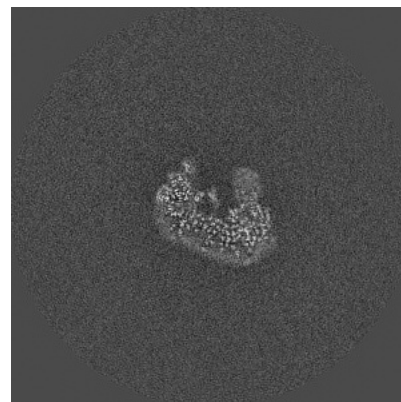
6.3.1 Primary map



X Index: 207

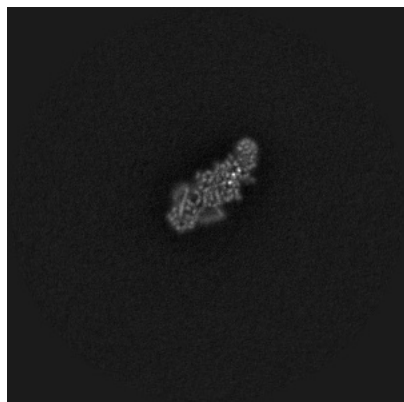


Y Index: 228

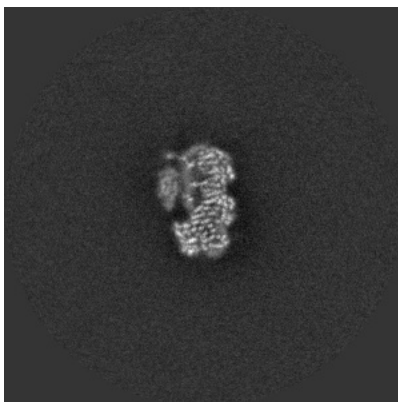


Z Index: 269

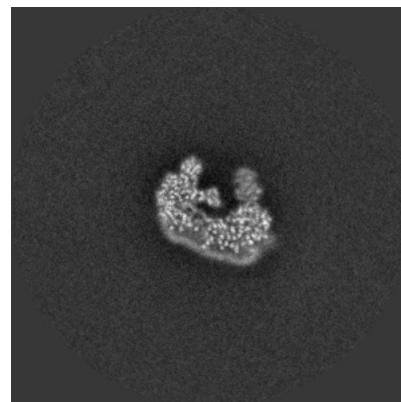
6.3.2 Raw map



X Index: 206



Y Index: 229

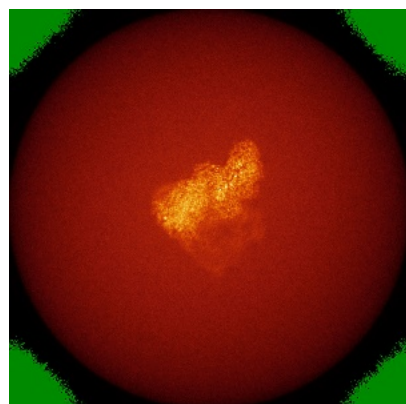


Z Index: 273

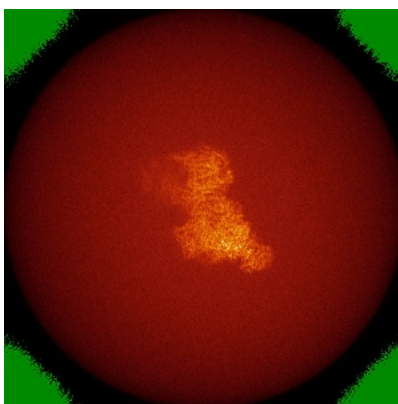
The images above show the largest variance slices of the map in three orthogonal directions.

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

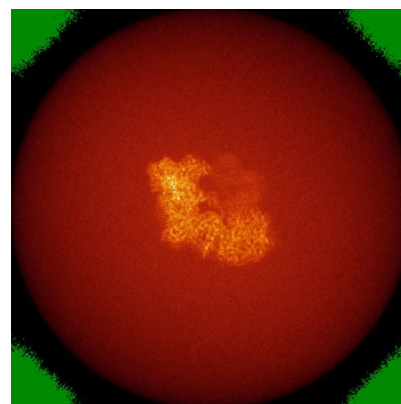
6.4.1 Primary map



X

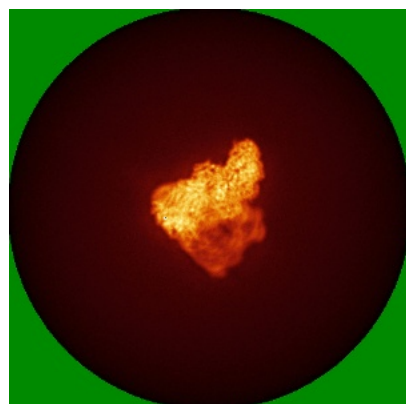


Y

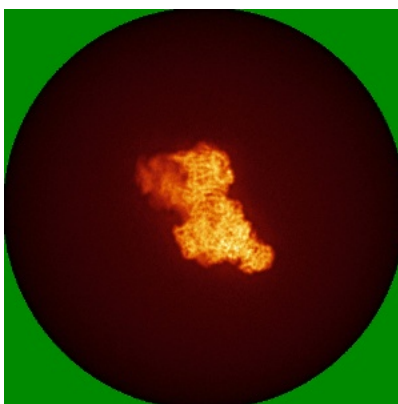


Z

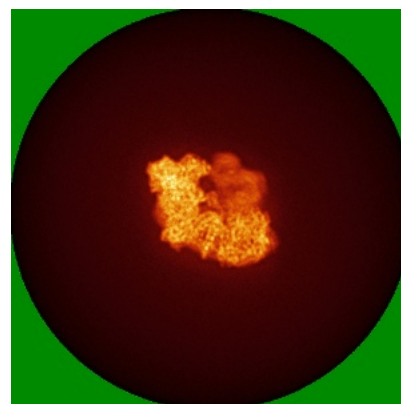
6.4.2 Raw map



X



Y

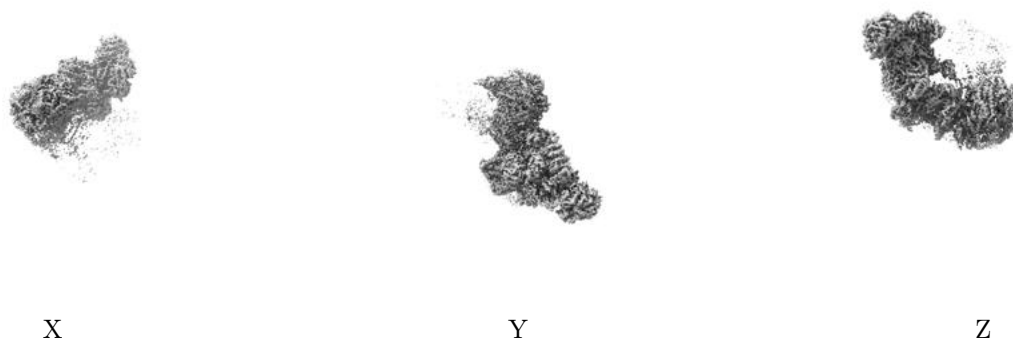


Z

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



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

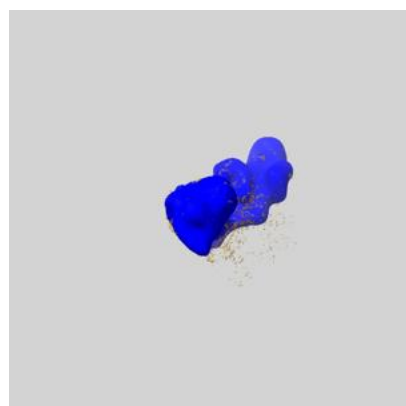
6.6 Mask visualisation [i](#)

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

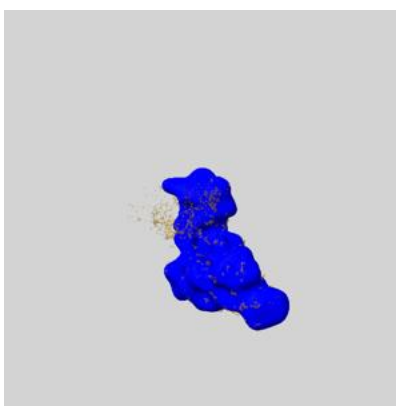
A mask typically either:

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

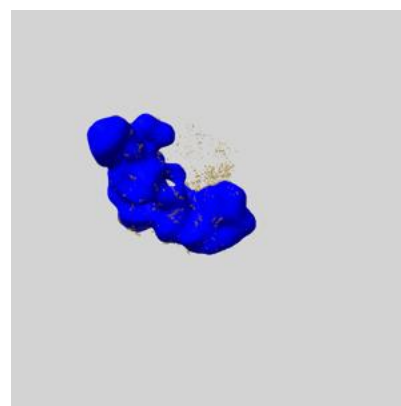
6.6.1 emd_4498_msk_1.map [i](#)



X



Y

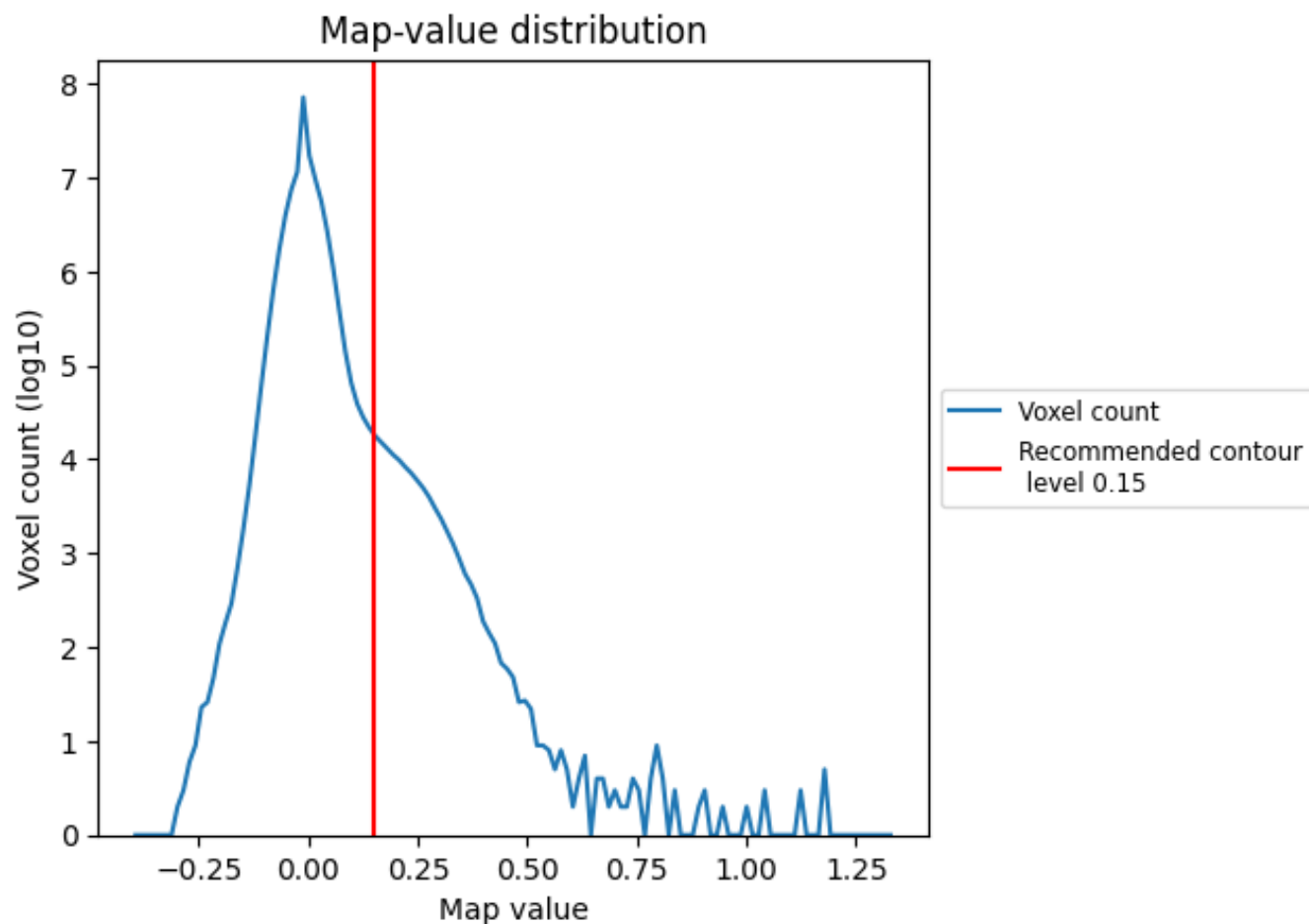


Z

7 Map analysis [i](#)

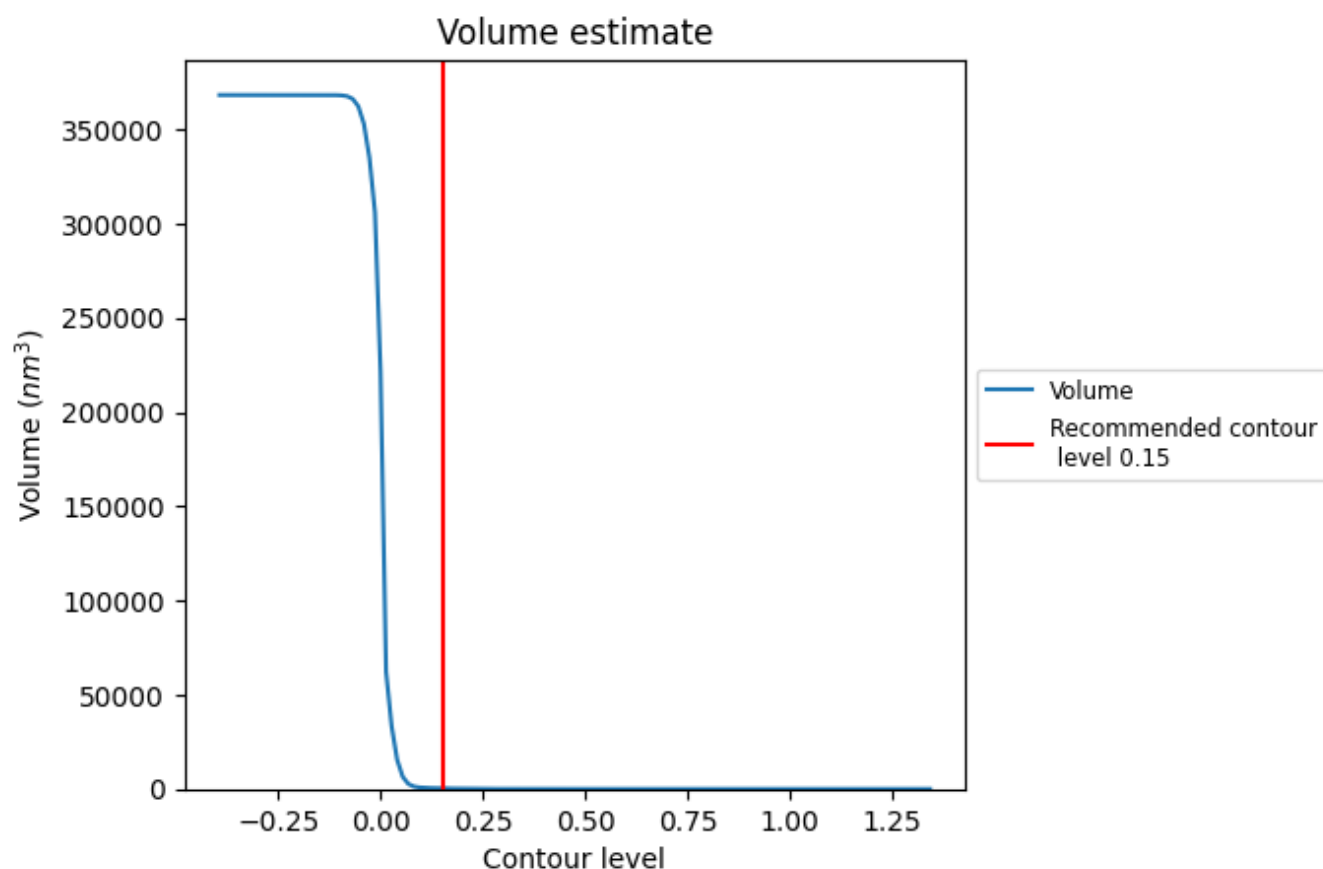
This section contains the results of statistical analysis of the map.

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.

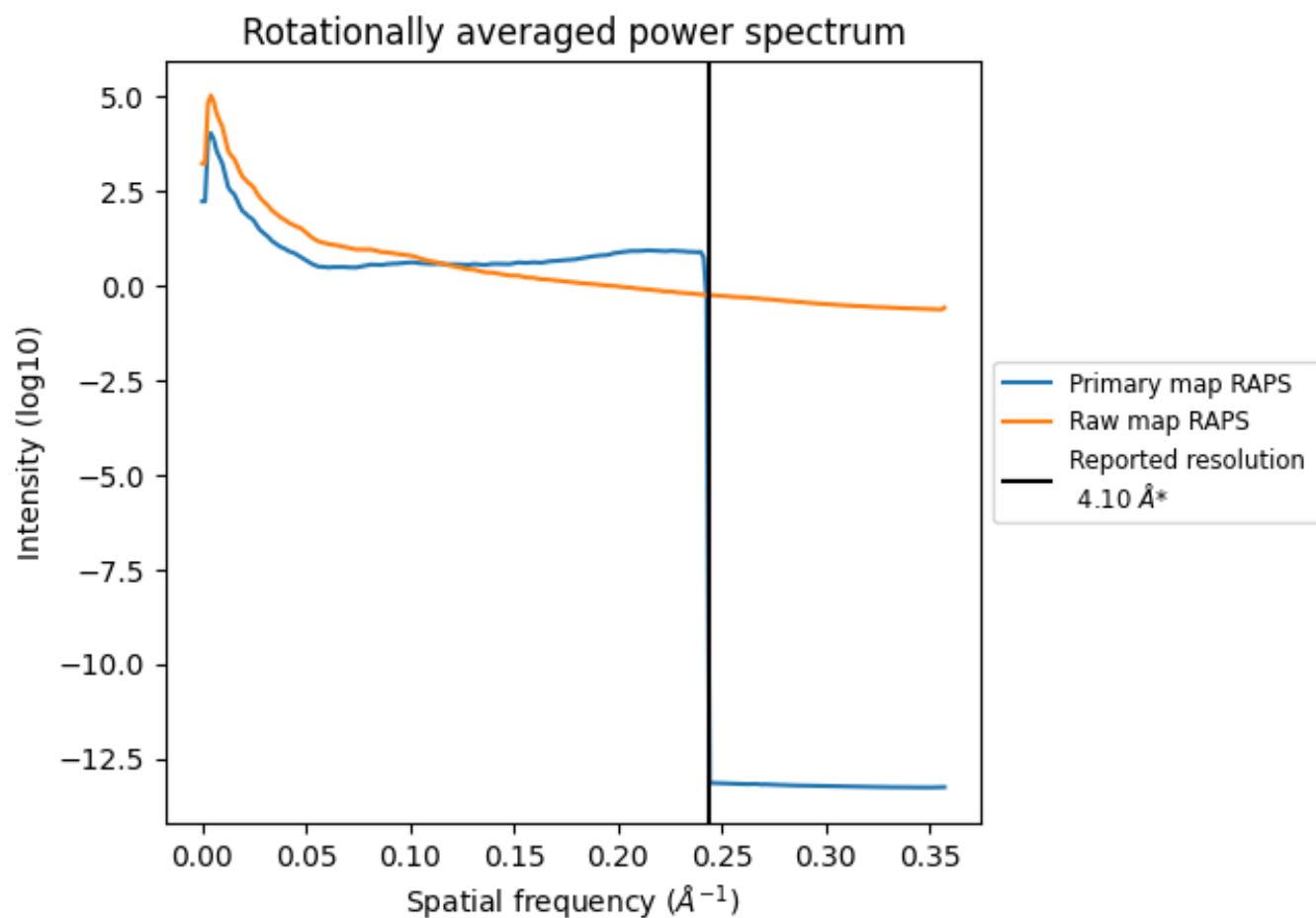
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 311 nm^3 ; this corresponds to an approximate mass of 281 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 ⓘ

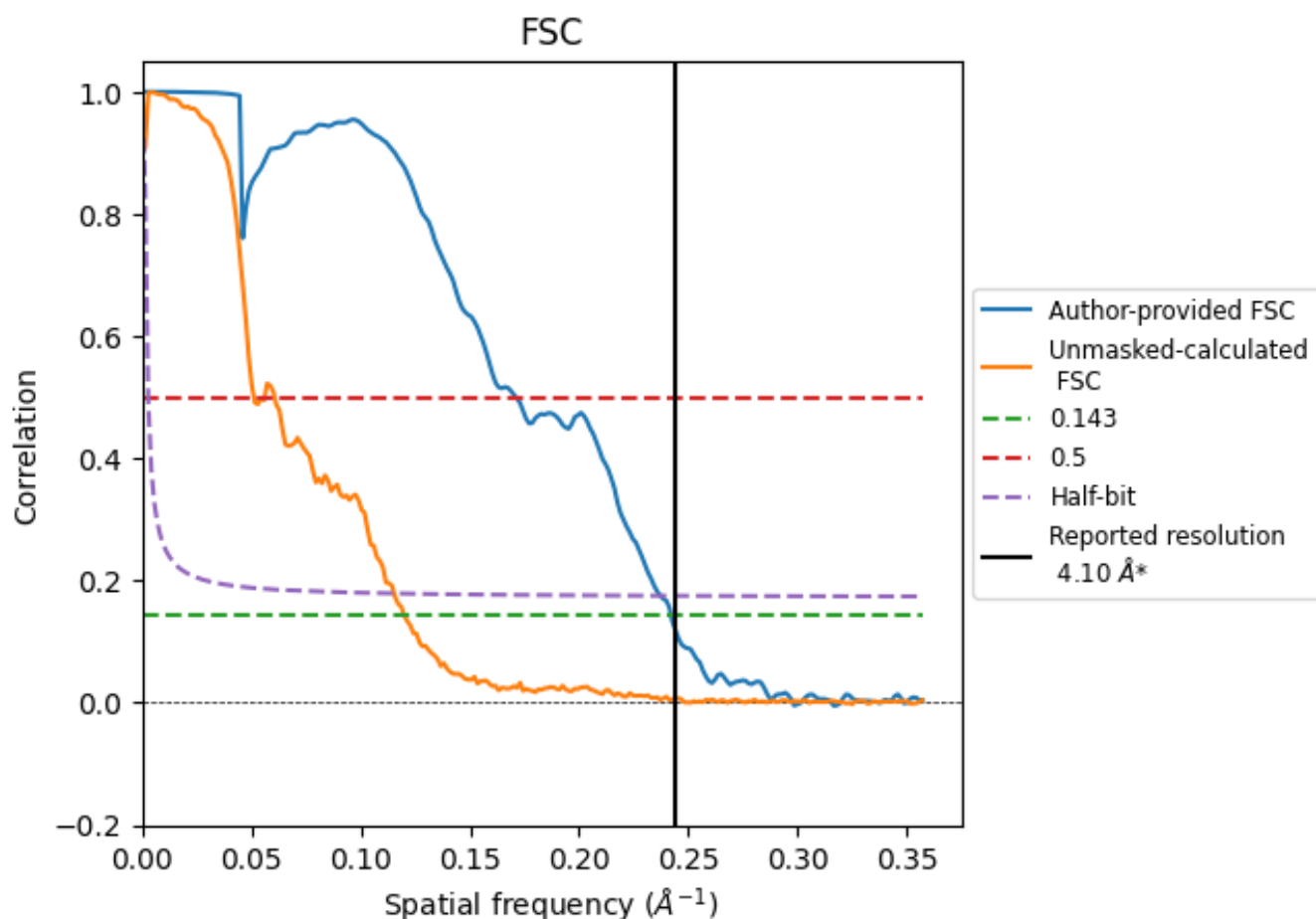


*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

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 Å⁻¹

8.2 Resolution estimates [i](#)

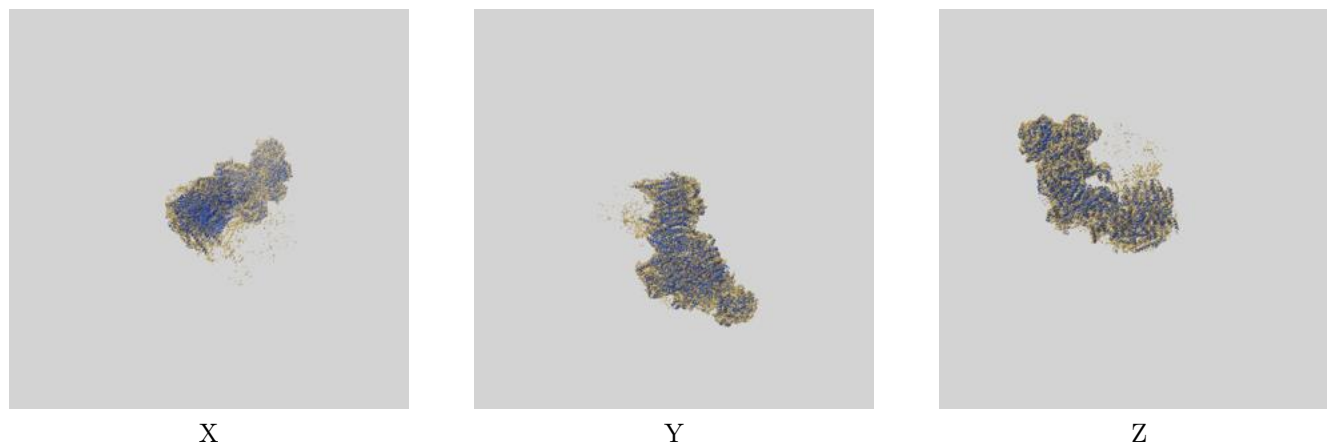
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.13	5.84	4.22
Unmasked-calculated*	8.34	19.53	8.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.34 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

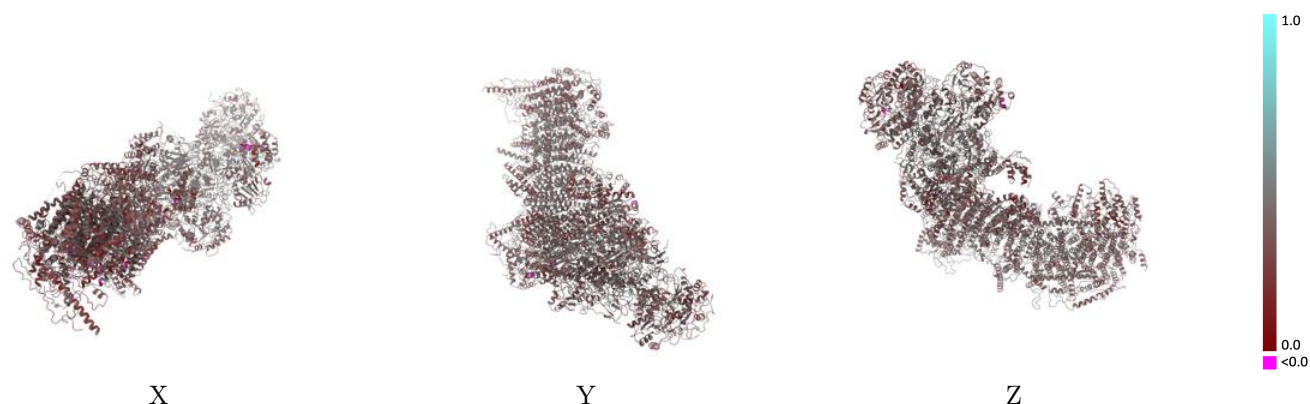
This section contains information regarding the fit between EMDB map EMD-4498 and PDB model 6QC6. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



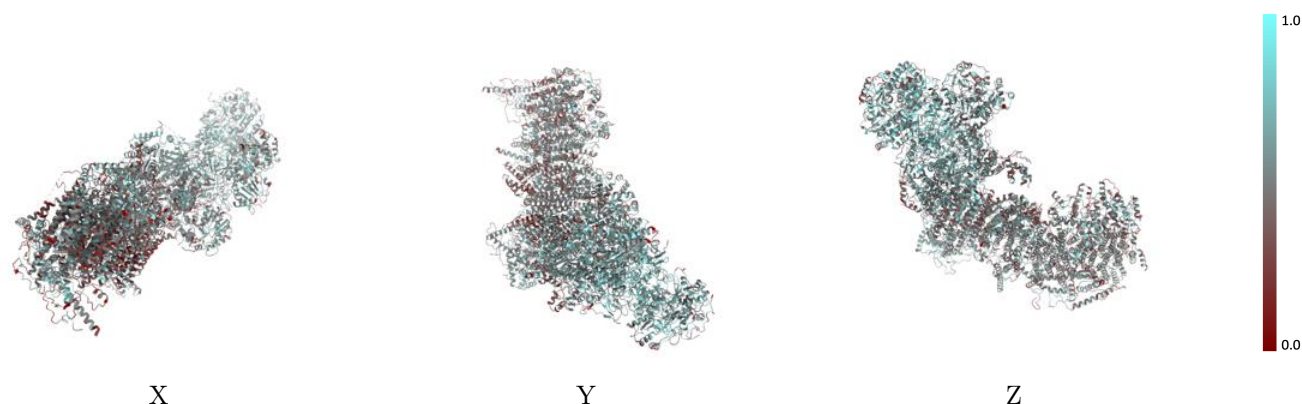
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



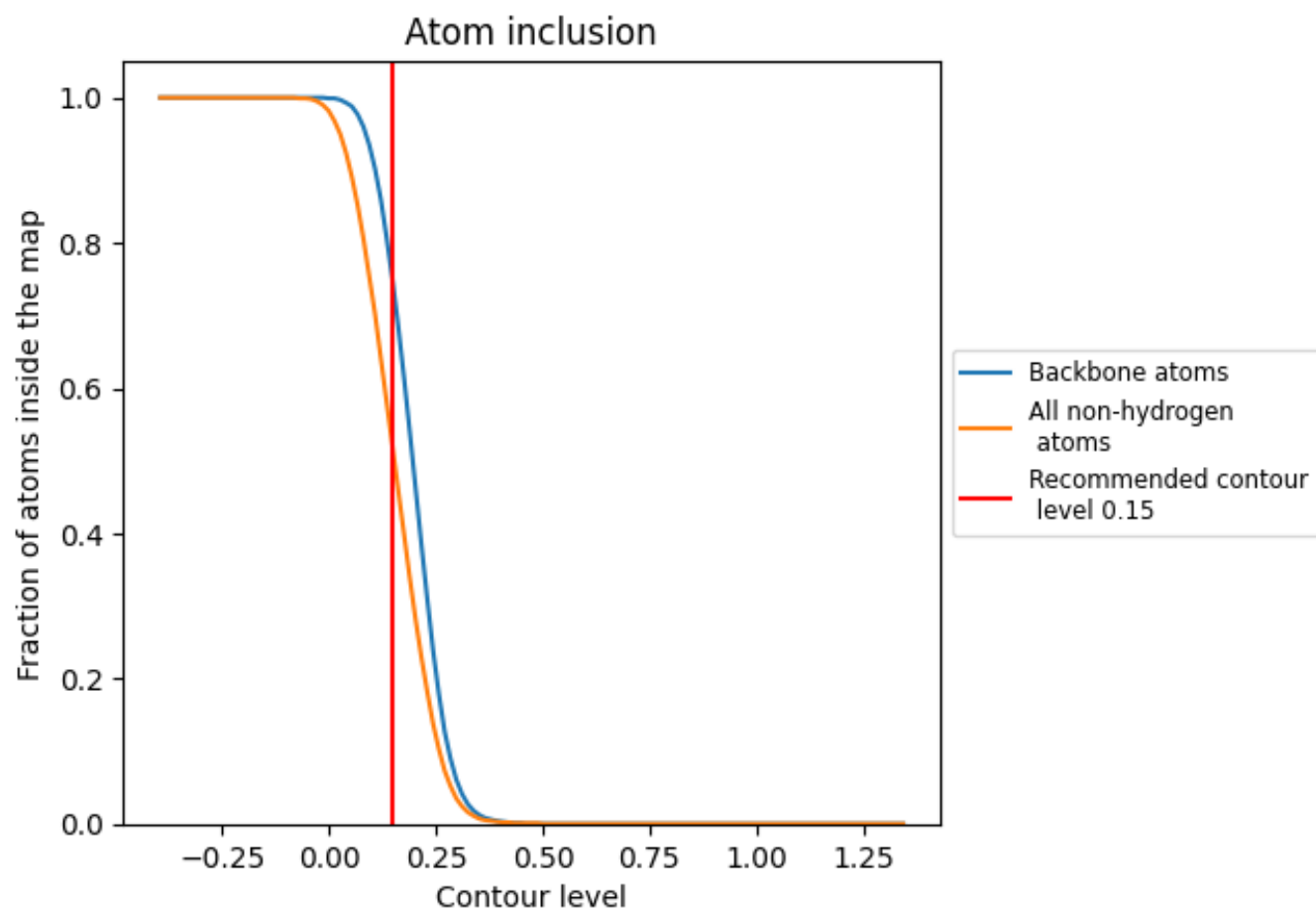
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 74% of all backbone atoms, 51% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5130	 0.3620
4L	 0.4300	 0.3560
A1	 0.5430	 0.3540
A2	 0.5490	 0.3280
A3	 0.5230	 0.3750
A5	 0.5650	 0.3640
A6	 0.5360	 0.3820
A7	 0.4710	 0.3660
A8	 0.5420	 0.3510
A9	 0.5290	 0.3660
AA	 0.4330	 0.3060
AB	 0.4370	 0.3220
AJ	 0.4940	 0.3560
AK	 0.3480	 0.3320
AL	 0.4830	 0.3690
AM	 0.5390	 0.3480
B1	 0.4360	 0.3480
B2	 0.4400	 0.3020
B3	 0.4150	 0.3350
B4	 0.4570	 0.3470
B5	 0.5260	 0.3650
B6	 0.4570	 0.3320
B7	 0.4560	 0.2950
B8	 0.4560	 0.3490
B9	 0.5180	 0.3340
BJ	 0.5220	 0.3430
BK	 0.4390	 0.3520
C1	 0.4790	 0.3450
C2	 0.4970	 0.3830
D1	 0.4810	 0.3630
D2	 0.4920	 0.3770
D3	 0.4360	 0.3480
D4	 0.4860	 0.3800
D5	 0.4510	 0.3480
D6	 0.3630	 0.3400



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
S1	 0.5870	 0.3840
S2	 0.5530	 0.3810
S3	 0.5990	 0.4040
S4	 0.5520	 0.4020
S5	 0.5280	 0.3610
S6	 0.5780	 0.3930
S7	 0.5960	 0.3930
S8	 0.6320	 0.3950
V1	 0.5950	 0.3530
V2	 0.5830	 0.3570
V3	 0.5590	 0.3500