



Full wwPDB EM Validation Report ⓘ

Mar 17, 2026 – 11:20 PM UTC

PDB ID : 6QC7 / pdb_00006qc7
EMDB ID : EMD-4499
Title : Ovine respiratory complex I FRC open class 3
Authors : Letts, J.A.; Sazanov, L.A.
Deposited on : 2018-12-27
Resolution : 4.40 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:

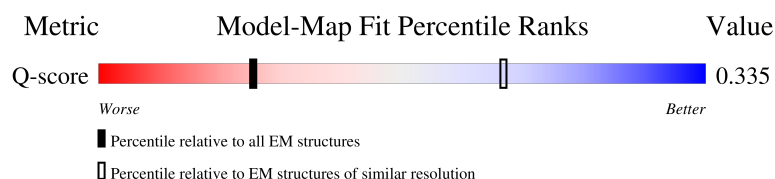
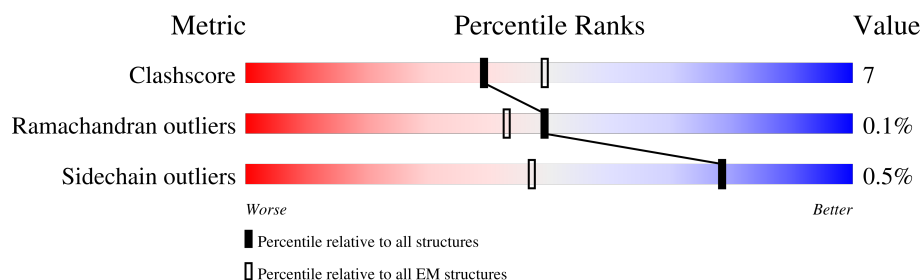
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

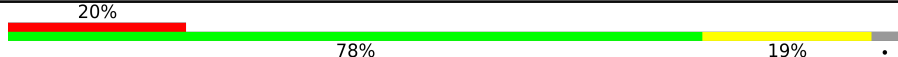
The reported resolution of this entry is 4.40 Å.

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	3132 (3.91 - 4.90)

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 65353 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 NDUFV2.

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 NDUFS2.

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 NDUFS7.

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 NDUFS8.

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 NDUFV3.

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

- Molecule 9 is a protein called NDUFS6.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S4	126	Total	C	N	O	S	0	0
			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 NDUF5.

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

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

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

- Molecule 15 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A7	96	Total	C	N	O	S	0	0
			766	478	146	139	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 NDUFA11.

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 subunit 8.

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

- Molecule 28 is a protein called NDUFB10.

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called NDUFA13.

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

- Molecule 36 is a protein called NDUF6.

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:ubiquinone oxidoreductase subunit B7.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B2	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 NDUF11.

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 NDUF1.

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

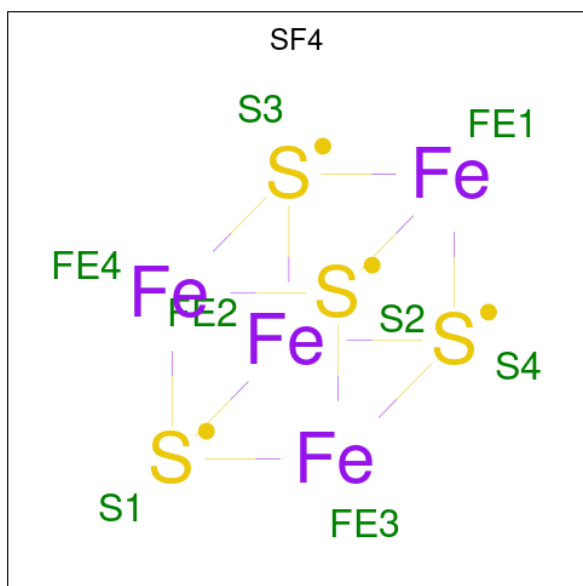
- Molecule 43 is a protein called NDUFB1.

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

- Molecule 44 is a protein called NDUFA1.

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

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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	

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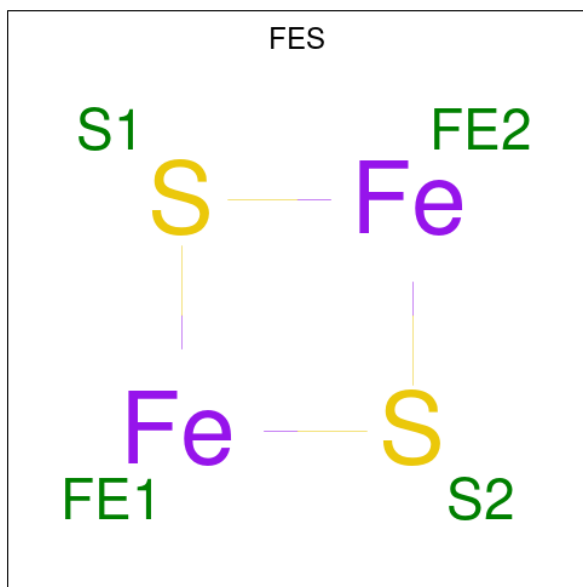
Mol	Chain	Residues	Atoms			AltConf
45	S8	1	Total	Fe	S	0
			8	4	4	
45	S8	1	Total	Fe	S	0
			8	4	4	

- 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).

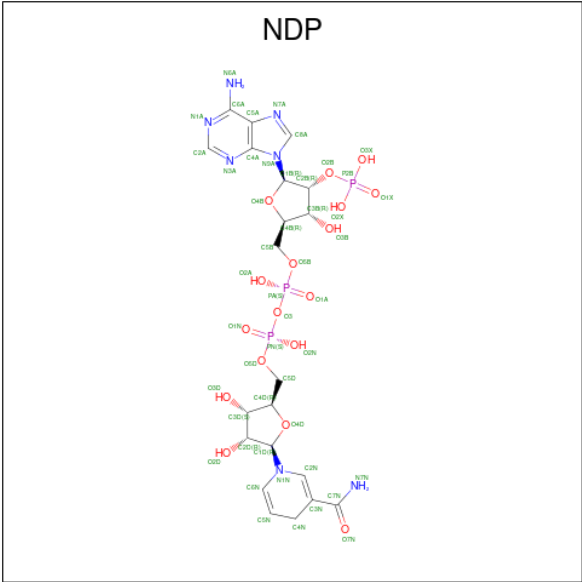


Mol	Chain	Residues	Atoms			AltConf
47	V2	1	Total	Fe	S	0
			4	2	2	
47	S1	1	Total	Fe	S	0
			4	2	2	

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

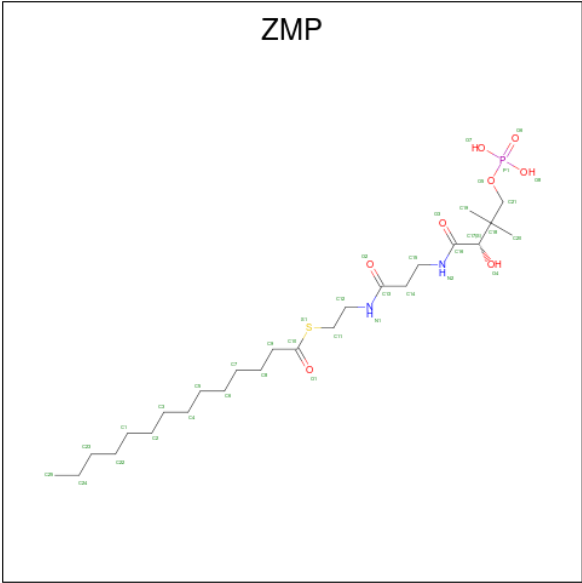
Mol	Chain	Residues	Atoms		AltConf
48	S6	1	Total	Zn	0
			1	1	

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



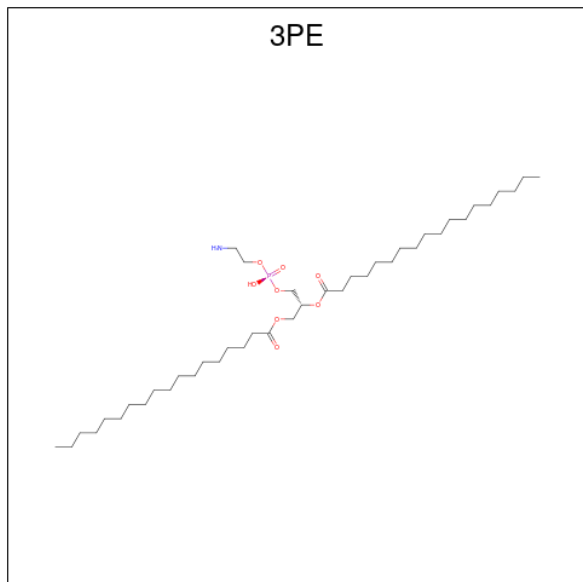
Mol	Chain	Residues	Atoms					AltConf
49	A9	1	Total	C	N	O	P	0
			48	21	7	17	3	

- 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).



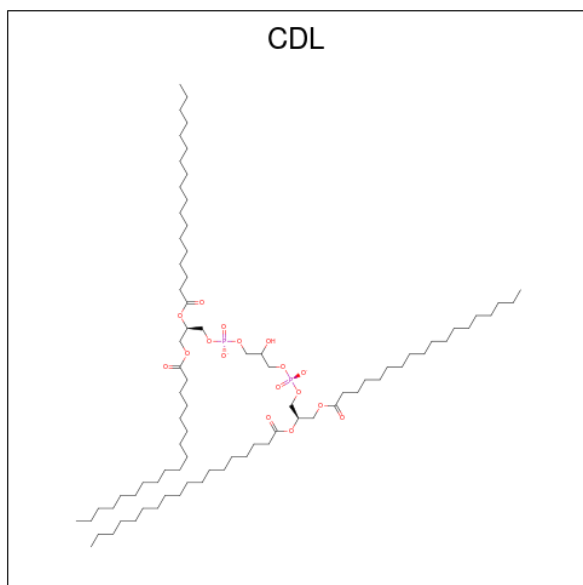
Mol	Chain	Residues	Atoms						AltConf
50	AA	1	Total 34	C 23	N 2	O 7	P 1	S 1	0
50	AB	1	Total 31	C 20	N 2	O 7	P 1	S 1	0

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



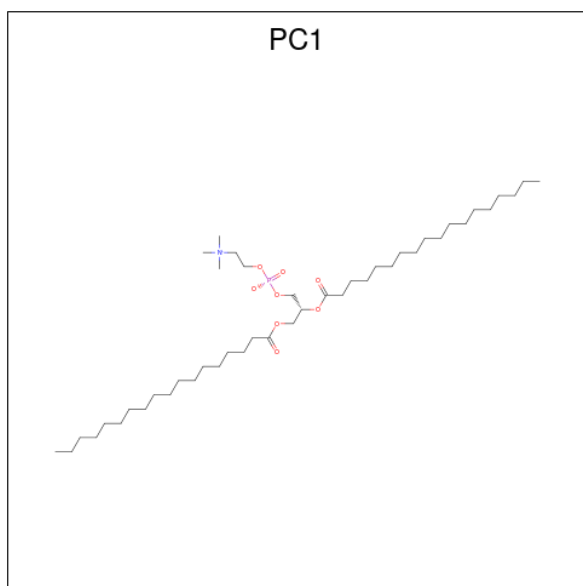
Mol	Chain	Residues	Atoms					AltConf
51	D1	1	Total	C	N	O	P	0
			26	16	1	8	1	
51	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	
51	D5	1	Total	C	N	O	P	0
			40	30	1	8	1	

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



Mol	Chain	Residues	Atoms				AltConf
52	D5	1	Total	C	O	P	0
			60	41	17	2	

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

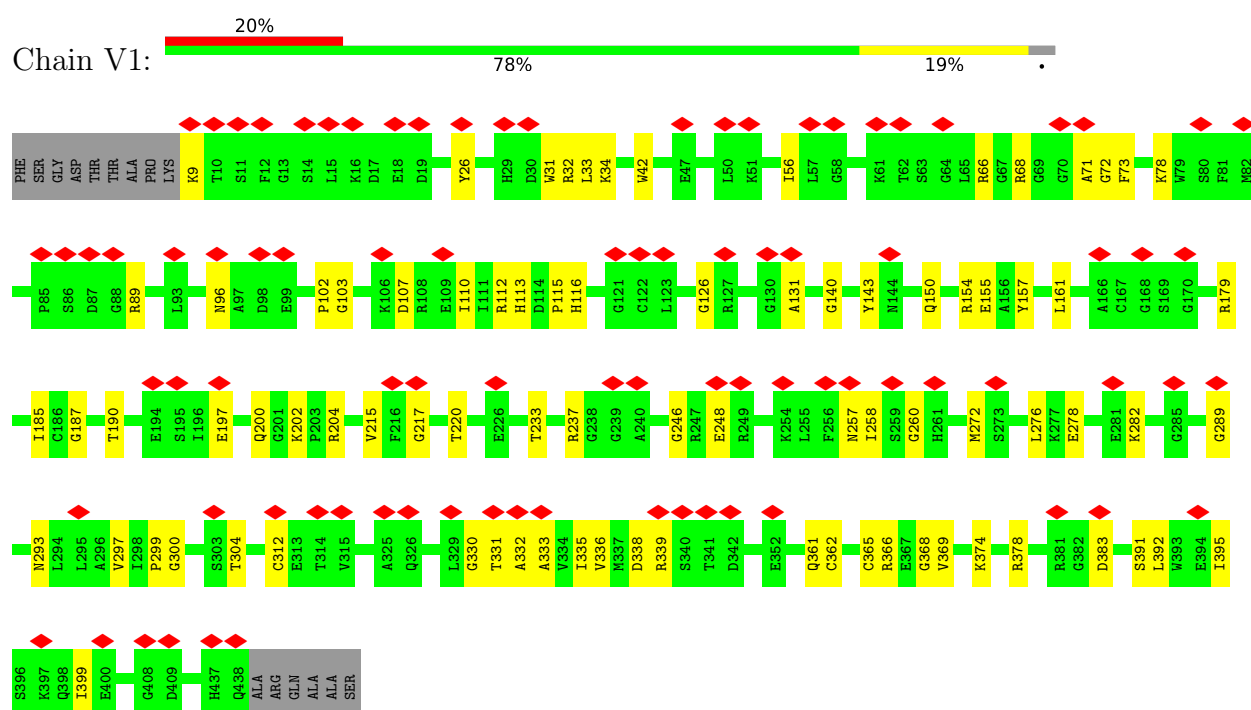


Mol	Chain	Residues	Atoms					AltConf
53	AK	1	Total	C	N	O	P	0
			28	18	1	8	1	

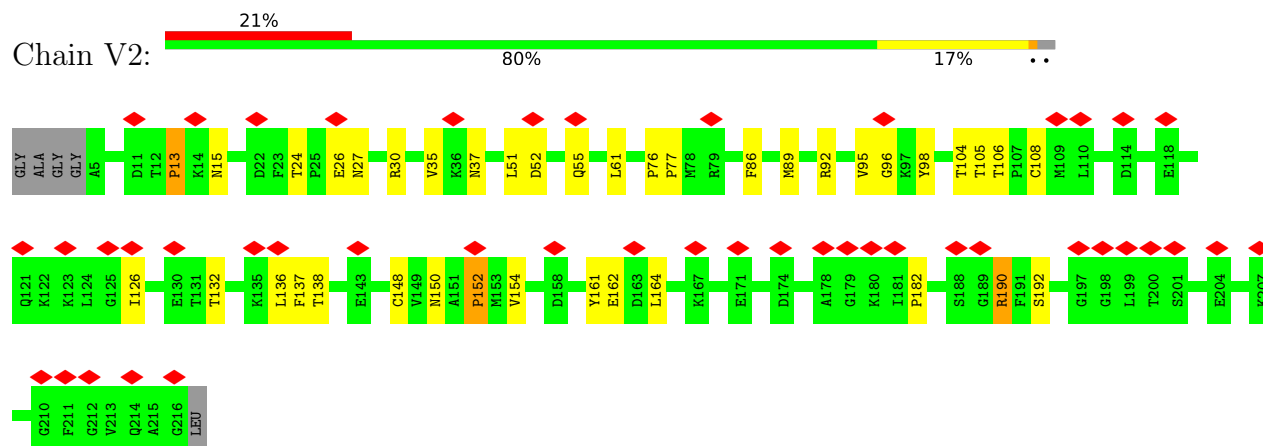
3 Residue-property plots

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

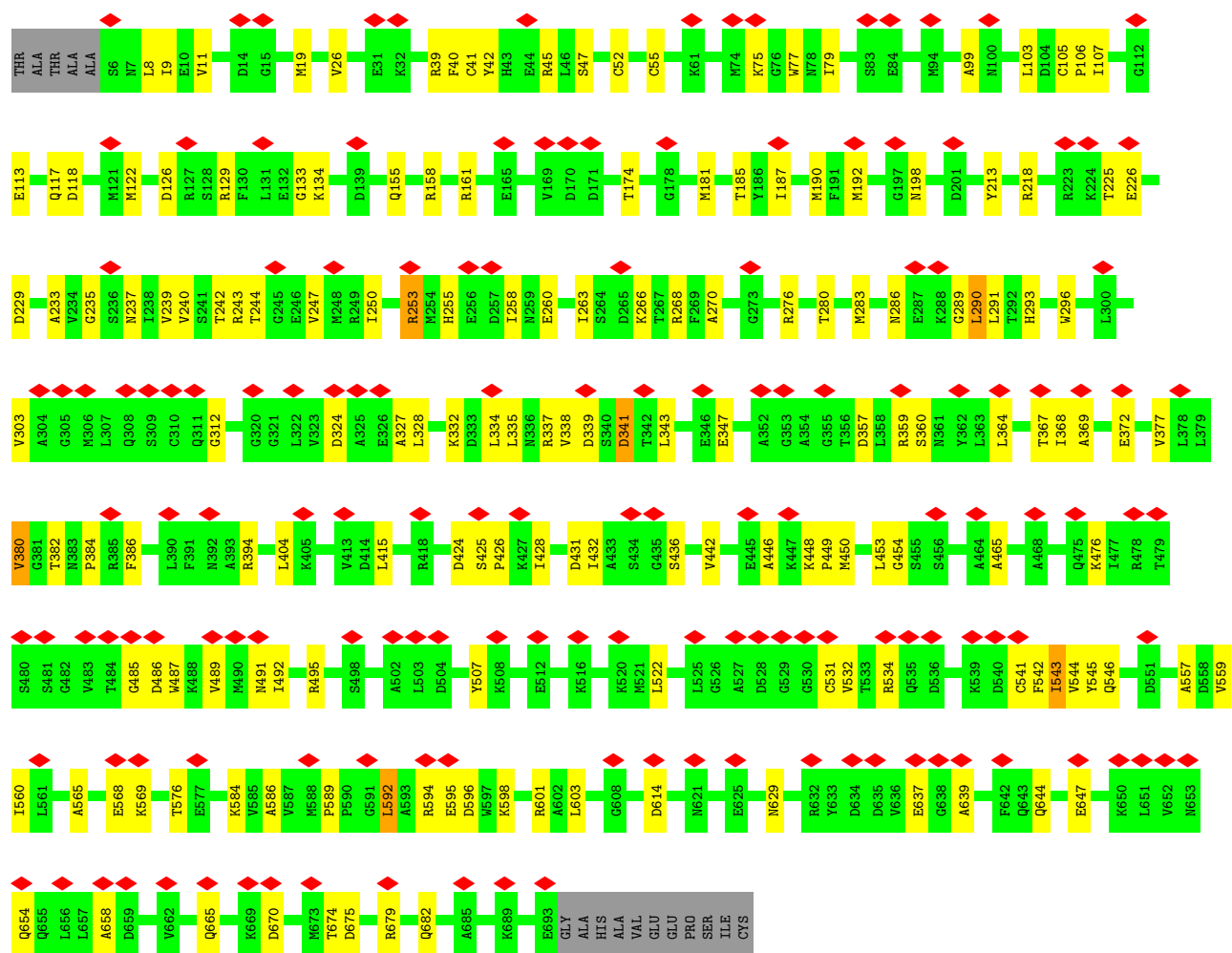


- Molecule 2: NDUFV2



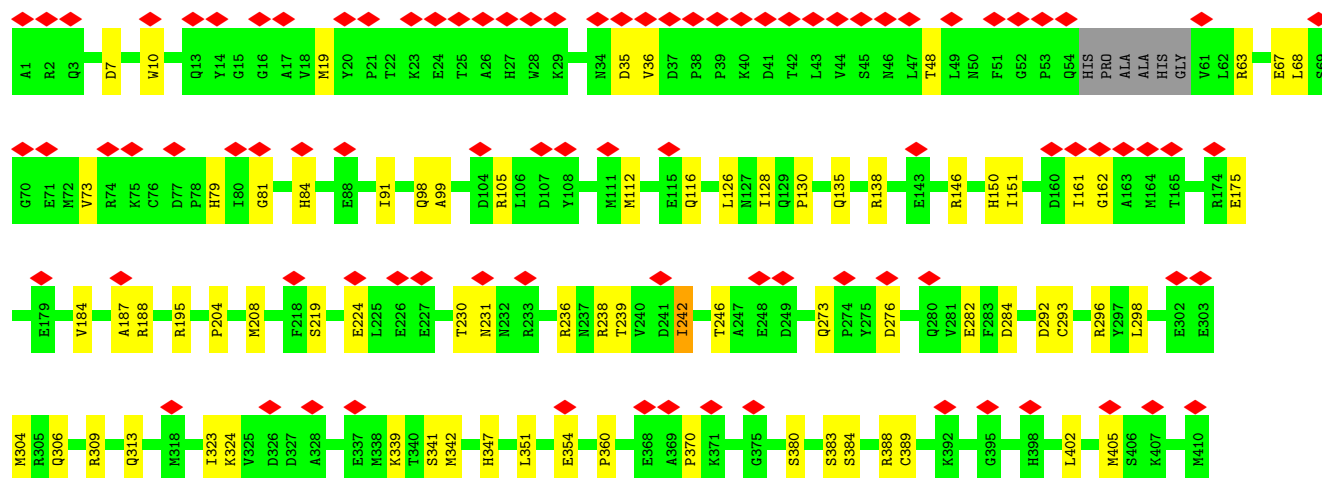
- Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain S1: 



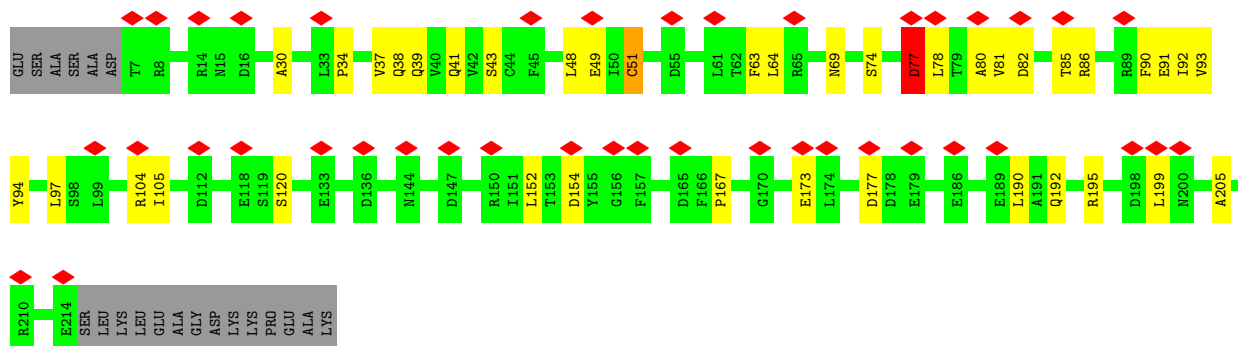
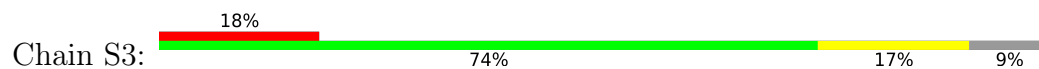
• Molecule 4: NDUF52

Chain S2: 

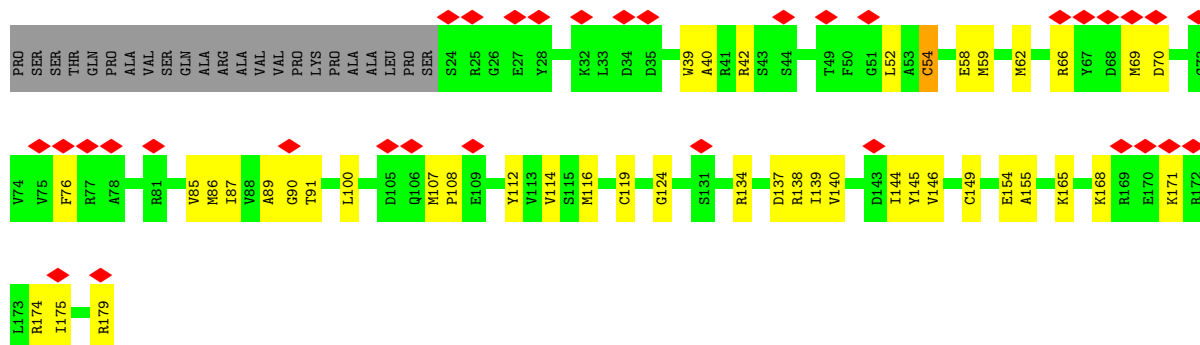




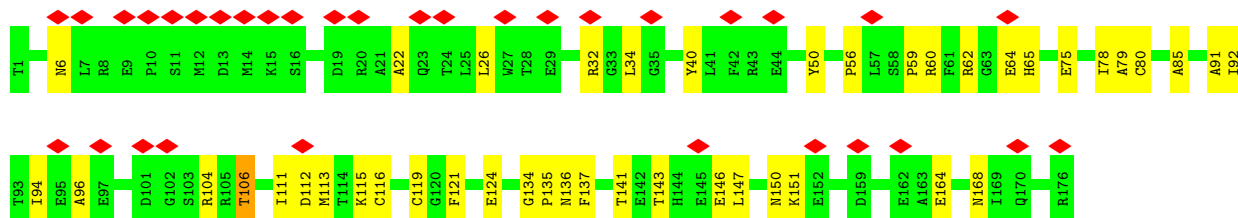
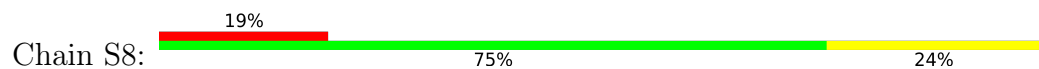
• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3



• Molecule 6: NDUF57

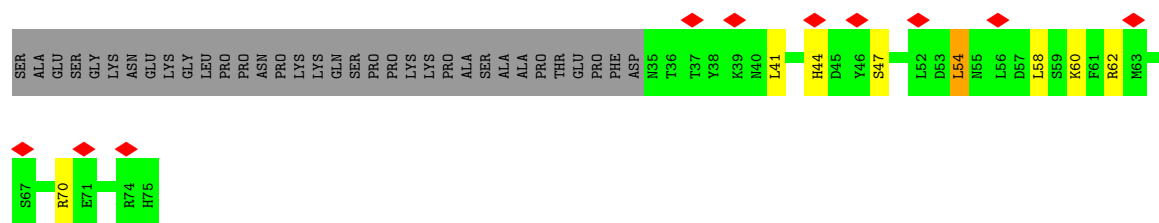


• Molecule 7: NDUF58

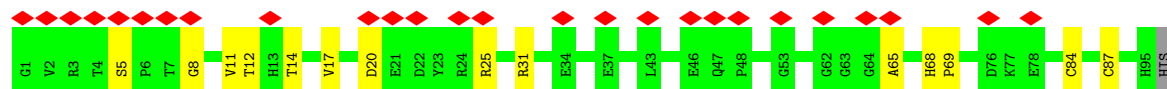
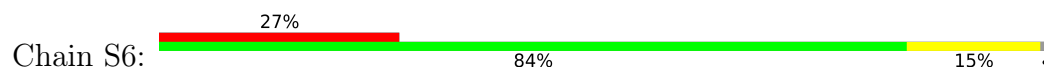


• Molecule 8: NDUFV3

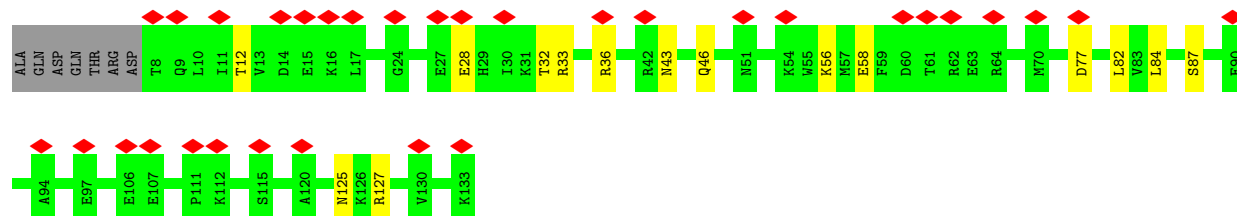
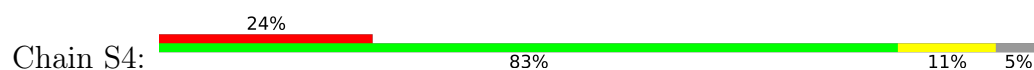




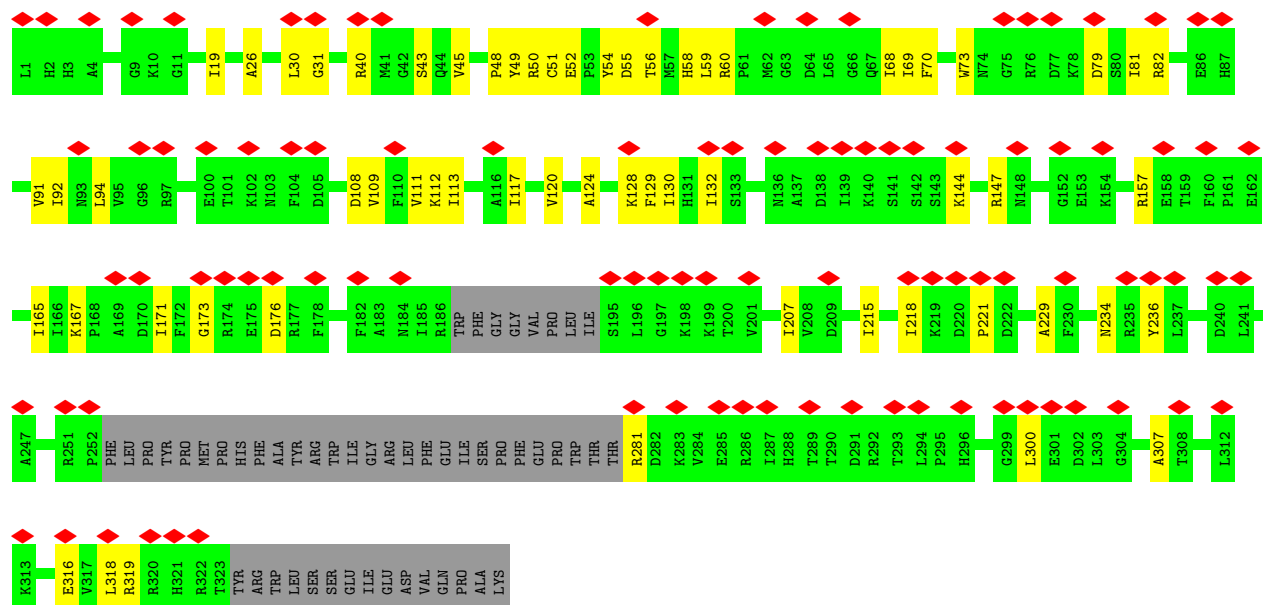
- Molecule 9: NDUFS6



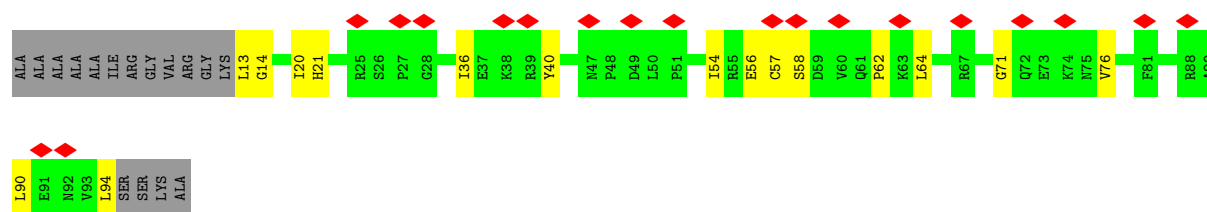
- Molecule 10: NADH:ubiquinone oxidoreductase subunit S4



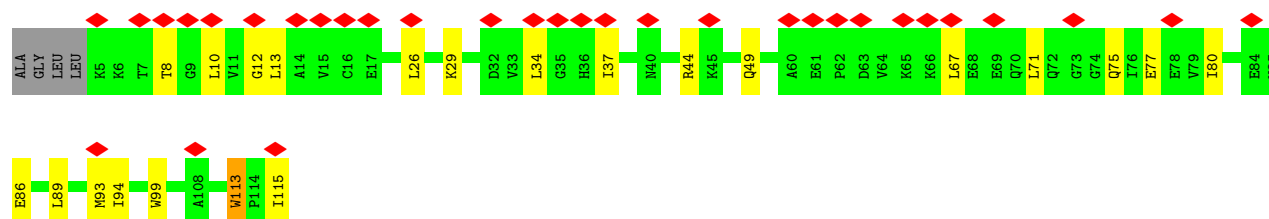
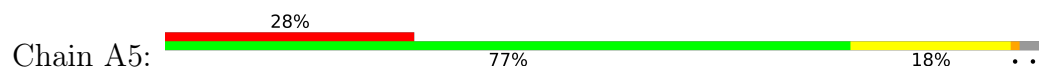
- Molecule 11: NADH:ubiquinone oxidoreductase subunit A9



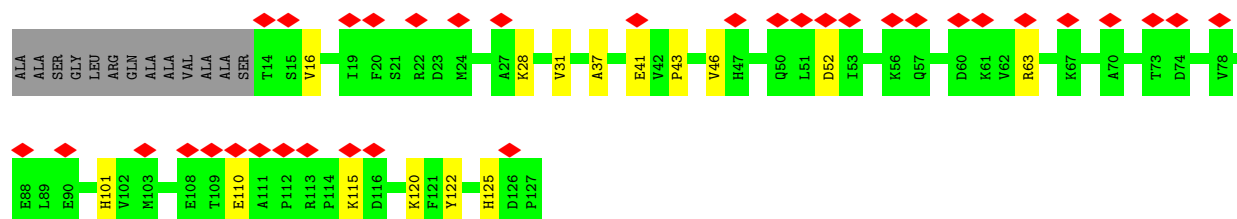
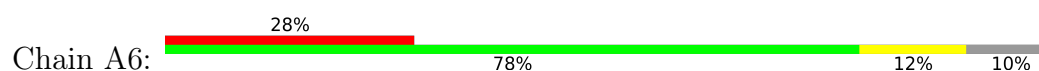
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



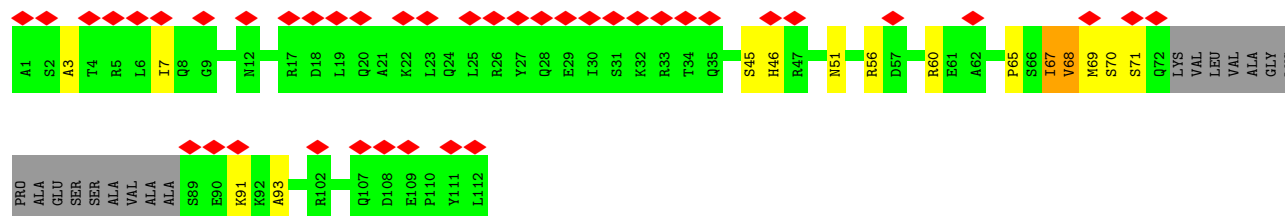
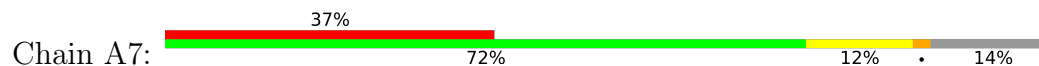
- Molecule 13: NDUFA5



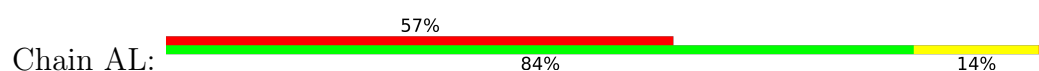
- Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

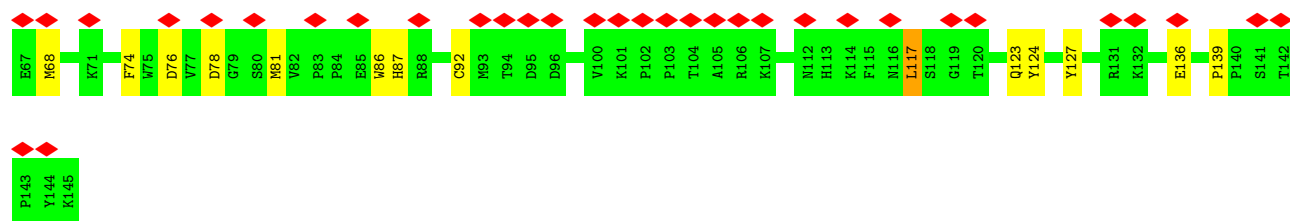


- Molecule 15: NDUFA7

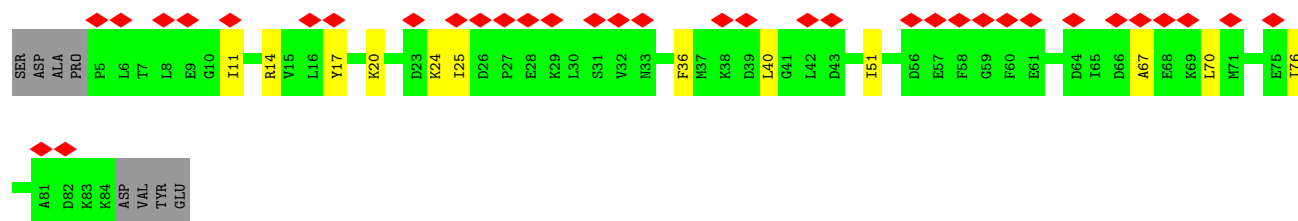
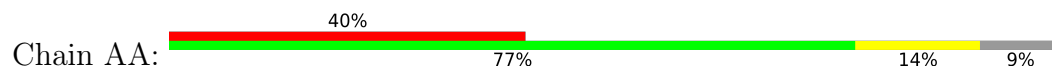


- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

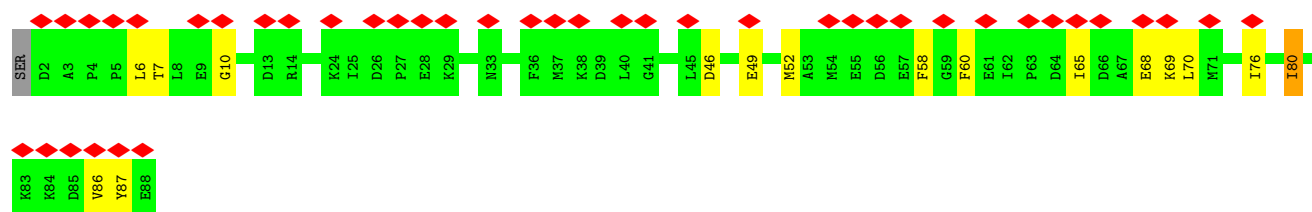
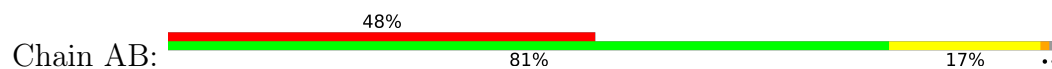




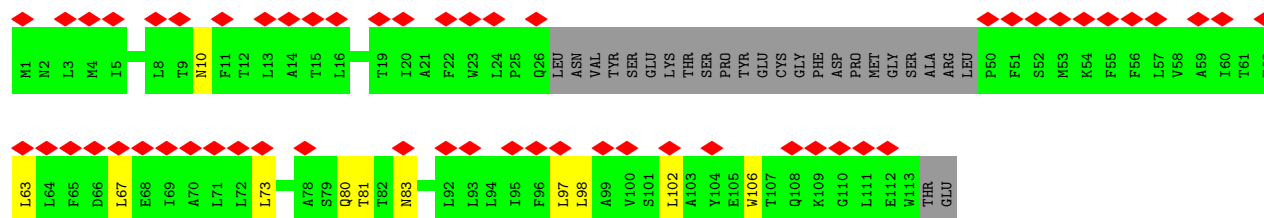
- Molecule 17: Acyl carrier protein



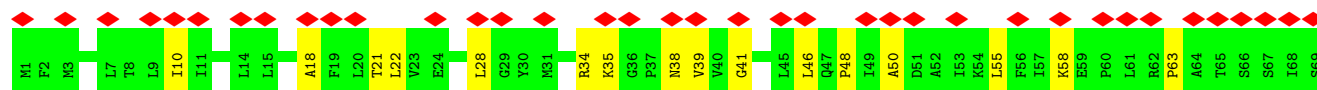
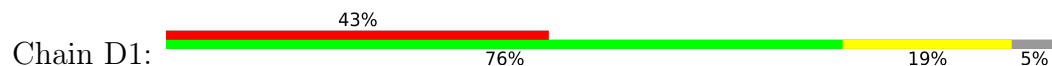
- Molecule 17: Acyl carrier protein

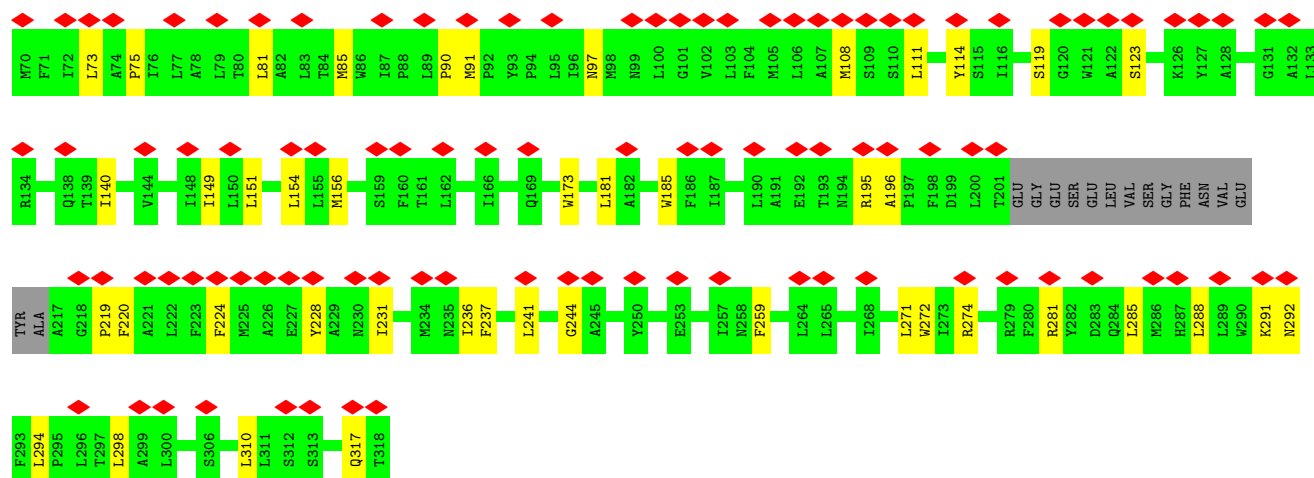


- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

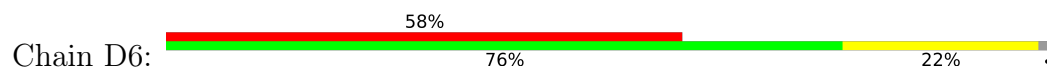


- Molecule 19: NADH-ubiquinone oxidoreductase chain 1

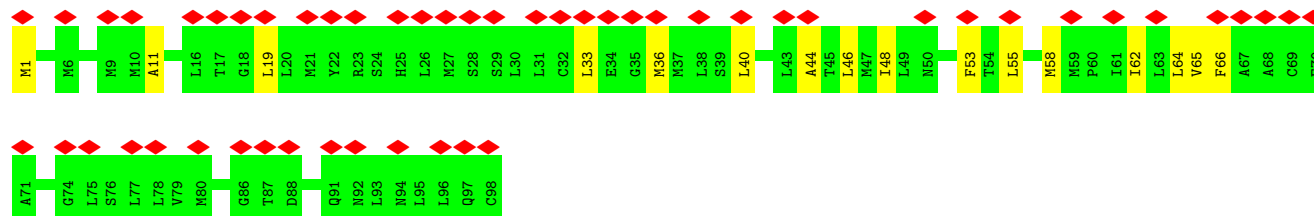
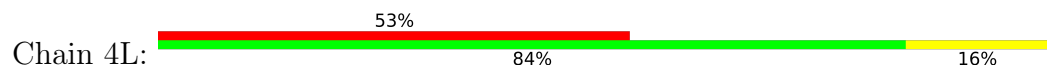




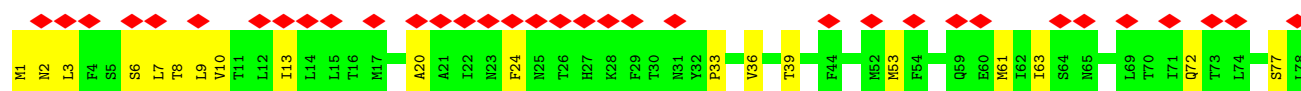
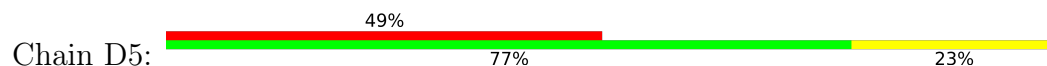
• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

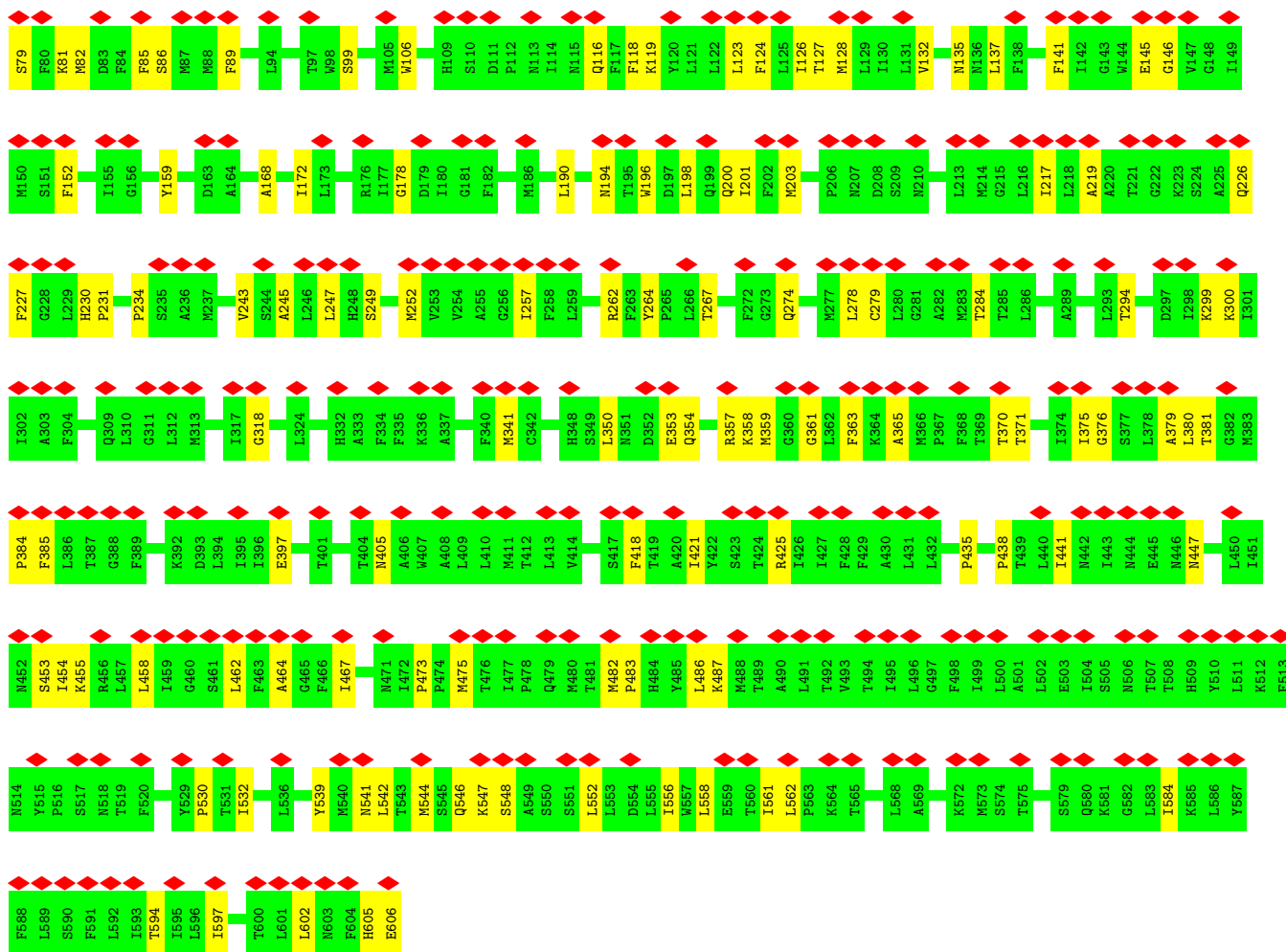


• Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

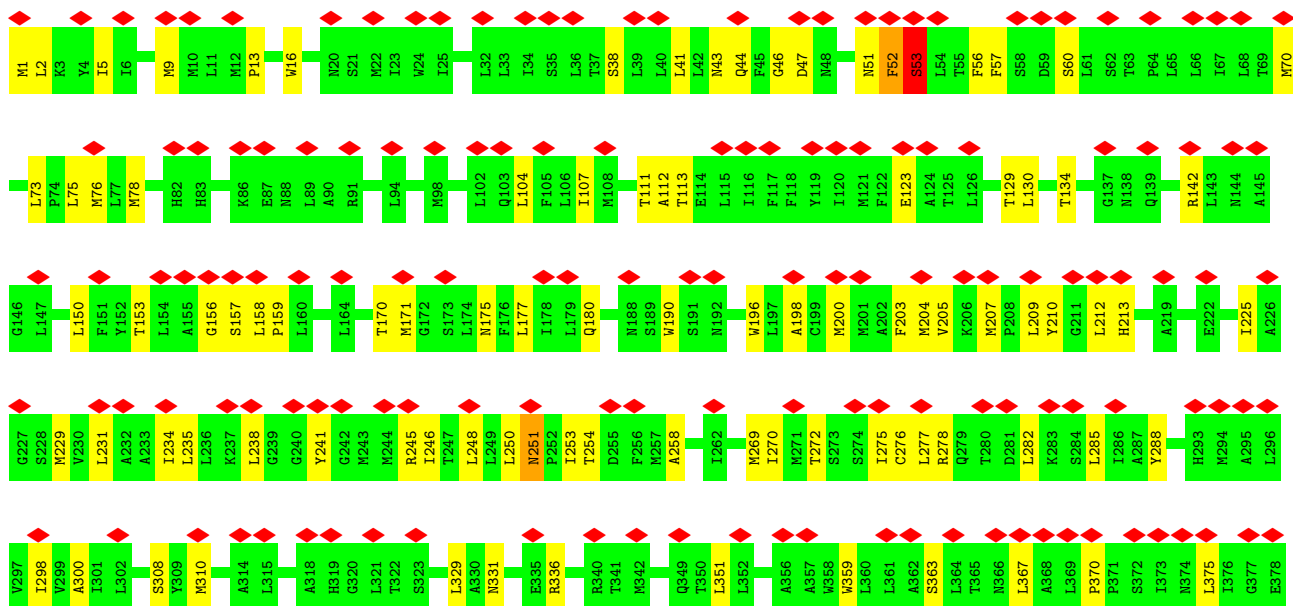
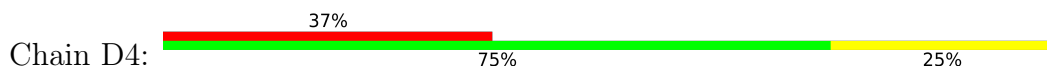


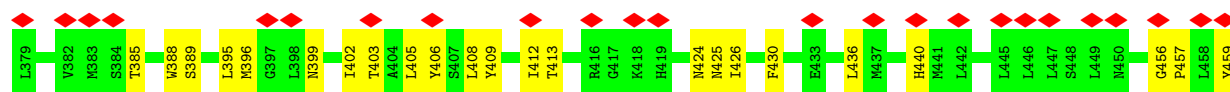
• Molecule 22: NADH-ubiquinone oxidoreductase chain 5



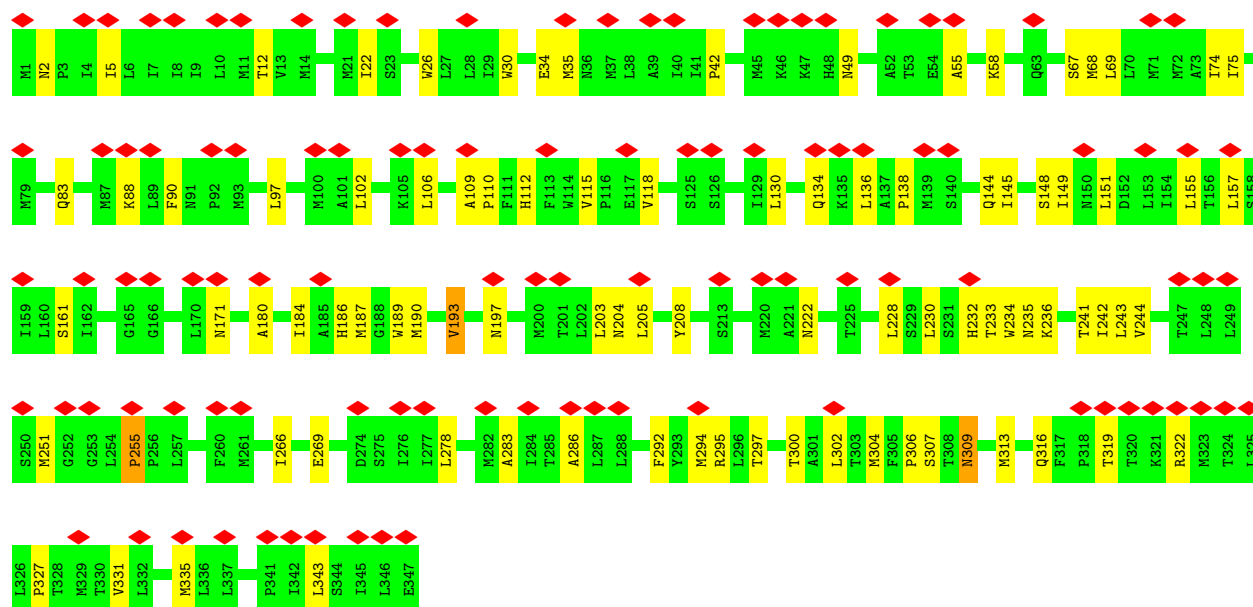
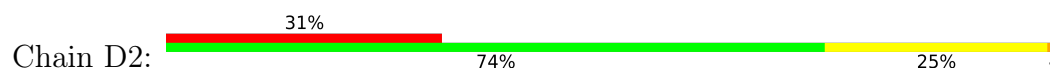


• Molecule 23: NADH-ubiquinone oxidoreductase chain 4

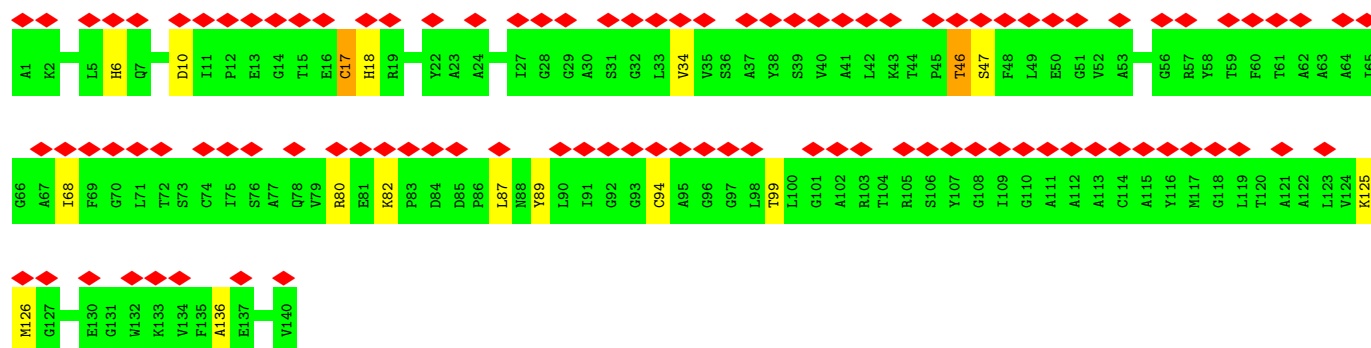
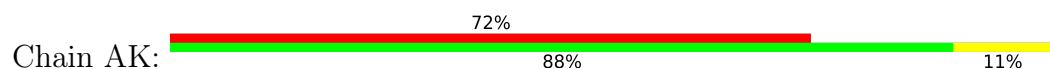




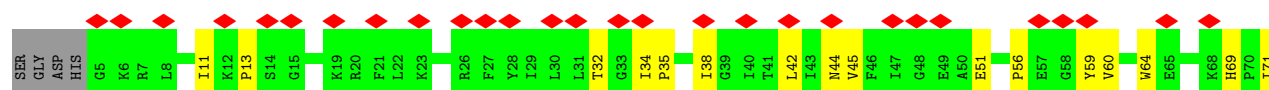
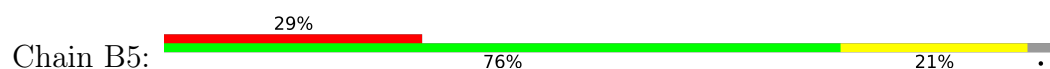
• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

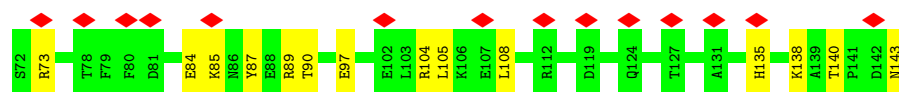


• Molecule 25: NDUFA11

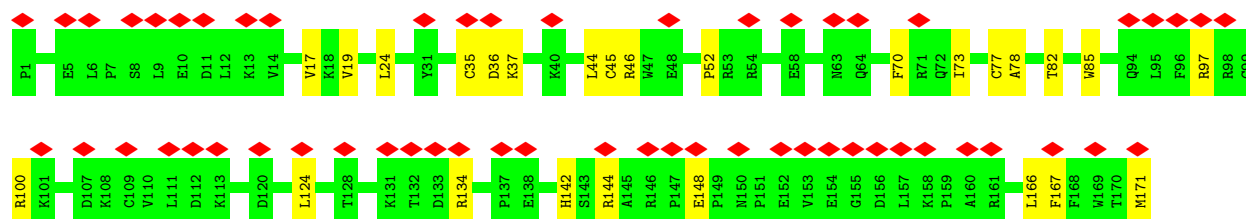
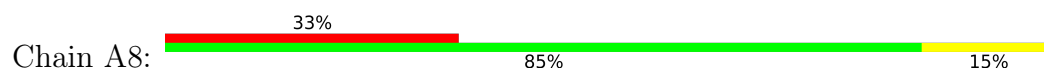


• Molecule 26: NADH:ubiquinone oxidoreductase subunit B5

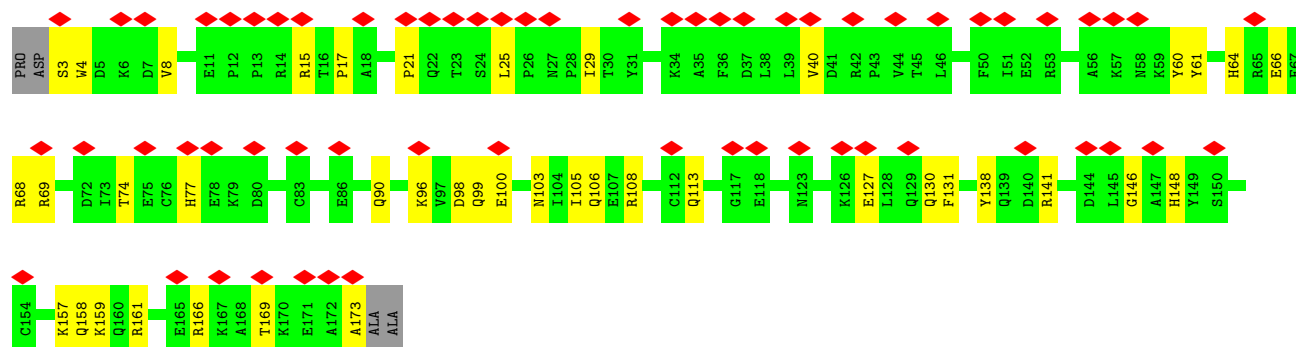
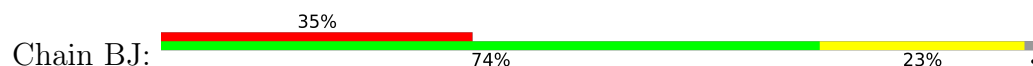




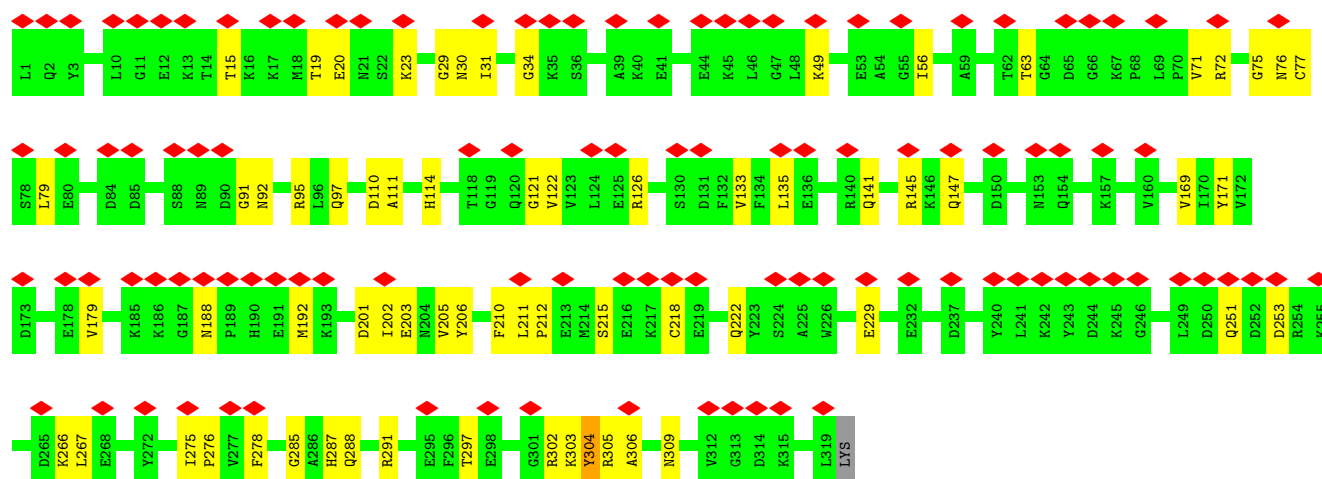
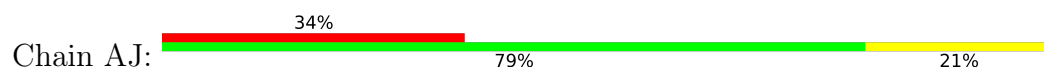
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



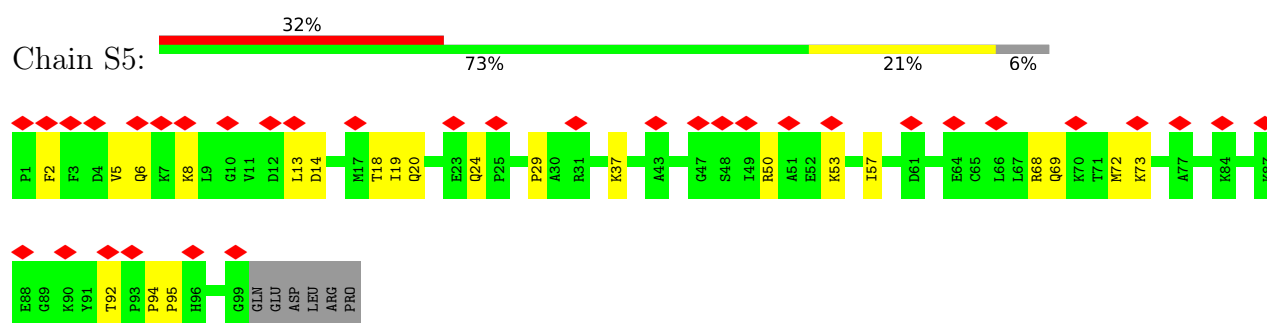
- Molecule 28: NDUFB10



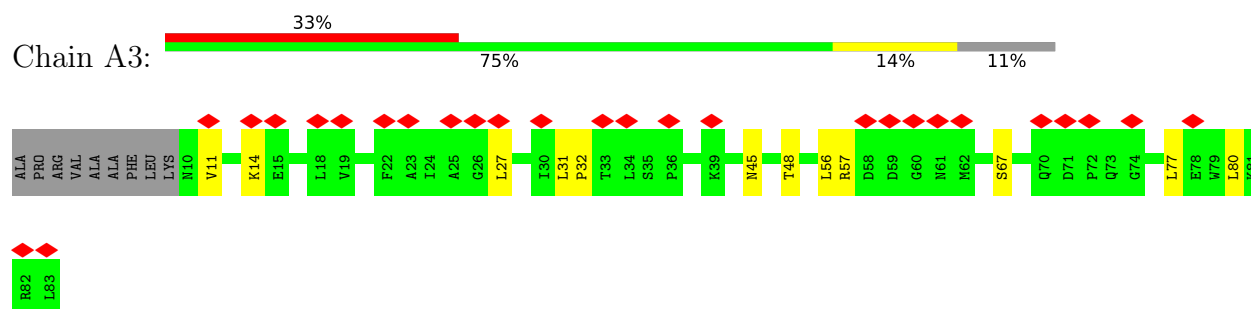
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



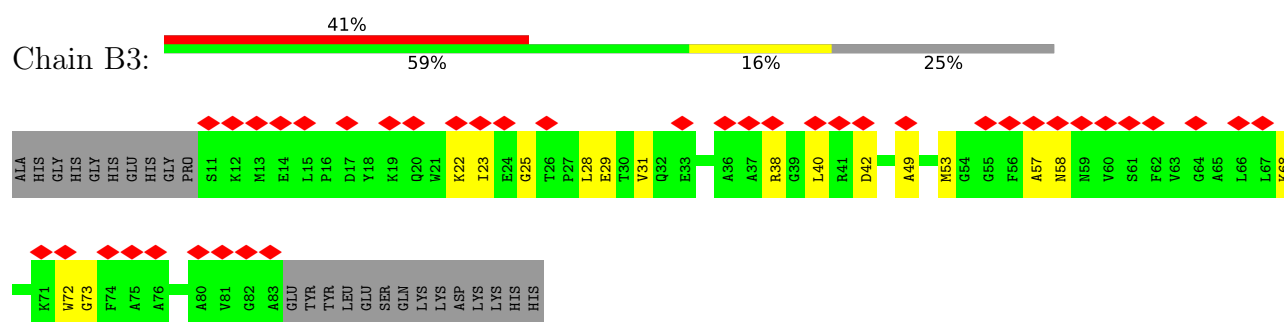
- Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



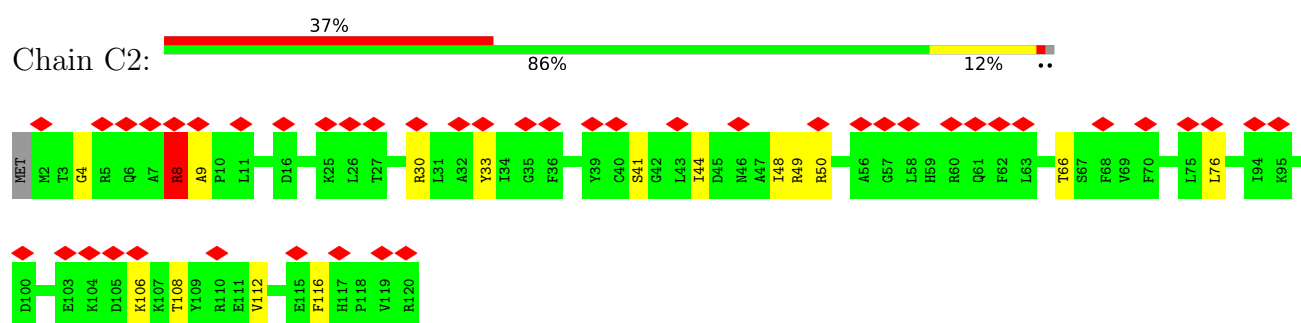
• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3



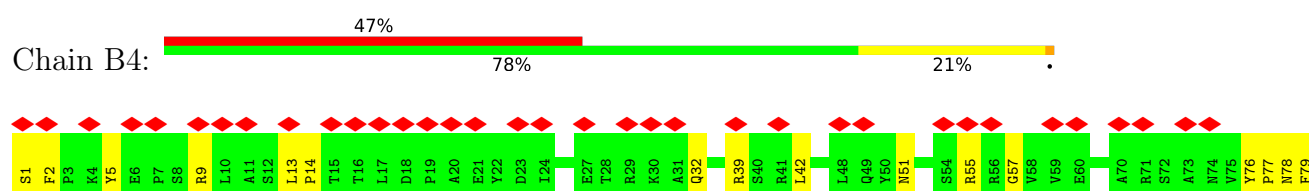
• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3

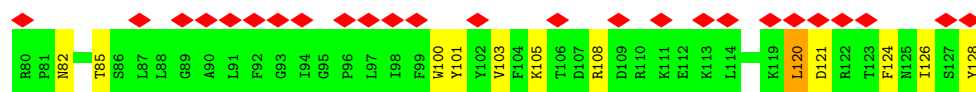


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

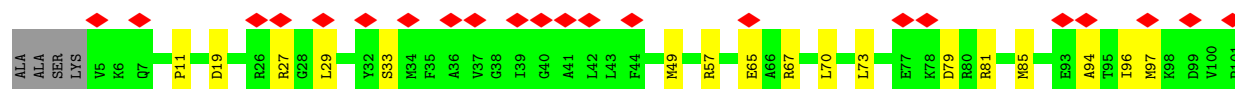
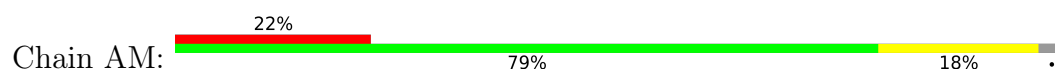


• Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

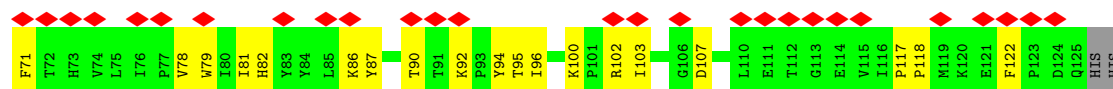




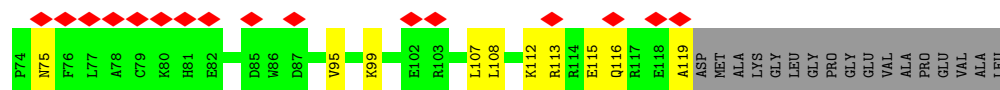
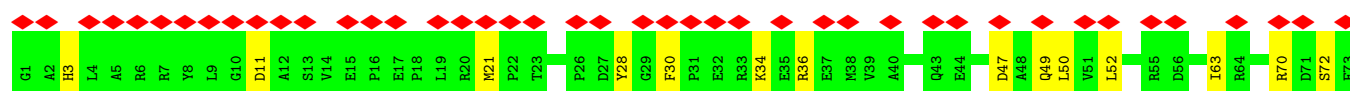
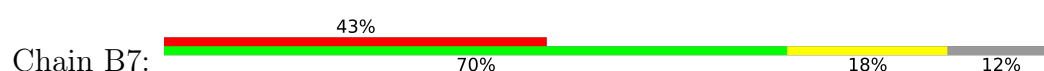
• Molecule 35: NDUFA13



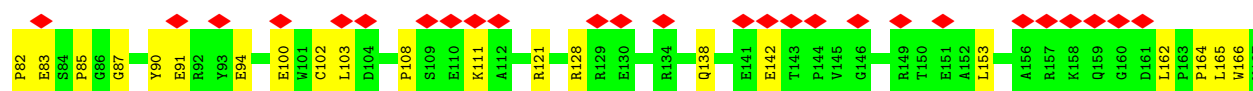
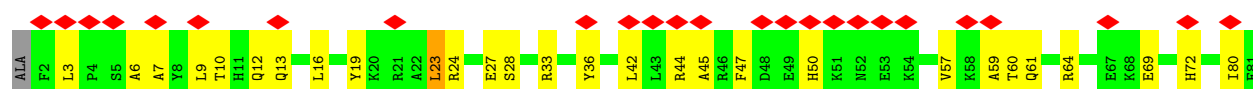
• Molecule 36: NDUF6

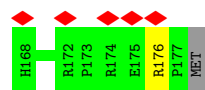


• Molecule 37: NADH:ubiquinone oxidoreductase subunit B7

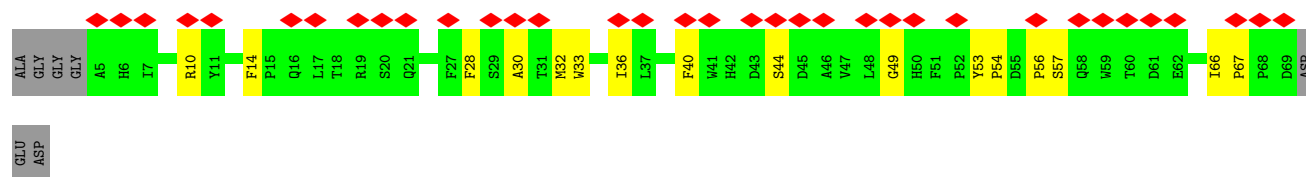


• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

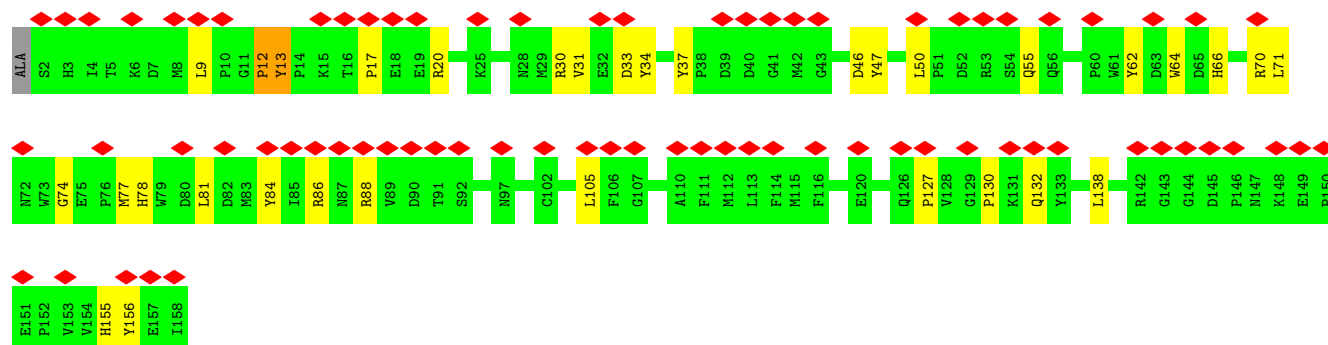
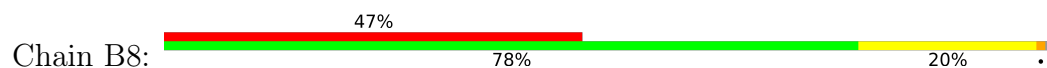




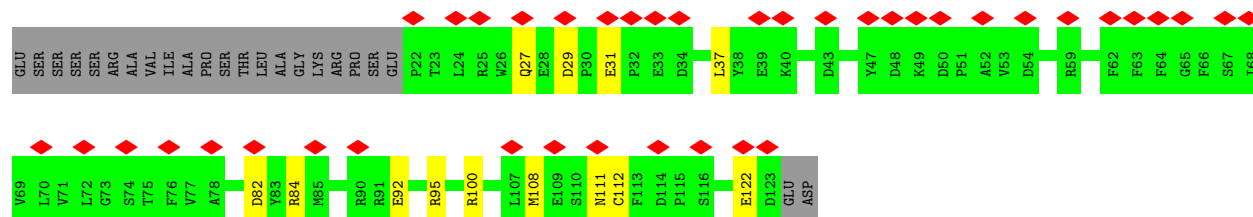
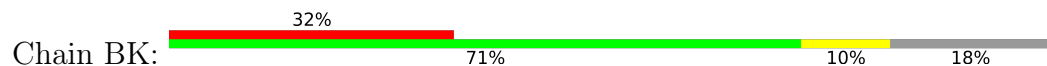
- Molecule 39: NADH:ubiquinone oxidoreductase subunit B2



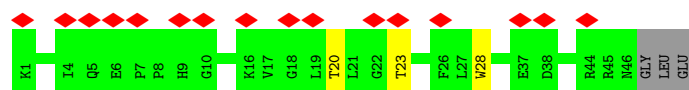
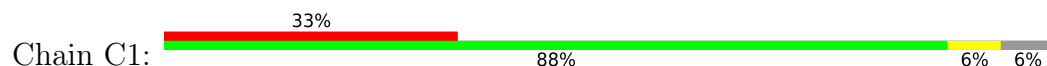
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



- Molecule 41: NDUFB11



- Molecule 42: NDUFC1



- Molecule 43: NDUFB1

- Molecule 44: NDUFA1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	21913	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	1.384	Depositor
Minimum map value	-0.360	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	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: FMN, NDP, SF4, 3PE, FES, CDL, ZMP, ZN, PC1

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	0.29	0/3386	0.63	0/4575
2	V2	0.28	0/1687	0.76	1/2295 (0.0%)
3	S1	0.28	0/5362	0.60	0/7266
4	S2	0.32	0/3502	0.63	2/4744 (0.0%)
5	S3	0.32	0/1776	0.69	1/2417 (0.0%)
6	S7	0.32	0/1278	0.64	0/1728
7	S8	0.34	0/1445	0.64	0/1956
8	V3	0.27	0/355	0.71	0/480
9	S6	0.25	0/749	0.54	0/1009
10	S4	0.26	0/1047	0.58	0/1415
11	A9	0.26	0/2343	0.69	2/3164 (0.1%)
12	A2	0.24	0/676	0.65	2/911 (0.2%)
13	A5	0.27	0/921	0.67	0/1249
14	A6	0.27	0/993	0.65	2/1336 (0.1%)
15	A7	0.23	0/784	0.66	0/1060
16	AL	0.26	0/1242	0.64	0/1688
17	AA	0.26	0/655	0.70	0/881
17	AB	0.24	0/714	0.55	0/963
18	D3	0.28	0/747	0.62	0/1022
19	D1	0.32	0/2487	0.73	2/3401 (0.1%)
20	D6	0.27	0/1339	0.65	0/1810
21	4L	0.31	0/758	0.68	0/1024
22	D5	0.30	0/4933	0.70	0/6710
23	D4	0.32	0/3740	0.73	0/5095
24	D2	0.33	0/2788	0.65	3/3795 (0.1%)
25	AK	0.26	0/1046	0.72	2/1419 (0.1%)
26	B5	0.25	0/1189	0.55	0/1607
27	A8	0.27	0/1441	0.65	0/1942
28	BJ	0.26	0/1475	0.66	3/1989 (0.2%)
29	AJ	0.26	0/2644	0.67	8/3579 (0.2%)
30	S5	0.27	0/843	0.66	1/1128 (0.1%)
31	A3	0.27	0/602	0.71	0/828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	B3	0.30	0/595	0.79	0/803
33	C2	0.29	0/1028	0.71	4/1388 (0.3%)
34	B4	0.23	0/1085	0.57	0/1467
35	AM	0.28	0/1172	0.69	0/1579
36	B6	0.29	0/841	0.75	0/1144
37	B7	0.27	0/1051	0.67	0/1408
38	B9	0.25	0/1568	0.64	2/2123 (0.1%)
39	B2	0.27	0/590	0.73	2/810 (0.2%)
40	B8	0.27	0/1379	0.80	5/1884 (0.3%)
41	BK	0.24	0/880	0.68	0/1196
42	C1	0.21	0/404	0.56	0/548
43	B1	0.22	0/462	0.59	0/624
44	A1	0.26	0/592	0.67	1/795 (0.1%)
All	All	0.28	0/66594	0.67	43/90255 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	V1	0	3
2	V2	0	3
3	S1	0	6
4	S2	0	3
5	S3	0	2
7	S8	0	1
13	A5	0	2
15	A7	0	4
19	D1	0	2
20	D6	0	1
22	D5	0	3
23	D4	0	2
25	AK	0	1
27	A8	0	1
29	AJ	0	1
30	S5	0	1
31	A3	0	1
32	B3	0	2
33	C2	0	1
36	B6	0	1
37	B7	0	1

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
39	B2	0	1
40	B8	0	1
43	B1	0	1
44	A1	0	1
All	All	0	46

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	B8	12	PRO	CA-C-N	8.74	130.47	120.06
40	B8	12	PRO	C-N-CA	8.74	130.47	120.06
19	D1	63	PRO	CA-C-N	8.37	136.76	121.70
19	D1	63	PRO	C-N-CA	8.37	136.76	121.70
29	AJ	229	GLU	CA-C-N	7.73	135.62	121.70
29	AJ	229	GLU	C-N-CA	7.73	135.62	121.70
28	BJ	21	PRO	CA-C-N	7.67	135.51	121.70
28	BJ	21	PRO	C-N-CA	7.67	135.51	121.70
14	A6	110	GLU	CA-C-N	7.23	134.71	121.70
14	A6	110	GLU	C-N-CA	7.23	134.71	121.70
33	C2	8	ARG	CA-C-N	7.12	134.52	121.70
33	C2	8	ARG	C-N-CA	7.12	134.52	121.70
39	B2	44	SER	CA-C-N	7.11	134.50	121.70
39	B2	44	SER	C-N-CA	7.11	134.50	121.70
44	A1	57	VAL	N-CA-C	-6.94	105.77	112.29
25	AK	17	CYS	CA-C-N	6.22	133.43	121.54
25	AK	17	CYS	C-N-CA	6.22	133.43	121.54
40	B8	13	TYR	N-CA-C	6.17	122.08	113.57
29	AJ	251	GLN	CA-C-N	5.80	132.14	121.70
29	AJ	251	GLN	C-N-CA	5.80	132.14	121.70
29	AJ	275	ILE	C-N-CD	-5.73	108.00	120.60
5	S3	77	ASP	N-CA-C	5.69	117.67	110.33
4	S2	230	THR	CA-C-N	5.69	132.40	121.54
4	S2	230	THR	C-N-CA	5.69	132.40	121.54
24	D2	309	ASN	CA-C-N	5.38	131.81	121.54
24	D2	309	ASN	C-N-CA	5.38	131.81	121.54
33	C2	4	GLY	CA-C-N	5.37	131.37	121.70
33	C2	4	GLY	C-N-CA	5.37	131.37	121.70
38	B9	9	LEU	CA-C-N	5.36	131.77	121.54
38	B9	9	LEU	C-N-CA	5.36	131.77	121.54
11	A9	221	PRO	CA-C-N	5.31	135.84	126.45
11	A9	221	PRO	C-N-CA	5.31	135.84	126.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	AJ	304	TYR	CA-CB-CG	5.30	123.45	113.90
40	B8	37	TYR	CA-C-N	5.30	139.71	127.00
40	B8	37	TYR	C-N-CA	5.30	139.71	127.00
28	BJ	25	LEU	C-N-CD	-5.28	108.98	120.60
12	A2	56	GLU	CA-C-N	-5.24	116.21	122.44
12	A2	56	GLU	C-N-CA	-5.24	116.21	122.44
24	D2	255	PRO	N-CA-C	5.14	116.97	110.70
30	S5	94	PRO	N-CA-C	5.05	116.86	110.70
2	V2	190	ARG	CA-CB-CG	5.03	124.17	114.10
29	AJ	275	ILE	CA-C-N	5.02	139.04	127.00
29	AJ	275	ILE	C-N-CA	5.02	139.04	127.00

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	A1	63	SER	Peptide
31	A3	57	ARG	Peptide
13	A5	113	TRP	Peptide
13	A5	93	MET	Peptide
15	A7	67	ILE	Peptide
15	A7	68	VAL	Mainchain,Peptide
15	A7	69	MET	Peptide
27	A8	52	PRO	Peptide
29	AJ	278	PHE	Peptide
25	AK	46	THR	Peptide
43	B1	52	GLU	Peptide
39	B2	56	PRO	Peptide
32	B3	22	LYS	Peptide
32	B3	58	ASN	Peptide
36	B6	122	PHE	Peptide
37	B7	30	PHE	Peptide
40	B8	86	ARG	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	159	TYR	Peptide
22	D5	359	MET	Peptide
22	D5	365	ALA	Peptide
20	D6	115	ILE	Peptide

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Mol	Chain	Res	Type	Group
3	S1	213	TYR	Peptide
3	S1	247	VAL	Peptide
3	S1	253	ARG	Peptide
3	S1	341	ASP	Peptide
3	S1	380	VAL	Peptide
3	S1	592	LEU	Peptide
4	S2	162	GLY	Peptide
4	S2	68	LEU	Peptide
4	S2	73	VAL	Peptide
5	S3	51	CYS	Peptide
5	S3	77	ASP	Peptide
30	S5	92	THR	Peptide
7	S8	106	THR	Peptide
1	V1	102	PRO	Peptide
1	V1	260	GLY	Peptide
1	V1	331	THR	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	50	0
2	V2	1647	0	1657	24	0
3	S1	5275	0	5300	112	0
4	S2	3414	0	3360	55	0
5	S3	1726	0	1676	37	0
6	S7	1247	0	1256	31	0
7	S8	1414	0	1371	33	0
8	V3	345	0	323	9	0
9	S6	737	0	710	9	0
10	S4	1024	0	1023	14	0
11	A9	2293	0	2326	36	0
12	A2	665	0	678	9	0
13	A5	901	0	936	13	0
14	A6	969	0	980	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A7	766	0	779	14	0
16	AL	1201	0	1170	17	0
17	AA	645	0	649	7	0
17	AB	702	0	692	12	0
18	D3	728	0	773	12	0
19	D1	2415	0	2542	36	0
20	D6	1308	0	1329	30	0
21	4L	748	0	794	19	0
22	D5	4805	0	4950	95	0
23	D4	3646	0	3850	82	0
24	D2	2724	0	2930	66	0
25	AK	1025	0	1033	10	0
26	B5	1156	0	1177	26	0
27	A8	1404	0	1384	19	0
28	BJ	1441	0	1417	34	0
29	AJ	2583	0	2547	40	0
30	S5	822	0	820	19	0
31	A3	582	0	583	8	0
32	B3	578	0	570	11	0
33	C2	997	0	983	18	0
34	B4	1059	0	1062	24	0
35	AM	1143	0	1137	24	0
36	B6	815	0	837	20	0
37	B7	1026	0	995	20	0
38	B9	1515	0	1469	38	0
39	B2	563	0	509	14	0
40	B8	1324	0	1219	23	0
41	BK	853	0	800	15	0
42	C1	391	0	391	2	0
43	B1	449	0	453	8	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	1	0
45	V1	8	0	0	1	0
46	V1	31	0	19	3	0
47	S1	4	0	0	1	0
47	V2	4	0	0	0	0
48	S6	1	0	0	0	0
49	A9	48	0	26	0	0
50	AA	34	0	40	1	0
50	AB	31	0	34	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	D1	26	0	26	0	0
51	D5	78	0	104	2	0
52	D5	60	0	64	3	0
53	AK	28	0	30	0	0
All	All	65353	0	65619	948	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 7.

All (948) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:80:ALA:HA	5:S3:91:GLU:O	1.19	1.31
5:S3:38:GLN:O	15:A7:70:SER:HA	1.46	1.16
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.57	1.03
50:AB:101:ZMP:O7	38:B9:12:GLN:NE2	1.94	1.00
5:S3:80:ALA:CA	5:S3:91:GLU:O	2.13	0.96
5:S3:38:GLN:HA	15:A7:70:SER:O	1.70	0.90
5:S3:38:GLN:O	15:A7:70:SER:CA	2.22	0.87
5:S3:80:ALA:HA	5:S3:91:GLU:C	2.03	0.82
50:AB:101:ZMP:O1	38:B9:50:HIS:NE2	2.14	0.80
50:AB:101:ZMP:H14	38:B9:59:ALA:HB1	1.67	0.75
22:D5:547:LYS:O	22:D5:552:LEU:HB2	1.87	0.74
4:S2:130:PRO:HG2	4:S2:135:GLN:HE21	1.52	0.73
50:AB:101:ZMP:O1	38:B9:50:HIS:CE1	2.42	0.73
29:AJ:304:TYR:H	33:C2:50:ARG:HH21	1.37	0.72
3:S1:568:GLU:HB3	3:S1:589:PRO:HG3	1.72	0.71
5:S3:85:THR:HG21	10:S4:87:SER:H	1.56	0.71
3:S1:255:HIS:HD2	3:S1:258:ILE:H	1.39	0.70
38:B9:80:ILE:HD12	38:B9:87:GLY:HA2	1.73	0.69
17:AB:7:THR:HG23	17:AB:10:GLY:H	1.56	0.69
3:S1:55:CYS:HB3	47:S1:803:FES:S2	2.33	0.68
3:S1:266:LYS:O	3:S1:270:ALA:HB2	1.93	0.68
23:D4:53:SER:HB2	23:D4:56:PHE:H	1.57	0.68
25:AK:6:HIS:O	25:AK:10:ASP:HB2	1.93	0.68
23:D4:231:LEU:O	23:D4:235:LEU:HB2	1.94	0.67
33:C2:30:ARG:HE	33:C2:76:LEU:HD11	1.58	0.67
16:AL:31:ASN:HD21	19:D1:39:VAL:HG22	1.60	0.66
10:S4:12:THR:HB	14:A6:16:VAL:H	1.60	0.66
24:D2:233:THR:HA	24:D2:236:LYS:HG2	1.77	0.65
23:D4:177:LEU:O	23:D4:180:GLN:C	2.39	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:382:THR:HB	3:S1:454:GLY:HA3	1.79	0.65
11:A9:92:ILE:HG22	11:A9:130:ILE:HB	1.78	0.65
24:D2:88:LYS:HG3	24:D2:148:SER:HB3	1.78	0.65
3:S1:117:GLN:NE2	45:S1:801:SF4:S3	2.69	0.65
23:D4:254:THR:O	23:D4:258:ALA:HB2	1.97	0.65
32:B3:25:GLY:O	32:B3:29:GLU:HB2	1.98	0.64
31:A3:27:LEU:O	31:A3:31:LEU:HB2	1.97	0.64
22:D5:279:CYS:SG	22:D5:405:ASN:ND2	2.70	0.64
3:S1:534:ARG:NH1	3:S1:541:CYS:SG	2.71	0.64
17:AB:70:LEU:HD23	17:AB:76:ILE:HG12	1.80	0.64
21:4L:1:MET:N	30:S5:72:MET:SD	2.71	0.63
22:D5:243:VAL:O	22:D5:247:LEU:HB2	1.97	0.63
5:S3:80:ALA:HB1	5:S3:90:PHE:HB3	1.80	0.63
3:S1:283:MET:HB2	3:S1:560:ILE:HB	1.79	0.63
26:B5:64:TRP:HB2	26:B5:73:ARG:HG3	1.81	0.62
17:AB:68:GLU:HB2	17:AB:69:LYS:HZ2	1.64	0.62
11:A9:51:CYS:SG	11:A9:52:GLU:N	2.71	0.62
13:A5:37:ILE:O	13:A5:44:ARG:NH1	2.32	0.62
5:S3:48:LEU:HB3	5:S3:105:ILE:HG22	1.81	0.62
3:S1:543:ILE:HD11	3:S1:557:ALA:HA	1.82	0.62
1:V1:32:ARG:HG3	1:V1:34:LYS:H	1.64	0.62
23:D4:170:THR:HG23	23:D4:171:MET:HG3	1.81	0.62
15:A7:70:SER:OG	15:A7:71:SER:N	2.33	0.62
22:D5:397:GLU:HB3	22:D5:482:MET:HE2	1.81	0.62
12:A2:21:HIS:O	12:A2:62:PRO:HA	1.99	0.61
37:B7:72:SER:HB2	37:B7:75:ASN:HB2	1.82	0.61
23:D4:204:MET:HB3	23:D4:209:LEU:HD22	1.82	0.61
24:D2:243:LEU:HD21	33:C2:44:ILE:HD11	1.82	0.61
37:B7:115:GLU:O	37:B7:119:ALA:HB3	1.99	0.61
1:V1:374:LYS:HE2	3:S1:133:GLY:HA2	1.83	0.61
6:S7:165:LYS:HE2	16:AL:76:ASP:HB2	1.82	0.61
23:D4:231:LEU:HA	23:D4:235:LEU:HD13	1.83	0.61
35:AM:96:ILE:HG23	35:AM:97:MET:HG2	1.83	0.61
5:S3:78:LEU:HA	5:S3:93:VAL:O	2.00	0.61
23:D4:388:TRP:O	34:B4:108:ARG:NH2	2.33	0.61
20:D6:133:SER:OG	35:AM:67:ARG:NH2	2.34	0.61
18:D3:10:ASN:HD21	19:D1:10:ILE:HG21	1.65	0.61
1:V1:200:GLN:NE2	3:S1:174:THR:OG1	2.33	0.60
20:D6:169:MET:HE1	20:D6:175:ASN:HD22	1.66	0.60
27:A8:97:ARG:HA	27:A8:100:ARG:HH21	1.66	0.60
8:V3:70:ARG:NH2	10:S4:125:ASN:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AJ:30:ASN:ND2	29:AJ:203:GLU:OE2	2.34	0.60
10:S4:33:ARG:NH2	10:S4:77:ASP:OD1	2.34	0.60
22:D5:116:GLN:NE2	52:D5:901:CDL:OB3	2.34	0.60
3:S1:106:PRO:O	3:S1:218:ARG:NH2	2.34	0.60
31:A3:48:THR:HG21	35:AM:57:ARG:HH21	1.65	0.60
40:B8:55:GLN:O	40:B8:70:ARG:NH2	2.35	0.60
22:D5:234:PRO:HB3	22:D5:300:LYS:HG2	1.84	0.60
19:D1:220:PHE:O	19:D1:224:PHE:HB2	2.02	0.60
27:A8:24:LEU:HG	35:AM:70:LEU:HD11	1.83	0.60
38:B9:102:CYS:SG	38:B9:103:LEU:N	2.73	0.60
1:V1:297:VAL:HG22	1:V1:336:VAL:HG12	1.84	0.60
24:D2:203:LEU:HD13	24:D2:343:LEU:HD12	1.84	0.60
11:A9:109:VAL:O	11:A9:113:ILE:HB	2.03	0.59
29:AJ:110:ASP:OD1	29:AJ:266:LYS:NZ	2.31	0.59
28:BJ:161:ARG:NH2	41:BK:111:ASN:OD1	2.35	0.59
3:S1:226:GLU:OE1	3:S1:253:ARG:NH2	2.35	0.59
18:D3:80:GLN:NE2	19:D1:317:GLN:O	2.30	0.59
14:A6:37:ALA:O	14:A6:41:GLU:HB2	2.03	0.59
22:D5:597:ILE:HD11	25:AK:34:VAL:HG22	1.84	0.59
1:V1:154:ARG:HD2	8:V3:54:LEU:HD21	1.84	0.59
27:A8:46:ARG:NH1	35:AM:79:ASP:OD2	2.36	0.59
4:S2:388:ARG:NH1	4:S2:389:CYS:O	2.35	0.59
17:AB:65:ILE:O	17:AB:69:LYS:NZ	2.35	0.59
3:S1:449:PRO:HG2	3:S1:489:VAL:HG22	1.85	0.58
20:D6:14:VAL:HG22	21:4L:11:ALA:HB2	1.85	0.58
30:S5:5:VAL:HA	30:S5:8:LYS:HB3	1.85	0.58
20:D6:58:LEU:O	20:D6:62:GLY:HA3	2.02	0.58
1:V1:233:THR:O	1:V1:237:ARG:HB2	2.04	0.58
23:D4:38:SER:OG	23:D4:70:MET:SD	2.55	0.58
22:D5:473:PRO:HB2	22:D5:475:MET:HE2	1.84	0.58
3:S1:40:PHE:O	3:S1:158:ARG:NH2	2.37	0.58
3:S1:113:GLU:OE2	10:S4:43:ASN:ND2	2.36	0.58
2:V2:27:ASN:OD1	2:V2:30:ARG:NH1	2.36	0.58
23:D4:175:ASN:ND2	26:B5:97:GLU:OE1	2.37	0.58
26:B5:85:LYS:HG2	26:B5:89:ARG:HH12	1.69	0.58
36:B6:87:TYR:HA	36:B6:90:THR:HG22	1.85	0.58
40:B8:30:ARG:HB3	40:B8:33:ASP:HB2	1.85	0.58
17:AB:52:MET:SD	38:B9:24:ARG:NH2	2.77	0.58
4:S2:360:PRO:HA	4:S2:380:SER:O	2.03	0.57
29:AJ:91:GLY:O	29:AJ:95:ARG:NH2	2.37	0.57
1:V1:89:ARG:NH1	1:V1:217:GLY:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D6:59:ILE:HG13	21:4L:64:LEU:HD21	1.86	0.57
22:D5:584:ILE:HD11	24:D2:58:LYS:HE2	1.86	0.57
23:D4:241:TYR:OH	23:D4:245:ARG:NH2	2.37	0.57
4:S2:116:GLN:HG3	4:S2:138:ARG:HD3	1.85	0.57
11:A9:108:ASP:O	11:A9:112:LYS:HB3	2.04	0.57
3:S1:243:ARG:HG2	3:S1:244:THR:HG23	1.85	0.57
4:S2:273:GLN:OE1	5:S3:104:ARG:NH2	2.35	0.57
5:S3:38:GLN:O	15:A7:70:SER:C	2.47	0.57
3:S1:118:ASP:OD2	10:S4:46:GLN:NE2	2.36	0.57
26:B5:60:VAL:HG11	43:B1:46:ARG:HD2	1.86	0.57
34:B4:39:ARG:NH1	40:B8:62:TYR:OH	2.38	0.57
1:V1:140:GLY:O	1:V1:179:ARG:NH2	2.37	0.57
21:4L:53:PHE:HD1	30:S5:20:GLN:HE21	1.53	0.57
23:D4:457:PRO:O	41:BK:84:ARG:NH1	2.34	0.57
5:S3:86:ARG:NH1	5:S3:91:GLU:OE2	2.37	0.57
18:D3:97:LEU:HD21	20:D6:162:LEU:HB2	1.87	0.57
3:S1:426:PRO:HD2	3:S1:658:ALA:HA	1.85	0.57
28:BJ:141:ARG:HD2	41:BK:112:CYS:HB3	1.87	0.57
2:V2:37:ASN:OD1	8:V3:62:ARG:NH1	2.37	0.56
3:S1:453:LEU:HB3	3:S1:492:ILE:HG22	1.86	0.56
11:A9:173:GLY:H	11:A9:176:ASP:HB2	1.70	0.56
22:D5:267:THR:O	22:D5:274:GLN:NE2	2.38	0.56
3:S1:237:ASN:HB3	3:S1:253:ARG:O	2.04	0.56
3:S1:432:ILE:O	3:S1:476:LYS:NZ	2.35	0.56
5:S3:80:ALA:HB2	5:S3:92:ILE:HD13	1.87	0.56
11:A9:108:ASP:HA	11:A9:111:VAL:HB	1.87	0.56
9:S6:20:ASP:OD1	9:S6:25:ARG:NH1	2.39	0.56
23:D4:156:GLY:HA3	23:D4:205:VAL:HG21	1.86	0.56
26:B5:51:GLU:H	28:BJ:61:TYR:HA	1.70	0.56
29:AJ:141:GLN:NE2	29:AJ:201:ASP:OD2	2.38	0.56
7:S8:65:HIS:NE2	7:S8:116:CYS:SG	2.73	0.56
11:A9:79:ASP:OD1	11:A9:82:ARG:NH1	2.38	0.56
13:A5:34:LEU:O	13:A5:44:ARG:NH1	2.38	0.56
15:A7:45:SER:O	15:A7:46:HIS:ND1	2.38	0.56
1:V1:362:CYS:N	45:V1:500:SF4:S2	2.77	0.56
3:S1:45:ARG:NE	3:S1:260:GLU:OE1	2.34	0.56
5:S3:74:SER:HB3	5:S3:97:LEU:O	2.05	0.56
8:V3:58:LEU:O	8:V3:62:ARG:NH2	2.39	0.56
3:S1:158:ARG:HA	3:S1:161:ARG:HH21	1.69	0.56
23:D4:210:TYR:O	23:D4:213:HIS:ND1	2.35	0.56
26:B5:140:THR:O	26:B5:143:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:77:SER:OG	22:D5:79:SER:OG	2.24	0.56
11:A9:319:ARG:NH2	14:A6:52:ASP:OD1	2.38	0.56
13:A5:34:LEU:HD11	13:A5:44:ARG:HA	1.87	0.56
23:D4:351:LEU:HD13	23:D4:426:ILE:HD11	1.88	0.56
37:B7:108:LEU:O	37:B7:112:LYS:HB2	2.05	0.56
22:D5:341:MET:HE3	22:D5:454:ILE:HD13	1.87	0.55
28:BJ:98:ASP:OD2	28:BJ:141:ARG:NH2	2.39	0.55
4:S2:105:ARG:NH1	6:S7:149:CYS:SG	2.66	0.55
4:S2:195:ARG:NH2	7:S8:124:GLU:OE1	2.39	0.55
5:S3:39:GLN:HB3	5:S3:51:CYS:HB2	1.89	0.55
14:A6:43:PRO:HA	14:A6:46:VAL:HG12	1.87	0.55
19:D1:196:ALA:HB3	19:D1:274:ARG:HG3	1.87	0.55
26:B5:135:HIS:HB3	30:S5:37:LYS:HE3	1.87	0.55
11:A9:56:THR:HA	11:A9:59:LEU:HG	1.88	0.55
19:D1:236:ILE:HG23	19:D1:259:PHE:HZ	1.69	0.55
24:D2:319:THR:HA	29:AJ:267:LEU:HD13	1.88	0.55
38:B9:24:ARG:NH1	38:B9:27:GLU:OE1	2.39	0.55
29:AJ:291:ARG:NH2	41:BK:29:ASP:OD2	2.39	0.55
1:V1:179:ARG:NH1	2:V2:52:ASP:OD2	2.38	0.55
24:D2:331:VAL:HG21	33:C2:41:SER:HB2	1.89	0.55
26:B5:44:ASN:HB3	26:B5:69:HIS:HE1	1.71	0.55
27:A8:35:CYS:SG	27:A8:36:ASP:N	2.78	0.55
40:B8:55:GLN:HG3	40:B8:84:TYR:HB3	1.89	0.55
3:S1:372:GLU:OE2	3:S1:394:ARG:NH1	2.38	0.55
23:D4:52:PHE:O	23:D4:56:PHE:HB2	2.07	0.55
16:AL:46:ASN:ND2	16:AL:48:TYR:OH	2.40	0.55
26:B5:56:PRO:HG2	26:B5:59:TYR:HB3	1.87	0.55
37:B7:34:LYS:NZ	40:B8:155:HIS:O	2.39	0.55
1:V1:33:LEU:HD23	1:V1:155:GLU:HB3	1.89	0.55
3:S1:312:GLY:N	3:S1:339:ASP:OD2	2.39	0.55
23:D4:123:GLU:HB2	24:D2:255:PRO:HG2	1.89	0.55
23:D4:389:SER:OG	34:B4:108:ARG:NH2	2.40	0.55
24:D2:102:LEU:HD22	24:D2:138:PRO:HB3	1.89	0.55
6:S7:70:ASP:OD2	19:D1:34:ARG:NH1	2.40	0.55
36:B6:103:ILE:HD11	37:B7:47:ASP:HB3	1.87	0.55
22:D5:358:LYS:HE2	22:D5:438:PRO:HD3	1.88	0.54
2:V2:95:VAL:HB	2:V2:138:THR:HG21	1.89	0.54
18:D3:81:THR:HG23	18:D3:83:ASN:H	1.72	0.54
20:D6:146:LEU:HD12	21:4L:58:MET:HG3	1.89	0.54
22:D5:547:LYS:O	22:D5:552:LEU:CB	2.54	0.54
3:S1:258:ILE:HG22	3:S1:368:ILE:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S2:105:ARG:NH1	45:S7:300:SF4:S3	2.79	0.54
20:D6:49:GLY:N	20:D6:139:GLU:OE2	2.33	0.54
38:B9:153:LEU:HD13	38:B9:164:PRO:HG2	1.89	0.54
36:B6:107:ASP:OD2	37:B7:70:ARG:NH2	2.40	0.54
1:V1:215:VAL:HG23	1:V1:220:THR:HG21	1.88	0.54
3:S1:243:ARG:NH2	7:S8:94:ILE:O	2.40	0.54
3:S1:601:ARG:NE	3:S1:614:ASP:OD1	2.40	0.54
2:V2:126:ILE:HG21	2:V2:132:THR:HA	1.90	0.54
3:S1:675:ASP:O	3:S1:679:ARG:HB2	2.07	0.54
23:D4:282:LEU:HD12	23:D4:285:LEU:HD12	1.89	0.54
26:B5:11:ILE:HG23	38:B9:103:LEU:HD13	1.88	0.54
1:V1:289:GLY:HA3	1:V1:293:ASN:HD22	1.71	0.54
7:S8:141:THR:HG21	7:S8:146:GLU:HB3	1.90	0.54
4:S2:187:ALA:HB2	7:S8:62:ARG:HH22	1.73	0.54
4:S2:188:ARG:NH1	6:S7:58:GLU:OE2	2.41	0.54
5:S3:39:GLN:NE2	5:S3:41:GLN:OE1	2.41	0.54
7:S8:135:PRO:HG3	7:S8:164:GLU:HG2	1.90	0.54
11:A9:120:VAL:O	11:A9:124:ALA:HB2	2.08	0.54
26:B5:89:ARG:HH21	43:B1:31:ASP:HB3	1.73	0.54
27:A8:37:LYS:NZ	31:A3:67:SER:O	2.40	0.54
4:S2:98:GLN:NE2	7:S8:85:ALA:O	2.39	0.54
16:AL:60:ARG:NH1	16:AL:92:CYS:SG	2.80	0.54
18:D3:81:THR:O	31:A3:45:ASN:ND2	2.41	0.54
29:AJ:297:THR:HB	29:AJ:303:LYS:HD2	1.90	0.54
33:C2:66:THR:OG1	42:C1:28:TRP:NE1	2.39	0.54
39:B2:10:ARG:NH1	39:B2:14:PHE:O	2.41	0.54
4:S2:224:GLU:OE1	7:S8:40:TYR:OH	2.25	0.53
5:S3:30:ALA:HA	5:S3:37:VAL:HG21	1.90	0.53
22:D5:561:ILE:HG23	22:D5:562:LEU:HG	1.89	0.53
27:A8:17:VAL:HG21	35:AM:73:LEU:HD21	1.88	0.53
3:S1:198:ASN:HD21	3:S1:263:ILE:H	1.56	0.53
6:S7:155:ALA:HB2	7:S8:137:PHE:HD2	1.72	0.53
19:D1:149:ILE:HG23	19:D1:181:LEU:HG	1.91	0.53
5:S3:41:GLN:HB3	15:A7:67:ILE:HG22	1.89	0.53
20:D6:159:TRP:HE1	24:D2:12:THR:HG22	1.73	0.53
50:AB:101:ZMP:H8	38:B9:47:PHE:CE1	2.42	0.53
1:V1:107:ASP:N	1:V1:107:ASP:OD1	2.39	0.53
20:D6:58:LEU:O	20:D6:62:GLY:CA	2.57	0.53
22:D5:72:GLN:OE1	28:BJ:99:GLN:NE2	2.41	0.53
1:V1:276:LEU:HD23	1:V1:312:CYS:HB2	1.90	0.53
7:S8:150:ASN:ND2	16:AL:127:TYR:O	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B7:28:TYR:HE2	39:B2:67:PRO:HD3	1.73	0.53
4:S2:63:ARG:HB3	4:S2:79:HIS:HB2	1.89	0.53
4:S2:238:ARG:HG3	4:S2:239:THR:HG23	1.90	0.53
5:S3:94:TYR:HH	5:S3:120:SER:HG	1.54	0.53
22:D5:441:ILE:HD11	39:B2:10:ARG:HG2	1.91	0.53
23:D4:251:ASN:OD1	23:D4:251:ASN:N	2.42	0.53
24:D2:228:LEU:HD23	29:AJ:276:PRO:HG2	1.89	0.53
29:AJ:287:HIS:ND1	41:BK:31:GLU:OE1	2.34	0.53
3:S1:347:GLU:OE2	3:S1:495:ARG:NH2	2.42	0.53
3:S1:442:VAL:O	3:S1:446:ALA:HB2	2.08	0.53
4:S2:19:MET:HG2	24:D2:295:ARG:HH12	1.72	0.53
20:D6:25:SER:HB3	20:D6:28:TYR:HD2	1.74	0.53
21:4L:40:LEU:HD22	24:D2:75:ILE:HD12	1.91	0.53
28:BJ:8:VAL:O	28:BJ:108:ARG:NH2	2.42	0.53
3:S1:26:VAL:HG13	3:S1:79:ILE:HD13	1.91	0.53
5:S3:41:GLN:NE2	5:S3:49:GLU:OE1	2.41	0.53
11:A9:52:GLU:HG2	11:A9:54:TYR:H	1.74	0.53
23:D4:177:LEU:O	23:D4:180:GLN:O	2.26	0.53
7:S8:143:THR:HA	11:A9:60:ARG:HH22	1.73	0.52
11:A9:26:ALA:HA	11:A9:31:GLY:HA3	1.91	0.52
23:D4:234:ILE:O	23:D4:238:LEU:HB2	2.09	0.52
1:V1:42:TRP:HE1	1:V1:116:HIS:HB3	1.74	0.52
5:S3:190:LEU:HD21	6:S7:134:ARG:HH21	1.72	0.52
23:D4:134:THR:O	23:D4:142:ARG:NH1	2.42	0.52
1:V1:78:LYS:NZ	46:V1:501:FMN:O1P	2.41	0.52
18:D3:63:LEU:HD12	20:D6:67:VAL:HG21	1.90	0.52
24:D2:26:TRP:HB3	24:D2:74:ILE:HD13	1.92	0.52
27:A8:171:MET:O	33:C2:30:ARG:NH1	2.43	0.52
29:AJ:77:CYS:O	29:AJ:92:ASN:ND2	2.39	0.52
3:S1:569:LYS:NZ	3:S1:596:ASP:OD2	2.43	0.52
3:S1:229:ASP:HB3	3:S1:235:GLY:HA2	1.92	0.52
22:D5:380:LEU:HD23	22:D5:381:THR:HG23	1.92	0.52
3:S1:250:ILE:HD11	3:S1:268:ARG:HA	1.91	0.52
22:D5:1:MET:HG2	22:D5:3:LEU:H	1.74	0.52
22:D5:172:ILE:HG21	23:D4:408:LEU:HD23	1.92	0.52
24:D2:136:LEU:HA	24:D2:205:LEU:HD21	1.90	0.52
40:B8:66:HIS:HB2	40:B8:71:LEU:HB2	1.90	0.52
2:V2:98:TYR:HD2	2:V2:136:LEU:HB2	1.73	0.52
11:A9:45:VAL:HB	11:A9:68:ILE:HG22	1.92	0.52
20:D6:167:VAL:HG22	24:D2:42:PRO:HG2	1.92	0.52
50:AB:101:ZMP:H8	38:B9:47:PHE:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:531:CYS:SG	3:S1:532:VAL:N	2.83	0.52
4:S2:35:ASP:O	24:D2:49:ASN:ND2	2.42	0.52
4:S2:126:LEU:HG	4:S2:128:ILE:HD12	1.92	0.52
7:S8:64:GLU:HB3	7:S8:134:GLY:HA3	1.92	0.52
22:D5:137:LEU:HB3	22:D5:196:TRP:HB2	1.92	0.52
23:D4:70:MET:HE2	23:D4:107:ILE:HD13	1.92	0.52
24:D2:109:ALA:HB2	24:D2:161:SER:HA	1.92	0.52
9:S6:68:HIS:HE1	9:S6:87:CYS:SG	2.19	0.52
22:D5:458:LEU:O	22:D5:462:LEU:HB2	2.11	0.52
24:D2:309:ASN:HD21	29:AJ:95:ARG:HG3	1.74	0.52
28:BJ:69:ARG:NH1	28:BJ:90:GLN:OE1	2.43	0.52
19:D1:281:ARG:O	19:D1:285:LEU:N	2.44	0.51
22:D5:546:GLN:OE1	23:D4:278:ARG:NH1	2.43	0.51
27:A8:166:LEU:HD23	27:A8:167:PHE:H	1.74	0.51
21:4L:48:ILE:HG23	21:4L:53:PHE:HB3	1.91	0.51
22:D5:33:PRO:HB3	22:D5:118:PHE:HE2	1.75	0.51
23:D4:57:PHE:HE1	23:D4:113:THR:HA	1.75	0.51
30:S5:95:PRO:O	35:AM:127:ARG:NH1	2.44	0.51
35:AM:124:TYR:HB3	35:AM:132:ILE:HG22	1.92	0.51
22:D5:371:THR:OG1	32:B3:68:LYS:NZ	2.42	0.51
26:B5:42:LEU:HA	26:B5:45:VAL:HG12	1.92	0.51
3:S1:105:CYS:SG	3:S1:117:GLN:NE2	2.83	0.51
16:AL:29:ARG:NH1	16:AL:74:PHE:O	2.43	0.51
19:D1:41:GLY:HA3	19:D1:46:LEU:HD11	1.91	0.51
4:S2:282:GLU:HB2	4:S2:313:GLN:HE22	1.76	0.51
22:D5:227:PHE:H	22:D5:284:THR:HG22	1.76	0.51
22:D5:264:TYR:HA	22:D5:267:THR:HG22	1.92	0.51
4:S2:91:ILE:HG12	4:S2:99:ALA:HB1	1.93	0.51
4:S2:341:SER:OG	4:S2:342:MET:N	2.44	0.51
24:D2:155:LEU:HD11	24:D2:278:LEU:HD21	1.93	0.51
1:V1:150:GLN:HB3	8:V3:54:LEU:HD12	1.92	0.51
5:S3:177:ASP:OD2	11:A9:40:ARG:NH2	2.39	0.51
11:A9:94:LEU:HG	11:A9:132:ILE:HG12	1.92	0.51
23:D4:269:MET:SD	23:D4:399:ASN:ND2	2.84	0.51
27:A8:148:GLU:OE1	30:S5:50:ARG:NH1	2.44	0.51
37:B7:36:ARG:NH1	40:B8:132:GLN:OE1	2.44	0.51
6:S7:89:ALA:HB2	6:S7:116:MET:HB3	1.93	0.51
7:S8:32:ARG:NH2	35:AM:27:ARG:O	2.44	0.51
17:AA:70:LEU:HD13	17:AA:76:ILE:HG12	1.93	0.51
24:D2:244:VAL:HG11	24:D2:300:THR:HG21	1.93	0.51
29:AJ:71:VAL:O	29:AJ:76:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:B3:40:LEU:HD21	38:B9:45:ALA:HB2	1.92	0.51
3:S1:185:THR:HG22	3:S1:187:ILE:H	1.76	0.51
26:B5:73:ARG:NH2	28:BJ:61:TYR:O	2.44	0.51
38:B9:100:GLU:O	38:B9:121:ARG:NH2	2.44	0.51
22:D5:61:MET:HE1	36:B6:96:ILE:HD12	1.93	0.50
1:V1:96:ASN:ND2	1:V1:187:GLY:O	2.44	0.50
23:D4:203:PHE:HB3	23:D4:207:MET:HE2	1.93	0.50
1:V1:257:ASN:HB2	1:V1:332:ALA:HA	1.92	0.50
2:V2:55:GLN:NE2	2:V2:89:MET:O	2.40	0.50
3:S1:240:VAL:HG12	3:S1:250:ILE:HG22	1.92	0.50
15:A7:3:ALA:HB1	15:A7:7:ILE:HD11	1.93	0.50
22:D5:119:LYS:NZ	52:D5:901:CDL:OB7	2.42	0.50
23:D4:153:THR:O	23:D4:157:SER:HB3	2.11	0.50
24:D2:197:ASN:ND2	24:D2:269:GLU:OE1	2.39	0.50
3:S1:225:THR:HB	3:S1:240:VAL:HG23	1.94	0.50
11:A9:300:LEU:HG	11:A9:307:ALA:HB2	1.93	0.50
12:A2:57:CYS:SG	12:A2:58:SER:N	2.76	0.50
4:S2:306:GLN:HE22	4:S2:309:ARG:HH11	1.59	0.50
6:S7:40:ALA:HA	19:D1:50:ALA:HB1	1.94	0.50
7:S8:79:ALA:HB2	7:S8:106:THR:HG22	1.93	0.50
23:D4:272:THR:HA	23:D4:275:ILE:HG22	1.93	0.50
4:S2:48:THR:HG22	4:S2:67:GLU:HG2	1.94	0.50
22:D5:10:VAL:HA	22:D5:13:ILE:HG22	1.92	0.50
24:D2:327:PRO:HB3	33:C2:44:ILE:HG23	1.93	0.50
28:BJ:68:ARG:NH1	43:B1:43:LEU:O	2.44	0.50
28:BJ:166:ARG:HH12	41:BK:122:GLU:HG2	1.76	0.50
34:B4:42:LEU:HD13	40:B8:74:GLY:HA3	1.94	0.50
2:V2:105:THR:OG1	2:V2:106:THR:N	2.45	0.50
3:S1:357:ASP:OD2	12:A2:40:TYR:OH	2.30	0.50
36:B6:67:SER:O	36:B6:71:PHE:HB2	2.12	0.50
37:B7:99:LYS:HG2	39:B2:57:SER:HB3	1.93	0.50
23:D4:73:LEU:HA	23:D4:76:MET:HE3	1.94	0.49
1:V1:185:ILE:HD11	2:V2:86:PHE:HZ	1.77	0.49
4:S2:36:VAL:HG22	24:D2:49:ASN:HB3	1.93	0.49
19:D1:140:ILE:HD12	20:D6:66:VAL:HG11	1.93	0.49
22:D5:127:THR:HG21	22:D5:146:GLY:HA3	1.95	0.49
23:D4:385:THR:HG21	23:D4:396:MET:HE3	1.93	0.49
24:D2:230:LEU:HB3	24:D2:300:THR:HG22	1.94	0.49
3:S1:324:ASP:HB2	3:S1:327:ALA:H	1.78	0.49
3:S1:450:MET:HA	3:S1:489:VAL:O	2.12	0.49
7:S8:80:CYS:N	45:S8:202:SF4:S1	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S6:12:THR:OG1	9:S6:14:THR:O	2.30	0.49
9:S6:84:CYS:HB3	9:S6:87:CYS:HB2	1.94	0.49
18:D3:98:LEU:HD22	19:D1:298:LEU:HD21	1.94	0.49
26:B5:104:ARG:NH2	27:A8:166:LEU:O	2.44	0.49
34:B4:32:GLN:HB3	38:B9:7:ALA:HB1	1.94	0.49
1:V1:246:GLY:HA3	1:V1:272:MET:HB3	1.94	0.49
1:V1:258:ILE:HG23	1:V1:335:ILE:HG22	1.93	0.49
1:V1:378:ARG:NH2	1:V1:383:ASP:O	2.38	0.49
23:D4:225:ILE:HG13	23:D4:229:MET:HE2	1.94	0.49
28:BJ:159:LYS:NZ	33:C2:112:VAL:O	2.45	0.49
38:B9:138:GLN:O	38:B9:142:GLU:CB	2.61	0.49
1:V1:42:TRP:HE3	1:V1:161:LEU:HD23	1.78	0.49
24:D2:297:THR:HG22	24:D2:302:LEU:HD13	1.93	0.49
17:AB:6:LEU:HB2	17:AB:86:VAL:HG11	1.95	0.49
1:V1:278:GLU:O	1:V1:282:LYS:HB2	2.13	0.49
3:S1:190:MET:HB3	3:S1:192:MET:HG2	1.95	0.49
7:S8:113:MET:HB2	7:S8:147:LEU:HB3	1.95	0.49
22:D5:375:ILE:HD12	39:B2:32:MET:HG3	1.94	0.49
24:D2:292:PHE:HA	24:D2:295:ARG:HG2	1.94	0.49
29:AJ:15:THR:OG1	29:AJ:253:ASP:OD1	2.30	0.49
1:V1:366:ARG:NH1	3:S1:155:GLN:OE1	2.46	0.49
3:S1:233:ALA:HB1	3:S1:576:THR:HB	1.94	0.49
11:A9:48:PRO:HB2	11:A9:73:TRP:CD1	2.48	0.49
24:D2:30:TRP:NE1	24:D2:67:SER:OG	2.46	0.49
37:B7:34:LYS:HG3	40:B8:156:TYR:HA	1.94	0.49
19:D1:149:ILE:HG21	19:D1:185:TRP:HB2	1.96	0.48
23:D4:46:GLY:HA2	41:BK:84:ARG:HD3	1.94	0.48
38:B9:108:PRO:HA	38:B9:111:LYS:HB2	1.95	0.48
38:B9:128:ARG:HA	38:B9:166:TRP:HZ2	1.77	0.48
39:B2:36:ILE:O	39:B2:40:PHE:HB2	2.13	0.48
1:V1:9:LYS:NZ	1:V1:248:GLU:OE2	2.46	0.48
1:V1:112:ARG:HH22	2:V2:192:SER:HB3	1.77	0.48
13:A5:8:THR:OG1	13:A5:75:GLN:OE1	2.28	0.48
17:AA:36:PHE:HA	17:AA:40:LEU:HD13	1.94	0.48
18:D3:73:LEU:HD21	20:D6:55:MET:HE1	1.94	0.48
22:D5:10:VAL:HG11	36:B6:78:VAL:HG22	1.95	0.48
32:B3:23:ILE:HD12	32:B3:49:ALA:HB2	1.93	0.48
4:S2:208:MET:HE1	35:AM:11:PRO:HD3	1.94	0.48
15:A7:51:ASN:HB2	15:A7:56:ARG:HH12	1.77	0.48
22:D5:203:MET:SD	28:BJ:113:GLN:NE2	2.86	0.48
22:D5:231:PRO:HB3	22:D5:530:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D4:363:SER:O	23:D4:367:LEU:HB2	2.13	0.48
40:B8:47:TYR:OH	40:B8:77:MET:O	2.28	0.48
5:S3:34:PRO:HD2	13:A5:99:TRP:HA	1.94	0.48
23:D4:51:ASN:HB2	26:B5:90:THR:HG22	1.94	0.48
23:D4:409:TYR:O	23:D4:413:THR:OG1	2.27	0.48
25:AK:89:TYR:CD2	25:AK:125:LYS:HB2	2.48	0.48
11:A9:30:LEU:HG	11:A9:207:ILE:HD11	1.96	0.48
31:A3:11:VAL:HG23	31:A3:14:LYS:HD3	1.95	0.48
3:S1:546:GLN:NE2	3:S1:596:ASP:OD1	2.46	0.48
6:S7:87:ILE:HG12	6:S7:114:VAL:HB	1.96	0.48
11:A9:81:ILE:HG21	11:A9:117:ILE:HG22	1.96	0.48
19:D1:156:MET:HB3	35:AM:49:MET:HE2	1.95	0.48
20:D6:114:GLU:HG2	20:D6:118:LYS:HA	1.96	0.48
23:D4:300:ALA:O	23:D4:308:SER:OG	2.28	0.48
50:AB:101:ZMP:H6A	38:B9:47:PHE:HE1	1.78	0.48
28:BJ:15:ARG:HB2	36:B6:100:LYS:HD3	1.95	0.48
3:S1:126:ASP:OD2	15:A7:56:ARG:NH2	2.46	0.48
10:S4:33:ARG:HH22	10:S4:77:ASP:HA	1.78	0.48
23:D4:270:ILE:HG13	23:D4:395:LEU:HD22	1.95	0.48
23:D4:459:TYR:O	28:BJ:96:LYS:NZ	2.47	0.48
5:S3:63:PHE:HD2	5:S3:64:LEU:HD12	1.79	0.48
7:S8:136:ASN:HB3	16:AL:87:HIS:CE1	2.49	0.48
21:4L:58:MET:HB3	21:4L:62:ILE:HD12	1.94	0.48
23:D4:129:THR:HG21	23:D4:231:LEU:HD13	1.96	0.48
24:D2:235:ASN:ND2	24:D2:307:SER:OG	2.45	0.48
2:V2:24:THR:HG22	2:V2:26:GLU:H	1.78	0.48
6:S7:179:ARG:HA	11:A9:50:ARG:HH12	1.78	0.48
7:S8:146:GLU:HG3	16:AL:124:TYR:HB3	1.95	0.48
22:D5:483:PRO:HD2	22:D5:486:LEU:HD22	1.96	0.48
24:D2:106:LEU:HD23	24:D2:138:PRO:HB2	1.96	0.48
4:S2:405:MET:SD	4:S2:421:GLN:NE2	2.87	0.48
6:S7:116:MET:HA	6:S7:146:VAL:HG23	1.96	0.48
11:A9:91:VAL:HG13	11:A9:129:PHE:HD1	1.78	0.48
22:D5:8:THR:HG21	22:D5:82:MET:HG2	1.96	0.48
23:D4:44:GLN:HE22	23:D4:60:SER:H	1.61	0.48
3:S1:335:LEU:HA	3:S1:338:VAL:HG12	1.96	0.47
4:S2:293:CYS:SG	4:S2:296:ARG:NH1	2.85	0.47
25:AK:80:ARG:HH12	25:AK:87:LEU:HB3	1.79	0.47
29:AJ:306:ALA:HA	29:AJ:309:ASN:HB2	1.96	0.47
4:S2:298:LEU:HD12	7:S8:6:ASN:HD21	1.79	0.47
22:D5:294:THR:H	22:D5:425:ARG:NH1	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D4:158:LEU:HD21	24:D2:283:ALA:HB1	1.96	0.47
25:AK:17:CYS:SG	25:AK:18:HIS:N	2.87	0.47
38:B9:85:PRO:HA	38:B9:90:TYR:HD1	1.77	0.47
38:B9:138:GLN:O	38:B9:142:GLU:HB2	2.14	0.47
4:S2:184:VAL:O	7:S8:60:ARG:NH2	2.40	0.47
26:B5:73:ARG:HH12	28:BJ:60:TYR:HB3	1.80	0.47
17:AB:87:TYR:HD2	36:B6:22:LEU:HD23	1.79	0.47
29:AJ:133:VAL:HG13	29:AJ:205:VAL:HG12	1.96	0.47
6:S7:124:GLY:HA2	7:S8:115:LYS:HA	1.96	0.47
20:D6:127:ILE:HG22	35:AM:119:MET:HB2	1.95	0.47
23:D4:250:LEU:HB3	23:D4:253:ILE:HD11	1.96	0.47
27:A8:142:HIS:ND1	35:AM:113:THR:O	2.45	0.47
35:AM:119:MET:HG2	35:AM:122:GLU:HG3	1.96	0.47
38:B9:91:GLU:HB3	38:B9:94:GLU:HB2	1.97	0.47
3:S1:155:GLN:NE2	3:S1:181:MET:O	2.47	0.47
4:S2:292:ASP:O	4:S2:296:ARG:N	2.45	0.47
11:A9:157:ARG:HH21	11:A9:165:ILE:HD13	1.79	0.47
18:D3:67:LEU:HD22	21:4L:65:VAL:HG23	1.96	0.47
17:AB:52:MET:HE3	38:B9:23:LEU:HD12	1.94	0.47
37:B7:113:ARG:NH2	37:B7:116:GLN:OE1	2.47	0.47
2:V2:150:ASN:OD1	2:V2:190:ARG:NH2	2.47	0.47
3:S1:359:ARG:NH2	3:S1:637:GLU:O	2.48	0.47
34:B4:77:PRO:HA	34:B4:78:ASN:HA	1.60	0.47
3:S1:380:VAL:HG23	3:S1:453:LEU:HA	1.96	0.47
4:S2:84:HIS:CD2	5:S3:152:LEU:HB3	2.50	0.47
6:S7:168:LYS:NZ	16:AL:76:ASP:OD2	2.38	0.47
7:S8:119:CYS:HB2	7:S8:121:PHE:H	1.79	0.47
13:A5:67:LEU:O	13:A5:71:LEU:N	2.43	0.47
22:D5:245:ALA:O	22:D5:249:SER:OG	2.27	0.47
23:D4:130:LEU:HD21	24:D2:294:MET:HE1	1.96	0.47
23:D4:403:THR:HA	23:D4:406:TYR:CE1	2.50	0.47
36:B6:102:ARG:HG2	37:B7:49:GLN:HB2	1.96	0.47
3:S1:283:MET:HA	3:S1:293:HIS:HA	1.96	0.47
22:D5:376:GLY:O	22:D5:379:ALA:N	2.47	0.47
24:D2:306:PRO:HB3	29:AJ:285:GLY:HA2	1.97	0.47
4:S2:383:SER:OG	4:S2:384:SER:N	2.48	0.47
6:S7:69:MET:HE1	6:S7:76:PHE:HB3	1.96	0.47
16:AL:42:ASP:OD2	16:AL:86:TRP:NE1	2.40	0.47
16:AL:117:LEU:HD13	16:AL:123:GLN:HA	1.96	0.47
23:D4:248:LEU:HG	28:BJ:148:HIS:HB3	1.97	0.47
19:D1:28:LEU:HG	19:D1:271:LEU:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:7:LEU:HA	22:D5:10:VAL:HG22	1.96	0.47
23:D4:277:LEU:HD12	23:D4:402:ILE:HG23	1.97	0.47
3:S1:39:ARG:HD2	3:S1:42:TYR:HB3	1.96	0.46
3:S1:242:THR:HG21	3:S1:586:ALA:HB1	1.96	0.46
19:D1:237:PHE:O	19:D1:241:LEU:HB2	2.15	0.46
24:D2:112:HIS:HB2	24:D2:184:ILE:HD13	1.97	0.46
24:D2:115:VAL:HG12	24:D2:180:ALA:HB1	1.97	0.46
34:B4:124:PHE:HB2	34:B4:126:ILE:HD11	1.97	0.46
3:S1:670:ASP:O	3:S1:674:THR:OG1	2.32	0.46
4:S2:339:LYS:HA	9:S6:69:PRO:HB3	1.97	0.46
6:S7:85:VAL:HG12	6:S7:112:TYR:HB2	1.97	0.46
17:AA:51:ILE:HG21	17:AA:67:ALA:HB1	1.96	0.46
22:D5:124:PHE:HZ	22:D5:252:MET:HB2	1.80	0.46
17:AB:49:GLU:OE2	38:B9:19:TYR:OH	2.32	0.46
3:S1:386:PHE:O	3:S1:665:GLN:NE2	2.44	0.46
13:A5:49:GLN:HE22	15:A7:91:LYS:HA	1.80	0.46
29:AJ:171:TYR:HD2	29:AJ:222:GLN:HG3	1.80	0.46
40:B8:64:TRP:NE1	40:B8:66:HIS:O	2.46	0.46
19:D1:111:LEU:HD13	19:D1:114:TYR:HD2	1.79	0.46
24:D2:189:TRP:HZ2	24:D2:286:ALA:HB2	1.81	0.46
24:D2:313:MET:HA	24:D2:316:GLN:HE22	1.80	0.46
28:BJ:64:HIS:NE2	41:BK:92:GLU:OE1	2.42	0.46
28:BJ:146:GLY:O	34:B4:128:TYR:OH	2.33	0.46
40:B8:30:ARG:HH11	40:B8:31:VAL:H	1.63	0.46
3:S1:522:LEU:HD21	3:S1:543:ILE:HG22	1.97	0.46
5:S3:69:ASN:ND2	15:A7:93:ALA:O	2.46	0.46
20:D6:160:SER:HB2	24:D2:35:MET:HE2	1.97	0.46
1:V1:126:GLY:HA2	1:V1:131:ALA:HB3	1.98	0.46
4:S2:204:PRO:HD3	7:S8:60:ARG:HH22	1.81	0.46
13:A5:77:GLU:HG3	13:A5:80:ILE:HD12	1.96	0.46
14:A6:28:LYS:HA	14:A6:31:VAL:HG12	1.98	0.46
14:A6:115:LYS:HA	14:A6:120:LYS:HE3	1.97	0.46
22:D5:357:ARG:NH1	38:B9:28:SER:O	2.49	0.46
23:D4:1:MET:HG2	23:D4:111:THR:HG21	1.96	0.46
3:S1:296:TRP:HE1	3:S1:592:LEU:HB3	1.81	0.46
3:S1:425:SER:HB3	3:S1:428:ILE:HG13	1.97	0.46
4:S2:161:ILE:HD11	4:S2:238:ARG:HE	1.81	0.46
9:S6:31:ARG:HH22	11:A9:69:ILE:HD11	1.80	0.46
11:A9:234:ASN:HB3	11:A9:236:TYR:HD1	1.80	0.46
22:D5:123:LEU:HA	22:D5:126:ILE:HD12	1.97	0.46
27:A8:70:PHE:HA	27:A8:73:ILE:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:AJ:210:PHE:HD2	29:AJ:211:LEU:HD22	1.79	0.46
43:B1:54:VAL:HG21	43:B1:57:LYS:HE2	1.97	0.46
2:V2:98:TYR:H	2:V2:136:LEU:HA	1.80	0.46
3:S1:367:THR:HG22	3:S1:369:ALA:H	1.81	0.46
3:S1:424:ASP:OD1	3:S1:424:ASP:N	2.48	0.46
13:A5:10:LEU:HD22	13:A5:13:LEU:HD13	1.98	0.46
13:A5:26:LEU:HA	13:A5:29:LYS:HZ1	1.81	0.46
29:AJ:305:ARG:HB2	33:C2:50:ARG:HB2	1.97	0.46
32:B3:25:GLY:O	32:B3:29:GLU:CB	2.63	0.46
3:S1:382:THR:HG23	3:S1:384:PRO:HD3	1.98	0.46
3:S1:584:LYS:HG3	10:S4:36:ARG:HH11	1.81	0.46
22:D5:418:PHE:HA	22:D5:421:ILE:HG12	1.98	0.46
4:S2:151:ILE:HD13	4:S2:304:MET:HE1	1.97	0.46
12:A2:20:ILE:HD12	12:A2:54:ILE:HG12	1.98	0.46
19:D1:288:LEU:O	19:D1:292:ASN:HB2	2.16	0.46
22:D5:20:ALA:O	22:D5:24:PHE:HB2	2.15	0.46
23:D4:424:ASN:OD1	34:B4:55:ARG:NH1	2.49	0.46
34:B4:100:TRP:HA	34:B4:103:VAL:HG22	1.98	0.46
3:S1:448:LYS:HB3	3:S1:487:TRP:CE2	2.51	0.45
22:D5:384:PRO:HA	22:D5:385:PHE:HA	1.63	0.45
24:D2:69:LEU:HD11	24:D2:97:LEU:HD22	1.97	0.45
3:S1:283:MET:HE2	3:S1:291:LEU:HG	1.96	0.45
26:B5:84:GLU:OE1	43:B1:55:THR:OG1	2.34	0.45
4:S2:231:ASN:OD1	4:S2:236:ARG:NH2	2.49	0.45
22:D5:82:MET:SD	22:D5:82:MET:N	2.90	0.45
29:AJ:19:THR:OG1	29:AJ:20:GLU:N	2.46	0.45
4:S2:19:MET:HB3	24:D2:171:ASN:HA	1.98	0.45
24:D2:151:LEU:HD22	25:AK:136:ALA:HB2	1.98	0.45
28:BJ:3:SER:OG	28:BJ:4:TRP:N	2.44	0.45
22:D5:9:LEU:HB3	36:B6:81:ILE:HD13	1.98	0.45
22:D5:558:LEU:HA	22:D5:561:ILE:HG22	1.98	0.45
24:D2:186:HIS:HB3	24:D2:190:MET:HE2	1.98	0.45
1:V1:71:ALA:HB1	1:V1:73:PHE:HD2	1.81	0.45
3:S1:286:ASN:O	3:S1:289:GLY:N	2.39	0.45
3:S1:290:LEU:HD13	3:S1:291:LEU:H	1.81	0.45
11:A9:49:TYR:HE1	11:A9:70:PHE:HB3	1.82	0.45
16:AL:68:MET:HE2	16:AL:81:MET:HE2	1.99	0.45
23:D4:2:LEU:HD23	43:B1:26:LEU:HD22	1.98	0.45
24:D2:193:VAL:HG21	24:D2:266:ILE:HG12	1.99	0.45
27:A8:45:CYS:HA	27:A8:134:ARG:HH12	1.82	0.45
38:B9:83:GLU:OE1	38:B9:176:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V1:68:ARG:O	46:V1:501:FMN:O3P	2.34	0.45
2:V2:61:LEU:HD11	2:V2:92:ARG:HG2	1.97	0.45
3:S1:465:ALA:HB2	3:S1:654:GLN:HB2	1.99	0.45
3:S1:644:GLN:HA	3:S1:647:GLU:HG2	1.97	0.45
24:D2:106:LEU:HB2	24:D2:187:MET:HE2	1.99	0.45
29:AJ:63:THR:HG23	29:AJ:302:ARG:HH12	1.81	0.45
38:B9:10:THR:HG23	38:B9:13:GLN:H	1.81	0.45
3:S1:107:ILE:HG22	7:S8:104:ARG:HD3	1.98	0.45
3:S1:283:MET:HG2	3:S1:293:HIS:HB3	1.98	0.45
5:S3:167:PRO:HA	10:S4:82:LEU:HD21	1.99	0.45
22:D5:81:LYS:HD3	22:D5:135:ASN:HD22	1.82	0.45
22:D5:217:ILE:HD13	22:D5:217:ILE:HA	1.82	0.45
28:BJ:66:GLU:OE2	41:BK:95:ARG:NH1	2.50	0.45
29:AJ:49:LYS:HD2	29:AJ:114:HIS:CE1	2.52	0.45
29:AJ:97:GLN:HG2	29:AJ:135:LEU:HD22	1.98	0.45
34:B4:51:ASN:HD22	38:B9:165:LEU:HD23	1.82	0.45
36:B6:92:LYS:O	36:B6:95:THR:OG1	2.33	0.45
41:BK:100:ARG:HH11	41:BK:108:MET:H	1.64	0.45
3:S1:360:SER:HB2	3:S1:639:ALA:HB3	1.99	0.45
4:S2:242:ILE:H	4:S2:242:ILE:HG13	1.70	0.45
22:D5:541:ASN:HD22	51:D5:902:3PE:H361	1.82	0.45
23:D4:370:PRO:HA	23:D4:375:LEU:HD13	1.98	0.45
29:AJ:72:ARG:HA	29:AJ:76:ASN:HD21	1.82	0.45
35:AM:19:ASP:OD1	35:AM:19:ASP:N	2.46	0.45
38:B9:61:GLN:HG3	38:B9:64:ARG:HH22	1.82	0.45
40:B8:34:TYR:OH	40:B8:46:ASP:O	2.35	0.45
2:V2:96:GLY:H	2:V2:138:THR:HG21	1.82	0.45
5:S3:77:ASP:O	5:S3:93:VAL:O	2.35	0.45
9:S6:11:VAL:HG12	9:S6:17:VAL:HB	1.99	0.45
22:D5:532:ILE:HD12	40:B8:105:LEU:HD13	1.98	0.45
23:D4:203:PHE:HE2	23:D4:246:ILE:HG12	1.81	0.45
24:D2:222:ASN:OD1	24:D2:222:ASN:N	2.48	0.45
24:D2:335:MET:O	33:C2:33:TYR:OH	2.32	0.45
35:AM:29:LEU:O	35:AM:33:SER:OG	2.34	0.45
3:S1:594:ARG:NH2	14:A6:122:TYR:O	2.46	0.44
4:S2:422:ASP:OD1	4:S2:422:ASP:N	2.50	0.44
11:A9:316:GLU:HG2	14:A6:52:ASP:HB3	2.00	0.44
29:AJ:56:ILE:HD11	29:AJ:79:LEU:HB2	1.98	0.44
2:V2:150:ASN:ND2	2:V2:162:GLU:OE1	2.33	0.44
3:S1:592:LEU:O	3:S1:594:ARG:NH1	2.51	0.44
21:4L:44:ALA:HB2	24:D2:75:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D4:5:ILE:HG23	23:D4:104:LEU:HD11	1.98	0.44
26:B5:138:LYS:HB3	30:S5:29:PRO:HD3	1.98	0.44
19:D1:195:ARG:HD2	19:D1:231:ILE:HD11	1.99	0.44
20:D6:126:VAL:HA	20:D6:127:ILE:HA	1.80	0.44
22:D5:299:LYS:H	22:D5:354:GLN:NE2	2.14	0.44
22:D5:544:MET:O	22:D5:548:SER:OG	2.35	0.44
26:B5:87:TYR:O	26:B5:90:THR:OG1	2.30	0.44
2:V2:76:PRO:HA	2:V2:77:PRO:HD3	1.80	0.44
4:S2:284:ASP:OD1	4:S2:284:ASP:N	2.49	0.44
6:S7:66:ARG:HH21	7:S8:56:PRO:HD2	1.82	0.44
10:S4:56:LYS:HA	10:S4:84:LEU:O	2.17	0.44
12:A2:64:LEU:HB3	12:A2:76:VAL:HG23	1.99	0.44
19:D1:97:ASN:H	35:AM:143:THR:HG22	1.82	0.44
20:D6:13:PHE:HD1	20:D6:39:VAL:HG23	1.82	0.44
22:D5:128:MET:HE2	22:D5:132:VAL:HG11	2.00	0.44
22:D5:556:ILE:HD11	34:B4:79:PHE:HB2	1.98	0.44
24:D2:157:LEU:O	24:D2:161:SER:OG	2.30	0.44
32:B3:38:ARG:HH12	38:B9:42:LEU:HD11	1.82	0.44
40:B8:13:TYR:HB2	40:B8:20:ARG:HE	1.81	0.44
3:S1:303:VAL:HA	3:S1:542:PHE:HZ	1.82	0.44
3:S1:404:LEU:H	10:S4:127:ARG:HH22	1.64	0.44
11:A9:55:ASP:O	11:A9:58:HIS:ND1	2.51	0.44
23:D4:196:TRP:CE2	23:D4:200:MET:HG3	2.53	0.44
24:D2:2:ASN:HB2	24:D2:5:ILE:HD12	1.99	0.44
26:B5:44:ASN:HB3	26:B5:69:HIS:CE1	2.53	0.44
3:S1:122:MET:HE2	5:S3:205:ALA:HB2	2.00	0.44
3:S1:280:THR:HG21	16:AL:136:GLU:HG2	2.00	0.44
4:S2:354:GLU:HA	5:S3:199:LEU:HD22	2.00	0.44
23:D4:298:ILE:HD13	23:D4:298:ILE:HA	1.70	0.44
34:B4:120:LEU:HD22	34:B4:121:ASP:H	1.82	0.44
19:D1:35:LYS:HB3	19:D1:38:ASN:HD21	1.83	0.44
22:D5:278:LEU:HB3	22:D5:318:GLY:HA3	1.99	0.44
23:D4:190:TRP:HB3	25:AK:126:MET:HE2	2.00	0.44
29:AJ:212:PRO:O	29:AJ:215:SER:OG	2.28	0.44
5:S3:173:GLU:OE2	6:S7:138:ARG:NH1	2.50	0.44
7:S8:22:ALA:O	7:S8:26:LEU:HB2	2.18	0.44
10:S4:28:GLU:O	10:S4:32:THR:OG1	2.31	0.44
24:D2:83:GLN:HE22	24:D2:90:PHE:HE2	1.64	0.44
3:S1:47:SER:O	3:S1:161:ARG:NH1	2.51	0.44
3:S1:99:ALA:O	3:S1:134:LYS:NZ	2.40	0.44
4:S2:246:THR:HG23	13:A5:12:GLY:HA3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S7:108:PRO:HG2	19:D1:58:LYS:HE2	2.00	0.44
17:AA:14:ARG:HA	17:AA:17:TYR:CE1	2.52	0.44
21:4L:33:LEU:HA	21:4L:36:MET:HE2	2.00	0.44
23:D4:253:ILE:H	23:D4:253:ILE:HG13	1.71	0.44
28:BJ:169:THR:O	28:BJ:173:ALA:HB3	2.18	0.44
3:S1:276:ARG:HE	3:S1:682:GLN:HE21	1.66	0.43
20:D6:44:VAL:HA	21:4L:46:LEU:HD21	2.00	0.43
20:D6:47:PHE:HD2	21:4L:46:LEU:HD22	1.82	0.43
22:D5:178:GLY:HA2	22:D5:219:ALA:HA	1.99	0.43
24:D2:130:LEU:O	24:D2:134:GLN:HB2	2.18	0.43
40:B8:50:LEU:HB2	40:B8:78:HIS:CD2	2.53	0.43
1:V1:197:GLU:OE2	1:V1:204:ARG:NH2	2.51	0.43
3:S1:334:LEU:HD21	3:S1:603:LEU:HD12	2.00	0.43
3:S1:341:ASP:OD1	3:S1:341:ASP:N	2.49	0.43
11:A9:215:ILE:HA	11:A9:218:ILE:HG22	2.00	0.43
19:D1:228:TYR:HD1	19:D1:231:ILE:HD12	1.82	0.43
20:D6:18:VAL:HG11	20:D6:96:GLY:HA3	2.00	0.43
22:D5:226:GLN:O	22:D5:230:HIS:N	2.51	0.43
24:D2:22:ILE:HD11	30:S5:5:VAL:H	1.83	0.43
29:AJ:169:VAL:HG23	29:AJ:218:CYS:HB3	2.00	0.43
11:A9:128:LYS:HD3	11:A9:218:ILE:HA	2.00	0.43
19:D1:173:TRP:NE1	19:D1:244:GLY:O	2.52	0.43
20:D6:119:PHE:HA	21:4L:1:MET:HG2	2.00	0.43
23:D4:329:LEU:HD23	23:D4:359:TRP:CD2	2.53	0.43
25:AK:68:ILE:HD13	25:AK:99:THR:HG21	1.99	0.43
28:BJ:100:GLU:HA	28:BJ:103:ASN:HD22	1.83	0.43
29:AJ:31:ILE:HG22	29:AJ:126:ARG:HH12	1.84	0.43
29:AJ:188:ASN:O	29:AJ:192:MET:N	2.51	0.43
37:B7:52:LEU:HD22	40:B8:138:LEU:HD21	2.00	0.43
38:B9:33:ARG:HA	38:B9:36:TYR:HB3	2.00	0.43
1:V1:392:LEU:HA	1:V1:395:ILE:HG22	2.00	0.43
3:S1:589:PRO:HD2	14:A6:125:HIS:HE1	1.83	0.43
4:S2:7:ASP:HB2	4:S2:10:TRP:HD1	1.83	0.43
51:D5:902:3PE:H332	23:D4:405:LEU:HD11	2.00	0.43
29:AJ:145:ARG:HE	29:AJ:147:GLN:HB3	1.83	0.43
34:B4:101:TYR:CZ	34:B4:105:LYS:HE2	2.53	0.43
3:S1:11:VAL:HG12	3:S1:77:TRP:HB2	2.00	0.43
13:A5:86:GLU:HA	13:A5:89:LEU:HG	2.01	0.43
17:AA:20:LYS:HA	17:AA:25:ILE:HG21	2.00	0.43
20:D6:71:THR:HA	20:D6:74:MET:HG3	2.01	0.43
20:D6:127:ILE:HG21	30:S5:68:ARG:HD2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D6:152:TRP:HB2	30:S5:13:LEU:HD12	2.00	0.43
23:D4:51:ASN:HD22	26:B5:90:THR:HG22	1.84	0.43
28:BJ:29:ILE:H	28:BJ:29:ILE:HG13	1.70	0.43
29:AJ:30:ASN:HD22	29:AJ:179:VAL:HG21	1.84	0.43
3:S1:485:GLY:HA2	3:S1:486:ASP:HA	1.67	0.43
6:S7:52:LEU:HB2	6:S7:90:GLY:HA3	2.01	0.43
6:S7:59:MET:HA	6:S7:62:MET:HG3	2.00	0.43
11:A9:318:LEU:HD13	11:A9:318:LEU:HA	1.89	0.43
24:D2:232:HIS:CE1	29:AJ:276:PRO:HG3	2.54	0.43
24:D2:322:ARG:HA	33:C2:49:ARG:HH22	1.83	0.43
36:B6:11:LEU:O	36:B6:15:ARG:HG2	2.18	0.43
1:V1:202:LYS:HB3	1:V1:361:GLN:NE2	2.33	0.43
21:4L:36:MET:HE3	24:D2:68:MET:HG3	2.01	0.43
22:D5:99:SER:OG	22:D5:453:SER:OG	2.34	0.43
22:D5:145:GLU:HB2	23:D4:370:PRO:HG3	2.00	0.43
22:D5:198:LEU:HD12	22:D5:201:ILE:HD12	2.01	0.43
29:AJ:202:ILE:O	29:AJ:206:TYR:HB2	2.18	0.43
34:B4:2:PHE:HE2	34:B4:5:TYR:HB2	1.82	0.43
44:A1:1:MET:HE3	44:A1:3:PHE:HB2	2.01	0.43
3:S1:328:LEU:HD22	3:S1:507:TYR:HE2	1.84	0.43
3:S1:359:ARG:HH11	3:S1:629:ASN:HD22	1.67	0.43
12:A2:36:ILE:HD12	12:A2:36:ILE:HA	1.88	0.43
17:AA:11:ILE:HA	17:AA:14:ARG:HG2	1.99	0.43
22:D5:363:PHE:HA	22:D5:370:THR:HG21	2.00	0.43
1:V1:66:ARG:NE	1:V1:72:GLY:O	2.44	0.43
2:V2:154:VAL:HG23	2:V2:164:LEU:HD21	2.01	0.43
5:S3:154:ASP:OD1	14:A6:101:HIS:NE2	2.46	0.43
16:AL:51:ASP:OD2	16:AL:54:GLN:NE2	2.48	0.43
22:D5:361:GLY:H	22:D5:435:PRO:HA	1.84	0.43
23:D4:205:VAL:HG22	23:D4:212:LEU:HD13	2.00	0.43
28:BJ:77:HIS:HB3	33:C2:106:LYS:HB3	2.00	0.43
31:A3:77:LEU:HB2	31:A3:80:LEU:HD23	2.00	0.43
8:V3:41:LEU:HG	8:V3:44:HIS:HB2	2.01	0.43
22:D5:10:VAL:HG12	36:B6:81:ILE:HD12	2.01	0.43
24:D2:234:TRP:CZ2	24:D2:304:MET:HG2	2.54	0.43
28:BJ:40:VAL:HG13	36:B6:79:TRP:HD1	1.84	0.43
29:AJ:111:ALA:HB1	29:AJ:122:VAL:HG21	2.01	0.43
36:B6:117:PRO:HA	36:B6:118:PRO:HD3	1.86	0.43
37:B7:34:LYS:HE3	37:B7:36:ARG:HB2	2.00	0.43
3:S1:544:VAL:HG22	3:S1:559:VAL:HB	2.01	0.42
22:D5:63:ILE:HG12	22:D5:82:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D4:203:PHE:O	23:D4:207:MET:HG2	2.18	0.42
23:D4:430:PHE:HE1	41:BK:37:LEU:HD22	1.83	0.42
24:D2:55:ALA:HB1	24:D2:118:VAL:HA	2.01	0.42
27:A8:44:LEU:HG	27:A8:134:ARG:HH21	1.85	0.42
28:BJ:157:LYS:HB2	33:C2:116:PHE:CE1	2.54	0.42
29:AJ:304:TYR:HA	33:C2:50:ARG:HB3	2.01	0.42
35:AM:57:ARG:HA	35:AM:57:ARG:HD2	1.82	0.42
1:V1:365:CYS:O	1:V1:369:VAL:HB	2.19	0.42
6:S7:114:VAL:HG22	6:S7:144:ILE:HB	2.00	0.42
6:S7:139:ILE:HG22	6:S7:140:VAL:HG13	2.01	0.42
23:D4:47:ASP:OD1	23:D4:47:ASP:N	2.48	0.42
23:D4:310:MET:HG2	23:D4:456:GLY:H	1.83	0.42
28:BJ:74:THR:O	33:C2:108:THR:OG1	2.33	0.42
30:S5:50:ARG:HA	30:S5:53:LYS:HB2	2.01	0.42
32:B3:53:MET:HA	32:B3:57:ALA:HB2	2.01	0.42
34:B4:82:ASN:HB2	34:B4:85:THR:HG23	2.02	0.42
43:B1:16:VAL:HG23	43:B1:17:PRO:HD3	2.00	0.42
44:A1:66:LEU:HD12	44:A1:69:ILE:HD11	2.01	0.42
1:V1:31:TRP:HE1	1:V1:115:PRO:HD2	1.84	0.42
3:S1:103:LEU:HD21	4:S2:342:MET:HA	2.02	0.42
4:S2:219:SER:OG	35:AM:19:ASP:O	2.30	0.42
5:S3:192:GLN:HE21	5:S3:195:ARG:HH12	1.67	0.42
6:S7:39:TRP:HD1	6:S7:42:ARG:HE	1.67	0.42
7:S8:34:LEU:HD12	19:D1:272:TRP:CE2	2.54	0.42
7:S8:59:PRO:HB3	7:S8:168:ASN:HD22	1.84	0.42
22:D5:2:ASN:O	22:D5:6:SER:OG	2.32	0.42
34:B4:13:LEU:HD22	34:B4:14:PRO:HD2	2.02	0.42
40:B8:12:PRO:HA	40:B8:46:ASP:HB3	2.01	0.42
1:V1:26:TYR:HA	1:V1:113:HIS:CE1	2.54	0.42
3:S1:122:MET:O	15:A7:60:ARG:NH2	2.52	0.42
7:S8:96:ALA:HA	7:S8:106:THR:HA	2.00	0.42
19:D1:18:ALA:O	19:D1:21:THR:OG1	2.30	0.42
22:D5:3:LEU:HD22	22:D5:53:MET:HE1	2.02	0.42
6:S7:39:TRP:HA	6:S7:42:ARG:HG2	2.01	0.42
6:S7:91:THR:HA	6:S7:119:CYS:HB3	2.02	0.42
7:S8:91:ALA:HB1	7:S8:112:ASP:H	1.84	0.42
21:4L:55:LEU:HD13	30:S5:24:GLN:HG3	2.02	0.42
22:D5:36:VAL:HA	22:D5:39:THR:HG22	2.01	0.42
22:D5:605:HIS:CD2	22:D5:606:GLU:HG3	2.55	0.42
23:D4:75:LEU:HD21	23:D4:440:HIS:CD2	2.54	0.42
2:V2:13:PRO:HA	2:V2:15:ASN:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V2:161:TYR:HE1	2:V2:182:PRO:HB2	1.85	0.42
4:S2:81:GLY:HA2	5:S3:152:LEU:HD23	2.02	0.42
4:S2:146:ARG:HG3	4:S2:370:PRO:HG3	2.02	0.42
6:S7:86:MET:HB2	6:S7:107:MET:HE1	2.01	0.42
30:S5:18:THR:HG22	30:S5:19:ILE:HG13	2.02	0.42
32:B3:28:LEU:HA	32:B3:31:VAL:HG12	2.00	0.42
35:AM:81:ARG:HG2	35:AM:85:MET:HE1	2.01	0.42
37:B7:11:ASP:OD1	37:B7:11:ASP:N	2.53	0.42
37:B7:95:VAL:HG22	39:B2:54:PRO:HG3	2.02	0.42
4:S2:150:HIS:CE1	4:S2:370:PRO:HB3	2.55	0.42
4:S2:292:ASP:OD1	4:S2:293:CYS:N	2.52	0.42
11:A9:19:ILE:O	11:A9:43:SER:OG	2.30	0.42
20:D6:112:GLU:OE1	30:S5:73:LYS:NZ	2.53	0.42
22:D5:85:PHE:O	22:D5:89:PHE:HB2	2.19	0.42
22:D5:594:THR:HG21	24:D2:110:PRO:HB3	2.00	0.42
24:D2:190:MET:HG2	24:D2:204:ASN:HB3	2.01	0.42
28:BJ:127:GLU:HA	28:BJ:130:GLN:HG2	2.01	0.42
32:B3:42:ASP:OD1	32:B3:42:ASP:N	2.53	0.42
38:B9:3:LEU:HD11	38:B9:6:ALA:HB3	2.00	0.42
4:S2:112:MET:HE3	4:S2:112:MET:HB3	1.95	0.42
11:A9:120:VAL:O	11:A9:124:ALA:CB	2.67	0.42
22:D5:86:SER:HB2	22:D5:262:ARG:HH22	1.85	0.42
22:D5:353:GLU:HA	38:B9:82:PRO:HG3	2.01	0.42
22:D5:556:ILE:HG13	34:B4:76:TYR:HD1	1.84	0.42
25:AK:80:ARG:HB3	25:AK:82:LYS:HZ2	1.83	0.42
28:BJ:138:TYR:HD1	41:BK:108:MET:HE1	1.84	0.42
28:BJ:158:GLN:OE1	28:BJ:161:ARG:NH2	2.53	0.42
33:C2:8:ARG:H	33:C2:9:ALA:HB3	1.84	0.42
34:B4:78:ASN:HD21	40:B8:12:PRO:HD3	1.84	0.42
2:V2:104:THR:HA	2:V2:108:CYS:HB2	2.01	0.42
3:S1:283:MET:HE1	16:AL:139:PRO:HB3	2.02	0.42
3:S1:364:LEU:HA	3:S1:491:ASN:HB2	2.01	0.42
3:S1:595:GLU:OE1	3:S1:598:LYS:NZ	2.53	0.42
4:S2:339:LYS:HG3	9:S6:65:ALA:HA	2.01	0.42
10:S4:36:ARG:NH2	10:S4:58:GLU:OE1	2.44	0.42
11:A9:167:LYS:O	11:A9:229:ALA:HA	2.20	0.42
22:D5:61:MET:HE3	22:D5:61:MET:HB2	1.94	0.42
22:D5:542:LEU:HD11	40:B8:88:ARG:HD2	2.01	0.42
28:BJ:17:PRO:HB3	36:B6:103:ILE:HG22	2.01	0.42
38:B9:57:VAL:HA	38:B9:60:THR:HG22	2.02	0.42
4:S2:276:ASP:N	4:S2:276:ASP:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:194:ASN:HB2	34:B4:126:ILE:HD13	2.02	0.42
23:D4:425:ASN:HD22	34:B4:57:GLY:HA2	1.85	0.42
27:A8:77:CYS:HA	27:A8:78:ALA:HA	1.66	0.42
29:AJ:23:LYS:H	29:AJ:121:GLY:HA2	1.84	0.42
36:B6:17:LEU:HD11	38:B9:162:LEU:HD22	2.01	0.42
1:V1:338:ASP:OD1	1:V1:339:ARG:N	2.53	0.41
1:V1:300:GLY:HA2	1:V1:330:GLY:H	1.84	0.41
3:S1:8:LEU:HD22	3:S1:19:MET:HB3	2.02	0.41
4:S2:175:GLU:OE2	4:S2:188:ARG:NH2	2.53	0.41
16:AL:78:ASP:HB2	16:AL:81:MET:HE3	2.01	0.41
19:D1:151:LEU:HD12	19:D1:154:LEU:HD11	2.02	0.41
22:D5:200:GLN:OE1	28:BJ:106:GLN:NE2	2.52	0.41
26:B5:32:THR:HA	26:B5:35:PRO:HD2	2.02	0.41
17:AB:58:PHE:HD2	17:AB:80:ILE:HG12	1.85	0.41
40:B8:81:LEU:HA	40:B8:84:TYR:HB2	2.02	0.41
1:V1:143:TYR:OH	8:V3:47:SER:O	2.27	0.41
3:S1:337:ARG:NH1	12:A2:71:GLY:O	2.53	0.41
3:S1:431:ASP:HB3	3:S1:436:SER:HB3	2.01	0.41
12:A2:13:LEU:HB3	12:A2:14:GLY:H	1.60	0.41
16:AL:117:LEU:H	16:AL:117:LEU:HG	1.75	0.41
22:D5:190:LEU:HD22	22:D5:196:TRP:HZ3	1.84	0.41
27:A8:82:THR:HA	27:A8:85:TRP:CD1	2.55	0.41
27:A8:144:ARG:HH22	30:S5:57:ILE:HD13	1.85	0.41
34:B4:1:SER:HB2	38:B9:69:GLU:HG2	2.02	0.41
3:S1:377:VAL:HG22	3:S1:450:MET:HB3	2.02	0.41
6:S7:175:ILE:O	6:S7:179:ARG:HB2	2.20	0.41
7:S8:92:ILE:HD13	7:S8:111:ILE:HG12	2.02	0.41
22:D5:141:PHE:HE2	23:D4:375:LEU:HD11	1.84	0.41
22:D5:247:LEU:HD12	22:D5:252:MET:HG2	2.01	0.41
22:D5:539:TYR:OH	34:B4:9:ARG:NH2	2.54	0.41
23:D4:41:LEU:O	23:D4:43:ASN:N	2.53	0.41
23:D4:159:PRO:HB2	23:D4:198:ALA:HB1	2.03	0.41
23:D4:336:ARG:HB3	23:D4:426:ILE:HG22	2.01	0.41
23:D4:436:LEU:O	23:D4:440:HIS:ND1	2.45	0.41
3:S1:41:CYS:HB3	3:S1:52:CYS:HB3	2.01	0.41
4:S2:323:ILE:HG22	4:S2:324:LYS:HG3	2.02	0.41
7:S8:75:GLU:OE2	7:S8:151:LYS:NZ	2.43	0.41
11:A9:144:LYS:HA	11:A9:147:ARG:HG2	2.02	0.41
22:D5:487:LYS:HE2	39:B2:49:GLY:HA2	2.02	0.41
26:B5:89:ARG:HG3	43:B1:34:LEU:HD23	2.03	0.41
17:AB:60:PHE:HZ	17:AB:80:ILE:HG13	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:BJ:77:HIS:HA	33:C2:108:THR:HA	2.03	0.41
37:B7:3:HIS:CE1	40:B8:127:PRO:HD3	2.56	0.41
41:BK:82:ASP:OD1	41:BK:82:ASP:N	2.54	0.41
1:V1:300:GLY:HA2	1:V1:330:GLY:N	2.36	0.41
50:AA:101:ZMP:H3A	50:AA:101:ZMP:H22A	1.76	0.41
22:D5:462:LEU:HD11	39:B2:32:MET:HG2	2.02	0.41
23:D4:13:PRO:HA	23:D4:16:TRP:HD1	1.85	0.41
23:D4:225:ILE:HD13	23:D4:331:ASN:HB2	2.03	0.41
28:BJ:105:ILE:HG22	28:BJ:131:PHE:HD1	1.85	0.41
32:B3:72:TRP:HB3	39:B2:30:ALA:HB1	2.03	0.41
36:B6:7:GLU:O	36:B6:11:LEU:HB2	2.21	0.41
1:V1:368:GLY:HA3	1:V1:399:ILE:HD11	2.03	0.41
2:V2:108:CYS:HB3	2:V2:152:PRO:HB3	2.01	0.41
3:S1:9:ILE:HG23	3:S1:75:LYS:HA	2.02	0.41
6:S7:100:LEU:HD23	6:S7:139:ILE:HG21	2.02	0.41
10:S4:28:GLU:O	10:S4:32:THR:CB	2.69	0.41
18:D3:81:THR:N	31:A3:45:ASN:HD21	2.17	0.41
19:D1:81:LEU:O	19:D1:85:MET:HB2	2.20	0.41
21:4L:66:PHE:HB3	24:D2:34:GLU:OE1	2.21	0.41
17:AB:46:ASP:OD2	38:B9:44:ARG:NH2	2.54	0.41
29:AJ:75:GLY:HA3	29:AJ:76:ASN:HA	1.68	0.41
29:AJ:288:GLN:OE1	41:BK:27:GLN:NE2	2.54	0.41
33:C2:44:ILE:O	33:C2:48:ILE:HG12	2.21	0.41
35:AM:94:ALA:HA	35:AM:103:TRP:HH2	1.86	0.41
36:B6:82:HIS:CE1	36:B6:86:LYS:HD2	2.56	0.41
1:V1:103:GLY:HA3	1:V1:333:ALA:HB2	2.01	0.41
1:V1:190:THR:HG21	1:V1:204:ARG:HB2	2.02	0.41
6:S7:137:ASP:OD1	6:S7:145:TYR:OH	2.37	0.41
9:S6:5:SER:OG	9:S6:8:GLY:N	2.53	0.41
18:D3:106:TRP:CD1	19:D1:291:LYS:HE2	2.55	0.41
19:D1:119:SER:O	19:D1:123:SER:OG	2.22	0.41
22:D5:123:LEU:HD21	52:D5:901:CDL:H741	2.01	0.41
23:D4:78:MET:HB2	23:D4:78:MET:HE3	1.79	0.41
23:D4:112:ALA:O	23:D4:245:ARG:NH1	2.52	0.41
24:D2:145:ILE:HD12	24:D2:149:ILE:HD11	2.02	0.41
35:AM:139:PHE:HB2	44:A1:45:TRP:CD1	2.56	0.41
37:B7:21:MET:HG3	40:B8:130:PRO:HD3	2.03	0.41
1:V1:391:SER:OG	3:S1:129:ARG:NH1	2.53	0.41
46:V1:501:FMN:H1'2	46:V1:501:FMN:H9	1.82	0.41
3:S1:198:ASN:ND2	3:S1:263:ILE:H	2.18	0.41
3:S1:338:VAL:HG13	3:S1:339:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V3:60:LYS:H	8:V3:60:LYS:HD2	1.86	0.41
11:A9:171:ILE:H	11:A9:171:ILE:HG13	1.70	0.41
19:D1:75:PRO:HG2	19:D1:219:PRO:HD2	2.03	0.41
22:D5:152:PHE:CD1	22:D5:168:ALA:HB1	2.56	0.41
22:D5:483:PRO:HG3	39:B2:53:TYR:CZ	2.56	0.41
23:D4:409:TYR:HA	23:D4:412:ILE:HG13	2.03	0.41
27:A8:124:LEU:HD12	35:AM:65:GLU:HB3	2.03	0.41
30:S5:6:GLN:HE22	30:S5:14:ASP:HB2	1.86	0.41
41:BK:92:GLU:OE1	41:BK:95:ARG:NH2	2.54	0.41
1:V1:299:PRO:HG2	1:V1:304:THR:HG21	2.03	0.41
2:V2:132:THR:HG21	2:V2:137:PHE:HB2	2.02	0.41
5:S3:43:SER:HA	15:A7:65:PRO:HB3	2.03	0.41
5:S3:82:ASP:OD1	5:S3:82:ASP:N	2.53	0.41
14:A6:63:ARG:HH22	17:AA:24:LYS:HE3	1.86	0.41
19:D1:310:LEU:HD11	31:A3:32:PRO:HG3	2.03	0.41
24:D2:208:TYR:HE1	24:D2:251:MET:HE1	1.86	0.41
24:D2:222:ASN:HD22	24:D2:233:THR:HG21	1.86	0.41
26:B5:34:ILE:HG23	26:B5:38:ILE:HD12	2.03	0.41
26:B5:69:HIS:CD2	26:B5:71:ILE:H	2.37	0.41
1:V1:103:GLY:N	2:V2:148:CYS:SG	2.82	0.40
1:V1:157:TYR:HD2	8:V3:58:LEU:HD12	1.86	0.40
3:S1:332:LYS:HA	3:S1:343:LEU:HD21	2.03	0.40
3:S1:415:LEU:HD23	3:S1:415:LEU:HA	1.94	0.40
3:S1:545:TYR:HB3	3:S1:560:ILE:HD13	2.02	0.40
6:S7:171:LYS:HA	6:S7:174:ARG:HE	1.86	0.40
19:D1:22:LEU:HB3	19:D1:48:PRO:HG2	2.03	0.40
22:D5:341:MET:SD	22:D5:453:SER:OG	2.68	0.40
23:D4:276:CYS:HB3	23:D4:288:TYR:HB2	2.03	0.40
24:D2:144:GLN:HG2	30:S5:2:PHE:HB2	2.04	0.40
29:AJ:29:GLY:HA3	29:AJ:34:GLY:HA3	2.02	0.40
3:S1:565:ALA:H	3:S1:568:GLU:HB2	1.86	0.40
18:D3:102:LEU:HD13	19:D1:294:LEU:HD23	2.03	0.40
21:4L:19:LEU:HD22	21:4L:36:MET:HE1	2.02	0.40
21:4L:55:LEU:HD13	30:S5:24:GLN:HA	2.03	0.40
24:D2:241:THR:OG1	24:D2:242:ILE:N	2.54	0.40
25:AK:46:THR:HA	25:AK:47:SER:HA	1.83	0.40
26:B5:105:LEU:HD23	26:B5:108:LEU:HD21	2.03	0.40
34:B4:1:SER:O	38:B9:72:HIS:ND1	2.54	0.40
35:AM:139:PHE:HB2	44:A1:45:TRP:CG	2.57	0.40
3:S1:364:LEU:HG	3:S1:491:ASN:HB2	2.04	0.40
6:S7:154:GLU:HG3	7:S8:50:TYR:HE1	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A5:113:TRP:O	13:A5:115:ILE:N	2.54	0.40
20:D6:163:ILE:HG13	24:D2:12:THR:HG21	2.03	0.40
22:D5:455:LYS:HG3	39:B2:28:PHE:CZ	2.56	0.40
22:D5:464:ALA:HA	22:D5:467:ILE:HB	2.03	0.40
4:S2:347:HIS:O	4:S2:351:LEU:HB2	2.19	0.40
23:D4:5:ILE:HG22	23:D4:9:MET:SD	2.62	0.40
32:B3:73:GLY:HA3	39:B2:33:TRP:HD1	1.85	0.40
37:B7:50:LEU:HD11	37:B7:63:ILE:HD11	2.03	0.40
12:A2:90:LEU:O	12:A2:94:LEU:CB	2.69	0.40
19:D1:85:MET:SD	19:D1:108:MET:HG3	2.62	0.40
20:D6:118:LYS:HB2	30:S5:69:GLN:HE21	1.85	0.40
22:D5:106:TRP:CG	22:D5:447:ASN:HD21	2.40	0.40
22:D5:245:ALA:O	22:D5:249:SER:CB	2.70	0.40
27:A8:17:VAL:HB	27:A8:19:VAL:HG22	2.02	0.40
36:B6:94:TYR:HD1	36:B6:94:TYR:HA	1.80	0.40
37:B7:107:LEU:HD21	39:B2:66:ILE:HA	2.03	0.40
42:C1:20:THR:HA	42:C1:23:THR:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V1	428/445 (96%)	382 (89%)	46 (11%)	0	100	100
2	V2	210/217 (97%)	165 (79%)	45 (21%)	0	100	100
3	S1	686/704 (97%)	605 (88%)	81 (12%)	0	100	100
4	S2	420/430 (98%)	370 (88%)	50 (12%)	0	100	100
5	S3	206/228 (90%)	176 (85%)	30 (15%)	0	100	100
6	S7	154/179 (86%)	138 (90%)	15 (10%)	1 (1%)	21	58
7	S8	174/176 (99%)	153 (88%)	21 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	V3	39/75 (52%)	31 (80%)	8 (20%)	0	100	100
9	S6	93/96 (97%)	83 (89%)	10 (11%)	0	100	100
10	S4	124/133 (93%)	109 (88%)	15 (12%)	0	100	100
11	A9	281/338 (83%)	244 (87%)	37 (13%)	0	100	100
12	A2	80/98 (82%)	68 (85%)	12 (15%)	0	100	100
13	A5	109/115 (95%)	96 (88%)	13 (12%)	0	100	100
14	A6	112/127 (88%)	104 (93%)	8 (7%)	0	100	100
15	A7	92/112 (82%)	74 (80%)	17 (18%)	1 (1%)	11	45
16	AL	142/145 (98%)	119 (84%)	23 (16%)	0	100	100
17	AA	78/88 (89%)	65 (83%)	13 (17%)	0	100	100
17	AB	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
18	D3	86/115 (75%)	80 (93%)	6 (7%)	0	100	100
19	D1	299/318 (94%)	262 (88%)	37 (12%)	0	100	100
20	D6	167/175 (95%)	143 (86%)	24 (14%)	0	100	100
21	4L	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
22	D5	604/606 (100%)	537 (89%)	67 (11%)	0	100	100
23	D4	457/459 (100%)	421 (92%)	35 (8%)	1 (0%)	43	77
24	D2	345/347 (99%)	320 (93%)	25 (7%)	0	100	100
25	AK	138/140 (99%)	128 (93%)	10 (7%)	0	100	100
26	B5	137/143 (96%)	124 (90%)	12 (9%)	1 (1%)	18	55
27	A8	169/171 (99%)	142 (84%)	27 (16%)	0	100	100
28	BJ	169/175 (97%)	150 (89%)	19 (11%)	0	100	100
29	AJ	317/320 (99%)	283 (89%)	34 (11%)	0	100	100
30	S5	97/105 (92%)	77 (79%)	20 (21%)	0	100	100
31	A3	72/83 (87%)	59 (82%)	13 (18%)	0	100	100
32	B3	71/97 (73%)	55 (78%)	16 (22%)	0	100	100
33	C2	117/120 (98%)	104 (89%)	13 (11%)	0	100	100
34	B4	126/128 (98%)	110 (87%)	16 (13%)	0	100	100
35	AM	137/143 (96%)	120 (88%)	17 (12%)	0	100	100
36	B6	92/127 (72%)	82 (89%)	10 (11%)	0	100	100
37	B7	117/136 (86%)	98 (84%)	19 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	B9	174/178 (98%)	147 (84%)	27 (16%)	0	100	100
39	B2	63/72 (88%)	53 (84%)	10 (16%)	0	100	100
40	B8	155/158 (98%)	122 (79%)	32 (21%)	1 (1%)	21	58
41	BK	100/125 (80%)	83 (83%)	17 (17%)	0	100	100
42	C1	44/49 (90%)	39 (89%)	5 (11%)	0	100	100
43	B1	50/57 (88%)	43 (86%)	6 (12%)	1 (2%)	6	31
44	A1	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
All	All	7980/8509 (94%)	6992 (88%)	982 (12%)	6 (0%)	49	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	S7	54	CYS
23	D4	53	SER
43	B1	53	GLU
15	A7	68	VAL
40	B8	17	PRO
26	B5	13	PRO

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%)	342 (99%)	2 (1%)	78	80
2	V2	182/183 (100%)	181 (100%)	1 (0%)	81	81
3	S1	578/588 (98%)	575 (100%)	3 (0%)	81	81
4	S2	368/371 (99%)	365 (99%)	3 (1%)	73	77
5	S3	189/204 (93%)	188 (100%)	1 (0%)	81	81
6	S7	132/150 (88%)	131 (99%)	1 (1%)	73	77
7	S8	151/151 (100%)	150 (99%)	1 (1%)	76	79
8	V3	40/68 (59%)	39 (98%)	1 (2%)	42	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	S6	79/80 (99%)	79 (100%)	0	100	100
10	S4	113/119 (95%)	113 (100%)	0	100	100
11	A9	246/292 (84%)	245 (100%)	1 (0%)	84	82
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	84/94 (89%)	84 (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%)	264 (99%)	2 (1%)	73	77
20	D6	140/144 (97%)	138 (99%)	2 (1%)	59	71
21	4L	87/87 (100%)	87 (100%)	0	100	100
22	D5	539/539 (100%)	536 (99%)	3 (1%)	78	80
23	D4	412/412 (100%)	410 (100%)	2 (0%)	81	81
24	D2	315/315 (100%)	314 (100%)	1 (0%)	86	84
25	AK	101/101 (100%)	100 (99%)	1 (1%)	68	76
26	B5	122/125 (98%)	122 (100%)	0	100	100
27	A8	154/154 (100%)	154 (100%)	0	100	100
28	BJ	155/157 (99%)	155 (100%)	0	100	100
29	AJ	283/284 (100%)	283 (100%)	0	100	100
30	S5	88/94 (94%)	88 (100%)	0	100	100
31	A3	65/71 (92%)	64 (98%)	1 (2%)	57	70
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
38	B9	159/160 (99%)	157 (99%)	2 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	B2	59/62 (95%)	59 (100%)	0	100	100
40	B8	142/142 (100%)	141 (99%)	1 (1%)	76	79
41	BK	93/112 (83%)	93 (100%)	0	100	100
42	C1	42/44 (96%)	42 (100%)	0	100	100
43	B1	48/53 (91%)	48 (100%)	0	100	100
44	A1	59/59 (100%)	59 (100%)	0	100	100
All	All	7073/7395 (96%)	7040 (100%)	33 (0%)	78	81

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V1	56	ILE
1	V1	110	ILE
2	V2	51	LEU
3	S1	239	VAL
3	S1	290	LEU
3	S1	543	ILE
4	S2	242	ILE
4	S2	402	LEU
4	S2	418	ILE
5	S3	81	VAL
6	S7	54	CYS
7	S8	78	ILE
8	V3	54	LEU
11	A9	281	ARG
13	A5	94	ILE
16	AL	117	LEU
19	D1	55	LEU
19	D1	73	LEU
20	D6	12	ILE
20	D6	54	LEU
22	D5	257	ILE
22	D5	350	LEU
22	D5	602	LEU
23	D4	150	LEU
23	D4	251	ASN
24	D2	193	VAL
25	AK	94	CYS
17	AB	80	ILE
31	A3	56	LEU

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Mol	Chain	Res	Type
34	B4	120	LEU
38	B9	16	LEU
38	B9	23	LEU
40	B8	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (132) such sidechains are listed below:

Mol	Chain	Res	Type
1	V1	37	GLN
1	V1	283	HIS
1	V1	293	ASN
1	V1	361	GLN
1	V1	431	GLN
2	V2	9	HIS
2	V2	155	GLN
2	V2	159	ASN
3	S1	308	GLN
3	S1	336	ASN
3	S1	361	ASN
3	S1	365	ASN
3	S1	401	HIS
3	S1	430	GLN
3	S1	499	GLN
3	S1	548	HIS
3	S1	682	GLN
4	S2	34	ASN
4	S2	50	ASN
4	S2	84	HIS
4	S2	135	GLN
4	S2	201	GLN
4	S2	306	GLN
4	S2	316	ASN
4	S2	409	HIS
5	S3	38	GLN
5	S3	102	ASN
5	S3	192	GLN
6	S7	127	HIS
7	S8	6	ASN
7	S8	168	ASN
9	S6	16	GLN
10	S4	43	ASN
11	A9	2	HIS

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Mol	Chain	Res	Type
12	A2	24	GLN
12	A2	47	ASN
13	A5	49	GLN
13	A5	110	GLN
14	A6	94	ASN
14	A6	125	HIS
15	A7	20	GLN
16	AL	31	ASN
16	AL	46	ASN
16	AL	59	HIS
16	AL	72	ASN
16	AL	116	ASN
18	D3	10	ASN
19	D1	157	ASN
19	D1	194	ASN
20	D6	175	ASN
21	4L	25	HIS
21	4L	83	ASN
22	D5	27	HIS
22	D5	59	GLN
22	D5	72	GLN
22	D5	199	GLN
22	D5	205	ASN
22	D5	295	GLN
22	D5	405	ASN
22	D5	434	GLN
22	D5	509	HIS
22	D5	541	ASN
22	D5	580	GLN
22	D5	605	HIS
23	D4	26	ASN
23	D4	81	GLN
23	D4	138	ASN
23	D4	144	ASN
23	D4	319	HIS
23	D4	390	ASN
23	D4	399	ASN
24	D2	2	ASN
24	D2	36	ASN
24	D2	63	GLN
24	D2	144	GLN
24	D2	186	HIS

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Mol	Chain	Res	Type
24	D2	204	ASN
24	D2	235	ASN
24	D2	309	ASN
24	D2	316	GLN
26	B5	69	HIS
26	B5	95	GLN
26	B5	143	ASN
17	AB	33	ASN
17	AB	47	GLN
27	A8	30	HIS
27	A8	150	ASN
28	BJ	77	HIS
28	BJ	99	GLN
28	BJ	103	ASN
28	BJ	113	GLN
28	BJ	114	GLN
28	BJ	120	HIS
28	BJ	122	GLN
29	AJ	76	ASN
29	AJ	92	ASN
29	AJ	97	GLN
29	AJ	114	HIS
29	AJ	151	HIS
29	AJ	200	GLN
29	AJ	204	ASN
29	AJ	251	GLN
29	AJ	271	ASN
30	S5	20	GLN
30	S5	69	GLN
31	A3	45	ASN
31	A3	70	GLN
32	B3	58	ASN
33	C2	117	HIS
34	B4	51	ASN
35	AM	60	GLN
35	AM	75	GLN
35	AM	89	ASN
36	B6	25	GLN
36	B6	82	HIS
37	B7	43	GLN
37	B7	83	GLN
38	B9	13	GLN

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Mol	Chain	Res	Type
38	B9	159	GLN
38	B9	168	HIS
39	B2	58	GLN
40	B8	56	GLN
40	B8	136	ASN
40	B8	137	ASN
40	B8	155	HIS
41	BK	27	GLN
41	BK	45	HIS
42	C1	34	GLN
44	A1	27	HIS
44	A1	31	ASN
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
45	SF4	S7	300	6	0,12,12	-	-	-		
46	FMN	V1	501	-	33,33,33	0.25	0	48,50,50	0.41	0
50	ZMP	AA	101	17	28,33,36	0.69	1 (3%)	32,40,45	1.15	3 (9%)
53	PC1	AK	201	-	27,27,53	0.39	0	33,35,61	0.40	0
50	ZMP	AB	101	17	25,30,36	0.80	1 (4%)	29,37,45	0.96	1 (3%)
51	3PE	D5	903	-	39,39,50	0.34	0	42,44,55	0.32	0
45	SF4	S1	802	3	0,12,12	-	-	-		
47	FES	S1	803	3	0,4,4	-	-	-		
51	3PE	D1	501	-	25,25,50	0.40	0	28,30,55	0.40	0
51	3PE	D5	902	-	37,37,50	0.35	0	40,42,55	0.34	0
47	FES	V2	300	2	0,4,4	-	-	-		
45	SF4	S1	801	3	0,12,12	-	-	-		
45	SF4	S8	201	7	0,12,12	-	-	-		
45	SF4	V1	500	1	0,12,12	-	-	-		
52	CDL	D5	901	-	59,59,99	0.39	0	65,71,111	0.52	1 (1%)
45	SF4	S8	202	7	0,12,12	-	-	-		
49	NDP	A9	401	-	51,52,52	0.41	0	71,80,80	0.58	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	S7	300	6	-	-	0/6/5/5
46	FMN	V1	501	-	-	8/18/18/18	0/3/3/3
50	ZMP	AA	101	17	-	10/38/40/43	-
53	PC1	AK	201	-	-	10/31/31/57	-
50	ZMP	AB	101	17	-	9/35/37/43	-
51	3PE	D5	903	-	-	10/43/43/54	-
45	SF4	S1	802	3	-	-	0/6/5/5
51	3PE	D1	501	-	-	3/28/28/54	-
51	3PE	D5	902	-	-	9/41/41/54	-
47	FES	S1	803	3	-	-	0/1/1/1
47	FES	V2	300	2	-	-	0/1/1/1
45	SF4	S1	801	3	-	-	0/6/5/5
45	SF4	S8	201	7	-	-	0/6/5/5
45	SF4	V1	500	1	-	-	0/6/5/5
52	CDL	D5	901	-	-	15/70/70/110	-
45	SF4	S8	202	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	NDP	A9	401	-	-	13/34/77/77	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	AB	101	ZMP	C9-C10	2.86	1.53	1.50
50	AA	101	ZMP	C9-C10	2.47	1.53	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	A9	401	NDP	P2B-O2B-C2B	2.74	130.76	123.43
50	AA	101	ZMP	C11-C12-N1	-2.63	106.92	112.41
50	AB	101	ZMP	O1-C10-C9	-2.62	120.96	123.98
50	AA	101	ZMP	O1-C10-C9	-2.55	121.03	123.98
50	AA	101	ZMP	C15-C14-C13	-2.47	108.28	112.39
52	D5	901	CDL	CB4-OB6-CB5	2.43	123.62	117.80

There are no chirality outliers.

All (87) 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-O2P
46	V1	501	FMN	C5'-O5'-P-O3P
49	A9	401	NDP	C5B-O5B-PA-O1A
49	A9	401	NDP	C5B-O5B-PA-O2A
49	A9	401	NDP	C5B-O5B-PA-O3
49	A9	401	NDP	C1B-C2B-O2B-P2B
49	A9	401	NDP	C2B-C1B-N9A-C8A
49	A9	401	NDP	C2B-C1B-N9A-C4A
50	AA	101	ZMP	O1-C10-S1-C11
50	AA	101	ZMP	C9-C10-S1-C11
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	C1-O11-P-O13
51	D1	501	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
51	D5	902	3PE	C1-O11-P-O13
51	D5	902	3PE	C11-O13-P-O11
51	D5	902	3PE	C11-O13-P-O12
51	D5	902	3PE	C11-O13-P-O14
51	D5	902	3PE	O13-C11-C12-N
51	D5	902	3PE	O21-C2-C3-O31
51	D5	903	3PE	C1-O11-P-O14
51	D5	903	3PE	C11-O13-P-O11
51	D5	903	3PE	C11-O13-P-O14
52	D5	901	CDL	CA2-OA2-PA1-OA3
52	D5	901	CDL	CA3-OA5-PA1-OA3
52	D5	901	CDL	CB2-OB2-PB2-OB4
52	D5	901	CDL	CB2-OB2-PB2-OB5
52	D5	901	CDL	CB3-OB5-PB2-OB2
53	AK	201	PC1	C11-O13-P-O12
53	AK	201	PC1	C11-O13-P-O11
53	AK	201	PC1	O13-C11-C12-N
50	AA	101	ZMP	C14-C13-N1-C12
50	AB	101	ZMP	C14-C13-N1-C12
52	D5	901	CDL	O1-C1-CA2-OA2
46	V1	501	FMN	C2'-C3'-C4'-C5'
50	AA	101	ZMP	O2-C13-N1-C12
50	AB	101	ZMP	O2-C13-N1-C12
51	D5	903	3PE	C28-C29-C2A-C2B
50	AB	101	ZMP	C5-C6-C7-C8
51	D5	902	3PE	C22-C23-C24-C25
51	D5	903	3PE	C39-C3A-C3B-C3C
50	AA	101	ZMP	C6-C7-C8-C9
52	D5	901	CDL	CB2-C1-CA2-OA2
51	D5	902	3PE	C1-C2-C3-O31
46	V1	501	FMN	C5'-O5'-P-O1P
49	A9	401	NDP	PN-O3-PA-O1A
52	D5	901	CDL	CA7-C31-C32-C33
53	AK	201	PC1	O11-C1-C2-O21
50	AB	101	ZMP	O3-C16-C17-O4
50	AA	101	ZMP	C2-C1-C22-C23
53	AK	201	PC1	O11-C1-C2-C3
46	V1	501	FMN	N10-C1'-C2'-O2'
50	AA	101	ZMP	C12-C11-S1-C10
50	AA	101	ZMP	C11-C12-N1-C13
49	A9	401	NDP	C2D-C1D-N1N-C6N
51	D5	902	3PE	C1-O11-P-O14

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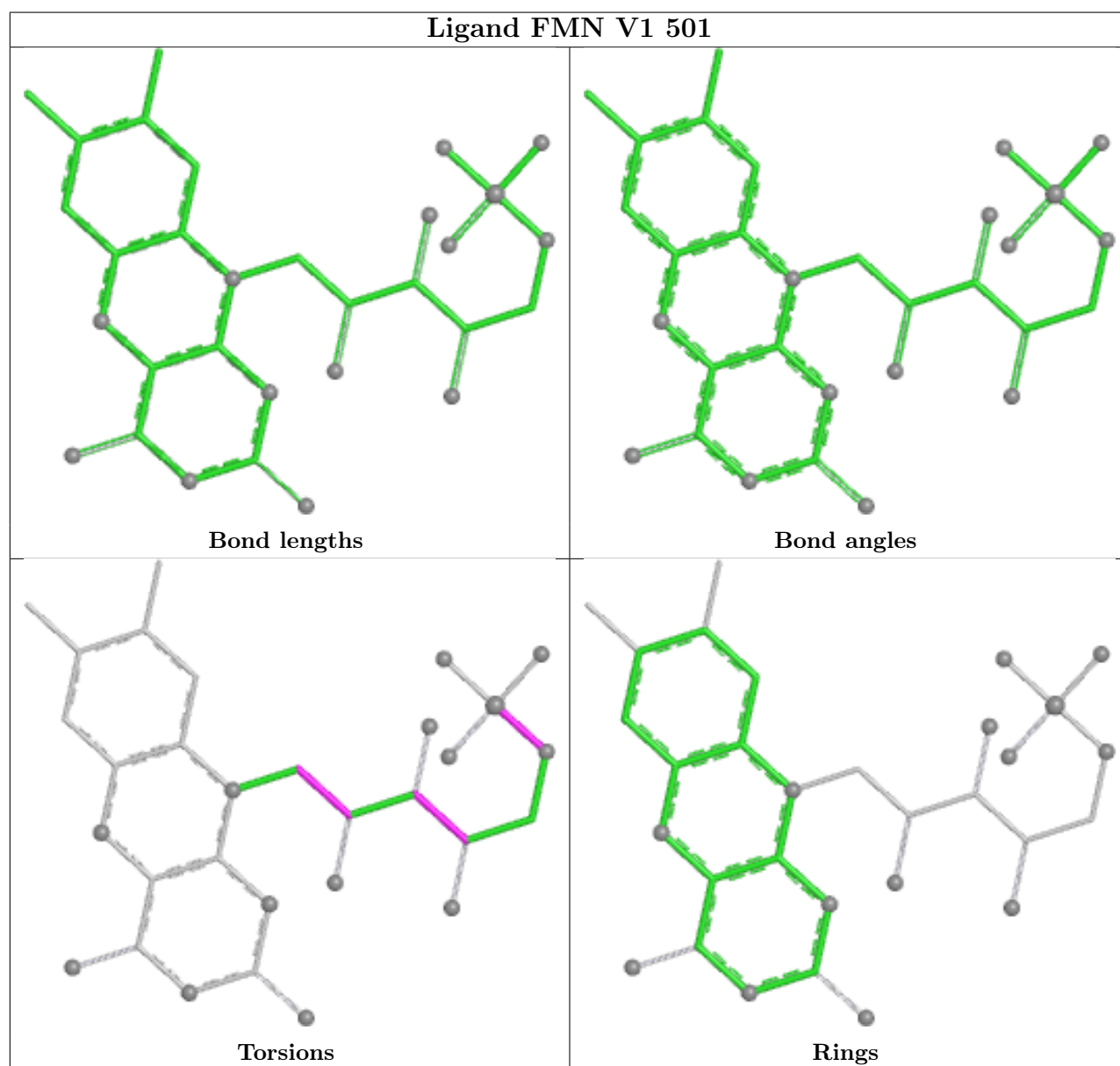
Mol	Chain	Res	Type	Atoms
51	D5	903	3PE	C1-O11-P-O13
52	D5	901	CDL	CA2-OA2-PA1-OA5
52	D5	901	CDL	CB3-OB5-PB2-OB3
52	D5	901	CDL	OB5-CB3-CB4-OB6
49	A9	401	NDP	C2D-C1D-N1N-C2N
49	A9	401	NDP	O4D-C1D-N1N-C6N
50	AB	101	ZMP	C3-C4-C5-C6
51	D5	903	3PE	C32-C33-C34-C35
49	A9	401	NDP	C4B-C5B-O5B-PA
53	AK	201	PC1	C31-C32-C33-C34
50	AA	101	ZMP	C5-C6-C7-C8
49	A9	401	NDP	O4D-C1D-N1N-C2N
53	AK	201	PC1	C12-C11-O13-P
52	D5	901	CDL	C12-C11-CA5-OA6
49	A9	401	NDP	PN-O3-PA-O2A
51	D5	903	3PE	O31-C31-C32-C33
50	AA	101	ZMP	C19-C18-C21-O5
52	D5	901	CDL	CB6-CB4-OB6-CB5
53	AK	201	PC1	O21-C21-C22-C23
51	D5	903	3PE	O32-C31-C32-C33
50	AB	101	ZMP	N2-C16-C17-O4
52	D5	901	CDL	C12-C11-CA5-OA7
51	D5	903	3PE	O21-C21-C22-C23
53	AK	201	PC1	O31-C31-C32-C33
52	D5	901	CDL	C32-C31-CA7-OA8
53	AK	201	PC1	O32-C31-C32-C33

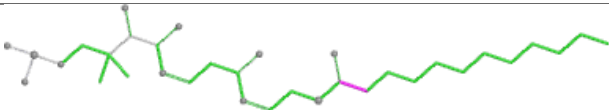
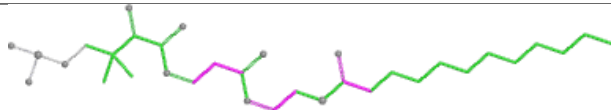
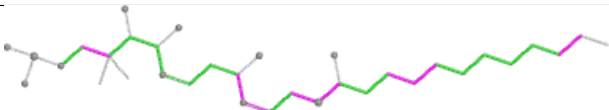
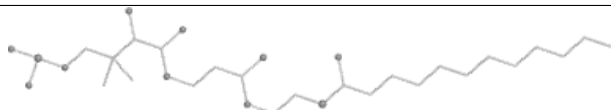
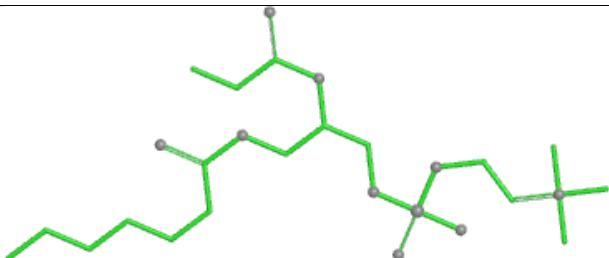
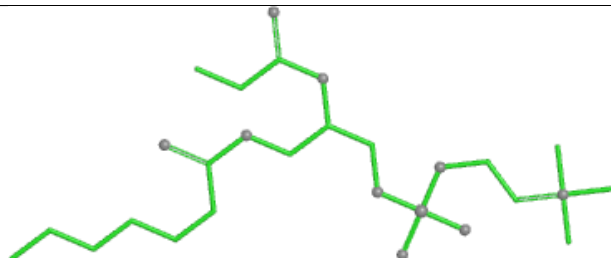
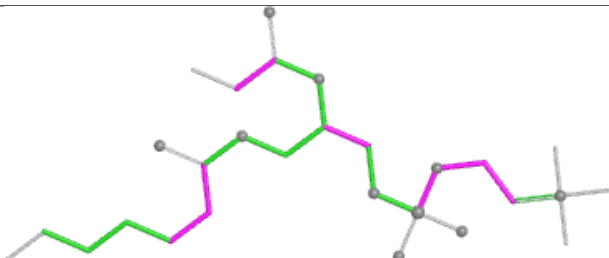
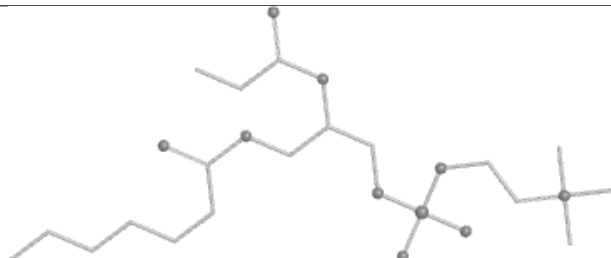
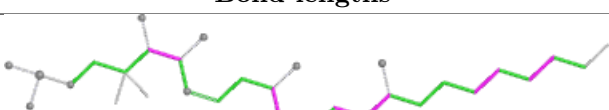
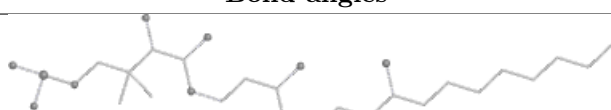
There are no ring outliers.

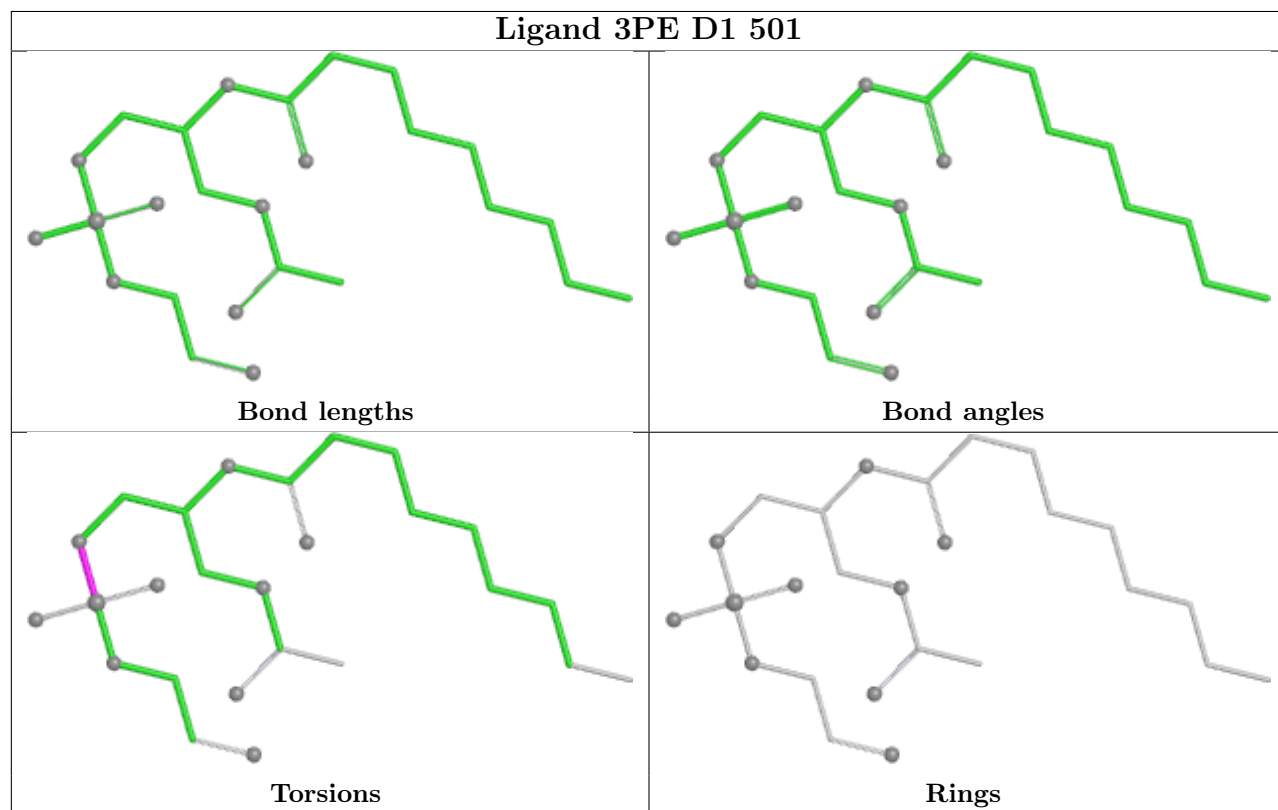
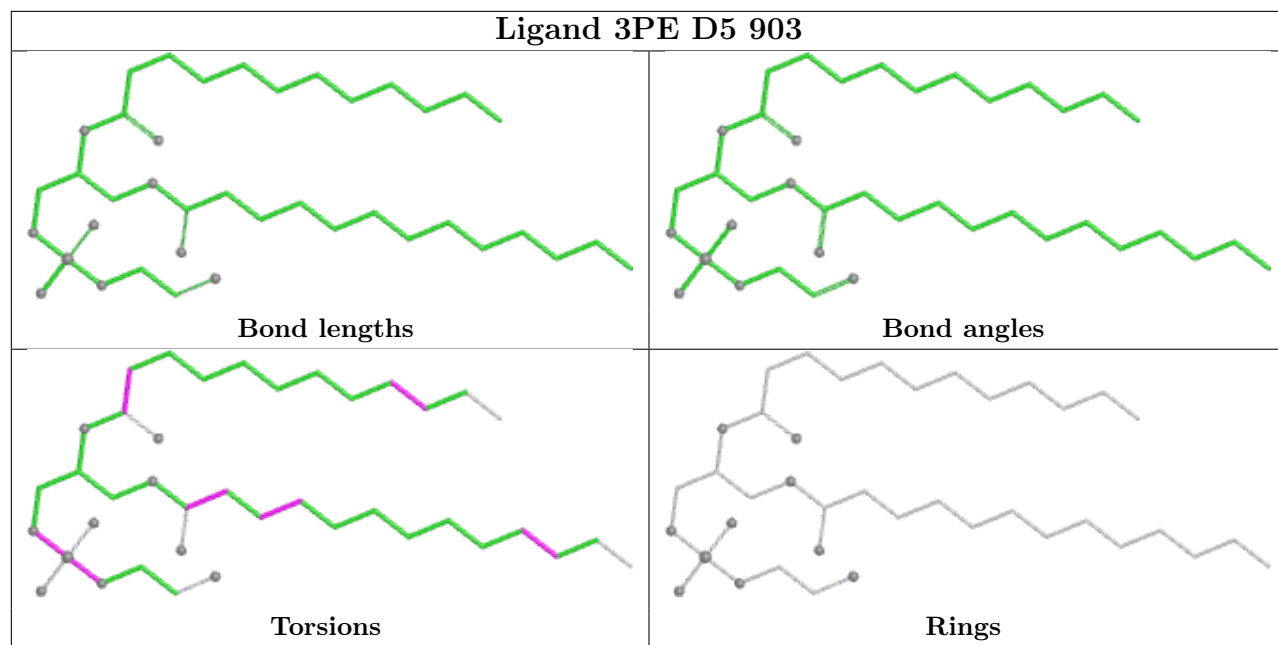
10 monomers are involved in 21 short contacts:

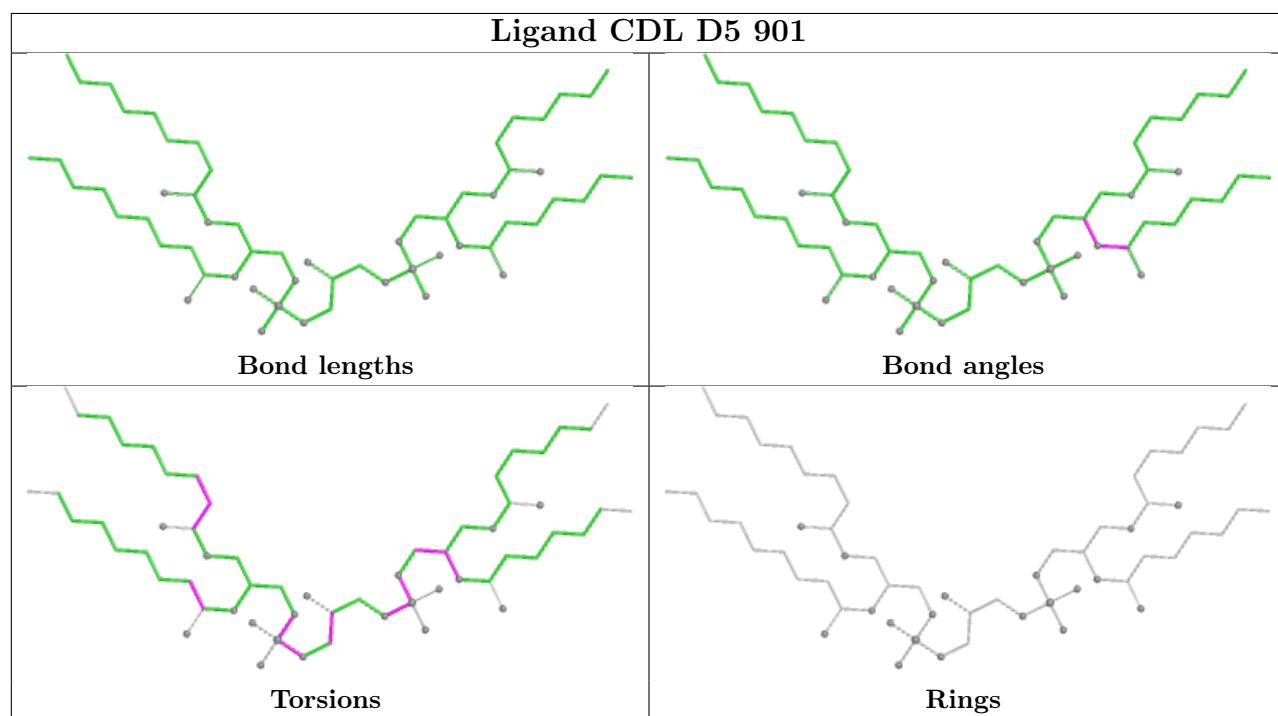
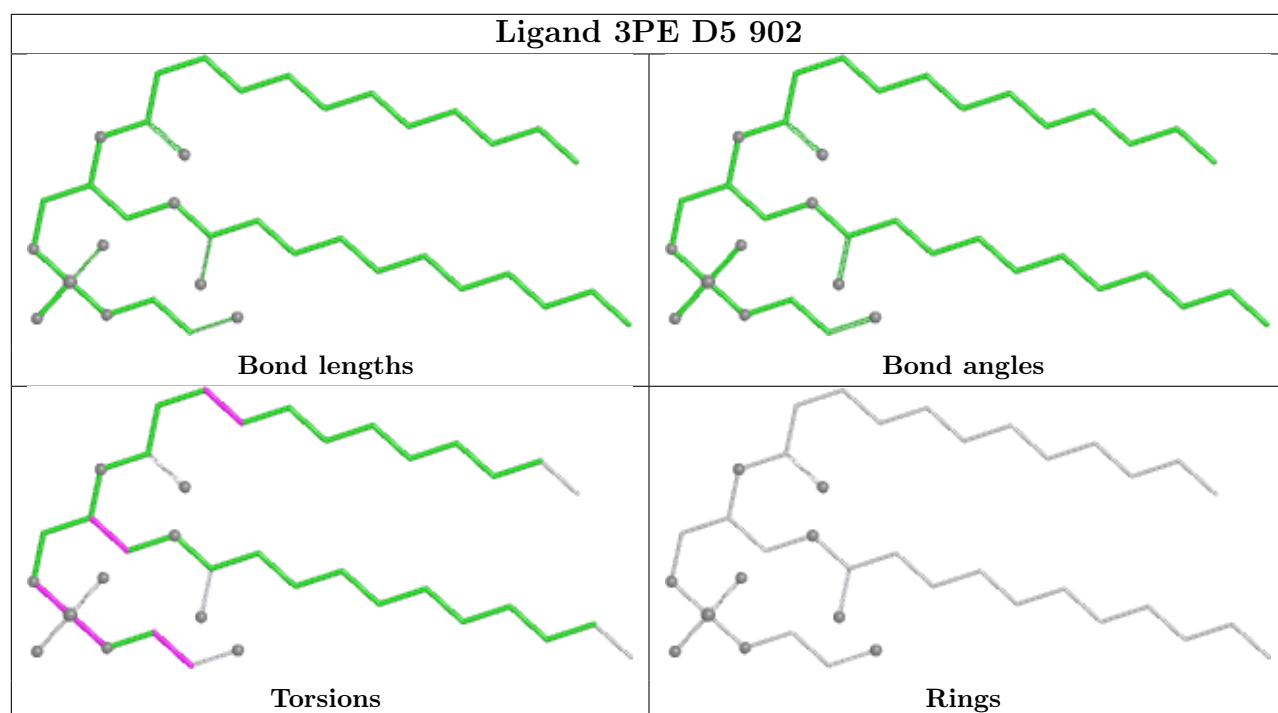
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	S7	300	SF4	1	0
46	V1	501	FMN	3	0
50	AA	101	ZMP	1	0
50	AB	101	ZMP	7	0
47	S1	803	FES	1	0
51	D5	902	3PE	2	0
45	S1	801	SF4	1	0
45	V1	500	SF4	1	0
52	D5	901	CDL	3	0
45	S8	202	SF4	1	0

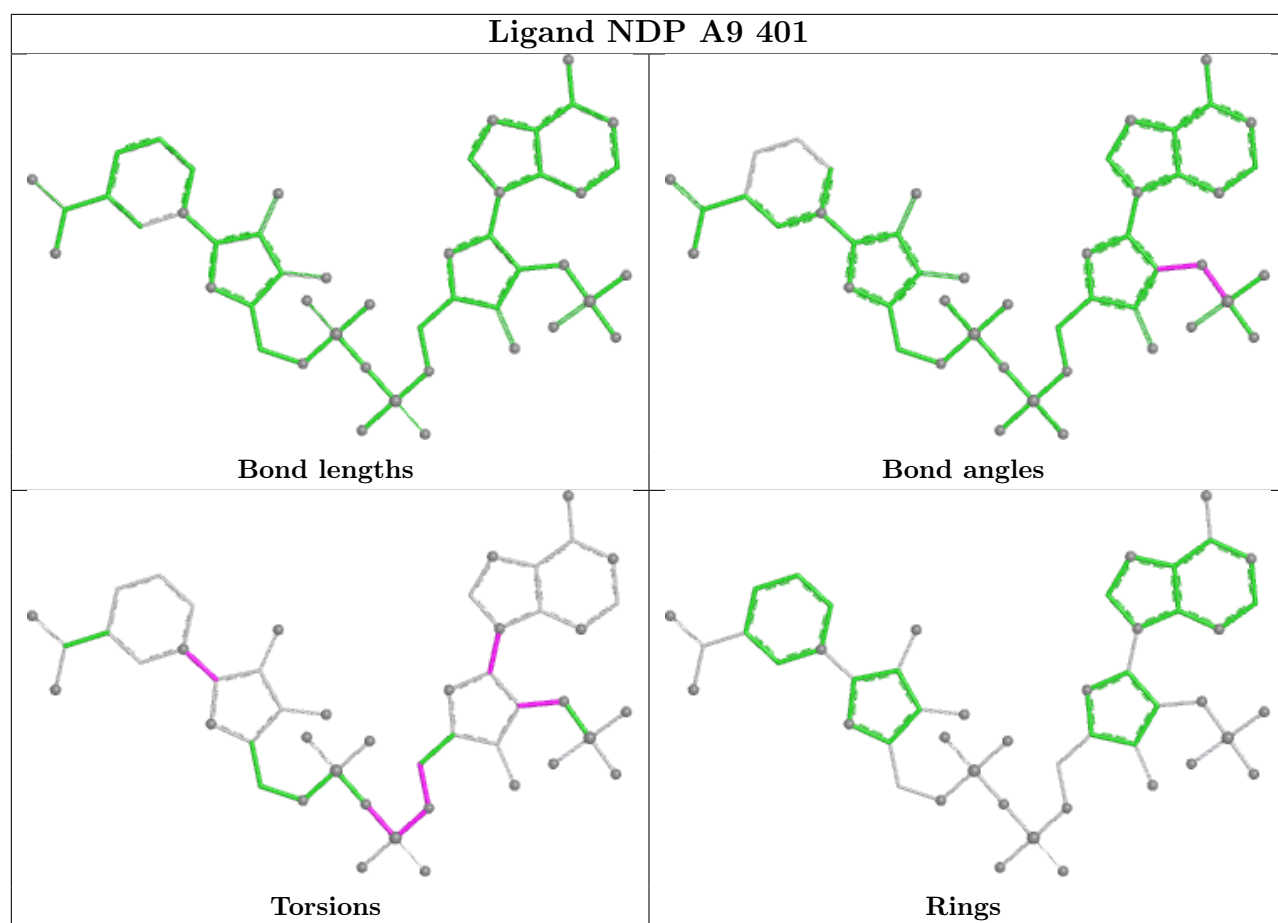
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ZMP AA 101	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PC1 AK 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand ZMP AB 101	
 Bond lengths	 Bond angles
 Torsions	 Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

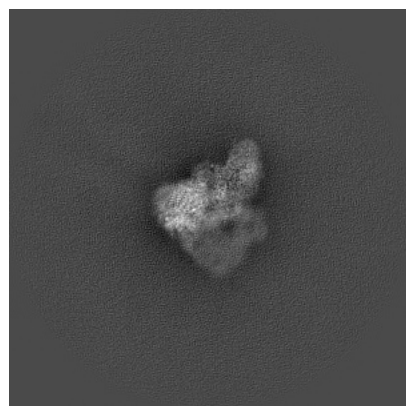
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4499. These allow visual inspection of the internal detail of the map and identification of artifacts.

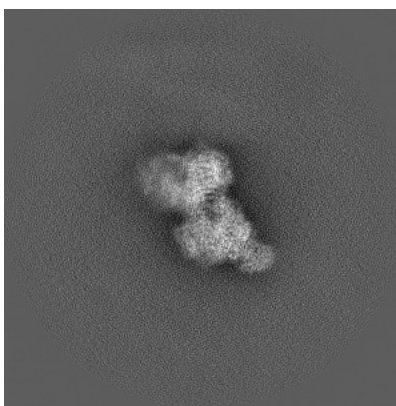
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

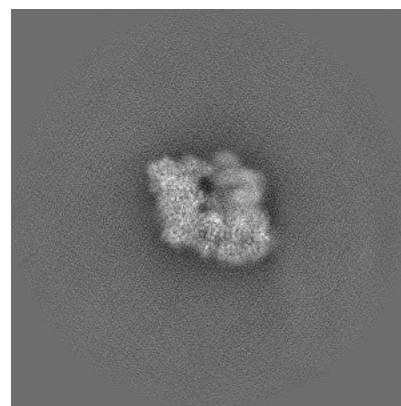
6.1.1 Primary map



X

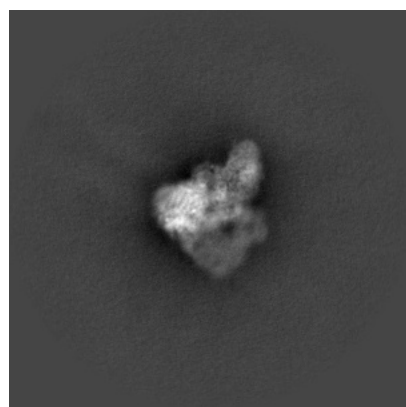


Y

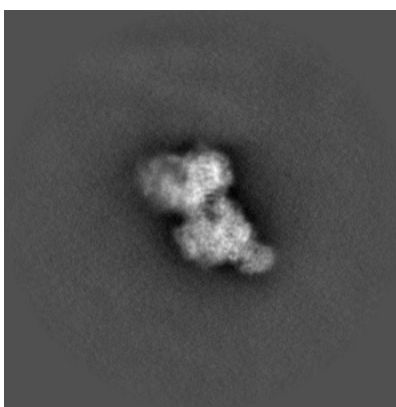


Z

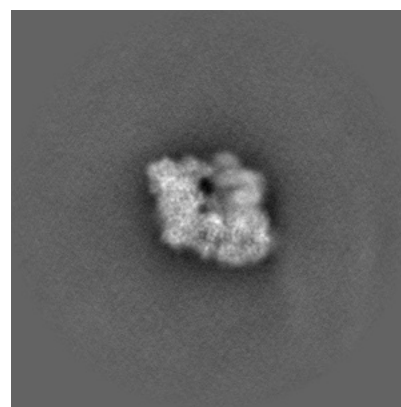
6.1.2 Raw map



X



Y

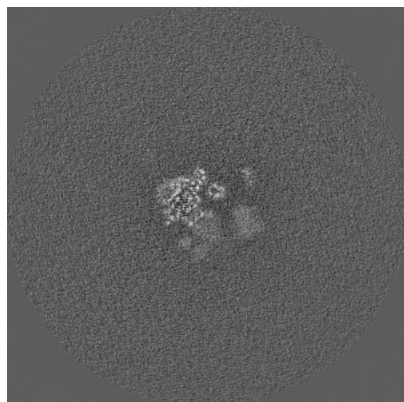


Z

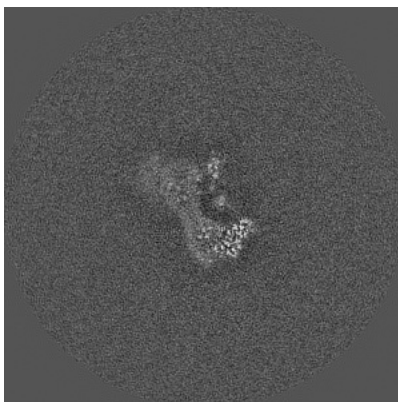
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

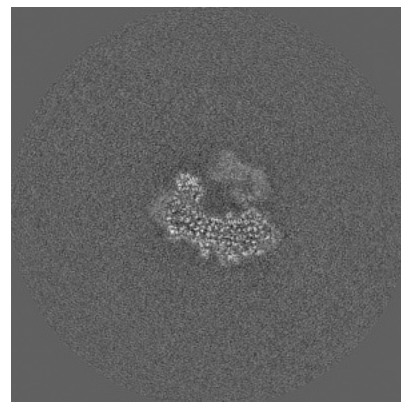
6.2.1 Primary map



X Index: 256

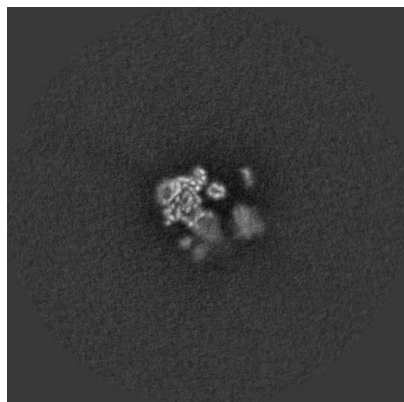


Y Index: 256

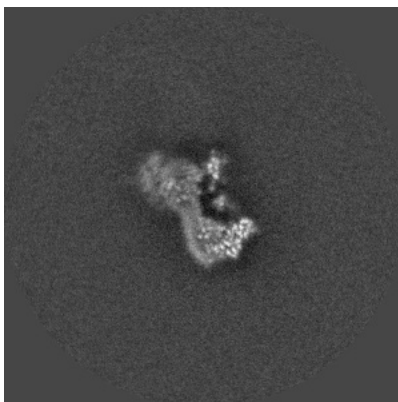


Z Index: 256

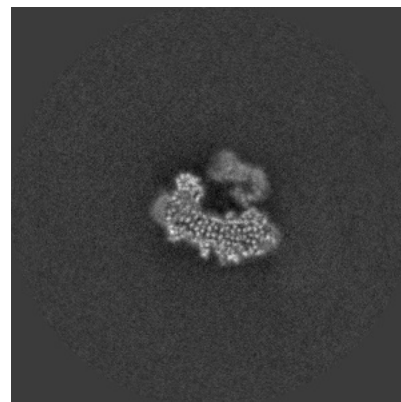
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

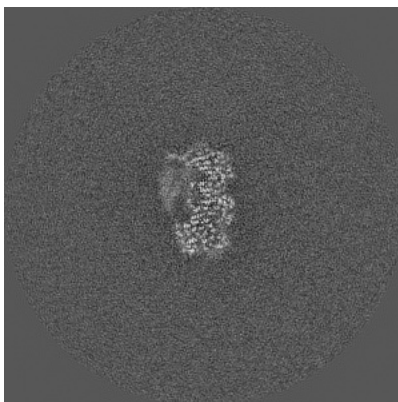
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

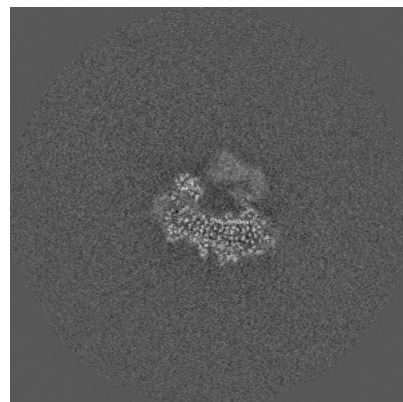
6.3.1 Primary map



X Index: 207

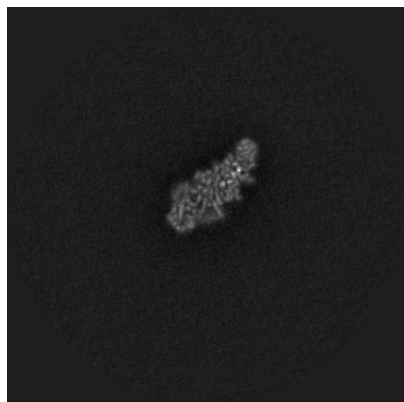


Y Index: 229

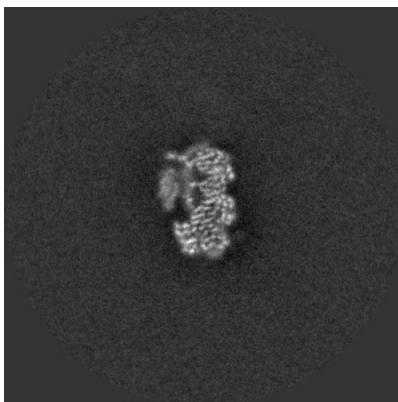


Z Index: 255

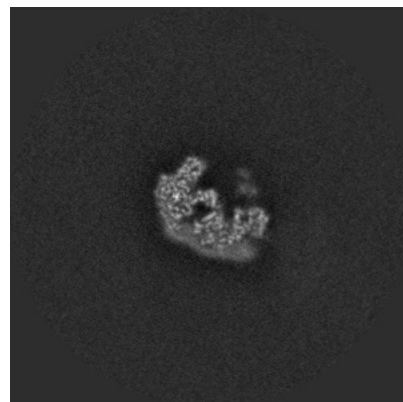
6.3.2 Raw map



X Index: 207



Y Index: 230

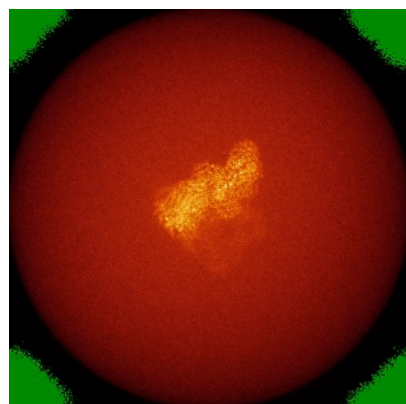


Z Index: 279

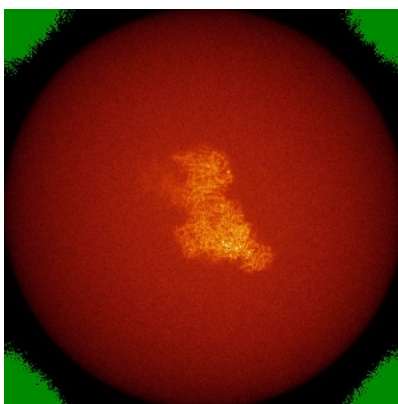
The images above show the largest variance slices of the map in three orthogonal directions.

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

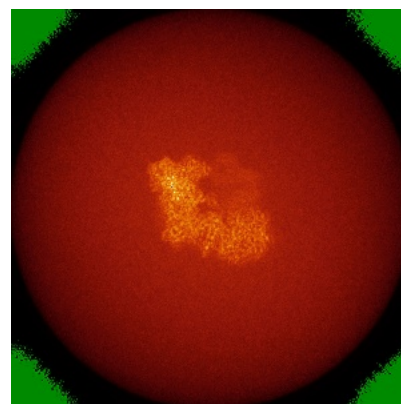
6.4.1 Primary map



X

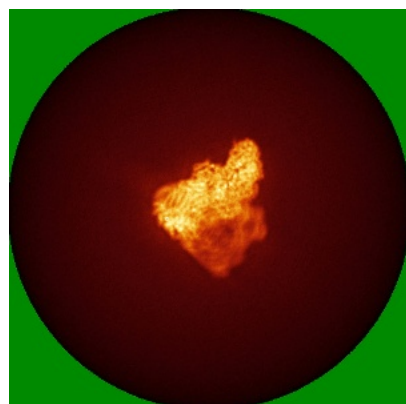


Y

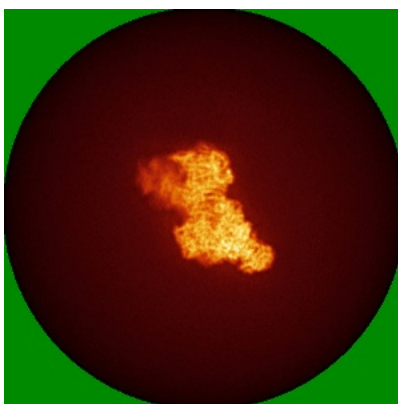


Z

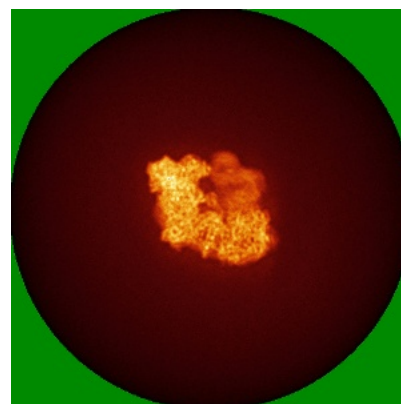
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

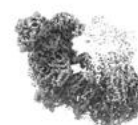
6.5.1 Primary map



X



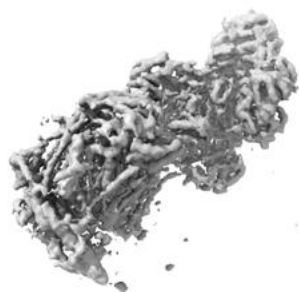
Y



Z

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

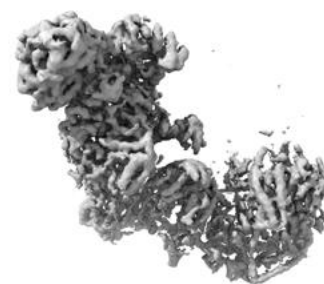
6.5.2 Raw map



X



Y



Z

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

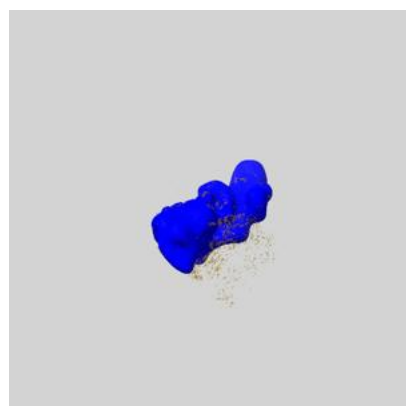
6.6 Mask visualisation [i](#)

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

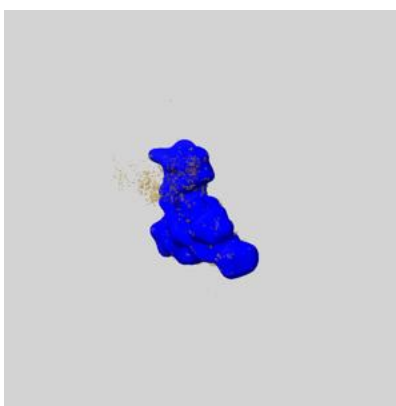
A mask typically either:

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

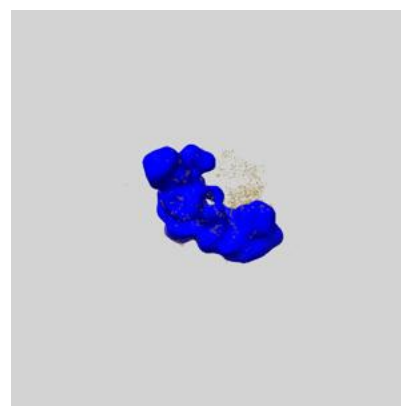
6.6.1 emd_4499_msk_1.map [i](#)



X



Y

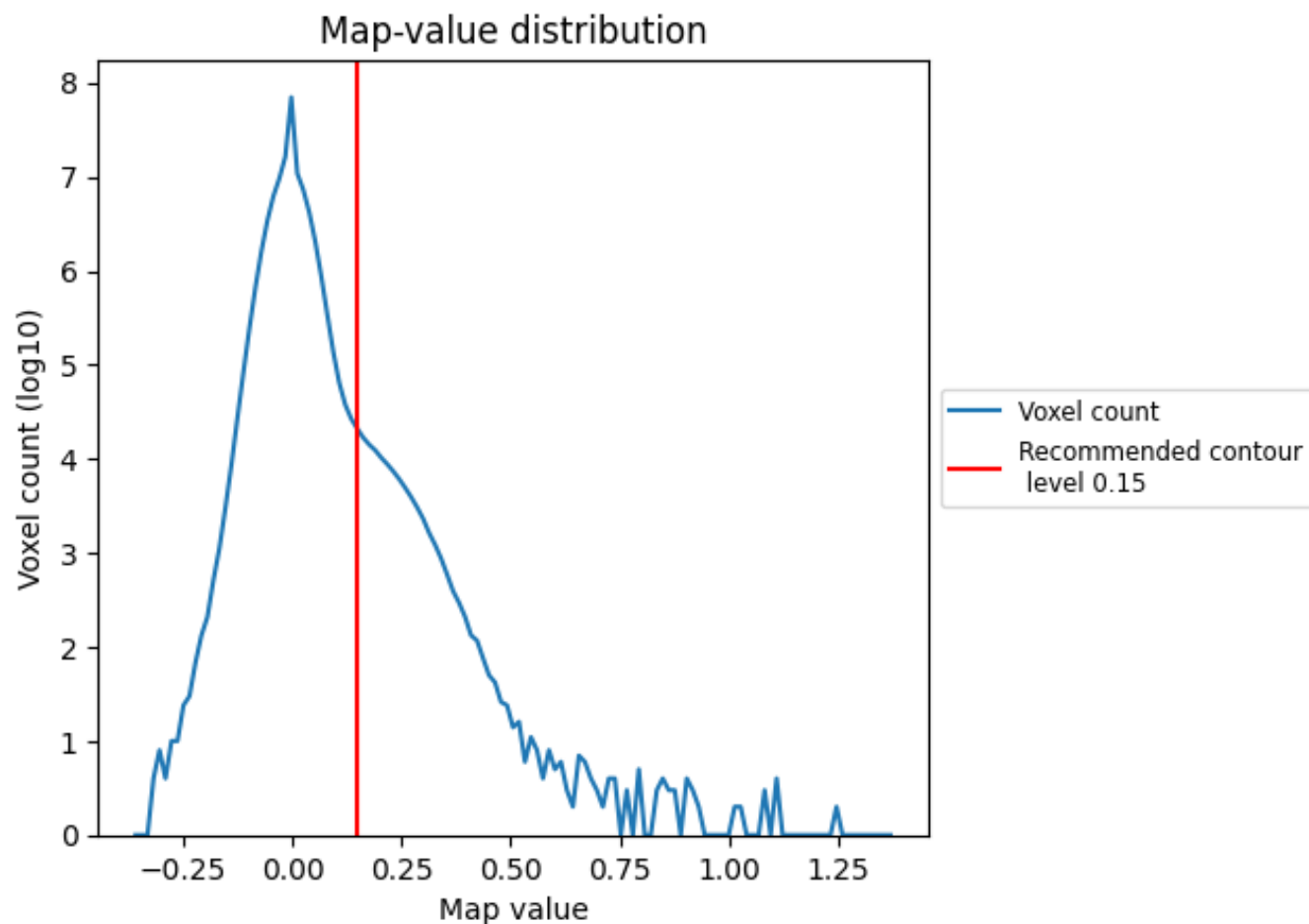


Z

7 Map analysis [i](#)

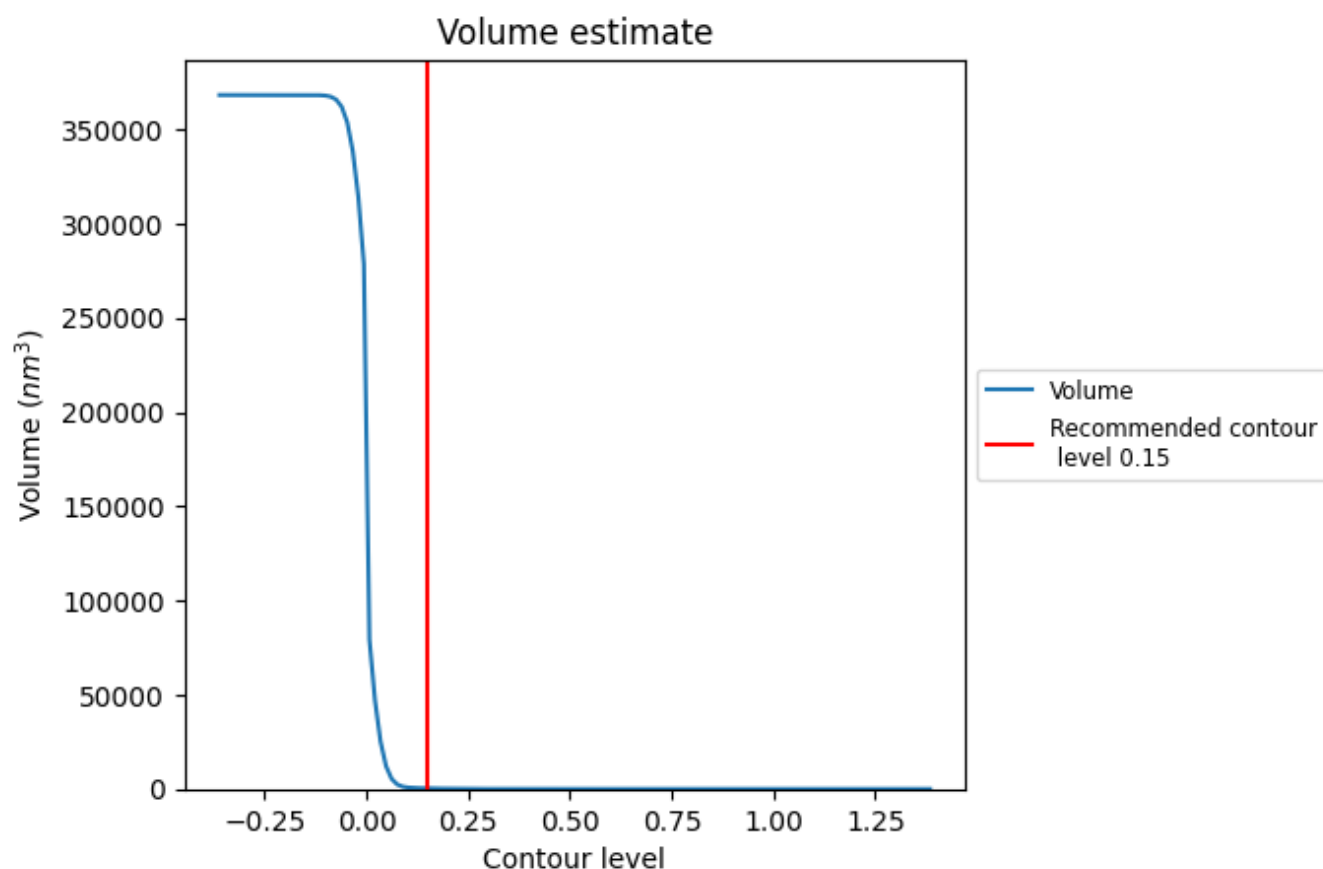
This section contains the results of statistical analysis of the map.

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.

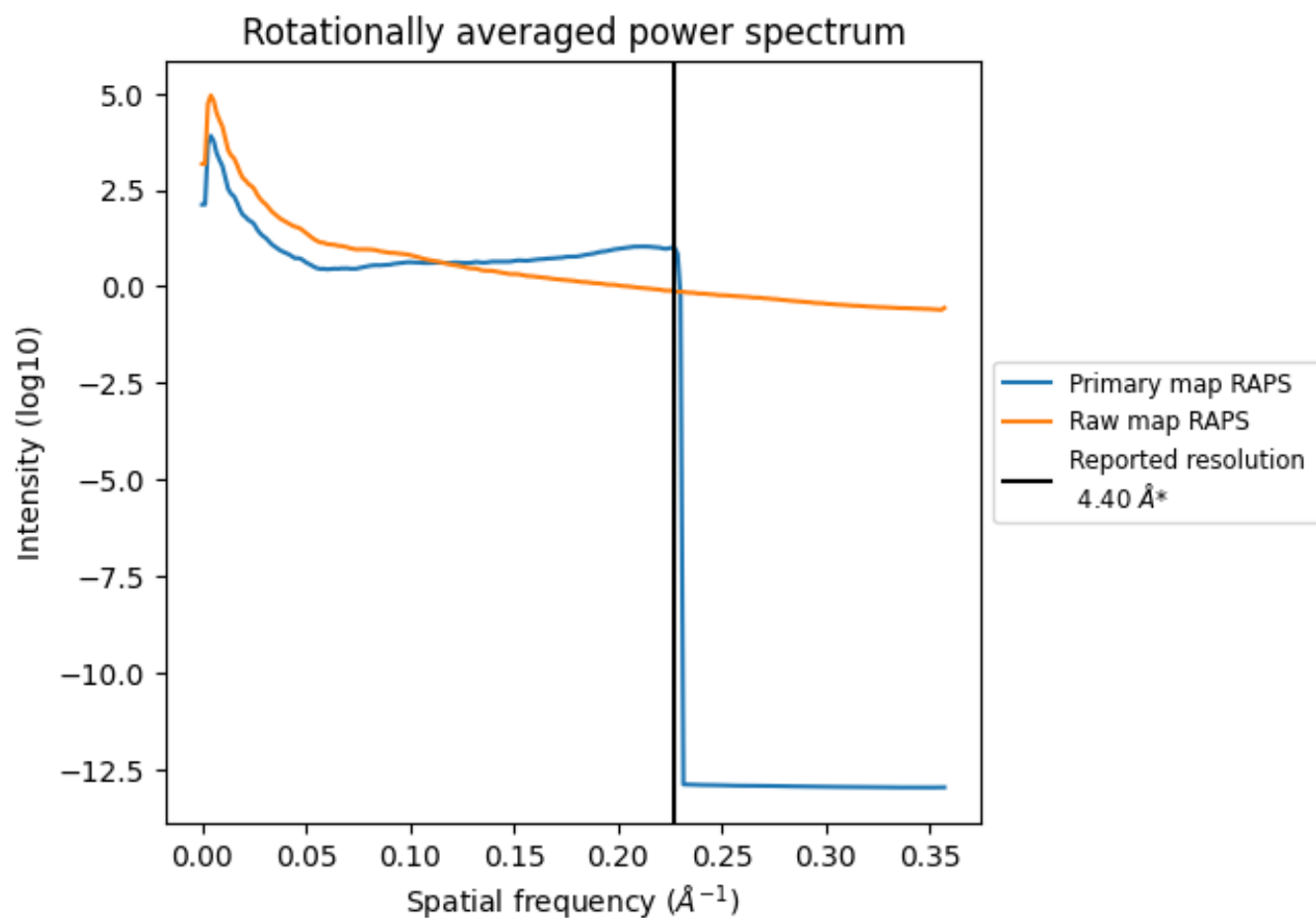
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 315 nm^3 ; this corresponds to an approximate mass of 285 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 ⓘ

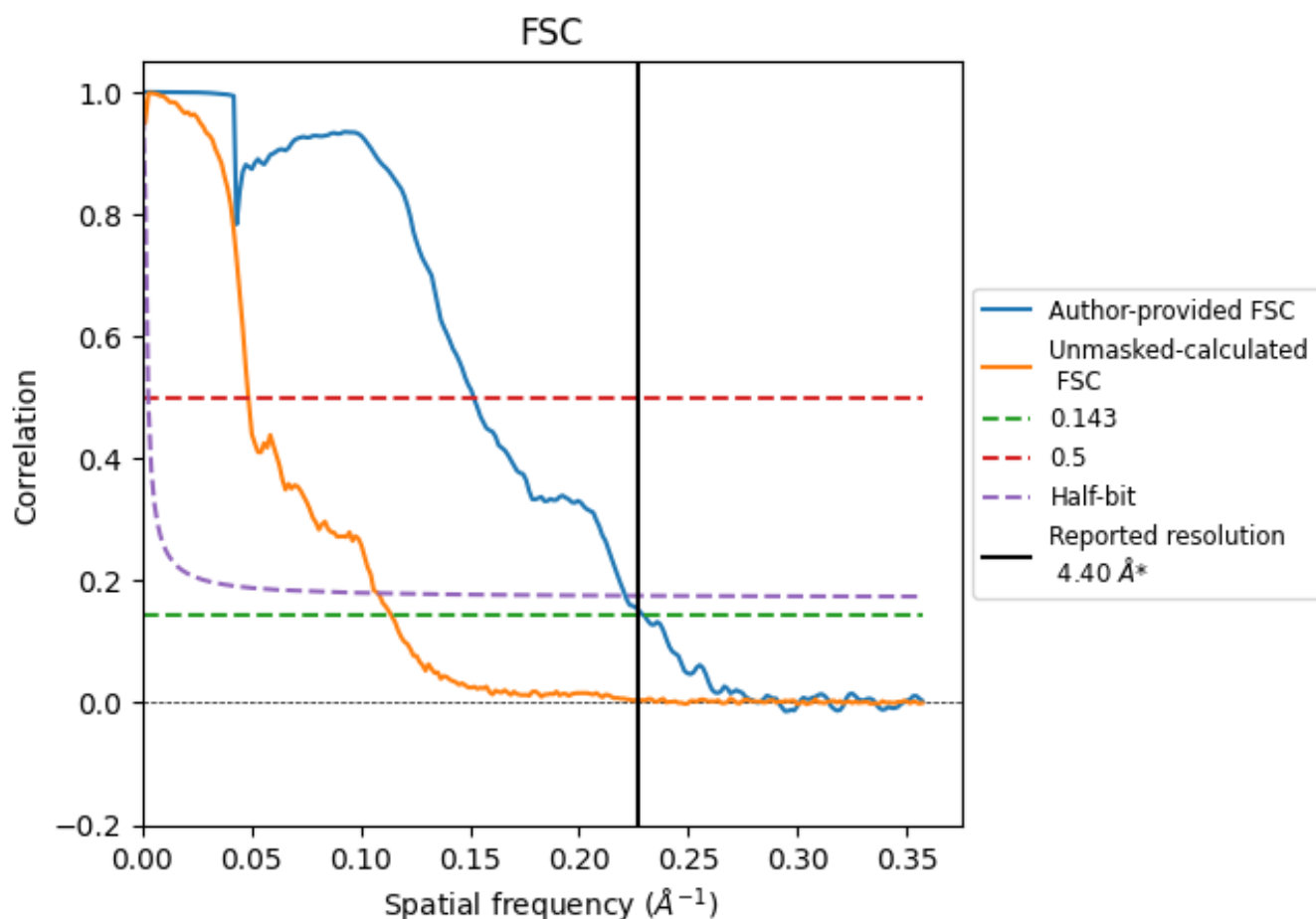


*Reported resolution corresponds to spatial frequency of 0.227 $\text{\AA}^{-1}$

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 0.227 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

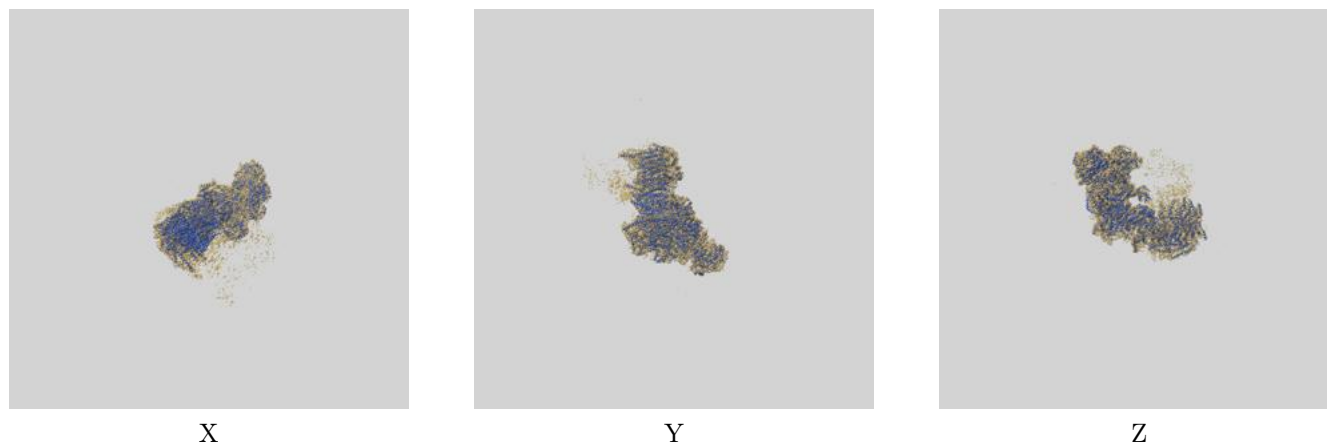
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.36	6.59	4.52
Unmasked-calculated*	8.77	20.58	9.28

*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 8.77 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

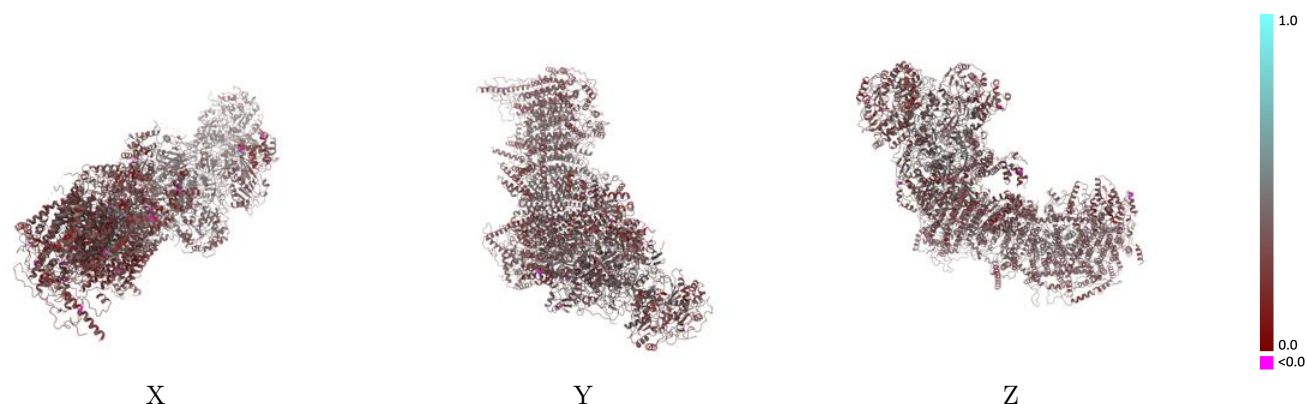
This section contains information regarding the fit between EMDB map EMD-4499 and PDB model 6QC7. Per-residue inclusion information can be found in [section 3](#) on [page 17](#).

9.1 Map-model overlay [i](#)



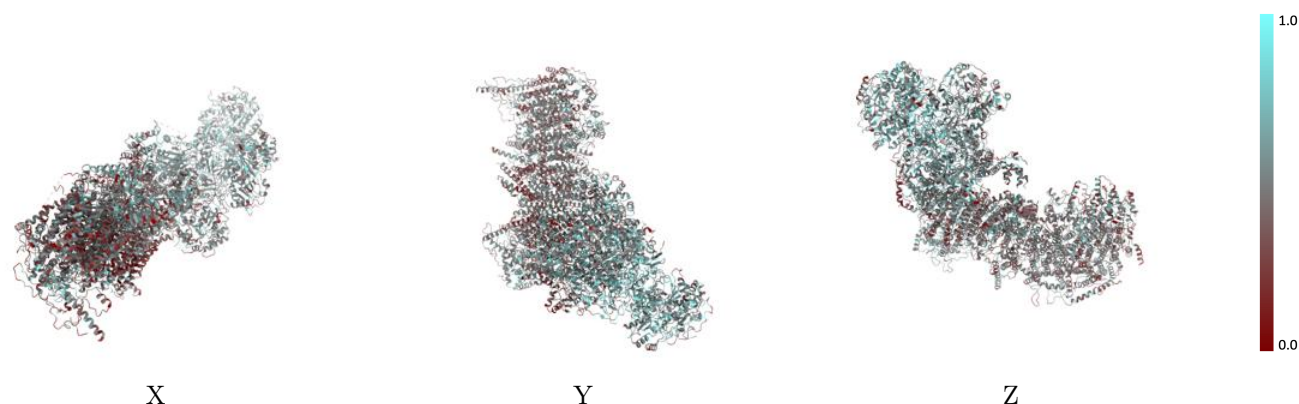
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



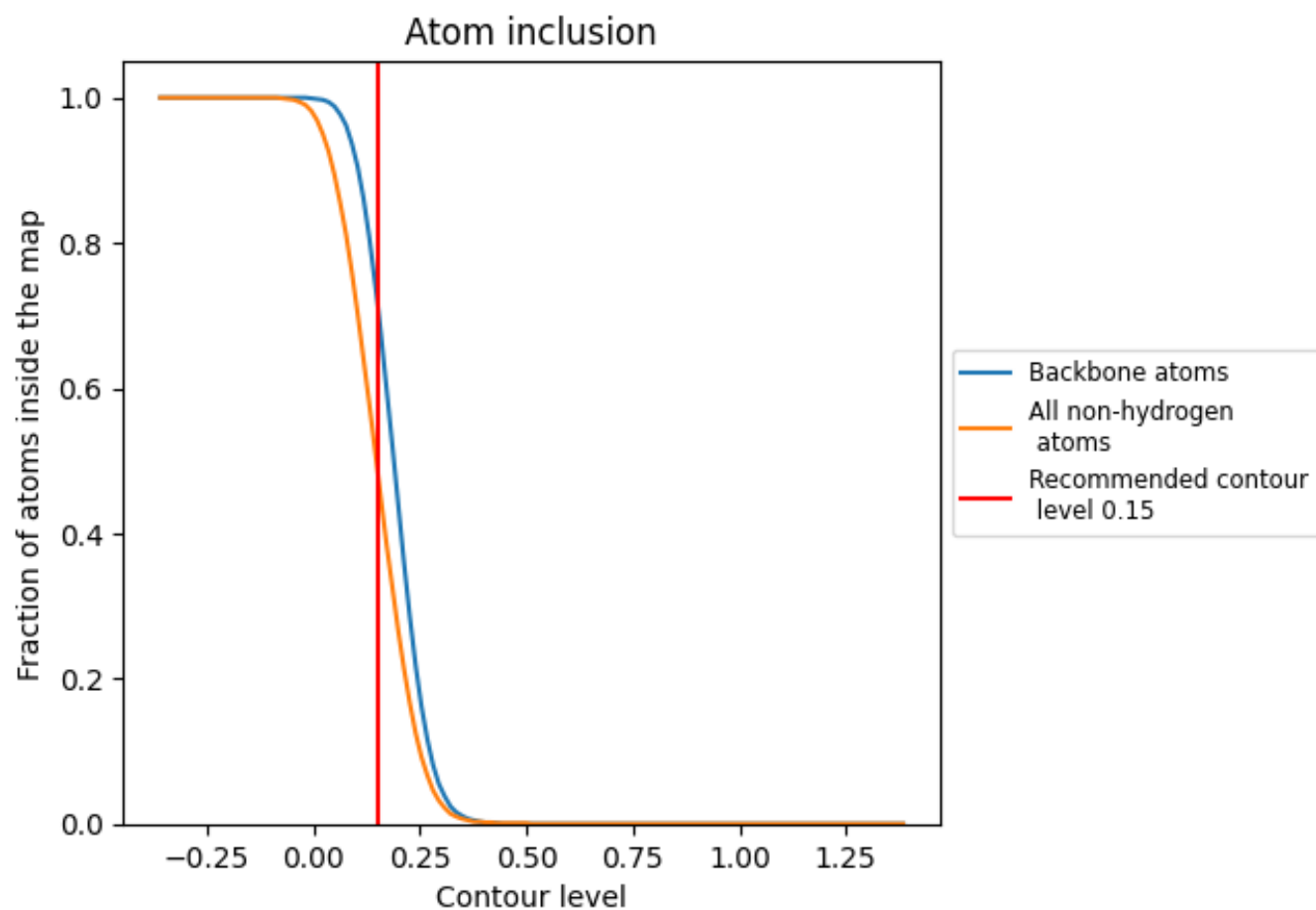
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 72% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.4860	 0.3350
4L	 0.3850	 0.3300
A1	 0.5310	 0.3410
A2	 0.5600	 0.3060
A3	 0.4700	 0.3310
A5	 0.5280	 0.3350
A6	 0.5220	 0.3440
A7	 0.4280	 0.3440
A8	 0.4930	 0.3260
A9	 0.5050	 0.3400
AA	 0.4350	 0.2830
AB	 0.4170	 0.2840
AJ	 0.4680	 0.3310
AK	 0.3110	 0.2960
AL	 0.3910	 0.3520
AM	 0.5390	 0.3340
B1	 0.3850	 0.3410
B2	 0.3940	 0.2920
B3	 0.3620	 0.2900
B4	 0.4310	 0.3120
B5	 0.5010	 0.3320
B6	 0.4230	 0.3270
B7	 0.4240	 0.2630
B8	 0.4410	 0.3180
B9	 0.5160	 0.3230
BJ	 0.4820	 0.3000
BK	 0.4480	 0.3100
C1	 0.4400	 0.2960
C2	 0.4640	 0.3310
D1	 0.4430	 0.3330
D2	 0.4870	 0.3520
D3	 0.3650	 0.3270
D4	 0.4590	 0.3410
D5	 0.4050	 0.3160
D6	 0.3510	 0.3070



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Chain	Atom inclusion	Q-score
S1	 0.5630	 0.3580
S2	 0.5370	 0.3600
S3	 0.5750	 0.3770
S4	 0.5470	 0.3870
S5	 0.4830	 0.3340
S6	 0.5700	 0.3860
S7	 0.5740	 0.3680
S8	 0.5950	 0.3800
V1	 0.5800	 0.3340
V2	 0.5730	 0.3240
V3	 0.5450	 0.3330