



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 05:08 AM UTC

PDB ID : 6RFS / pdb_00006rfs
EMDB ID : EMD-4874
Title : Cryo-EM structure of a respiratory complex I mutant lacking NDUF54
Authors : Parey, K.; Vonck, J.
Deposited on : 2019-04-16
Resolution : 4.04 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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:

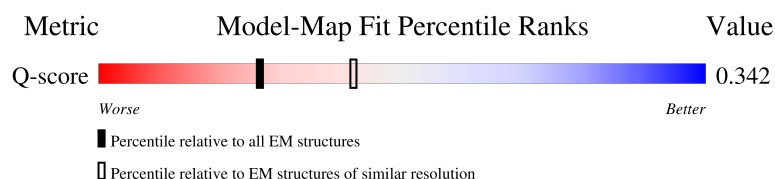
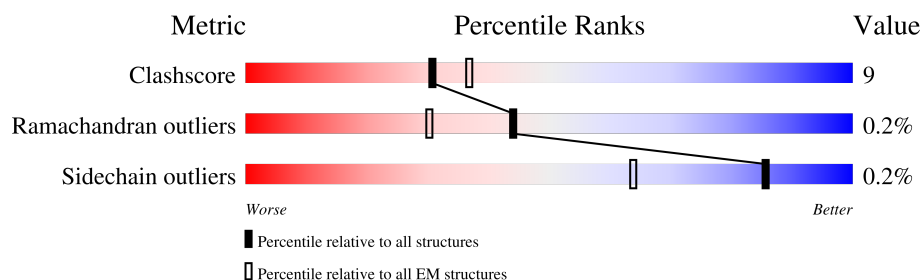
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.04 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	6625 (3.54 - 4.54)

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	A	728	14% 71% 23% 5%
2	B	488	17% 71% 22% 7%
3	C	466	9% 58% 24% 17%
4	D	87	22% 72% 26% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	375	
6	F	144	
7	G	281	
8	H	243	
9	I	229	
10	J	198	
11	K	210	
12	L	89	
13	M	136	
14	O	109	
15	P	124	
16	Q	132	
17	R	109	
18	S	249	
19	U	172	
20	W	123	
21	X	169	
22	Z	182	
23	a	149	
24	b	74	
25	c	60	
26	d	92	
27	e	67	
28	f	87	
29	g	78	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	h	138	
31	i	90	
32	j	93	
33	n	120	
34	1	341	
35	2	469	
36	3	128	
37	4	486	
38	5	655	
39	6	185	
40	8	99	
41	9	89	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
42	SF4	A	802	-	-	X	-
42	SF4	B	501	-	-	X	-
42	SF4	I	301	-	-	X	-
42	SF4	I	302	-	-	X	-
42	SF4	K	301	-	-	X	-
43	FES	H	301	-	-	X	-

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 60966 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 Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	692	Total	C	N	O	S	0	0
			5258	3263	926	1040	29		

- Molecule 2 is a protein called Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	456	Total	C	N	O	S	0	0
			3528	2229	621	654	24		

- Molecule 3 is a protein called Subunit NUCM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	387	Total	C	N	O	S	0	0
			3052	1948	522	561	21		

- Molecule 4 is a protein called Subunit NIMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	86	Total	C	N	O	S	0	0
			682	432	127	120	3		

- Molecule 5 is a protein called Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	331	Total	C	N	O	S	0	0
			2650	1683	464	494	9		

- Molecule 6 is a protein called Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I).

plex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	121	Total	C	N	O	S	0	0
			990	629	166	193	2		

- Molecule 7 is a protein called Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1978	1272	336	366	4		

- Molecule 8 is a protein called Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	213	Total	C	N	O	S	0	0
			1664	1043	279	324	18		

- Molecule 9 is a protein called Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	190	Total	C	N	O	S	0	0
			1519	966	254	289	10		

- Molecule 10 is a protein called Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	116	Total	C	N	O	S	0	0
			790	495	146	147	2		

- Molecule 11 is a protein called Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	170	Total	C	N	O	S	0	0
			1347	857	236	239	15		

- Molecule 12 is a protein called Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	83	Total	C	N	O	S	0	0
			645	434	102	106	3		

- Molecule 13 is a protein called Subunit NUMM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	117	Total	C	N	O	S	0	0
			912	568	163	176	5		

- Molecule 14 is a protein called Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	77	Total	C	N	O	0	0
			591	373	93	125		

- Molecule 15 is a protein called Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	123	Total	C	N	O	S	0	0
			1037	667	182	186	2		

- Molecule 16 is a protein called Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	85	Total	C	N	O	S	0	0
			648	405	103	138	2		

- Molecule 17 is a protein called Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	106	Total	C	N	O	S	0	0
			885	562	168	152	3		

- Molecule 18 is a protein called Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	174	Total	C	N	O	S	0	0
			1430	920	245	263	2		

- Molecule 19 is a protein called Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	171	Total	C	N	O	S	0	0
			1346	847	236	253	10		

- Molecule 20 is a protein called Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	121	Total	C	N	O	S	0	0
			974	623	178	168	5		

- Molecule 21 is a protein called Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	167	Total	C	N	O	S	0	0
			1300	842	222	232	4		

- Molecule 22 is a protein called Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	181	Total	C	N	O	S	0	0
			1390	893	240	256	1		

- Molecule 23 is a protein called Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	124	Total	C	N	O	S	0	0
			1030	669	165	194	2		

- Molecule 24 is a protein called Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
24	b	64	Total	C	N	O	0	0
			490	326	83	81		

- Molecule 25 is a protein called Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
25	c	44	Total	C	N	O	0	0
			353	229	67	57		

- Molecule 26 is a protein called Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	90	Total	C	N	O	S	0	0
			761	472	137	149	3		

- Molecule 27 is a protein called Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	e	52	Total	C	N	O	S	0	0
			436	293	75	65	3		

- Molecule 28 is a protein called Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
28	f	80	Total	C	N	O	S	0	0
			629	394	119	115	1		

- Molecule 29 is a protein called Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms				AltConf	Trace
29	g	76	Total	C	N	O	0	0
			617	405	112	100		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	71	GLY	GLN	conflict	UNP A0A1D8NJR0

- Molecule 30 is a protein called Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	136	Total	C	N	O	S	0	0
			1130	727	193	208	2		

- Molecule 31 is a protein called Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
31	i	83	Total	C	N	O	S	0	0
			646	413	117	115	1		

- Molecule 32 is a protein called Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	90	Total	C	N	O	S	0	0
			724	465	132	127			

- Molecule 33 is a protein called Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
33	n	113	Total	C	N	O	S	0	0
			904	582	153	168	1		

- Molecule 34 is a protein called Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1	340	Total	C	N	O	S	0	0
			2682	1826	393	456	7		

- Molecule 35 is a protein called Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
35	2	469	Total	C	N	O	S	0	0
			3775	2557	550	656	12		

- Molecule 36 is a protein called Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
36	3	116	Total	C	N	O	S	0	0
			911	623	136	150	2		

- Molecule 37 is a protein called Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
37	4	486	Total	C	N	O	S	0	0
			3856	2600	586	655	15		

- Molecule 38 is a protein called Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
38	5	632	Total	C	N	O	S	0	0
			4954	3306	756	867	25		

- Molecule 39 is a protein called Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
39	6	138	Total	C	N	O	S	0	0
			1096	752	154	183	7		

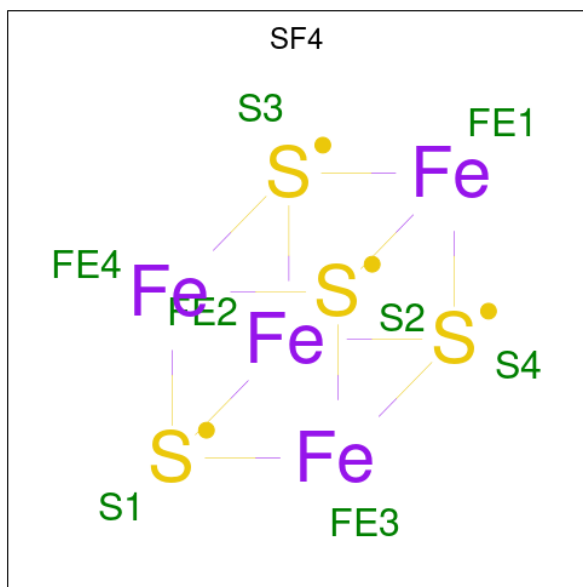
- Molecule 40 is a protein called Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I).

Mol	Chain	Residues	Atoms					AltConf	Trace
40	8	80	Total	C	N	O	S	0	0
			662	420	120	114	8		

- Molecule 41 is a protein called Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I).

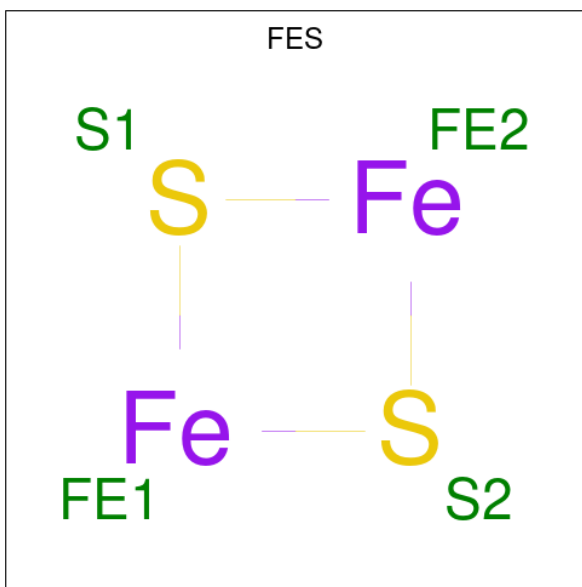
Mol	Chain	Residues	Atoms					AltConf	Trace
41	9	66	Total	C	N	O	S	0	0
			528	325	99	98	6		

- Molecule 42 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



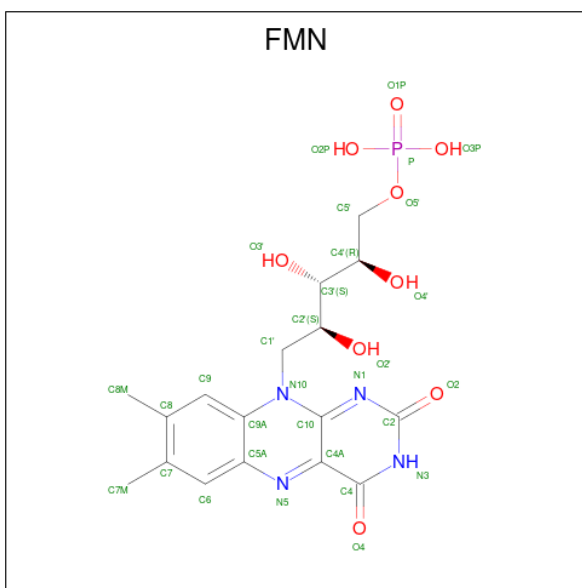
Mol	Chain	Residues	Atoms			AltConf
42	A	1	Total	Fe	S	0
			8	4	4	
42	A	1	Total	Fe	S	0
			8	4	4	
42	B	1	Total	Fe	S	0
			8	4	4	
42	I	1	Total	Fe	S	0
			8	4	4	
42	I	1	Total	Fe	S	0
			8	4	4	
42	K	1	Total	Fe	S	0
			8	4	4	

- Molecule 43 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
43	A	1	Total 4	Fe 2	S 2	0
43	H	1	Total 4	Fe 2	S 2	0

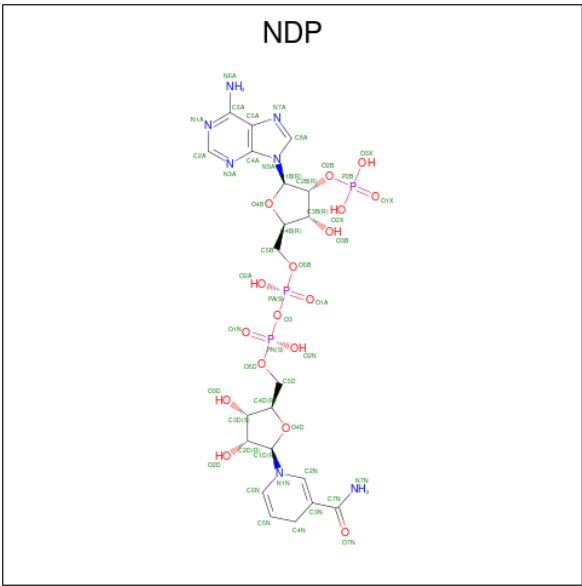
- Molecule 44 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

- Molecule 45 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

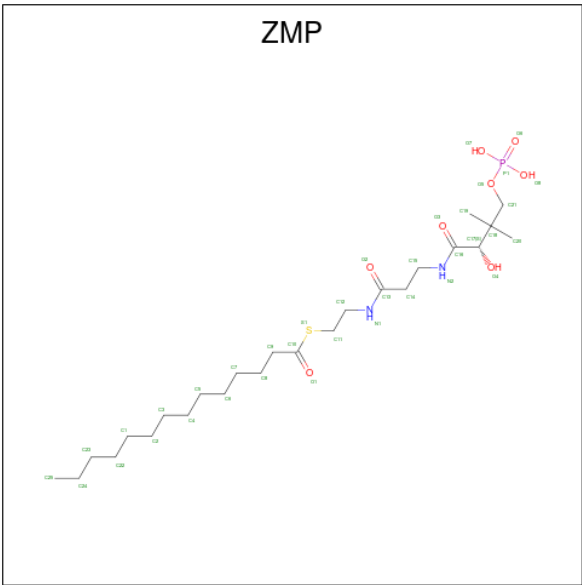


Mol	Chain	Residues	Atoms					AltConf
45	E	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 46 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
46	M	1	Total	Zn	0
			1	1	

- Molecule 47 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
47	O	1	Total	C	N	O	P	S	0
			30	19	2	7	1	1	

3 Residue-property plots

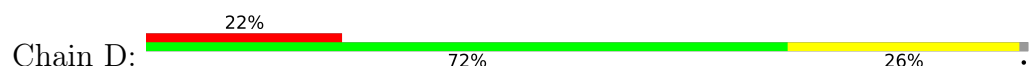
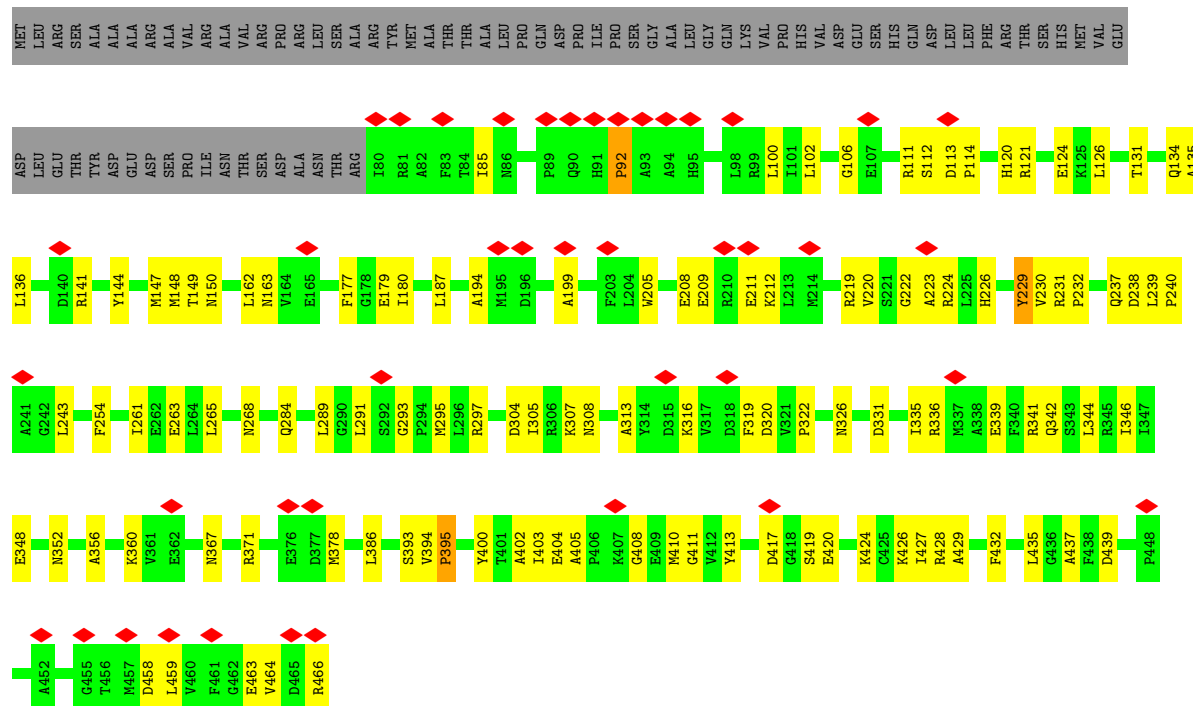
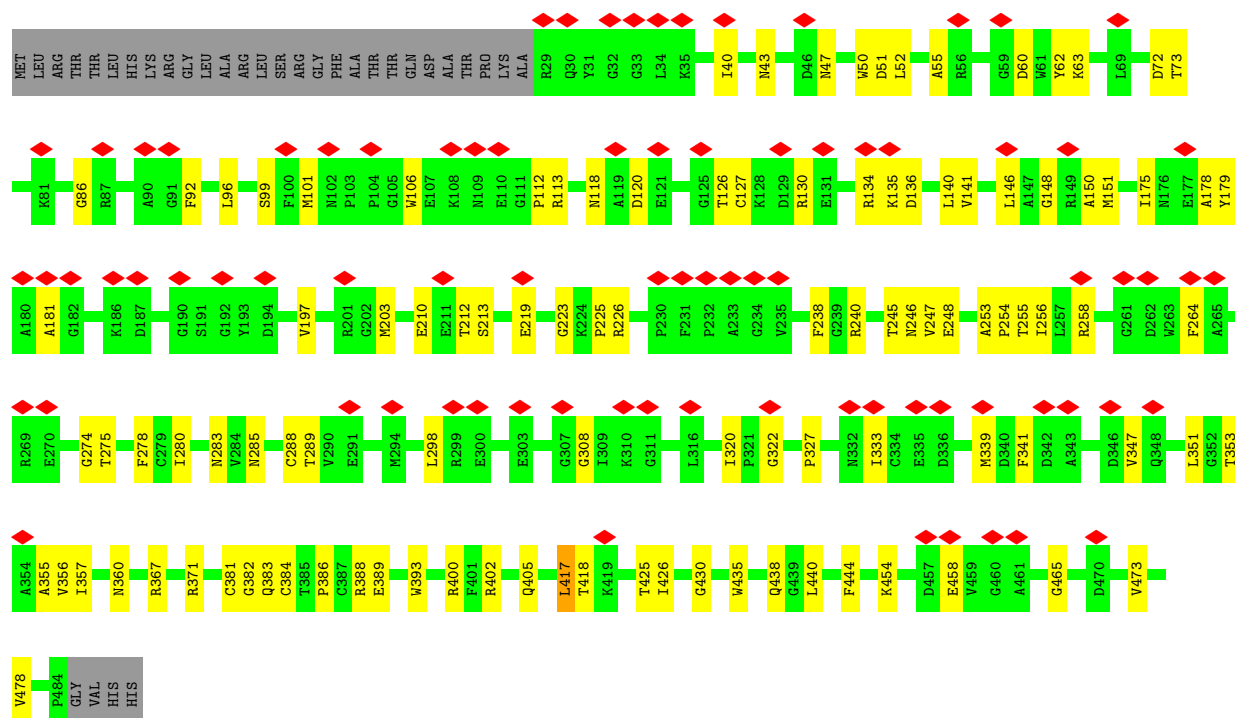
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

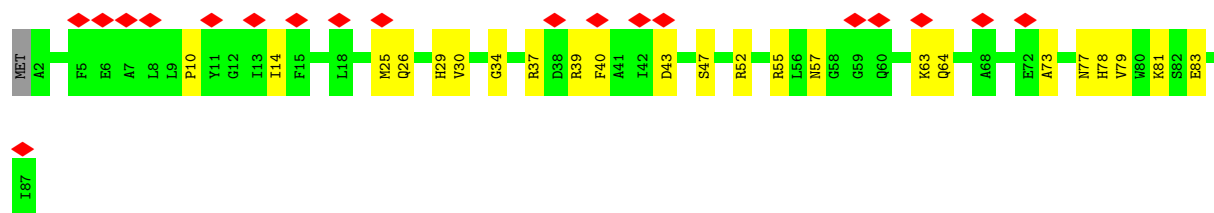
- Molecule 1: Subunit NUAM of NADH:Ubiquinone Oxidoreductase (Complex I)



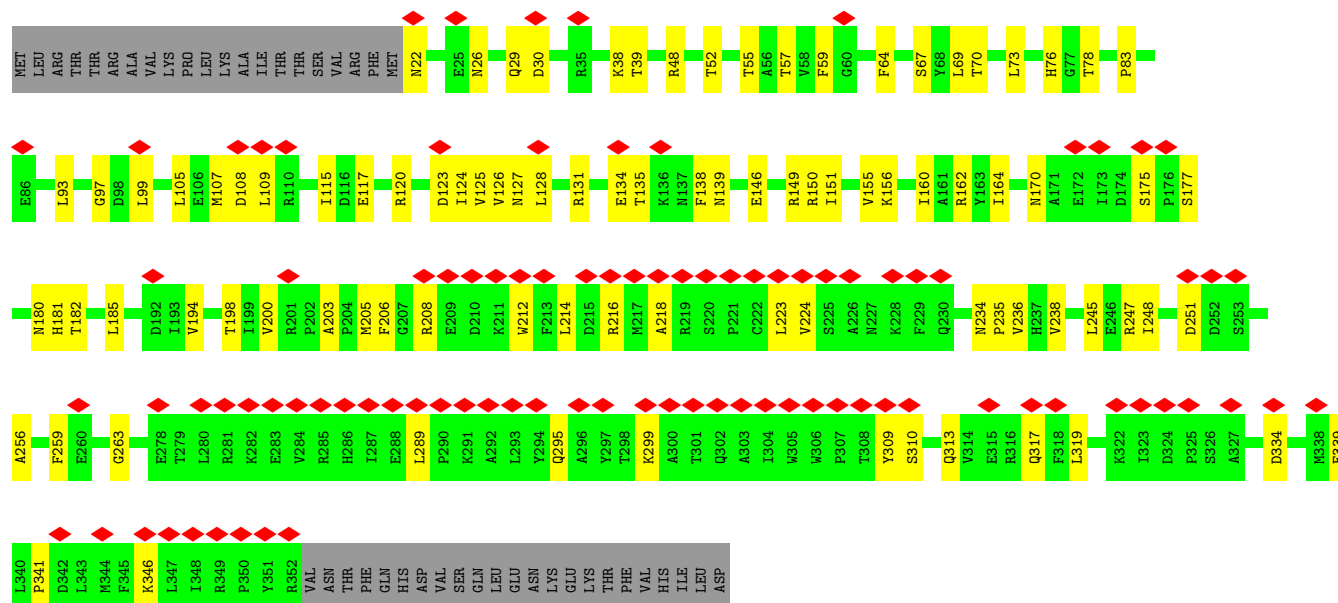
- Molecule 2: Subunit NUBM of NADH:Ubiquinone Oxidoreductase (Complex I)



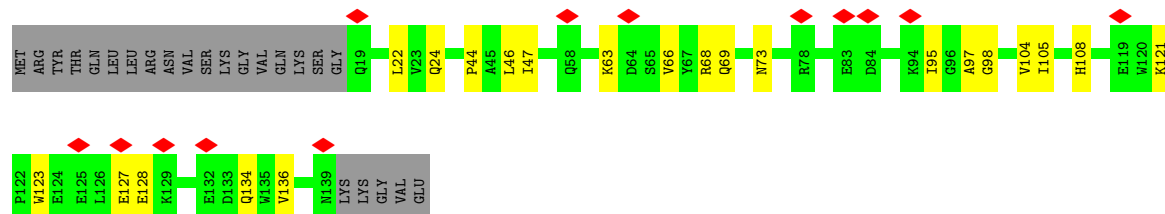




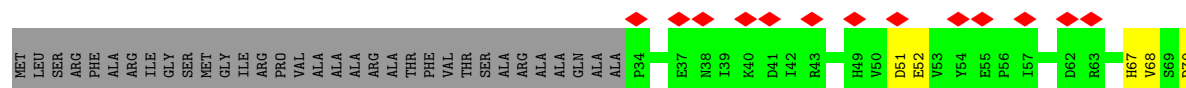
• Molecule 5: Subunit NUEM of NADH:Ubiquinone Oxidoreductase (Complex I)

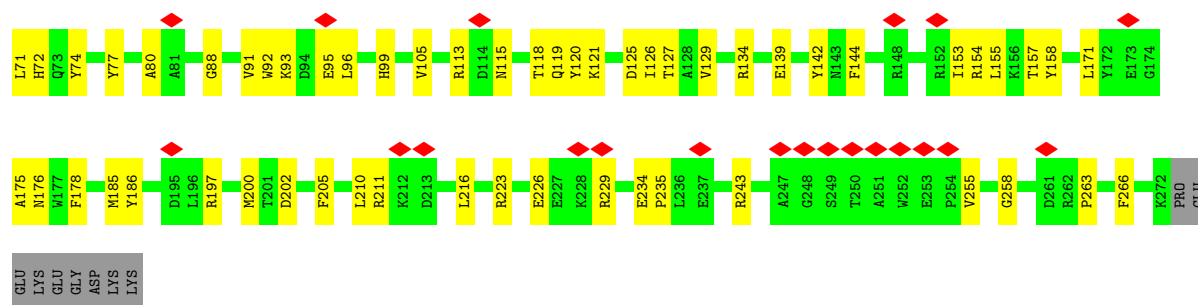


• Molecule 6: Subunit NUFM of NADH:Ubiquinone Oxidoreductase (Complex I)

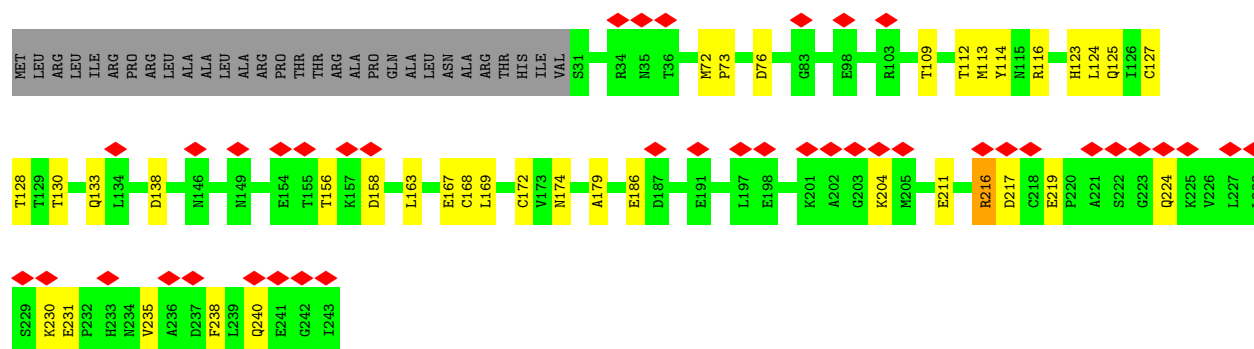


• Molecule 7: Subunit NUGM of NADH:Ubiquinone Oxidoreductase (Complex I)

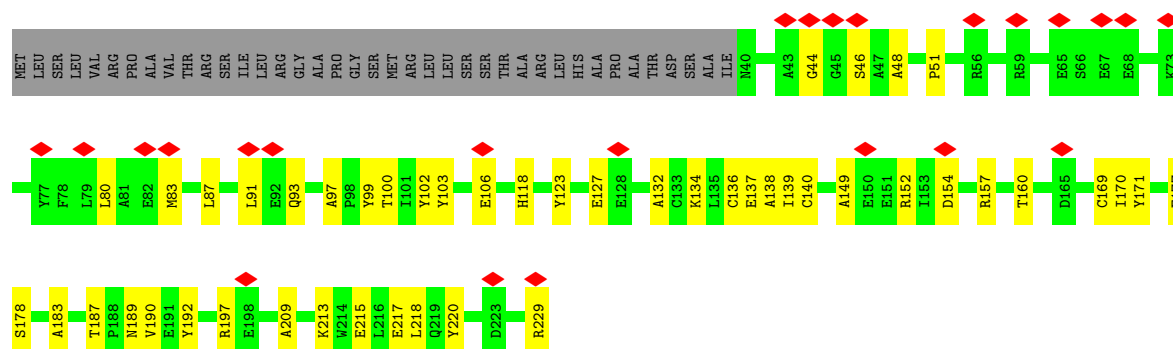




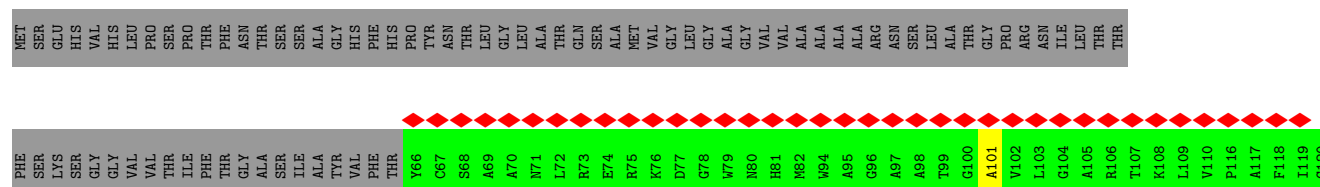
• Molecule 8: Subunit NUHM of NADH:Ubiquinone Oxidoreductase (Complex I)

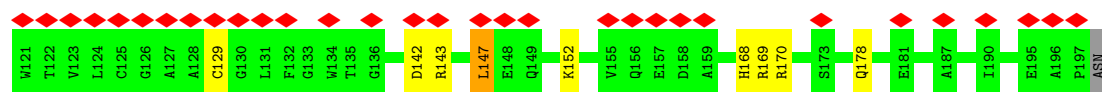


• Molecule 9: Subunit NUIM of NADH:Ubiquinone Oxidoreductase (Complex I)

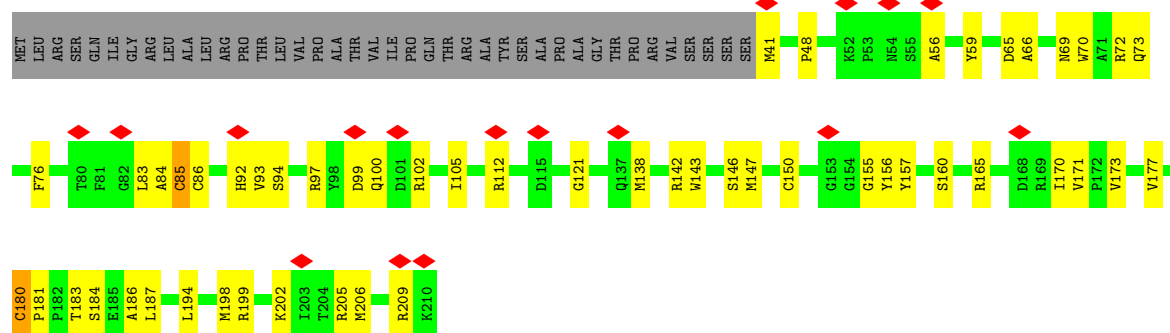


• Molecule 10: Subunit NUJM of NADH:Ubiquinone Oxidoreductase (Complex I)

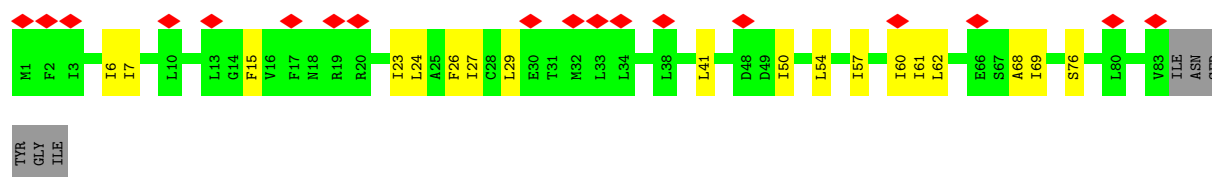
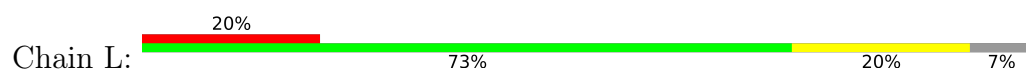




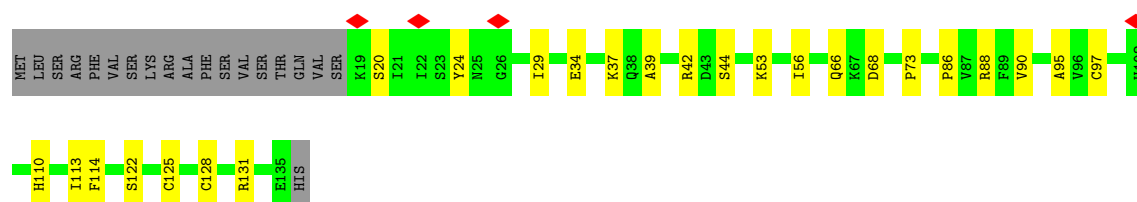
- Molecule 11: Subunit NUKM of NADH:Ubiquinone Oxidoreductase (Complex I)



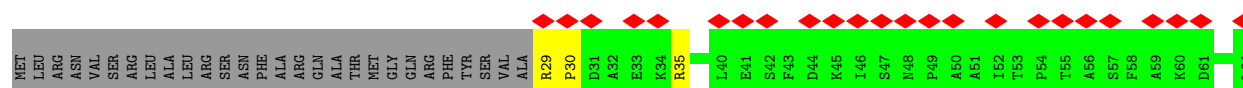
- Molecule 12: Subunit NULM of NADH:Ubiquinone Oxidoreductase (Complex I)

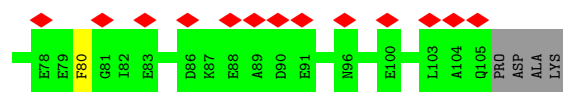


- Molecule 13: Subunit NUMM of NADH:Ubiquinone Oxidoreductase (Complex I)

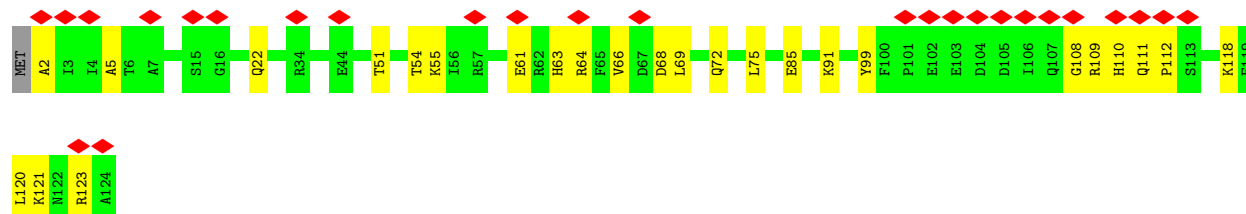
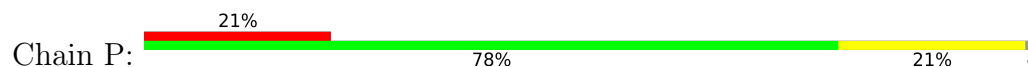


- Molecule 14: Acyl carrier protein ACPM1 of NADH:Ubiquinone Oxidoreductase (Complex I)

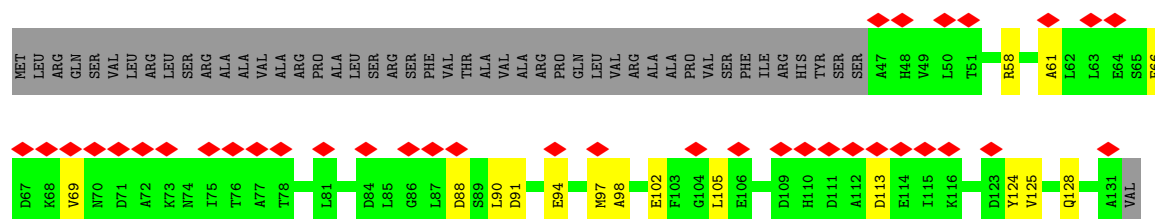




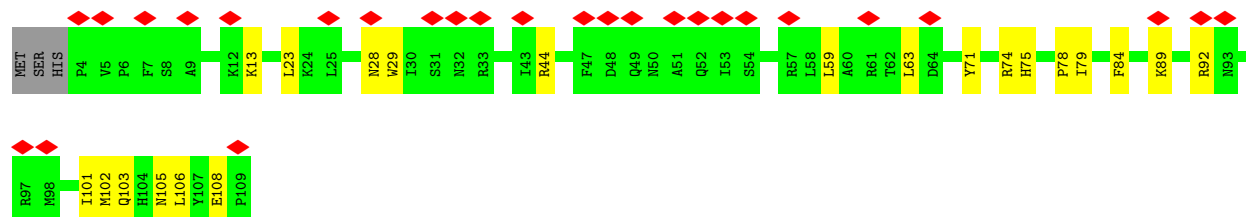
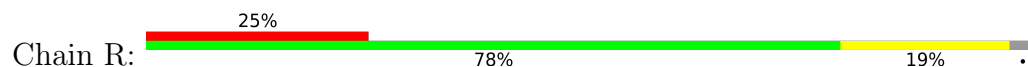
- Molecule 15: Subunit NB4M of protein NADH:Ubiquinone Oxidoreductase (Complex I)



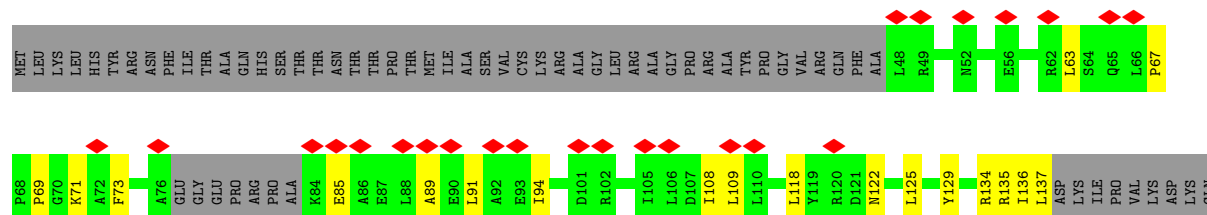
- Molecule 16: Acyl carrier protein ACPM2 of NADH:Ubiquinone Oxidoreductase (Complex I)

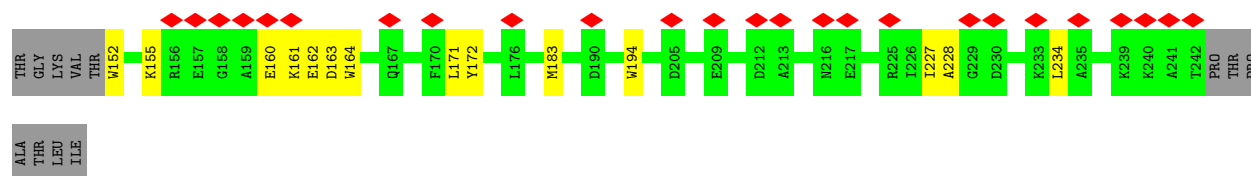


- Molecule 17: Subunit NI2M of NADH:Ubiquinone Oxidoreductase (Complex I)

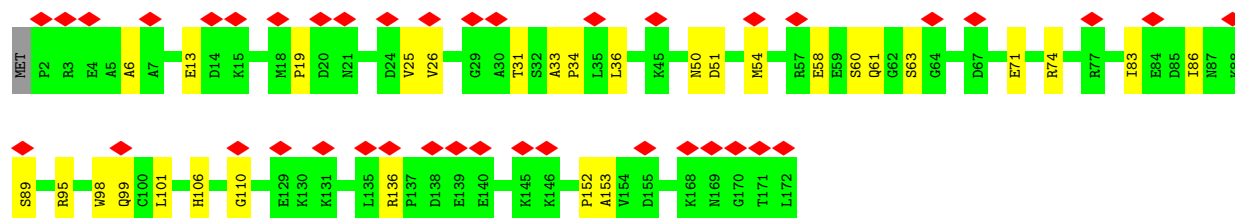
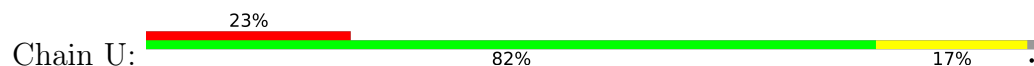


- Molecule 18: Subunit NESM of NADH:Ubiquinone Oxidoreductase (Complex I)

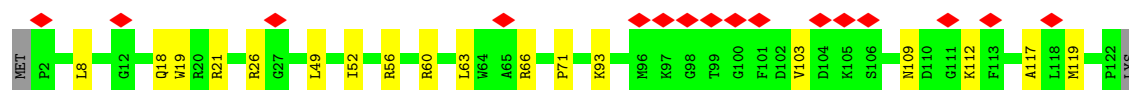
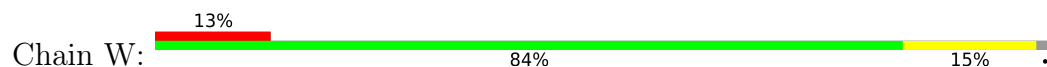




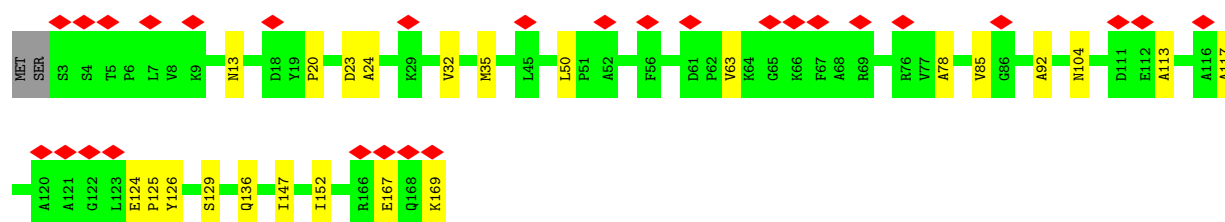
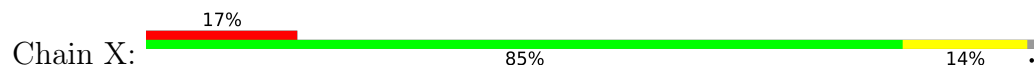
- Molecule 19: Subunit NUPM of NADH:Ubiquinone Oxidoreductase (Complex I)



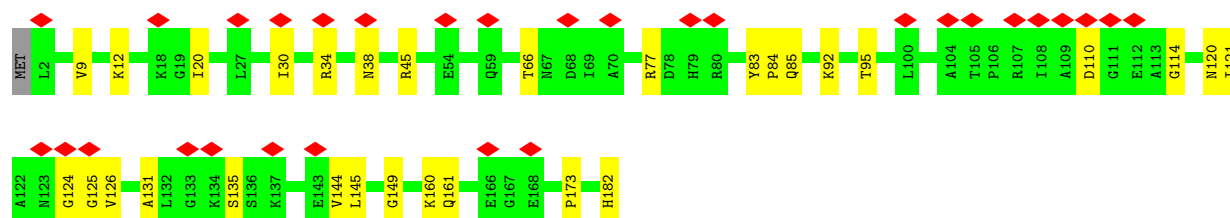
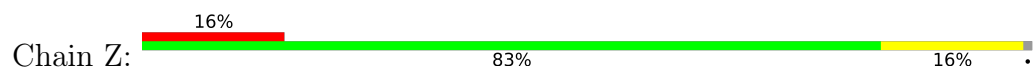
- Molecule 20: Subunit NB6M of NADH:Ubiquinone Oxidoreductase (Complex I)



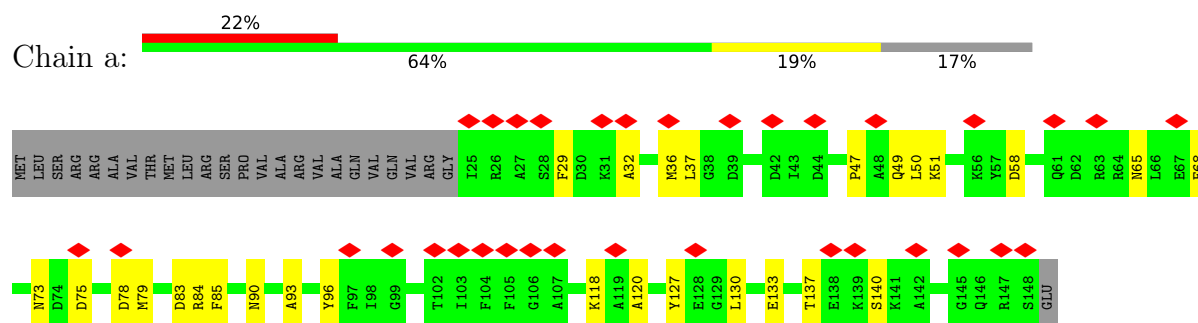
- Molecule 21: Subunit NUXM of NADH:Ubiquinone Oxidoreductase (Complex I)



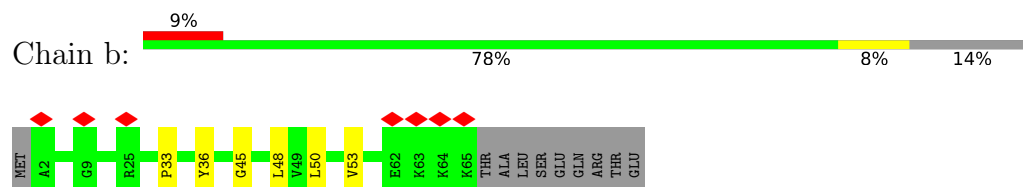
- Molecule 22: Subunit NUZM of NADH:Ubiquinone Oxidoreductase (Complex I)



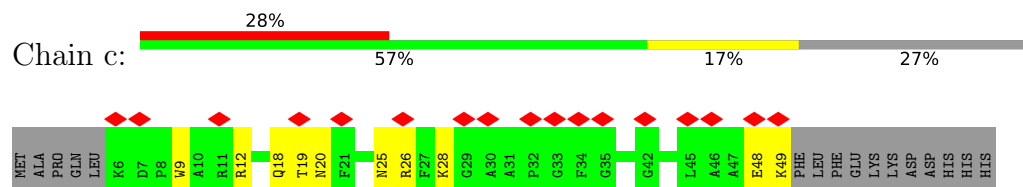
- Molecule 23: Subunit NIAM of NADH:Ubiquinone Oxidoreductase (Complex I)



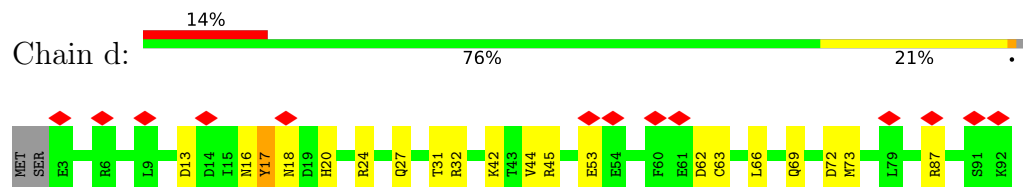
- Molecule 24: Subunit NEBM of NADH:Ubiquinone Oxidoreductase (Complex I)



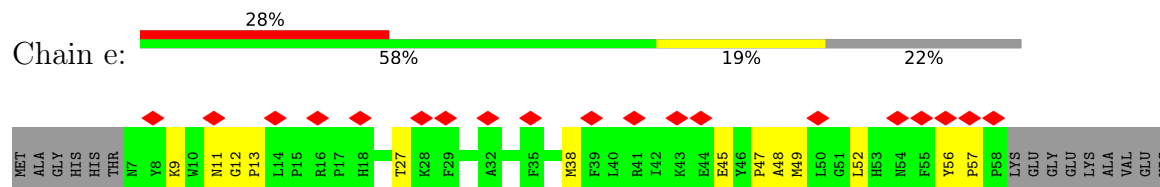
- Molecule 25: Subunit NB2M of NADH:Ubiquinone Oxidoreductase (Complex I)



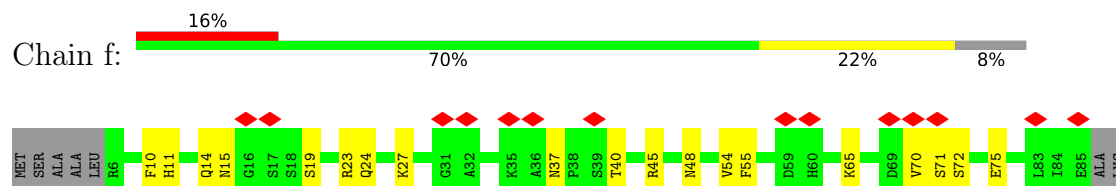
- Molecule 26: Subunit NIDM of NADH:Ubiquinone Oxidoreductase (Complex I)



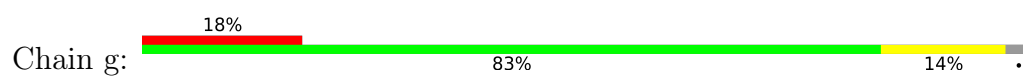
- Molecule 27: Subunit NUVM of NADH:Ubiquinone Oxidoreductase (Complex I)



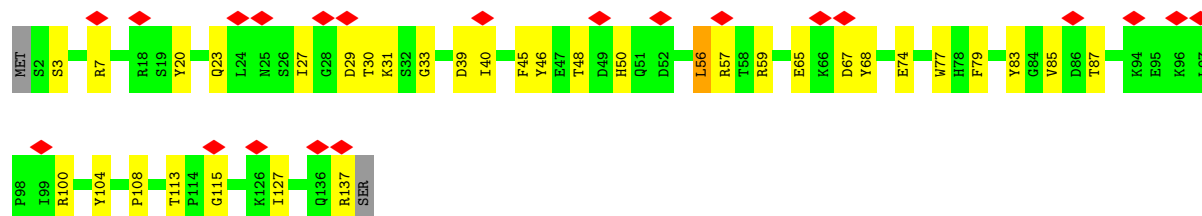
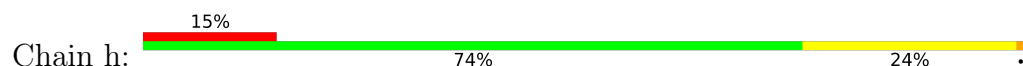
- Molecule 28: Subunit NI8M of NADH:Ubiquinone Oxidoreductase (Complex I)



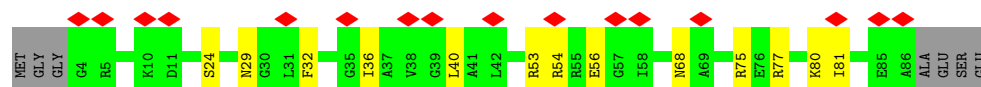
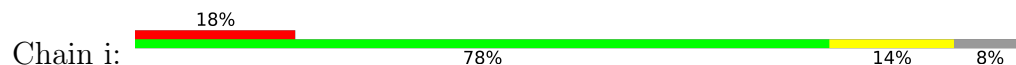
- Molecule 29: Subunit NI9M of NADH:Ubiquinone Oxidoreductase (Complex I)



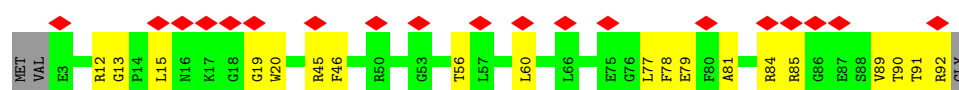
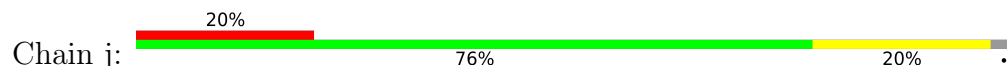
- Molecule 30: Subunit N7BM of NADH:Ubiquinone Oxidoreductase (Complex I)



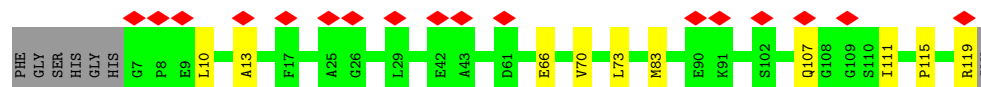
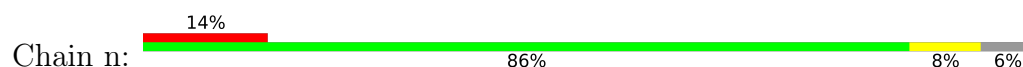
- Molecule 31: Subunit NUUM of NADH:Ubiquinone Oxidoreductase (Complex I)



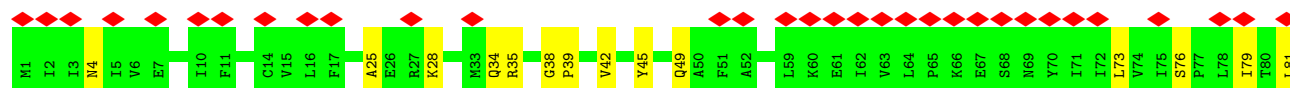
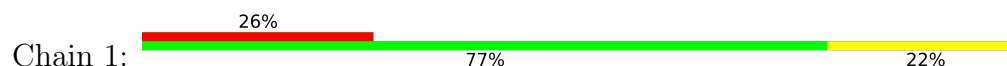
- Molecule 32: Subunit NB5M of NADH:Ubiquinone Oxidoreductase (Complex I)

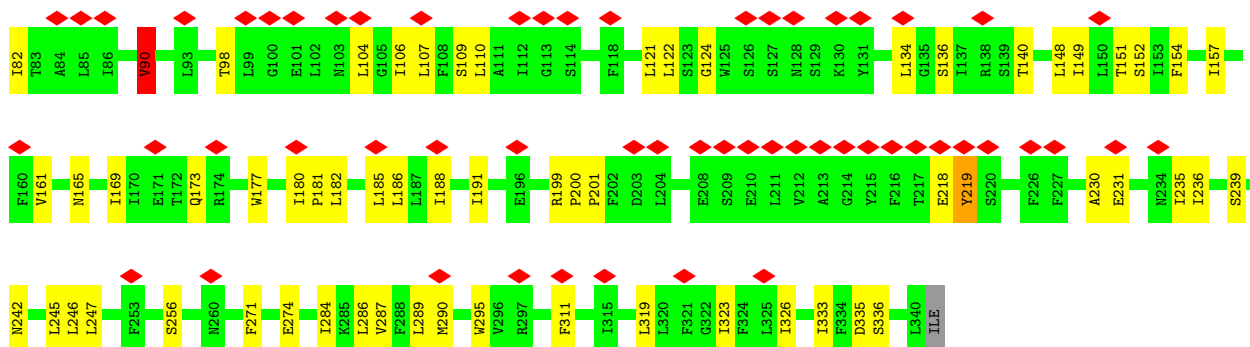


- Molecule 33: Subunit NUNM of NADH:Ubiquinone Oxidoreductase (Complex I)

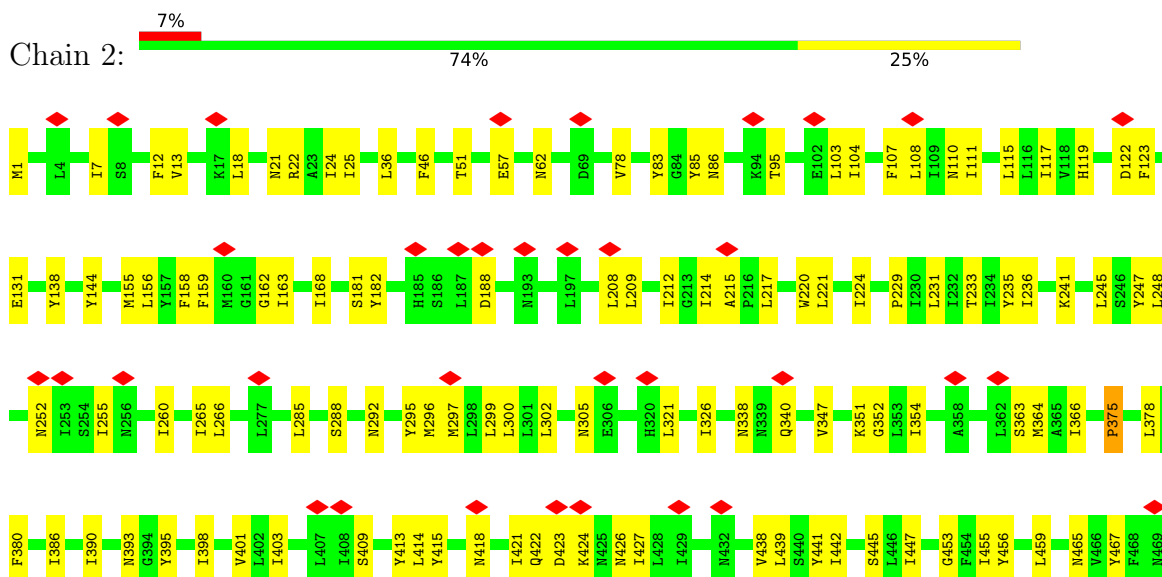


- Molecule 34: Subunit NU1M of NADH:Ubiquinone Oxidoreductase (Complex I)

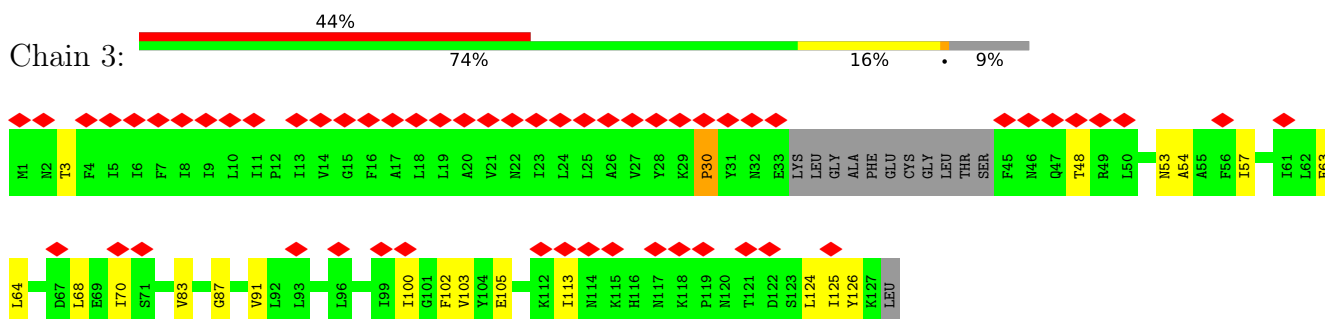




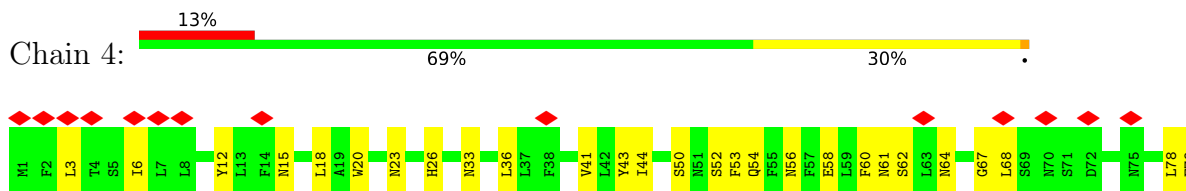
• Molecule 35: Subunit NU2M of NADH:Ubiquinone Oxidoreductase (Complex I)

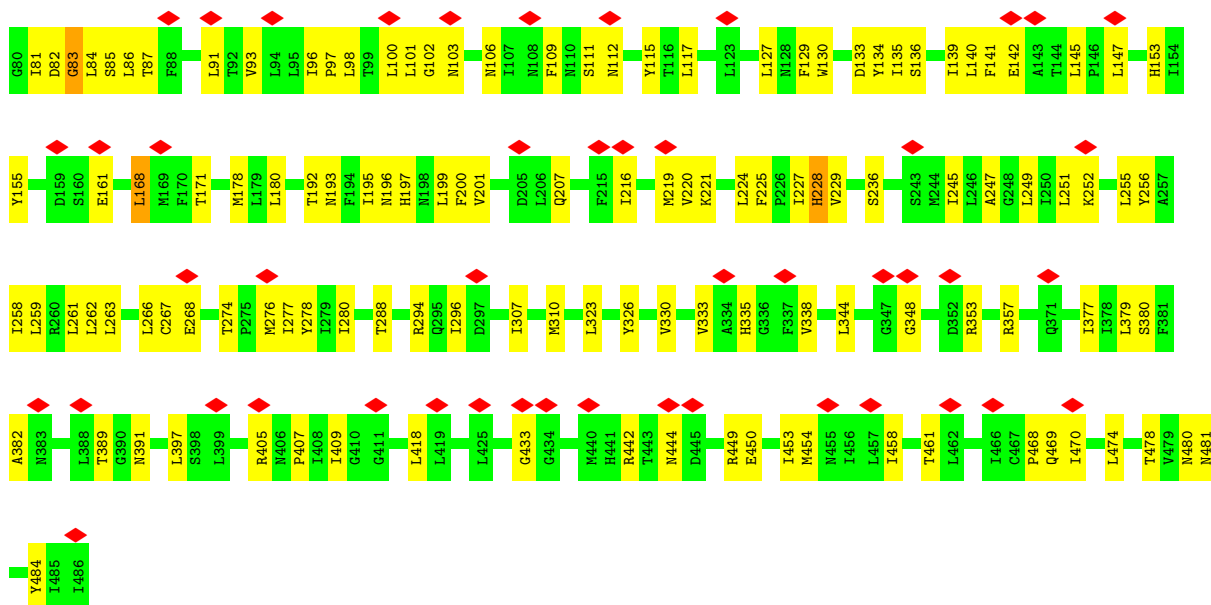


• Molecule 36: Subunit NU3M of NADH:Ubiquinone Oxidoreductase (Complex I)

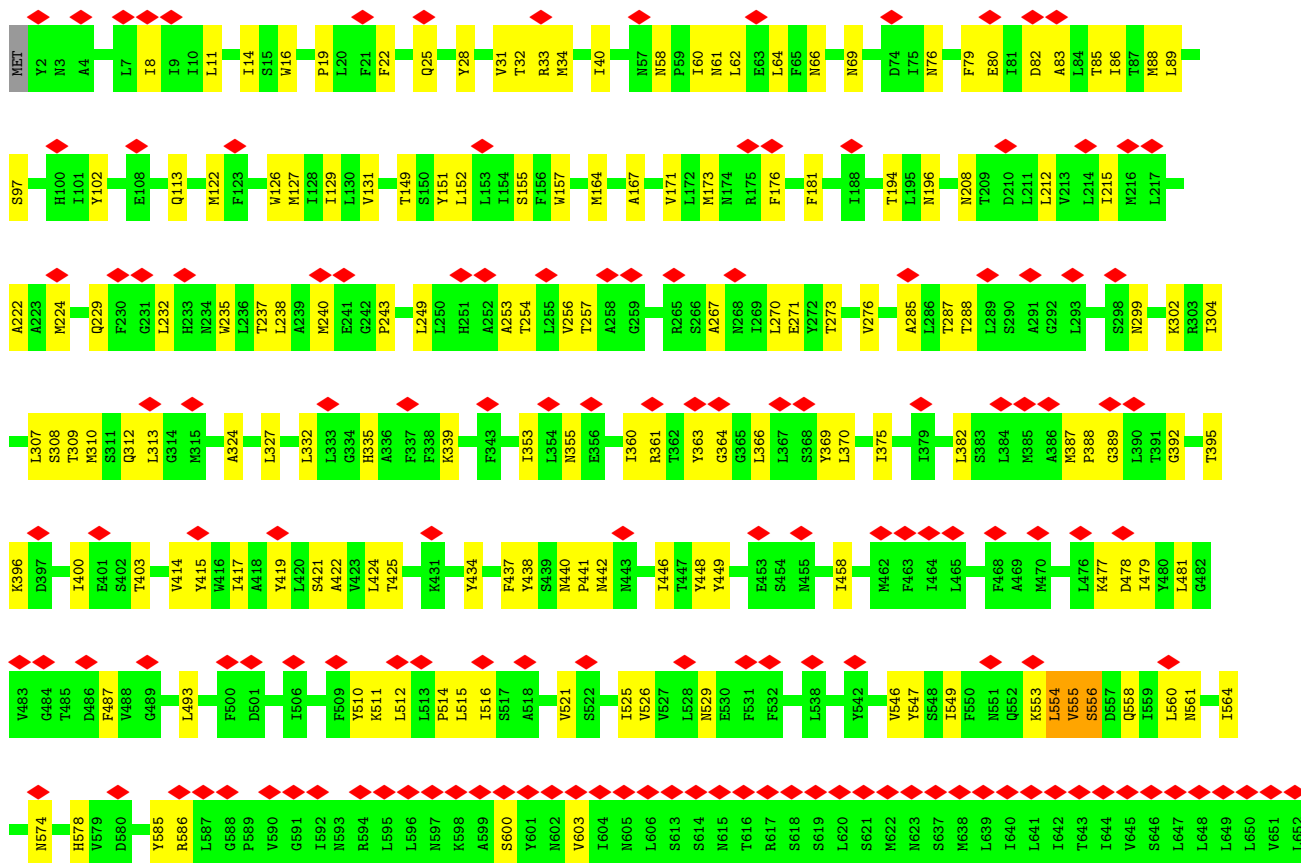


• Molecule 37: Subunit NU4M of NADH:Ubiquinone Oxidoreductase (Complex I)



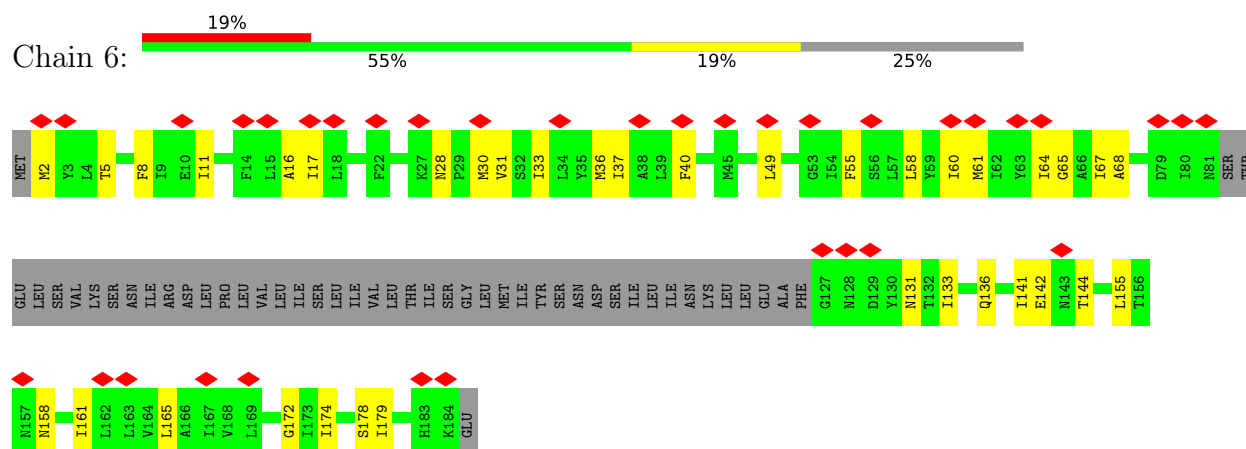


• Molecule 38: Subunit NU5M of NADH:Ubiquinone Oxidoreductase (Complex I)

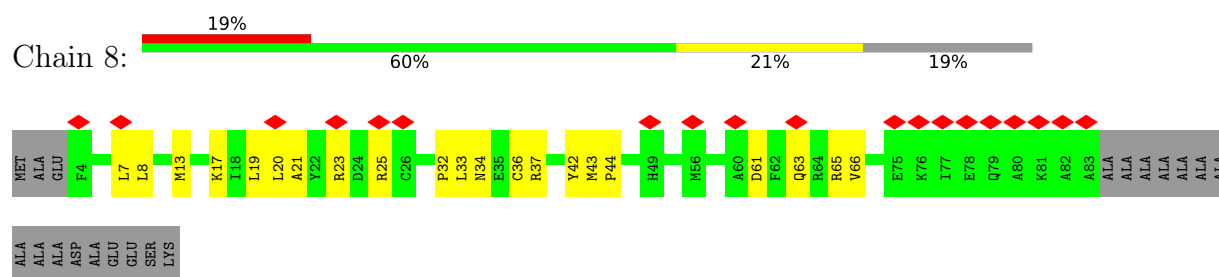


ASN
PHE
ILE
ILE
VAL
ILE
PRO
VAL
LEU
SER
SER
ILE
TTR
ILE
PHE
SER

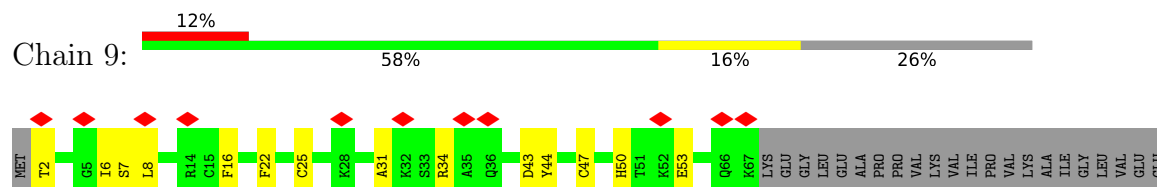
- Molecule 39: Subunit NU6M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 40: Subunit NB8M of NADH:Ubiquinone Oxidoreductase (Complex I)



- Molecule 41: Subunit NIPM of NADH:Ubiquinone Oxidoreductase (Complex I)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	145767	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	-2000	Depositor
Maximum defocus (nm)	-3000	Depositor
Magnification	45872	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.099	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	497.04, 497.04, 497.04	wwPDB
Map dimensions	456, 456, 456	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.42	0/5351	0.67	0/7262
2	B	0.41	0/3605	0.66	1/4865 (0.0%)
3	C	0.56	1/3122 (0.0%)	0.77	2/4225 (0.0%)
4	D	0.38	0/698	0.56	0/940
5	E	0.36	0/2709	0.66	0/3671
6	F	0.34	0/1011	0.67	0/1371
7	G	0.46	0/2040	0.69	2/2781 (0.1%)
8	H	0.35	0/1700	0.70	2/2307 (0.1%)
9	I	0.53	0/1557	0.75	1/2110 (0.0%)
10	J	0.32	0/805	0.71	0/1096
11	K	0.51	0/1385	0.70	0/1883
12	L	0.46	0/653	0.70	0/883
13	M	0.41	0/935	0.63	0/1268
14	O	0.27	0/598	0.53	0/813
15	P	0.40	0/1062	0.68	0/1427
16	Q	0.29	0/654	0.51	0/890
17	R	0.34	0/910	0.66	0/1229
18	S	0.34	0/1454	0.70	0/1960
19	U	0.42	0/1375	0.73	0/1856
20	W	0.35	0/998	0.61	0/1346
21	X	0.38	0/1339	0.61	0/1814
22	Z	0.38	0/1431	0.66	0/1955
23	a	0.35	0/1064	0.62	0/1439
24	b	0.40	0/503	0.63	0/679
25	c	0.27	0/364	0.48	0/491
26	d	0.41	0/777	0.59	0/1043
27	e	0.30	0/456	0.66	0/619
28	f	0.33	0/639	0.69	0/856
29	g	0.36	0/643	0.57	0/880
30	h	0.41	0/1168	0.72	1/1589 (0.1%)
31	i	0.31	0/666	0.54	0/907
32	j	0.37	0/745	0.60	1/1006 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	n	0.37	0/932	0.72	2/1264 (0.2%)
34	1	0.47	0/2755	0.80	2/3764 (0.1%)
35	2	0.54	0/3855	0.77	2/5252 (0.0%)
36	3	0.40	0/930	0.78	1/1269 (0.1%)
37	4	0.49	0/3950	0.77	1/5392 (0.0%)
38	5	0.41	0/5078	0.68	0/6934
39	6	0.44	0/1117	0.69	0/1524
40	8	0.32	0/676	0.65	0/904
41	9	0.38	0/537	0.61	0/717
All	All	0.43	1/62247 (0.0%)	0.69	18/84481 (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	A	0	2
3	C	0	3
5	E	0	1
8	H	0	1
11	K	0	1
18	S	0	1
22	Z	0	1
30	h	0	1
34	1	0	3
35	2	0	1
36	3	0	1
37	4	0	3
38	5	0	3
All	All	0	22

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	395	PRO	CA-C	9.02	1.56	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	n	10	LEU	CA-C-N	8.80	134.05	120.68
33	n	10	LEU	C-N-CA	8.80	134.05	120.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	3	30	PRO	N-CA-CB	7.29	110.91	103.25
3	C	395	PRO	O-C-N	7.11	124.58	121.31
3	C	92	PRO	N-CA-CB	6.39	109.96	103.25
32	j	19	GLY	N-CA-C	5.91	117.53	111.56
9	I	103	TYR	CA-CB-CG	-5.82	103.43	113.90
8	H	240	GLN	CA-C-N	5.77	132.56	121.54
8	H	240	GLN	C-N-CA	5.77	132.56	121.54
35	2	215	ALA	N-CA-C	5.44	121.83	109.81
37	4	67	GLY	N-CA-C	5.29	116.91	111.56
30	h	56	LEU	CA-CB-CG	5.22	134.58	116.30
35	2	375	PRO	N-CA-C	5.19	117.03	110.70
2	B	417	LEU	CA-CB-CG	-5.16	98.26	116.30
34	1	90	VAL	CA-C-N	-5.07	111.88	120.70
34	1	90	VAL	C-N-CA	-5.07	111.88	120.70
7	G	93	LYS	CA-C-N	5.03	131.14	121.54
7	G	93	LYS	C-N-CA	5.03	131.14	121.54

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	1	200	PRO	Peptide
34	1	219	TYR	Peptide
34	1	90	VAL	Peptide
35	2	338	ASN	Peptide
36	3	48	THR	Peptide
37	4	106	ASN	Peptide
37	4	228	HIS	Peptide
37	4	81	ILE	Peptide
38	5	253	ALA	Peptide
38	5	554	LEU	Peptide
38	5	64	LEU	Peptide
1	A	162	THR	Peptide
1	A	222	ASN	Peptide
3	C	106	GLY	Peptide
3	C	222	GLY	Peptide
3	C	229	TYR	Peptide
5	E	175	SER	Peptide
8	H	204	LYS	Peptide
11	K	180	CYS	Peptide
18	S	160	GLU	Peptide
22	Z	9	VAL	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
30	h	68	TYR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5258	0	5159	126	0
2	B	3528	0	3489	73	0
3	C	3052	0	3000	89	0
4	D	682	0	671	19	0
5	E	2650	0	2634	63	0
6	F	990	0	977	16	0
7	G	1978	0	1908	44	0
8	H	1664	0	1633	31	0
9	I	1519	0	1460	46	0
10	J	790	0	696	8	0
11	K	1347	0	1325	53	0
12	L	645	0	709	19	0
13	M	912	0	869	20	0
14	O	591	0	585	2	0
15	P	1037	0	1018	16	0
16	Q	648	0	637	14	0
17	R	885	0	893	20	0
18	S	1430	0	1463	23	0
19	U	1346	0	1327	24	0
20	W	974	0	987	19	0
21	X	1300	0	1276	13	0
22	Z	1390	0	1395	23	0
23	a	1030	0	967	20	0
24	b	490	0	509	4	0
25	c	353	0	343	8	0
26	d	761	0	721	17	0
27	e	436	0	426	11	0
28	f	629	0	640	13	0
29	g	617	0	597	9	0
30	h	1130	0	1084	25	0
31	i	646	0	630	13	0
32	j	724	0	706	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	n	904	0	873	11	0
34	1	2682	0	2766	54	0
35	2	3775	0	4005	74	0
36	3	911	0	956	17	0
37	4	3856	0	4054	110	0
38	5	4954	0	4974	107	0
39	6	1096	0	1182	28	0
40	8	662	0	667	17	0
41	9	528	0	515	9	0
42	A	16	0	0	5	0
42	B	8	0	0	2	0
42	I	16	0	0	5	0
42	K	8	0	0	2	0
43	A	4	0	0	0	0
43	H	4	0	0	2	0
44	B	31	0	19	2	0
45	E	48	0	26	2	0
46	M	1	0	0	0	0
47	O	30	0	32	1	0
All	All	60966	0	60803	1086	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 9.

All (1086) 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)
8:H:211:GLU:OE1	8:H:211:GLU:N	2.08	0.85
1:A:222:ASN:HD22	1:A:723:LYS:HE2	1.43	0.82
9:I:169:CYS:HA	42:I:301:SF4:S3	2.22	0.80
35:2:252:ASN:CG	35:2:255:ILE:HD11	2.08	0.77
11:K:86:CYS:HB2	11:K:121:GLY:HA2	1.67	0.76
20:W:112:LYS:HG3	33:n:119:ARG:HH12	1.51	0.76
2:B:393:TRP:HE1	2:B:417:LEU:HD13	1.50	0.75
18:S:69:PRO:HG3	18:S:129:TYR:HE1	1.52	0.75
11:K:100:GLN:HB2	11:K:105:ILE:HB	1.69	0.73
21:X:92:ALA:HA	21:X:147:ILE:HD11	1.71	0.73
1:A:233:CYS:HA	42:A:802:SF4:S2	2.28	0.72
30:h:3:SER:HA	30:h:7:ARG:HH21	1.52	0.72
1:A:326:ASP:HB2	5:E:29:GLN:HE22	1.56	0.71
35:2:217:LEU:HB3	35:2:220:TRP:HE1	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:TRP:HB2	2:B:113:ARG:HH22	1.55	0.70
30:h:33:GLY:HA3	30:h:46:TYR:HB3	1.75	0.69
3:C:265:LEU:HA	3:C:268:ASN:HD22	1.57	0.69
3:C:150:ASN:ND2	3:C:410:MET:SD	2.66	0.69
9:I:139:ILE:HD11	9:I:178:SER:HB3	1.74	0.69
18:S:171:LEU:HD12	37:4:33:ASN:HB3	1.75	0.69
35:2:252:ASN:ND2	35:2:255:ILE:HD11	2.06	0.69
35:2:363:SER:HB2	35:2:447:ILE:HD13	1.73	0.69
11:K:86:CYS:HB2	11:K:121:GLY:CA	2.21	0.68
37:4:219:MET:HG3	37:4:224:LEU:HB2	1.73	0.68
17:R:28:ASN:HD22	17:R:78:PRO:HA	1.58	0.68
37:4:50:SER:HB2	37:4:52:SER:HB3	1.76	0.68
17:R:79:ILE:HD11	38:5:361:ARG:HE	1.59	0.67
1:A:68:TYR:HB2	1:A:80:CYS:HB2	1.77	0.67
8:H:133:GLN:HE22	8:H:138:ASP:HB2	1.59	0.67
31:i:56:GLU:HB3	38:5:58:ASN:HD22	1.58	0.67
37:4:97:PRO:O	37:4:101:LEU:N	2.28	0.67
1:A:67:ARG:HD2	1:A:70:TYR:HB3	1.76	0.67
8:H:168:CYS:HA	43:H:301:FES:S1	2.35	0.66
1:A:69:CYS:SG	1:A:80:CYS:HB3	2.34	0.66
2:B:381:CYS:SG	2:B:382:GLY:N	2.68	0.66
30:h:74:GLU:HB3	30:h:77:TRP:HD1	1.60	0.66
1:A:126:LEU:HD21	1:A:144:LEU:HD21	1.78	0.66
34:1:106:ILE:HD11	34:1:169:ILE:HD11	1.77	0.66
38:5:235:TRP:HA	38:5:238:LEU:HB2	1.77	0.66
4:D:25:MET:O	4:D:29:HIS:ND1	2.29	0.66
7:G:186:TYR:O	7:G:211:ARG:NH2	2.28	0.66
12:L:61:ILE:HG23	36:3:68:LEU:HD11	1.78	0.65
5:E:126:VAL:HG12	5:E:164:ILE:HB	1.77	0.65
1:A:494:ALA:O	1:A:497:PHE:HB3	1.95	0.65
8:H:125:GLN:HB2	8:H:179:ALA:HB3	1.78	0.65
6:F:24:GLN:HB3	36:3:124:LEU:HD23	1.79	0.65
8:H:230:LYS:HG3	8:H:231:GLU:HG2	1.78	0.64
8:H:169:LEU:N	43:H:301:FES:S1	2.71	0.64
5:E:107:MET:HE1	5:E:115:ILE:HG13	1.79	0.64
29:g:60:GLN:HB3	33:n:111:ILE:HG13	1.78	0.64
33:n:73:LEU:HD11	37:4:78:LEU:HD11	1.79	0.64
3:C:284:GLN:HE22	6:F:105:ILE:HG21	1.60	0.64
20:W:63:LEU:HD11	39:6:141:ILE:HD12	1.79	0.64
34:1:110:LEU:HD21	34:1:151:THR:HG23	1.80	0.64
35:2:299:LEU:O	35:2:305:ASN:ND2	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:4:379:LEU:HD22	37:4:454:MET:HE1	1.77	0.64
5:E:115:ILE:HG12	5:E:151:ILE:HG22	1.79	0.64
21:X:13:ASN:HD21	21:X:167:GLU:HG2	1.63	0.64
4:D:39:ARG:HH12	19:U:106:HIS:HD2	1.46	0.63
9:I:215:GLU:HB3	30:h:100:ARG:HH21	1.63	0.63
35:2:78:VAL:HG11	35:2:321:LEU:HD21	1.80	0.63
38:5:240:MET:HG2	38:5:302:LYS:HB3	1.80	0.63
36:3:100:ILE:HA	36:3:103:VAL:HG22	1.78	0.63
23:a:75:ASP:OD1	37:4:294:ARG:NH1	2.31	0.63
19:U:61:GLN:HG2	33:n:119:ARG:H	1.63	0.63
8:H:73:PRO:O	8:H:76:ASP:HB3	1.99	0.63
9:I:44:GLY:H	9:I:46:SER:HB3	1.63	0.63
26:d:87:ARG:HE	37:4:201:VAL:HG12	1.64	0.63
1:A:73:LYS:HE3	1:A:290:GLU:HB2	1.81	0.62
3:C:224:ARG:HH12	11:K:184:SER:H	1.46	0.62
18:S:228:ALA:O	31:i:77:ARG:NH1	2.33	0.62
4:D:52:ARG:HG3	4:D:55:ARG:HH21	1.63	0.62
16:Q:58:ARG:NH2	16:Q:102:GLU:O	2.32	0.62
38:5:194:THR:HG22	38:5:196:ASN:H	1.64	0.62
11:K:147:MET:HA	11:K:177:VAL:HB	1.81	0.62
1:A:552:LEU:HB2	1:A:571:TYR:HA	1.81	0.62
2:B:384:CYS:HB3	2:B:386:PRO:HD2	1.81	0.62
5:E:309:TYR:OH	5:E:317:GLN:NE2	2.33	0.62
1:A:127:GLN:HE21	2:B:389:GLU:HB3	1.65	0.61
1:A:222:ASN:HD22	1:A:723:LYS:CE	2.11	0.61
2:B:371:ARG:HH12	8:H:167:GLU:HG2	1.64	0.61
8:H:211:GLU:H	8:H:211:GLU:CD	2.05	0.61
1:A:491:ARG:HG2	1:A:493:ASP:H	1.65	0.61
18:S:69:PRO:HG3	18:S:129:TYR:CE1	2.35	0.61
35:2:352:GLY:HA3	35:2:424:LYS:HB2	1.82	0.61
1:A:402:ALA:HA	1:A:427:ARG:HH12	1.66	0.61
11:K:85:CYS:HB2	42:K:301:SF4:S1	2.41	0.61
3:C:124:GLU:OE1	3:C:466:ARG:NH1	2.34	0.61
8:H:235:VAL:HA	8:H:238:PHE:HB2	1.83	0.61
2:B:384:CYS:N	42:B:501:SF4:S4	2.73	0.61
9:I:187:THR:HG22	9:I:189:ASN:H	1.66	0.61
1:A:233:CYS:CB	42:A:802:SF4:S2	2.88	0.61
26:d:63:CYS:HB2	26:d:66:LEU:HB2	1.83	0.61
3:C:428:ARG:NH1	3:C:429:ALA:O	2.34	0.61
5:E:105:LEU:HB2	13:M:66:GLN:HG3	1.83	0.61
3:C:141:ARG:NH2	11:K:180:CYS:SG	2.73	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:42:VAL:HG21	34:1:49:GLN:HB2	1.81	0.60
38:5:85:THR:HG23	38:5:131:VAL:HG12	1.82	0.60
2:B:203:MET:HB3	8:H:113:MET:HB2	1.83	0.60
3:C:147:MET:SD	3:C:147:MET:N	2.73	0.60
3:C:163:ASN:HD22	22:Z:83:TYR:HA	1.66	0.60
11:K:93:VAL:HG21	11:K:187:LEU:HD23	1.83	0.60
28:f:72:SER:H	28:f:75:GLU:HB2	1.65	0.60
37:4:23:ASN:ND2	37:4:111:SER:OG	2.34	0.60
38:5:478:ASP:HB2	40:8:44:PRO:HG3	1.84	0.60
4:D:79:VAL:HG12	19:U:13:GLU:HB3	1.83	0.60
29:g:29:ALA:HB2	34:1:319:LEU:HD22	1.82	0.60
11:K:86:CYS:HB2	11:K:121:GLY:N	2.17	0.60
35:2:378:LEU:HD12	35:2:453:GLY:HA3	1.83	0.60
9:I:149:ALA:HA	9:I:160:THR:H	1.66	0.60
1:A:158:PHE:HZ	1:A:163:GLY:HA2	1.66	0.60
38:5:237:THR:HA	38:5:240:MET:HE1	1.82	0.60
37:4:109:PHE:O	37:4:155:TYR:OH	2.20	0.60
26:d:31:THR:HG23	37:4:480:ASN:HD22	1.67	0.60
31:i:24:SER:HB3	33:n:13:ALA:HB2	1.84	0.60
38:5:478:ASP:OD1	40:8:37:ARG:NH2	2.32	0.60
39:6:8:PHE:HB3	39:6:49:LEU:HD21	1.84	0.60
38:5:173:MET:HB3	38:5:232:LEU:HD13	1.83	0.59
1:A:217:LEU:HD22	1:A:219:LYS:HB3	1.83	0.59
1:A:458:THR:HG22	1:A:460:ALA:H	1.66	0.59
37:4:278:TYR:HB3	37:4:409:ILE:HG12	1.84	0.59
1:A:189:CYS:SG	1:A:190:VAL:N	2.75	0.59
7:G:71:LEU:HD21	7:G:96:LEU:HB2	1.84	0.59
27:e:47:PRO:HA	27:e:52:LEU:HD12	1.84	0.59
2:B:384:CYS:HB2	42:B:501:SF4:S4	2.42	0.59
26:d:53:GLU:OE2	31:i:53:ARG:NH1	2.35	0.59
26:d:62:ASP:O	31:i:68:ASN:ND2	2.35	0.59
16:Q:91:ASP:OD1	17:R:44:ARG:NH2	2.36	0.59
35:2:260:ILE:HG21	35:2:300:LEU:HD22	1.85	0.59
40:8:61:ASP:OD2	40:8:65:ARG:NH2	2.35	0.59
38:5:256:VAL:HG11	38:5:313:LEU:HD11	1.84	0.59
7:G:74:TYR:O	7:G:77:TYR:HB3	2.01	0.59
5:E:162:ARG:NH1	5:E:251:ASP:O	2.35	0.59
2:B:288:CYS:SG	2:B:289:THR:N	2.75	0.59
3:C:429:ALA:HB1	3:C:463:GLU:HB3	1.83	0.59
12:L:29:LEU:HD11	35:2:162:GLY:HA3	1.85	0.59
13:M:53:LYS:HD2	13:M:56:ILE:HD12	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:HA	1:A:197:ALA:HB3	1.85	0.58
34:1:181:PRO:HB2	34:1:182:LEU:HD12	1.85	0.58
1:A:556:ASP:OD2	1:A:705:ARG:NH2	2.36	0.58
30:h:45:PHE:HE2	30:h:77:TRP:HB3	1.69	0.58
20:W:56:ARG:HH12	34:1:335:ASP:HB3	1.68	0.58
23:a:118:LYS:NZ	23:a:120:ALA:O	2.36	0.58
1:A:484:VAL:HB	1:A:521:VAL:HG12	1.84	0.58
16:Q:90:LEU:HB3	17:R:44:ARG:HH12	1.68	0.58
20:W:60:ARG:NH1	29:g:56:SER:O	2.35	0.58
1:A:575:ASN:ND2	1:A:702:SER:O	2.36	0.58
5:E:150:ARG:HH12	11:K:41:MET:HB2	1.69	0.58
12:L:7:ILE:HD11	39:6:16:ALA:HB1	1.85	0.58
34:1:148:LEU:HB2	36:3:63:PHE:HE1	1.67	0.58
2:B:101:MET:O	2:B:113:ARG:NH1	2.36	0.58
6:F:63:LYS:HA	6:F:68:ARG:HD3	1.86	0.58
9:I:140:CYS:HA	42:I:301:SF4:S2	2.44	0.58
23:a:49:GLN:NE2	23:a:83:ASP:OD1	2.36	0.58
37:4:135:ILE:HG13	37:4:192:THR:HG21	1.86	0.58
11:K:48:PRO:O	11:K:202:LYS:NZ	2.37	0.57
32:j:85:ARG:HA	38:5:208:ASN:HB3	1.86	0.57
9:I:171:TYR:OH	9:I:192:TYR:OH	2.21	0.57
37:4:139:ILE:HD12	37:4:140:LEU:HG	1.86	0.57
37:4:236:SER:O	37:4:357:ARG:NH2	2.37	0.57
3:C:219:ARG:HD2	3:C:243:LEU:HD13	1.87	0.57
21:X:20:PRO:O	21:X:104:ASN:ND2	2.33	0.57
32:j:85:ARG:HG2	38:5:208:ASN:HA	1.87	0.57
8:H:216:ARG:NE	8:H:219:GLU:OE2	2.25	0.57
9:I:93:GLN:HE21	34:1:35:ARG:HD2	1.69	0.57
16:Q:94:GLU:HG2	25:c:9:TRP:HE1	1.69	0.57
25:c:20:ASN:ND2	38:5:369:TYR:OH	2.36	0.57
1:A:393:SER:HA	1:A:398:ASN:HD21	1.68	0.57
9:I:136:CYS:HB3	42:I:302:SF4:S3	2.44	0.57
27:e:27:THR:HA	38:5:375:ILE:HG21	1.85	0.57
38:5:62:LEU:HD11	38:5:79:PHE:HD2	1.70	0.57
11:K:94:SER:OG	11:K:100:GLN:NE2	2.37	0.57
7:G:92:TRP:NE1	22:Z:84:PRO:O	2.35	0.57
19:U:136:ARG:NH2	29:g:54:ASP:O	2.37	0.57
28:f:14:GLN:NE2	28:f:48:ASN:OD1	2.37	0.57
33:n:66:GLU:OE2	37:4:53:PHE:N	2.37	0.57
37:4:50:SER:OG	37:4:54:GLN:NE2	2.37	0.57
37:4:251:LEU:HD23	37:4:310:MET:HG3	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:5:224:MET:HG3	38:5:229:GLN:HB2	1.86	0.57
1:A:442:VAL:HG22	1:A:455:LEU:HB2	1.87	0.57
34:1:104:LEU:HD12	34:1:107:LEU:HD23	1.87	0.57
35:2:221:LEU:HA	35:2:224:ILE:HD12	1.85	0.57
37:4:101:LEU:O	37:4:449:ARG:NH1	2.35	0.57
1:A:187:THR:N	42:A:802:SF4:S4	2.76	0.56
30:h:59:ARG:HB2	30:h:83:TYR:HE1	1.69	0.56
16:Q:98:ALA:HB1	25:c:12:ARG:HH12	1.70	0.56
1:A:186:CYS:N	42:A:802:SF4:S4	2.79	0.56
1:A:233:CYS:HB2	42:A:802:SF4:S2	2.45	0.56
5:E:146:GLU:OE2	5:E:149:ARG:NH1	2.37	0.56
11:K:85:CYS:CB	42:K:301:SF4:S1	2.93	0.56
15:P:66:VAL:O	15:P:72:GLN:NE2	2.38	0.56
20:W:26:ARG:NH2	22:Z:30:ILE:O	2.37	0.56
35:2:95:THR:OG1	35:2:340:GLN:NE2	2.38	0.56
38:5:151:TYR:HB2	38:5:171:VAL:HG21	1.87	0.56
1:A:116:GLN:HG3	1:A:120:ASN:HD21	1.70	0.56
1:A:254:LYS:HB2	1:A:269:ARG:HD3	1.86	0.56
1:A:549:MET:HG3	1:A:568:PHE:HD2	1.70	0.56
2:B:127:CYS:SG	8:H:172:CYS:N	2.78	0.56
38:5:151:TYR:HD2	38:5:152:LEU:HD12	1.71	0.56
1:A:564:PRO:O	30:h:137:ARG:NH2	2.33	0.56
1:A:284:VAL:HG23	1:A:291:GLU:HB2	1.86	0.56
6:F:134:GLN:O	7:G:134:ARG:NH1	2.38	0.56
17:R:108:GLU:OE1	18:S:134:ARG:NH1	2.38	0.56
1:A:646:ARG:HE	1:A:657:VAL:HG13	1.69	0.56
1:A:717:PHE:HA	1:A:723:LYS:CD	2.36	0.56
3:C:85:ILE:HD11	3:C:102:LEU:HD12	1.88	0.56
24:b:45:GLY:O	24:b:48:LEU:HB2	2.06	0.56
11:K:206:MET:O	11:K:209:ARG:NH1	2.32	0.56
17:R:29:TRP:HE3	17:R:75:HIS:HD2	1.53	0.56
1:A:75:ALA:O	1:A:191:ARG:NH1	2.38	0.56
3:C:313:ALA:HB1	3:C:316:LYS:HB2	1.88	0.56
32:j:77:LEU:HA	32:j:91:THR:HG22	1.88	0.56
11:K:112:ARG:HH11	34:1:218:GLU:HG3	1.71	0.56
2:B:72:ASP:HB2	2:B:150:ALA:HA	1.87	0.55
6:F:136:VAL:O	7:G:134:ARG:NH1	2.38	0.55
31:i:36:ILE:O	31:i:40:LEU:N	2.38	0.55
1:A:415:THR:HG23	1:A:417:PRO:HD3	1.87	0.55
7:G:263:PRO:HG2	7:G:266:PHE:HB2	1.89	0.55
35:2:22:ARG:NH1	35:2:86:ASN:OD1	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:5:299:ASN:OD1	38:5:547:TYR:OH	2.23	0.55
38:5:421:SER:O	38:5:425:THR:N	2.39	0.55
33:n:107:GLN:HA	41:9:16:PHE:HZ	1.70	0.55
35:2:25:ILE:HG21	35:2:83:TYR:HB2	1.87	0.55
1:A:185:HIS:HB2	2:B:388:ARG:HH12	1.71	0.55
35:2:209:LEU:HB3	35:2:214:ILE:HG13	1.87	0.55
2:B:333:ILE:HG21	2:B:347:VAL:HG11	1.88	0.55
34:1:4:ASN:HB2	36:3:3:THR:HB	1.88	0.55
34:1:28:LYS:HD2	34:1:38:GLY:HA3	1.88	0.55
37:4:103:ASN:O	37:4:115:TYR:OH	2.22	0.55
2:B:134:ARG:CZ	8:H:217:ASP:OD2	2.55	0.55
22:Z:120:ASN:O	22:Z:125:GLY:N	2.40	0.55
26:d:42:LYS:HG2	26:d:45:ARG:HH12	1.71	0.55
35:2:13:VAL:HG22	35:2:24:ILE:HD13	1.87	0.55
37:4:91:LEU:HD23	37:4:333:VAL:HG23	1.88	0.55
2:B:367:ARG:HH21	2:B:402:ARG:HH12	1.55	0.55
20:W:117:ALA:HA	39:6:133:ILE:HB	1.89	0.55
38:5:66:ASN:HA	38:5:76:ASN:HD22	1.71	0.55
4:D:83:GLU:HG3	19:U:6:ALA:HB2	1.89	0.55
17:R:105:ASN:ND2	17:R:108:GLU:O	2.40	0.55
23:a:36:MET:SD	23:a:36:MET:N	2.79	0.55
3:C:179:GLU:HG3	3:C:346:ILE:HG21	1.89	0.55
12:L:57:ILE:HA	12:L:60:ILE:HD12	1.89	0.55
35:2:302:LEU:HD12	35:2:393:ASN:HD22	1.72	0.55
38:5:127:MET:HE3	38:5:254:THR:HB	1.89	0.55
2:B:327:PRO:HD3	2:B:435:TRP:HB3	1.89	0.54
19:U:153:ALA:O	34:1:256:SER:OG	2.25	0.54
38:5:422:ALA:O	38:5:425:THR:HB	2.06	0.54
1:A:83:CYS:SG	1:A:97:CYS:N	2.80	0.54
35:2:354:ILE:HB	35:2:421:ILE:HG22	1.88	0.54
1:A:392:ARG:NH1	1:A:663:GLU:OE2	2.38	0.54
17:R:101:ILE:HD11	37:4:444:ASN:HA	1.89	0.54
35:2:351:LYS:NZ	35:2:423:ASP:O	2.41	0.54
37:4:23:ASN:HA	37:4:112:ASN:HD21	1.72	0.54
5:E:30:ASP:HB2	15:P:121:LYS:HA	1.89	0.54
38:5:554:LEU:O	38:5:556:SER:N	2.39	0.54
2:B:120:ASP:O	44:B:502:FMN:N3	2.39	0.54
2:B:425:THR:HG21	2:B:430:GLY:HA3	1.90	0.54
17:R:71:TYR:O	17:R:74:ARG:NH1	2.38	0.54
34:1:185:LEU:HD12	34:1:188:ILE:HD11	1.88	0.54
3:C:121:ARG:HD3	11:K:157:TYR:CZ	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:5:446:ILE:HA	38:5:449:TYR:HD2	1.71	0.54
3:C:211:GLU:OE2	11:K:92:HIS:ND1	2.41	0.54
17:R:106:LEU:HD22	32:j:20:TRP:HB2	1.89	0.54
3:C:360:LYS:HB3	3:C:367:ASN:HD21	1.72	0.54
3:C:424:LYS:HZ1	7:G:127:THR:HG21	1.72	0.54
9:I:139:ILE:HD11	9:I:178:SER:CB	2.37	0.54
36:3:53:ASN:HD22	36:3:113:ILE:HG13	1.72	0.54
36:3:83:VAL:HB	36:3:87:GLY:HA3	1.90	0.54
38:5:257:THR:HG23	38:5:332:LEU:HD21	1.90	0.54
3:C:111:ARG:NH1	15:P:5:ALA:O	2.41	0.54
20:W:93:LYS:HA	20:W:103:VAL:HG21	1.90	0.54
38:5:16:TRP:CD1	38:5:122:MET:HB3	2.43	0.54
37:4:382:ALA:O	37:4:391:ASN:ND2	2.41	0.54
3:C:113:ASP:OD1	7:G:197:ARG:NH2	2.41	0.53
37:4:83:GLY:HA2	37:4:474:LEU:HB3	1.90	0.53
40:8:34:ASN:O	40:8:37:ARG:HB2	2.08	0.53
5:E:200:VAL:HA	5:E:259:PHE:HB2	1.89	0.53
5:E:205:MET:HB3	5:E:238:VAL:HG22	1.90	0.53
7:G:119:GLN:HB2	7:G:121:LYS:HE2	1.90	0.53
8:H:124:LEU:HB2	8:H:163:LEU:HA	1.91	0.53
26:d:24:ARG:NH2	26:d:27:GLN:OE1	2.41	0.53
5:E:38:LYS:HE2	13:M:24:TYR:HD2	1.74	0.53
27:e:9:LYS:O	38:5:449:TYR:OH	2.24	0.53
30:h:56:LEU:HA	30:h:83:TYR:HE2	1.73	0.53
34:1:186:LEU:HA	34:1:246:LEU:HD21	1.90	0.53
8:H:186:GLU:HB2	8:H:211:GLU:HB3	1.91	0.53
11:K:102:ARG:HA	34:1:39:PRO:HA	1.89	0.53
35:2:285:LEU:O	35:2:288:SER:OG	2.23	0.53
15:P:85:GLU:HB3	15:P:91:LYS:HG3	1.90	0.53
22:Z:92:LYS:NZ	22:Z:121:ILE:O	2.41	0.53
34:1:151:THR:HG22	36:3:70:ILE:HG21	1.90	0.53
3:C:194:ALA:HB1	3:C:199:ALA:HB3	1.88	0.53
9:I:102:TYR:O	9:I:106:GLU:N	2.37	0.53
18:S:227:ILE:HG12	26:d:44:VAL:HG22	1.90	0.53
38:5:40:ILE:HD13	38:5:97:SER:HB2	1.91	0.53
39:6:158:ASN:HB3	39:6:161:ILE:HD12	1.89	0.53
1:A:570:VAL:HG22	1:A:585:VAL:HB	1.90	0.53
6:F:46:LEU:HD13	6:F:104:VAL:HG22	1.91	0.53
41:9:50:HIS:HB3	41:9:53:GLU:HB3	1.90	0.53
31:i:56:GLU:OE2	40:8:17:LYS:NZ	2.39	0.53
34:1:199:ARG:NH2	34:1:231:GLU:OE2	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:5:212:LEU:HA	38:5:215:ILE:HD12	1.90	0.53
2:B:225:PRO:O	2:B:383:GLN:NE2	2.31	0.53
39:6:8:PHE:O	39:6:11:ILE:HB	2.09	0.53
2:B:178:ALA:HA	2:B:181:ALA:HB3	1.90	0.53
13:M:97:CYS:HB3	13:M:125:CYS:SG	2.49	0.53
38:5:271:GLU:HB3	38:5:493:LEU:HG	1.89	0.53
2:B:55:ALA:HB1	2:B:60:ASP:HB2	1.90	0.52
18:S:73:PHE:HB3	18:S:136:ILE:HG13	1.92	0.52
37:4:87:THR:O	37:4:91:LEU:N	2.41	0.52
37:4:153:HIS:HE1	37:4:161:GLU:HG2	1.74	0.52
1:A:207:ARG:NH2	8:H:112:THR:OG1	2.42	0.52
3:C:121:ARG:NH2	11:K:157:TYR:OH	2.41	0.52
1:A:199:ALA:HB2	1:A:223:THR:HB	1.92	0.52
1:A:419:ARG:HD3	1:A:694:ILE:HD11	1.91	0.52
18:S:91:LEU:HD23	18:S:94:ILE:HD12	1.92	0.52
19:U:58:GLU:O	19:U:61:GLN:NE2	2.42	0.52
28:f:10:PHE:HB3	28:f:54:VAL:HG22	1.92	0.52
35:2:85:TYR:HB2	35:2:439:LEU:HD12	1.92	0.52
38:5:392:GLY:HA2	38:5:395:THR:HG22	1.90	0.52
40:8:33:LEU:O	40:8:36:CYS:HB3	2.09	0.52
1:A:348:ALA:HA	1:A:551:TRP:HB3	1.91	0.52
3:C:131:THR:O	3:C:135:ALA:N	2.43	0.52
3:C:393:SER:HA	3:C:420:GLU:HG2	1.91	0.52
4:D:14:ILE:HG21	34:1:290:MET:HE1	1.92	0.52
11:K:86:CYS:CB	11:K:121:GLY:N	2.73	0.52
25:c:19:THR:O	25:c:25:ASN:ND2	2.32	0.52
1:A:700:THR:H	1:A:704:SER:HB2	1.74	0.52
2:B:298:LEU:HB2	2:B:339:MET:HE3	1.92	0.52
3:C:126:LEU:HD23	7:G:216:LEU:HD11	1.92	0.52
12:L:62:LEU:HD13	35:2:131:GLU:HG3	1.92	0.52
37:4:15:ASN:HA	37:4:18:LEU:HD12	1.90	0.52
37:4:458:ILE:O	37:4:461:THR:OG1	2.28	0.52
1:A:385:PRO:O	1:A:387:HIS:ND1	2.43	0.52
4:D:40:PHE:O	34:1:165:ASN:ND2	2.42	0.52
4:D:64:GLN:HA	19:U:31:THR:HG21	1.91	0.52
13:M:86:PRO:O	13:M:88:ARG:NH2	2.42	0.52
37:4:117:LEU:HG	37:4:147:LEU:HD22	1.91	0.52
37:4:323:LEU:HD22	37:4:397:LEU:HD22	1.91	0.52
41:9:22:PHE:O	41:9:25:CYS:HB3	2.09	0.52
3:C:149:THR:HG21	3:C:405:ALA:HA	1.91	0.52
3:C:231:ARG:NH1	9:I:177:GLU:OE1	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:W:109:ASN:N	41:9:43:ASP:OD1	2.38	0.52
2:B:418:THR:HG21	2:B:438:GLN:HG3	1.92	0.52
5:E:99:LEU:HB2	9:I:197:ARG:HH11	1.74	0.52
18:S:162:GLU:OE1	18:S:164:TRP:NE1	2.42	0.52
30:h:85:VAL:HG22	30:h:87:THR:H	1.73	0.52
32:j:89:VAL:HG13	32:j:90:THR:HG23	1.92	0.52
15:P:55:LYS:HE2	15:P:99:TYR:HB3	1.91	0.52
22:Z:110:ASP:O	22:Z:114:GLY:N	2.39	0.52
35:2:366:ILE:HD11	35:2:447:ILE:HG23	1.92	0.52
38:5:434:TYR:HA	38:5:438:TYR:HB2	1.92	0.52
3:C:205:TRP:HE3	3:C:261:ILE:HG22	1.75	0.52
14:O:29:ARG:HD3	14:O:30:PRO:HD2	1.92	0.52
28:f:71:SER:HB3	28:f:75:GLU:HG3	1.91	0.52
35:2:103:LEU:HG	35:2:107:PHE:HE2	1.75	0.52
1:A:249:PRO:HA	1:A:252:LEU:HD23	1.92	0.51
3:C:417:ASP:HB3	3:C:419:SER:H	1.74	0.51
5:E:295:GLN:HE21	5:E:299:LYS:HE3	1.75	0.51
37:4:58:GLU:HG2	37:4:78:LEU:HD23	1.92	0.51
37:4:197:HIS:HA	37:4:200:PHE:HD2	1.75	0.51
1:A:357:GLU:HG3	1:A:645:VAL:HG11	1.91	0.51
19:U:36:LEU:HD23	19:U:101:LEU:HD21	1.91	0.51
23:a:93:ALA:HB1	38:5:555:VAL:HG11	1.92	0.51
29:g:47:ARG:NE	34:1:333:ILE:O	2.43	0.51
34:1:121:LEU:HD22	34:1:140:THR:HG21	1.91	0.51
35:2:108:LEU:HD23	35:2:111:ILE:HD12	1.92	0.51
38:5:312:GLN:HE22	38:5:396:LYS:HD2	1.75	0.51
2:B:322:GLY:N	2:B:355:ALA:O	2.42	0.51
7:G:95:GLU:HB3	7:G:154:ARG:HH12	1.74	0.51
10:J:147:LEU:HD12	10:J:152:LYS:HD3	1.91	0.51
21:X:50:LEU:HB3	21:X:78:ALA:HB1	1.92	0.51
5:E:22:ASN:ND2	7:G:235:PRO:O	2.41	0.51
7:G:88:GLY:O	7:G:99:HIS:HB2	2.10	0.51
7:G:226:GLU:O	7:G:229:ARG:NH1	2.37	0.51
18:S:63:LEU:HD13	18:S:125:LEU:HD12	1.92	0.51
18:S:183:MET:HE2	37:4:470:ILE:HG22	1.92	0.51
34:1:157:ILE:HG13	34:1:245:LEU:HD13	1.92	0.51
39:6:55:PHE:HA	39:6:58:LEU:HB2	1.92	0.51
2:B:473:VAL:HG22	2:B:478:VAL:HG12	1.91	0.51
19:U:86:ILE:HA	19:U:89:SER:HB3	1.92	0.51
21:X:32:VAL:HA	21:X:35:MET:HE3	1.91	0.51
37:4:56:ASN:HA	37:4:79:PHE:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:4:377:ILE:O	37:4:380:SER:OG	2.25	0.51
1:A:111:THR:HG22	1:A:113:ARG:H	1.75	0.51
3:C:320:ASP:HA	22:Z:182:HIS:HB2	1.92	0.51
12:L:23:ILE:HA	12:L:26:PHE:HD2	1.76	0.51
17:R:103:GLN:OE1	18:S:135:ARG:NH2	2.43	0.51
21:X:129:SER:OG	21:X:136:GLN:NE2	2.43	0.51
1:A:398:ASN:N	1:A:520:ASN:OD1	2.42	0.51
3:C:293:GLY:HA3	3:C:408:GLY:HA2	1.93	0.51
38:5:273:THR:HG22	38:5:276:VAL:H	1.75	0.51
1:A:159:THR:HG23	2:B:465:GLY:HA3	1.93	0.51
35:2:18:LEU:O	35:2:21:ASN:ND2	2.44	0.51
36:3:91:VAL:HG23	39:6:155:LEU:HD11	1.93	0.51
37:4:220:VAL:HA	37:4:227:ILE:HG21	1.93	0.51
37:4:274:THR:OG1	37:4:405:ARG:NH1	2.44	0.51
1:A:717:PHE:HA	1:A:723:LYS:HD3	1.93	0.51
30:h:27:ILE:HG13	30:h:29:ASP:H	1.76	0.51
32:j:13:GLY:O	35:2:427:ILE:N	2.41	0.51
2:B:43:ASN:HD21	2:B:50:TRP:HA	1.76	0.51
7:G:115:ASN:HB3	7:G:118:THR:HB	1.91	0.51
20:W:49:LEU:HD22	34:1:336:SER:HB2	1.93	0.51
11:K:56:ALA:HA	11:K:59:TYR:HD2	1.76	0.50
27:e:45:GLU:HB2	27:e:49:MET:HE3	1.93	0.50
3:C:297:ARG:NH2	3:C:339:GLU:OE2	2.45	0.50
5:E:55:THR:O	5:E:123:ASP:N	2.45	0.50
9:I:170:ILE:HG21	11:K:156:TYR:HD1	1.75	0.50
16:Q:61:ALA:O	27:e:11:ASN:ND2	2.44	0.50
39:6:8:PHE:HA	39:6:11:ILE:HD12	1.94	0.50
1:A:135:VAL:HA	9:I:157:ARG:HH11	1.77	0.50
9:I:190:VAL:HB	11:K:186:ALA:HB2	1.94	0.50
38:5:304:ILE:O	38:5:308:SER:OG	2.26	0.50
1:A:217:LEU:HD13	1:A:219:LYS:HD2	1.93	0.50
3:C:205:TRP:HE1	34:1:34:GLN:HA	1.77	0.50
7:G:120:TYR:HB3	7:G:144:PHE:HB3	1.92	0.50
33:n:83:MET:HE2	35:2:465:ASN:HB3	1.93	0.50
41:9:7:SER:OG	41:9:8:LEU:N	2.45	0.50
7:G:142:TYR:HB2	7:G:155:LEU:HB3	1.93	0.50
15:P:118:LYS:HB3	15:P:123:ARG:HG2	1.93	0.50
18:S:136:ILE:HG22	18:S:137:LEU:HG	1.94	0.50
23:a:47:PRO:HG2	23:a:50:LEU:HB2	1.93	0.50
37:4:335:HIS:HA	37:4:338:VAL:HG12	1.94	0.50
37:4:353:ARG:NH1	37:4:450:GLU:OE1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:254:PHE:HD2	3:C:344:LEU:HD12	1.76	0.50
5:E:170:ASN:HD21	5:E:319:LEU:HD12	1.76	0.50
1:A:197:ALA:HB1	1:A:223:THR:HG21	1.93	0.50
2:B:101:MET:HG3	2:B:113:ARG:HH11	1.76	0.50
5:E:214:LEU:O	5:E:218:ALA:N	2.44	0.50
12:L:26:PHE:HZ	35:2:155:MET:HE1	1.76	0.50
20:W:18:GLN:OE1	22:Z:12:LYS:NZ	2.45	0.50
37:4:98:LEU:HD12	37:4:453:ILE:HG23	1.93	0.50
1:A:575:ASN:ND2	1:A:706:SER:OG	2.45	0.50
9:I:132:ALA:O	9:I:157:ARG:NH2	2.45	0.50
9:I:217:GLU:HA	9:I:220:TYR:HD2	1.76	0.50
12:L:50:ILE:O	12:L:54:LEU:N	2.45	0.50
32:j:91:THR:HG23	32:j:92:ARG:HG3	1.94	0.50
35:2:403:ILE:HG13	37:4:180:LEU:HD11	1.93	0.50
37:4:389:THR:HG23	37:4:391:ASN:H	1.76	0.50
3:C:177:PHE:HA	3:C:180:ILE:HG12	1.93	0.50
4:D:39:ARG:HH12	19:U:106:HIS:CD2	2.27	0.50
7:G:243:ARG:NH1	9:I:137:GLU:OE2	2.45	0.50
9:I:123:TYR:HD2	9:I:127:GLU:HB3	1.77	0.50
11:K:86:CYS:CB	11:K:121:GLY:H	2.24	0.50
20:W:49:LEU:HD23	20:W:52:ILE:HD12	1.93	0.50
25:c:25:ASN:HA	25:c:28:LYS:HB2	1.93	0.50
35:2:12:PHE:HE2	35:2:24:ILE:HG12	1.77	0.50
39:6:37:ILE:HA	39:6:40:PHE:HD2	1.77	0.50
3:C:219:ARG:HB3	3:C:240:PRO:HG2	1.94	0.49
38:5:421:SER:HA	38:5:424:LEU:HB2	1.93	0.49
40:8:32:PRO:O	40:8:36:CYS:N	2.37	0.49
13:M:125:CYS:HB3	13:M:128:CYS:SG	2.52	0.49
16:Q:113:ASP:OD2	17:R:13:LYS:NZ	2.46	0.49
32:j:46:PHE:O	38:5:586:ARG:NH2	2.45	0.49
34:1:110:LEU:HD22	34:1:154:PHE:HD2	1.76	0.49
37:4:247:ALA:HA	37:4:251:LEU:HD13	1.94	0.49
40:8:8:LEU:HB2	40:8:13:MET:HE2	1.95	0.49
5:E:198:THR:HG22	5:E:256:ALA:H	1.76	0.49
16:Q:124:TYR:O	16:Q:128:GLN:NE2	2.45	0.49
38:5:149:THR:O	38:5:152:LEU:N	2.45	0.49
2:B:283:ASN:HD22	2:B:360:ASN:HB2	1.77	0.49
3:C:304:ASP:N	3:C:308:ASN:OD1	2.42	0.49
6:F:95:ILE:HG22	6:F:97:ALA:H	1.76	0.49
11:K:170:ILE:HG22	11:K:171:VAL:HG13	1.94	0.49
1:A:69:CYS:SG	1:A:80:CYS:N	2.85	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:ILE:HG23	2:B:255:THR:HG21	1.94	0.49
3:C:428:ARG:HG3	7:G:125:ASP:HB2	1.93	0.49
9:I:152:ARG:HD2	9:I:154:ASP:H	1.76	0.49
34:1:124:GLY:HA3	34:1:136:SER:HB2	1.94	0.49
35:2:144:TYR:HD2	35:2:229:PRO:HG3	1.77	0.49
3:C:305:ILE:HB	3:C:404:GLU:HB2	1.94	0.49
6:F:127:GLU:HG3	6:F:128:GLU:HG3	1.94	0.49
12:L:61:ILE:HD13	39:6:165:LEU:HD21	1.94	0.49
30:h:39:ASP:OD1	30:h:40:ILE:N	2.45	0.49
31:i:53:ARG:HH11	38:5:61:ASN:HD21	1.59	0.49
37:4:478:THR:HA	37:4:481:ASN:HB2	1.95	0.49
6:F:66:VAL:HG21	7:G:80:ALA:HB1	1.92	0.49
12:L:68:ALA:HB2	36:3:64:LEU:HD22	1.93	0.49
35:2:347:VAL:HG11	35:2:415:TYR:HE2	1.78	0.49
37:4:98:LEU:O	37:4:102:GLY:N	2.45	0.49
38:5:415:TYR:OH	38:5:510:TYR:O	2.30	0.49
1:A:363:LYS:NZ	1:A:534:ILE:O	2.46	0.49
2:B:86:GLY:N	2:B:92:PHE:O	2.46	0.49
15:P:63:HIS:HB3	15:P:75:LEU:HD21	1.93	0.49
28:f:70:VAL:HG22	28:f:75:GLU:HB3	1.94	0.49
38:5:419:TYR:HE1	38:5:514:PRO:HA	1.77	0.49
1:A:137:ASP:OD2	1:A:239:THR:OG1	2.31	0.49
2:B:130:ARG:O	2:B:134:ARG:N	2.35	0.49
2:B:246:ASN:ND2	2:B:248:GLU:HB3	2.27	0.49
4:D:55:ARG:O	4:D:77:ASN:ND2	2.46	0.49
7:G:176:ASN:HD21	15:P:2:ALA:HB3	1.77	0.49
11:K:202:LYS:HD3	11:K:206:MET:HE3	1.95	0.49
1:A:389:ILE:HG13	1:A:537:THR:HG21	1.95	0.49
9:I:91:LEU:HB2	34:1:295:TRP:HE1	1.78	0.49
11:K:76:PHE:HD2	11:K:105:ILE:HG12	1.78	0.49
37:4:196:ASN:HB3	37:4:200:PHE:HE2	1.77	0.49
37:4:207:GLN:HE22	37:4:268:GLU:H	1.61	0.49
38:5:479:ILE:HG12	40:8:42:TYR:HD2	1.77	0.49
2:B:148:GLY:HA2	2:B:151:MET:HB2	1.94	0.48
21:X:113:ALA:O	21:X:117:ALA:N	2.45	0.48
37:4:145:LEU:HD21	37:4:171:THR:HG21	1.94	0.48
1:A:306:THR:HG23	1:A:307:GLN:HG3	1.95	0.48
1:A:601:ASN:OD1	1:A:604:GLY:N	2.46	0.48
3:C:211:GLU:HB3	11:K:97:ARG:HE	1.78	0.48
2:B:219:GLU:OE2	2:B:226:ARG:NH1	2.47	0.48
7:G:144:PHE:HB2	7:G:153:ILE:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:66:ALA:O	11:K:70:TRP:HB2	2.13	0.48
23:a:78:ASP:OD1	23:a:79:MET:N	2.46	0.48
26:d:17:TYR:HB3	37:4:199:LEU:HD22	1.95	0.48
30:h:29:ASP:OD1	30:h:30:THR:N	2.46	0.48
2:B:140:LEU:HD13	2:B:247:VAL:HG23	1.95	0.48
16:Q:97:MET:HE3	17:R:23:LEU:HB2	1.95	0.48
28:f:37:ASN:HB3	28:f:40:THR:HG22	1.94	0.48
30:h:48:THR:HG22	30:h:50:HIS:H	1.78	0.48
1:A:455:LEU:HD13	1:A:465:ALA:HB1	1.96	0.48
6:F:108:HIS:HE1	36:3:126:TYR:CG	2.31	0.48
26:d:16:ASN:O	26:d:18:ASN:N	2.45	0.48
38:5:11:LEU:HA	38:5:14:ILE:HD12	1.95	0.48
38:5:414:VAL:HA	38:5:417:ILE:HB	1.95	0.48
40:8:19:LEU:HD13	40:8:21:ALA:H	1.78	0.48
1:A:627:ARG:HA	1:A:637:LEU:HD12	1.96	0.48
2:B:51:ASP:OD1	2:B:52:LEU:N	2.46	0.48
35:2:456:TYR:HD1	35:2:459:LEU:HD12	1.78	0.48
1:A:67:ARG:HA	1:A:82:MET:HB3	1.95	0.48
5:E:131:ARG:NH1	45:E:401:NDP:H2B	2.29	0.48
11:K:76:PHE:HE1	11:K:198:MET:HE1	1.79	0.48
13:M:90:VAL:HG21	13:M:95:ALA:HB2	1.96	0.48
18:S:85:GLU:HB3	18:S:89:ALA:HB2	1.96	0.48
37:4:178:MET:HE3	37:4:261:LEU:HD11	1.96	0.48
37:4:252:LYS:NZ	37:4:335:HIS:HD2	2.12	0.48
1:A:347:LYS:O	1:A:551:TRP:N	2.42	0.48
7:G:175:ALA:HA	7:G:178:PHE:HD2	1.79	0.48
8:H:124:LEU:HG	8:H:163:LEU:HD23	1.96	0.48
11:K:72:ARG:HD3	11:K:143:TRP:HH2	1.78	0.48
37:4:245:ILE:O	37:4:249:LEU:HB2	2.14	0.48
1:A:550:VAL:N	1:A:568:PHE:O	2.46	0.48
29:g:6:PRO:O	29:g:10:ASN:ND2	2.39	0.48
38:5:28:TYR:HA	38:5:31:VAL:HG12	1.95	0.48
1:A:392:ARG:HD2	28:f:45:ARG:HG3	1.96	0.48
2:B:341:PHE:HE1	2:B:351:LEU:HD12	1.78	0.48
21:X:85:VAL:HA	35:2:1:MET:HE1	1.95	0.48
35:2:375:PRO:HA	35:2:380:PHE:CG	2.49	0.48
37:4:134:TYR:HD2	37:4:192:THR:HA	1.78	0.48
38:5:366:LEU:H	38:5:437:PHE:HA	1.79	0.48
39:6:36:MET:HE3	39:6:40:PHE:HE2	1.79	0.48
1:A:459:HIS:CE1	1:A:497:PHE:HA	2.48	0.47
2:B:47:ASN:OD1	8:H:224:GLN:NE2	2.41	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:322:PRO:HG2	3:C:335:ILE:HG13	1.96	0.47
3:C:326:ASN:N	3:C:331:ASP:OD2	2.46	0.47
34:1:157:ILE:HG21	34:1:245:LEU:HB2	1.96	0.47
7:G:185:MET:HB3	7:G:210:LEU:HD12	1.95	0.47
23:a:127:TYR:HB2	23:a:130:LEU:HD23	1.95	0.47
37:4:53:PHE:O	37:4:56:ASN:ND2	2.47	0.47
37:4:258:ILE:HA	37:4:262:LEU:HD13	1.95	0.47
5:E:73:LEU:O	5:E:78:THR:OG1	2.29	0.47
27:e:48:ALA:O	38:5:511:LYS:NZ	2.34	0.47
34:1:149:ILE:HA	34:1:152:SER:HB3	1.94	0.47
35:2:438:VAL:HA	35:2:441:TYR:HB3	1.95	0.47
38:5:88:MET:HE3	38:5:88:MET:HB2	1.67	0.47
1:A:710:MET:HA	1:A:713:SER:HB3	1.96	0.47
7:G:71:LEU:HD22	7:G:91:VAL:HG21	1.95	0.47
8:H:123:HIS:CE1	8:H:125:GLN:HE21	2.31	0.47
9:I:97:ALA:HB3	22:Z:38:ASN:HD21	1.79	0.47
11:K:202:LYS:HE2	11:K:205:ARG:HH21	1.79	0.47
2:B:179:TYR:OH	2:B:197:VAL:O	2.32	0.47
2:B:393:TRP:NE1	2:B:417:LEU:HD13	2.26	0.47
5:E:48:ARG:NH1	5:E:97:GLY:O	2.48	0.47
7:G:202:ASP:HB3	7:G:205:PHE:HB2	1.97	0.47
10:J:143:ARG:HH12	35:2:255:ILE:HG22	1.79	0.47
11:K:160:SER:O	11:K:165:ARG:NH2	2.47	0.47
13:M:110:HIS:CD2	13:M:128:CYS:HB3	2.48	0.47
18:S:109:LEU:HG	37:4:12:TYR:HE2	1.79	0.47
22:Z:120:ASN:O	22:Z:124:GLY:N	2.47	0.47
1:A:479:ASN:OD1	1:A:516:TRP:NE1	2.48	0.47
3:C:120:HIS:CD2	7:G:200:MET:HB2	2.50	0.47
7:G:68:VAL:HG12	7:G:72:HIS:HE1	1.79	0.47
8:H:72:MET:O	8:H:114:TYR:OH	2.27	0.47
8:H:113:MET:HE1	8:H:125:GLN:HE22	1.79	0.47
22:Z:92:LYS:O	22:Z:95:THR:OG1	2.26	0.47
32:j:78:PHE:HB2	37:4:407:PRO:HG3	1.96	0.47
1:A:123:GLU:OE2	1:A:157:ARG:NE	2.47	0.47
1:A:346:PHE:HE2	1:A:366:THR:HG22	1.80	0.47
3:C:395:PRO:HA	7:G:255:VAL:HG21	1.96	0.47
4:D:81:LYS:HE3	39:6:136:GLN:HE21	1.80	0.47
5:E:29:GLN:HG2	15:P:120:LEU:HB3	1.96	0.47
9:I:93:GLN:NE2	34:1:35:ARG:HD2	2.29	0.47
11:K:84:ALA:C	11:K:86:CYS:N	2.73	0.47
18:S:194:TRP:HH2	26:d:32:ARG:HH21	1.61	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Z:45:ARG:HH12	30:h:83:TYR:HB3	1.79	0.47
22:Z:144:VAL:HG12	22:Z:145:LEU:HD12	1.96	0.47
23:a:137:THR:N	23:a:140:SER:OG	2.47	0.47
29:g:64:LEU:HD11	33:n:115:PRO:HG3	1.96	0.47
38:5:560:LEU:HA	38:5:564:ILE:HD12	1.96	0.47
39:6:60:ILE:HG23	39:6:64:ILE:HD11	1.96	0.47
1:A:302:ASP:HB3	1:A:707:SER:HB2	1.96	0.47
1:A:322:ASN:ND2	5:E:39:THR:OG1	2.41	0.47
5:E:70:THR:HA	5:E:73:LEU:HB3	1.96	0.47
19:U:51:ASP:OD2	29:g:67:ARG:NH2	2.47	0.47
38:5:388:PRO:HG3	38:5:515:LEU:HD21	1.97	0.47
5:E:162:ARG:NH2	5:E:248:ILE:O	2.36	0.47
37:4:225:PHE:HA	37:4:228:HIS:CE1	2.50	0.47
37:4:261:LEU:HB2	37:4:262:LEU:HD12	1.97	0.47
37:4:454:MET:HE3	37:4:458:ILE:HD11	1.96	0.47
38:5:307:LEU:HA	38:5:310:MET:HG2	1.97	0.47
39:6:142:GLU:HG3	39:6:144:THR:HG23	1.95	0.47
19:U:33:ALA:HB1	19:U:98:TRP:HB2	1.98	0.47
21:X:125:PRO:HG2	21:X:169:LYS:HE2	1.96	0.47
28:f:15:ASN:O	28:f:23:ARG:NH1	2.48	0.47
29:g:17:ARG:O	29:g:21:HIS:ND1	2.41	0.47
35:2:409:SER:HB2	35:2:413:TYR:HE2	1.80	0.47
9:I:100:THR:HG21	11:K:99:ASP:HB2	1.96	0.46
37:4:225:PHE:HA	37:4:228:HIS:HE1	1.80	0.46
38:5:32:THR:OG1	38:5:33:ARG:N	2.48	0.46
1:A:410:ILE:HG22	1:A:481:LEU:H	1.79	0.46
3:C:307:LYS:HE3	22:Z:160:LYS:HE2	1.97	0.46
5:E:120:ARG:HH11	13:M:29:ILE:HG22	1.81	0.46
37:4:258:ILE:HG13	37:4:262:LEU:HD22	1.97	0.46
37:4:418:LEU:HD12	38:5:176:PHE:HA	1.95	0.46
38:5:22:PHE:HA	38:5:25:GLN:HE21	1.80	0.46
9:I:118:HIS:NE2	9:I:169:CYS:SG	2.65	0.46
19:U:25:VAL:HG12	19:U:26:VAL:H	1.80	0.46
19:U:98:TRP:HA	19:U:101:LEU:HB3	1.96	0.46
35:2:51:THR:HG23	35:2:62:ASN:HB3	1.98	0.46
37:4:207:GLN:HE21	37:4:266:LEU:HA	1.80	0.46
38:5:22:PHE:HA	38:5:25:GLN:NE2	2.31	0.46
1:A:135:VAL:HG12	9:I:157:ARG:HD3	1.97	0.46
2:B:126:THR:HB	2:B:353:THR:HG21	1.98	0.46
3:C:112:SER:HB3	3:C:439:ASP:HB3	1.98	0.46
3:C:238:ASP:OD1	3:C:239:LEU:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:67:PRO:HB2	18:S:71:LYS:HD2	1.97	0.46
38:5:309:THR:HG23	38:5:335:HIS:HE1	1.81	0.46
1:A:294:ASN:HD21	1:A:697:PHE:HZ	1.61	0.46
3:C:148:MET:HE1	3:C:229:TYR:CD2	2.51	0.46
5:E:212:TRP:HE3	5:E:216:ARG:HD2	1.80	0.46
6:F:22:LEU:HB3	36:3:125:ILE:HD13	1.97	0.46
9:I:80:LEU:HD22	9:I:83:MET:HG3	1.96	0.46
21:X:23:ASP:OD1	21:X:24:ALA:N	2.48	0.46
30:h:20:TYR:OH	34:1:45:TYR:OH	2.26	0.46
34:1:284:ILE:HA	34:1:287:VAL:HG12	1.98	0.46
38:5:324:ALA:HB1	38:5:327:LEU:HD12	1.96	0.46
4:D:43:ASP:O	4:D:47:SER:N	2.47	0.46
5:E:206:PHE:HD1	5:E:235:PRO:HB2	1.80	0.46
35:2:414:LEU:HD11	37:4:168:LEU:HG	1.98	0.46
37:4:229:VAL:HG13	38:5:585:TYR:CE1	2.50	0.46
11:K:183:THR:O	11:K:187:LEU:N	2.43	0.46
35:2:247:TYR:HD2	35:2:248:LEU:HD22	1.81	0.46
37:4:433:GLY:HA3	38:5:164:MET:HG3	1.98	0.46
38:5:477:LYS:HG3	38:5:481:LEU:HD12	1.97	0.46
3:C:424:LYS:HD2	7:G:129:VAL:HG22	1.97	0.46
15:P:61:GLU:OE2	15:P:64:ARG:NH2	2.39	0.46
1:A:164:LYS:H	13:M:114:PHE:HE2	1.64	0.46
1:A:308:ARG:HD3	30:h:127:ILE:HG21	1.97	0.46
5:E:182:THR:HA	5:E:185:LEU:HD12	1.98	0.46
27:e:38:MET:HA	38:5:389:GLY:HA3	1.97	0.46
38:5:366:LEU:HD12	38:5:370:LEU:HD13	1.98	0.46
11:K:146:SER:HB2	11:K:173:VAL:HG11	1.98	0.46
34:1:90:VAL:HG13	34:1:98:THR:HG21	1.98	0.46
35:2:57:GLU:HB3	41:9:2:THR:HG23	1.98	0.46
3:C:187:LEU:HD21	3:C:209:GLU:HB2	1.98	0.45
3:C:319:PHE:CE1	3:C:342:GLN:HB3	2.51	0.45
4:D:37:ARG:NH1	34:1:274:GLU:OE1	2.49	0.45
5:E:52:THR:OG1	5:E:76:HIS:O	2.33	0.45
5:E:339:GLU:HB3	5:E:341:PRO:HD2	1.98	0.45
10:J:170:ARG:NH2	10:J:178:GLN:OE1	2.49	0.45
11:K:76:PHE:CD2	11:K:105:ILE:HG12	2.51	0.45
20:W:119:MET:HB3	39:6:133:ILE:HD11	1.98	0.45
31:i:29:ASN:HA	31:i:32:PHE:HD2	1.81	0.45
32:j:12:ARG:HD3	35:2:426:ASN:HB3	1.98	0.45
35:2:455:ILE:HG12	37:4:60:PHE:HE1	1.81	0.45
38:5:126:TRP:HE3	38:5:129:ILE:HD11	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1:79:ILE:HA	34:1:82:ILE:HG12	1.97	0.45
37:4:288:THR:HG21	37:4:307:ILE:HG21	1.97	0.45
38:5:249:LEU:O	38:5:254:THR:OG1	2.33	0.45
38:5:442:ASN:N	38:5:448:TYR:OH	2.37	0.45
1:A:696:ASN:HD22	1:A:699:MET:HE2	1.81	0.45
2:B:43:ASN:ND2	2:B:135:LYS:O	2.50	0.45
3:C:336:ARG:NH2	3:C:458:ASP:OD2	2.48	0.45
3:C:432:PHE:HA	3:C:464:VAL:HG13	1.99	0.45
5:E:247:ARG:HH21	15:P:108:GLY:HA2	1.82	0.45
9:I:213:LYS:HA	30:h:104:TYR:HE1	1.81	0.45
13:M:42:ARG:HE	13:M:44:SER:HB2	1.80	0.45
13:M:122:SER:HB2	13:M:131:ARG:HB3	1.98	0.45
47:O:201:ZMP:H19B	15:P:22:GLN:HG3	1.97	0.45
23:a:73:ASN:OD1	37:4:294:ARG:NH1	2.43	0.45
38:5:102:TYR:HE1	38:5:458:ILE:HG23	1.82	0.45
38:5:574:ASN:HA	38:5:578:HIS:HD2	1.82	0.45
5:E:64:PHE:HE2	5:E:238:VAL:HG21	1.81	0.45
7:G:68:VAL:O	7:G:72:HIS:ND1	2.50	0.45
11:K:84:ALA:C	11:K:86:CYS:H	2.23	0.45
21:X:124:GLU:HG2	21:X:126:TYR:H	1.81	0.45
37:4:64:ASN:ND2	37:4:68:LEU:O	2.35	0.45
38:5:181:PHE:HB2	38:5:222:ALA:HB2	1.98	0.45
5:E:177:SER:HB2	5:E:180:ASN:HB2	1.97	0.45
19:U:50:ASN:HB3	20:W:71:PRO:HG2	1.98	0.45
36:3:64:LEU:HD11	39:6:67:ILE:HG22	1.98	0.45
37:4:193:ASN:HD21	37:4:195:ILE:HB	1.82	0.45
37:4:259:LEU:HA	37:4:263:LEU:HD12	1.99	0.45
38:5:82:ASP:OD1	38:5:83:ALA:N	2.49	0.45
3:C:419:SER:OG	3:C:420:GLU:N	2.50	0.45
34:1:236:ILE:HA	34:1:239:SER:HB2	1.98	0.45
1:A:222:ASN:ND2	1:A:723:LYS:HE2	2.23	0.45
3:C:121:ARG:HH22	3:C:141:ARG:HB3	1.82	0.45
3:C:220:VAL:O	3:C:237:GLN:NE2	2.49	0.45
3:C:426:LYS:NZ	3:C:427:ILE:O	2.38	0.45
7:G:72:HIS:HB3	7:G:266:PHE:HD2	1.81	0.45
7:G:200:MET:HE2	7:G:200:MET:HB3	1.79	0.45
19:U:33:ALA:HB2	19:U:106:HIS:HE1	1.82	0.45
38:5:400:ILE:O	38:5:403:THR:OG1	2.23	0.45
5:E:234:ASN:ND2	5:E:263:GLY:O	2.50	0.45
12:L:6:ILE:HG21	39:6:17:ILE:HG12	1.99	0.45
19:U:83:ILE:HA	19:U:86:ILE:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:h:65:GLU:HG2	30:h:67:ASP:H	1.82	0.45
38:5:353:ILE:HG22	38:5:355:ASN:H	1.82	0.45
1:A:248:ARG:NH2	9:I:157:ARG:HH12	2.15	0.45
1:A:494:ALA:O	1:A:498:PHE:N	2.49	0.45
4:D:30:VAL:O	4:D:34:GLY:N	2.44	0.45
4:D:57:ASN:HD22	4:D:63:LYS:H	1.65	0.45
9:I:136:CYS:CB	42:I:302:SF4:S3	3.05	0.45
35:2:122:ASP:OD1	35:2:123:PHE:N	2.49	0.45
38:5:309:THR:HA	38:5:339:LYS:HE3	1.99	0.45
3:C:344:LEU:HD22	20:W:19:TRP:HB3	1.98	0.45
23:a:84:ARG:H	38:5:561:ASN:HD21	1.64	0.45
30:h:7:ARG:HH22	30:h:57:ARG:HH22	1.65	0.45
35:2:168:ILE:HG12	35:2:208:LEU:HD22	1.99	0.45
38:5:364:GLY:HA3	38:5:441:PRO:HA	1.99	0.45
40:8:7:LEU:HD13	40:8:25:ARG:HD3	1.99	0.45
1:A:377:ASP:HB3	1:A:528:ARG:HH11	1.82	0.44
5:E:203:ALA:HB3	5:E:236:VAL:HG23	2.00	0.44
8:H:127:CYS:SG	8:H:128:THR:N	2.91	0.44
10:J:169:ARG:NH1	26:d:13:ASP:OD1	2.46	0.44
18:S:163:ASP:HB3	37:4:26:HIS:HE1	1.81	0.44
38:5:229:GLN:HA	38:5:287:THR:HG21	2.00	0.44
2:B:213:SER:OG	2:B:223:GLY:O	2.35	0.44
6:F:63:LYS:O	6:F:69:GLN:NE2	2.50	0.44
17:R:89:LYS:HA	17:R:92:ARG:HD2	1.99	0.44
23:a:37:LEU:HA	32:j:45:ARG:HD3	1.98	0.44
30:h:113:THR:HG22	30:h:115:GLY:H	1.82	0.44
1:A:116:GLN:HG3	1:A:120:ASN:ND2	2.32	0.44
2:B:440:LEU:HD12	2:B:444:PHE:HB2	2.00	0.44
5:E:134:GLU:HG2	5:E:139:ASN:HA	1.99	0.44
5:E:224:VAL:HG21	5:E:289:LEU:HG	1.99	0.44
7:G:223:ARG:NH1	7:G:234:GLU:OE2	2.50	0.44
19:U:110:GLY:HA2	19:U:152:PRO:HB3	1.99	0.44
23:a:93:ALA:HA	23:a:96:TYR:HD2	1.82	0.44
38:5:546:VAL:HA	38:5:549:ILE:HD12	2.00	0.44
40:8:34:ASN:HA	40:8:37:ARG:HD2	1.98	0.44
1:A:205:SER:HB2	8:H:109:THR:HG21	2.00	0.44
16:Q:66:PHE:HD2	16:Q:69:VAL:HG13	1.82	0.44
16:Q:105:LEU:HD21	16:Q:125:VAL:HG13	2.00	0.44
37:4:82:ASP:O	37:4:85:SER:N	2.44	0.44
39:6:174:ILE:O	39:6:178:SER:N	2.47	0.44
1:A:122:MET:HE1	1:A:147:GLN:HG2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:115:ILE:HG21	5:E:151:ILE:HA	1.98	0.44
8:H:130:THR:HA	8:H:133:GLN:HB3	2.00	0.44
18:S:118:LEU:HD13	18:S:122:ASN:HD21	1.82	0.44
1:A:224:GLU:HG3	1:A:418:ARG:HG2	2.00	0.44
3:C:226:HIS:HD2	11:K:181:PRO:HB3	1.82	0.44
5:E:208:ARG:HH11	5:E:346:LYS:HE2	1.82	0.44
9:I:48:ALA:HB1	22:Z:161:GLN:HE21	1.82	0.44
25:c:18:GLN:HG3	27:e:13:PRO:HA	1.99	0.44
25:c:48:GLU:HG2	25:c:49:LYS:HG2	1.98	0.44
34:1:161:VAL:HG21	34:1:169:ILE:HG12	2.00	0.44
37:4:227:ILE:HG22	37:4:228:HIS:H	1.82	0.44
1:A:145:GLN:HG2	3:C:386:LEU:HD11	2.00	0.44
12:L:15:PHE:HZ	35:2:159:PHE:HB3	1.83	0.44
1:A:220:ASN:H	1:A:722:LYS:HB3	1.82	0.44
2:B:278:PHE:O	2:B:289:THR:HA	2.18	0.44
9:I:209:ALA:HB2	13:M:73:PRO:HB3	1.98	0.44
19:U:60:SER:HB2	19:U:63:SER:HB2	2.00	0.44
26:d:72:ASP:OD1	32:j:84:ARG:NH2	2.50	0.44
37:4:141:PHE:HZ	37:4:221:LYS:HG3	1.82	0.44
38:5:19:PRO:HG3	38:5:34:MET:HE1	2.00	0.44
1:A:36:GLU:HG2	1:A:49:GLU:HA	2.00	0.44
8:H:174:ASN:HB3	8:H:186:GLU:HB3	2.00	0.44
28:f:19:SER:O	28:f:23:ARG:N	2.49	0.44
39:6:30:MET:HG3	39:6:33:ILE:HD11	1.98	0.44
2:B:51:ASP:O	2:B:55:ALA:N	2.51	0.43
2:B:112:PRO:O	2:B:240:ARG:NE	2.47	0.43
5:E:124:ILE:HG22	5:E:162:ARG:HB2	1.99	0.43
12:L:41:LEU:HD13	12:L:41:LEU:HA	1.77	0.43
19:U:34:PRO:HG3	19:U:98:TRP:CE2	2.53	0.43
28:f:11:HIS:CE1	28:f:45:ARG:HB2	2.52	0.43
34:1:173:GLN:HE22	34:1:247:LEU:C	2.25	0.43
35:2:375:PRO:HG2	37:4:142:GLU:HB2	2.00	0.43
3:C:224:ARG:NH1	11:K:184:SER:H	2.14	0.43
34:1:177:TRP:HB2	34:1:180:ILE:HG22	1.99	0.43
35:2:212:ILE:HD12	35:2:241:LYS:HD3	2.00	0.43
2:B:40:ILE:HD13	2:B:275:THR:HG21	2.01	0.43
2:B:320:ILE:HB	2:B:357:ILE:HB	2.00	0.43
3:C:305:ILE:HG21	3:C:403:ILE:HA	1.99	0.43
5:E:57:THR:O	5:E:125:VAL:HA	2.18	0.43
11:K:138:MET:O	11:K:142:ARG:NH2	2.34	0.43
27:e:56:TYR:HD1	40:8:66:VAL:HG11	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:2:115:LEU:HD23	35:2:115:LEU:HA	1.85	0.43
35:2:418:ASN:O	35:2:422:GLN:NE2	2.52	0.43
38:5:122:MET:HE3	38:5:126:TRP:HE1	1.82	0.43
1:A:129:HIS:HD2	3:C:378:MET:HE2	1.83	0.43
1:A:157:ARG:H	1:A:157:ARG:HD3	1.83	0.43
1:A:248:ARG:HD3	1:A:249:PRO:HD2	2.00	0.43
2:B:400:ARG:HG3	2:B:405:GLN:HB2	2.01	0.43
3:C:291:LEU:HD23	3:C:291:LEU:HA	1.86	0.43
3:C:371:ARG:HD3	9:I:229:ARG:HB3	1.99	0.43
9:I:170:ILE:HG21	11:K:156:TYR:CD1	2.53	0.43
20:W:119:MET:N	39:6:131:ASN:O	2.51	0.43
31:i:75:ARG:NH1	31:i:81:ILE:O	2.51	0.43
37:4:255:LEU:HB2	37:4:310:MET:HE1	2.00	0.43
38:5:238:LEU:HD12	38:5:553:LYS:HE2	1.99	0.43
1:A:702:SER:O	1:A:706:SER:OG	2.33	0.43
2:B:255:THR:OG1	2:B:258:ARG:NH1	2.51	0.43
3:C:194:ALA:O	3:C:199:ALA:N	2.51	0.43
3:C:289:LEU:HD13	3:C:437:ALA:HB1	1.99	0.43
3:C:426:LYS:HD2	3:C:466:ARG:HH11	1.83	0.43
9:I:134:LYS:O	9:I:138:ALA:N	2.51	0.43
31:i:75:ARG:HG3	31:i:80:LYS:HD2	2.00	0.43
34:1:287:VAL:HA	34:1:290:MET:HG2	2.00	0.43
35:2:7:ILE:HD12	36:3:100:ILE:HD11	2.01	0.43
35:2:138:TYR:CE1	35:2:158:PHE:HA	2.53	0.43
35:2:181:SER:OG	35:2:182:TYR:N	2.52	0.43
35:2:245:LEU:HD13	35:2:296:MET:HG3	2.01	0.43
41:9:44:TYR:O	41:9:47:CYS:HB3	2.18	0.43
1:A:82:MET:HG2	1:A:147:GLN:NE2	2.33	0.43
3:C:121:ARG:H	3:C:121:ARG:HG2	1.59	0.43
3:C:239:LEU:HD22	3:C:243:LEU:HD23	2.00	0.43
4:D:10:PRO:HB2	34:1:25:ALA:HB2	2.00	0.43
5:E:155:VAL:HG13	5:E:160:ILE:HB	2.01	0.43
13:M:68:ASP:HB3	30:h:115:GLY:HA2	2.00	0.43
31:i:40:LEU:HD12	38:5:14:ILE:HD11	2.00	0.43
2:B:134:ARG:HD3	8:H:217:ASP:OD2	2.19	0.43
5:E:310:SER:HB2	5:E:313:GLN:HB2	1.99	0.43
9:I:152:ARG:HE	9:I:154:ASP:HB2	1.83	0.43
34:1:242:ASN:HB3	34:1:289:LEU:HD21	2.00	0.43
37:4:61:ASN:OD1	37:4:62:SER:N	2.50	0.43
37:4:330:VAL:HA	37:4:333:VAL:HG12	2.01	0.43
8:H:156:THR:HG22	8:H:158:ASP:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:194:LEU:HG	11:K:198:MET:HE3	2.00	0.43
18:S:91:LEU:HA	18:S:94:ILE:HD12	2.01	0.43
19:U:54:MET:HE3	33:n:115:PRO:HG2	2.01	0.43
28:f:24:GLN:HG2	28:f:27:LYS:HD2	2.01	0.43
31:i:54:ARG:HA	38:5:60:ILE:HD13	2.00	0.43
38:5:28:TYR:HB2	38:5:113:GLN:HE21	1.83	0.43
1:A:329:LEU:HA	1:A:332:ILE:HD12	2.00	0.43
7:G:67:HIS:O	7:G:70:ASP:HB3	2.19	0.43
7:G:126:ILE:HG12	7:G:178:PHE:HB3	2.01	0.43
21:X:63:VAL:O	35:2:86:ASN:ND2	2.45	0.43
23:a:85:PHE:HD2	38:5:558:GLN:HB2	1.84	0.43
23:a:130:LEU:HD22	23:a:133:GLU:HG3	2.01	0.43
35:2:233:THR:HA	35:2:236:ILE:HG13	2.01	0.43
37:4:127:LEU:HA	37:4:130:TRP:HD1	1.84	0.43
37:4:267:CYS:HB3	37:4:484:TYR:CG	2.54	0.43
37:4:276:MET:HE3	37:4:280:ILE:HD11	2.01	0.43
37:4:326:TYR:OH	37:4:468:PRO:O	2.36	0.43
38:5:360:ILE:HA	38:5:363:TYR:HD2	1.84	0.43
9:I:87:LEU:HB3	34:1:295:TRP:CZ2	2.54	0.43
35:2:46:PHE:HE2	35:2:467:TYR:HB3	1.83	0.43
36:3:54:ALA:HA	36:3:57:ILE:HG22	2.01	0.43
37:4:216:ILE:HA	37:4:219:MET:HB3	2.00	0.43
1:A:225:LEU:HB2	1:A:228:ASN:ND2	2.33	0.42
1:A:314:ILE:HG12	1:A:585:VAL:HG22	2.00	0.42
1:A:533:ASP:HA	28:f:45:ARG:HH11	1.84	0.42
2:B:118:ASN:N	2:B:245:THR:O	2.47	0.42
5:E:120:ARG:HH11	13:M:29:ILE:HA	1.84	0.42
36:3:64:LEU:O	36:3:68:LEU:HB2	2.19	0.42
37:4:98:LEU:O	37:4:101:LEU:HB3	2.18	0.42
38:5:155:SER:HB3	38:5:167:ALA:HB2	2.01	0.42
4:D:73:ALA:O	4:D:77:ASN:N	2.50	0.42
24:b:45:GLY:HA2	24:b:48:LEU:HD23	2.01	0.42
32:j:79:GLU:O	32:j:81:ALA:N	2.47	0.42
37:4:344:LEU:HA	37:4:348:GLY:HA3	2.00	0.42
2:B:146:LEU:HG	2:B:254:PRO:HB3	2.00	0.42
12:L:69:ILE:HD11	39:6:172:GLY:HA2	2.02	0.42
19:U:71:GLU:HA	19:U:74:ARG:HE	1.84	0.42
34:1:73:LEU:HD11	34:1:219:TYR:HB2	2.01	0.42
2:B:72:ASP:OD1	2:B:73:THR:N	2.53	0.42
3:C:134:GLN:NE2	9:I:139:ILE:HA	2.35	0.42
5:E:128:LEU:HB2	45:E:401:NDP:H4D	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:65:ASP:OD1	11:K:69:ASN:ND2	2.53	0.42
15:P:109:ARG:HG2	15:P:110:HIS:CD2	2.54	0.42
35:2:104:ILE:HA	35:2:107:PHE:HD2	1.83	0.42
39:6:2:MET:O	39:6:5:THR:OG1	2.28	0.42
39:6:28:ASN:HB2	39:6:31:VAL:HG23	2.01	0.42
2:B:353:THR:HG23	2:B:355:ALA:H	1.84	0.42
5:E:156:LYS:HB2	5:E:194:VAL:HB	2.00	0.42
18:S:172:TYR:CD1	37:4:36:LEU:HD11	2.55	0.42
24:b:50:LEU:O	24:b:53:VAL:HB	2.18	0.42
2:B:253:ALA:HA	2:B:256:ILE:HG22	2.00	0.42
4:D:55:ARG:HD2	4:D:78:HIS:HA	2.02	0.42
5:E:59:PHE:HB2	5:E:127:ASN:HA	2.02	0.42
5:E:155:VAL:HA	5:E:160:ILE:HD12	2.01	0.42
9:I:80:LEU:HB3	9:I:83:MET:HB2	2.02	0.42
34:1:76:SER:HB3	34:1:122:LEU:HD22	2.02	0.42
38:5:309:THR:HG23	38:5:335:HIS:CE1	2.54	0.42
1:A:158:PHE:HD1	2:B:393:TRP:HZ3	1.68	0.42
1:A:345:GLU:HA	1:A:547:PRO:HA	2.00	0.42
3:C:208:GLU:OE2	3:C:212:LYS:NZ	2.53	0.42
3:C:348:GLU:O	3:C:352:ASN:ND2	2.53	0.42
20:W:21:ARG:NH2	22:Z:173:PRO:HD2	2.33	0.42
22:Z:66:THR:O	22:Z:77:ARG:NH2	2.47	0.42
23:a:51:LYS:NZ	23:a:68:GLU:OE2	2.52	0.42
35:2:442:ILE:O	35:2:445:SER:OG	2.29	0.42
37:4:101:LEU:HD21	37:4:449:ARG:HB2	2.01	0.42
1:A:188:ARG:HG2	1:A:232:LEU:HG	2.02	0.42
1:A:550:VAL:HB	1:A:569:VAL:HG12	2.01	0.42
3:C:100:LEU:HA	3:C:114:PRO:HA	2.02	0.42
11:K:177:VAL:HG21	11:K:187:LEU:HD12	2.01	0.42
17:R:106:LEU:HD13	32:j:20:TRP:CG	2.54	0.42
32:j:56:THR:HA	32:j:60:LEU:HD23	2.01	0.42
34:1:199:ARG:HB3	34:1:201:PRO:HD2	2.02	0.42
37:4:41:VAL:HA	37:4:44:ILE:HD12	2.01	0.42
37:4:43:TYR:HE1	37:4:474:LEU:HD11	1.85	0.42
38:5:83:ALA:HB1	38:5:487:PHE:CE2	2.54	0.42
38:5:285:ALA:O	38:5:288:THR:OG1	2.30	0.42
1:A:183:CYS:SG	1:A:184:ILE:N	2.93	0.42
1:A:187:THR:HG22	1:A:191:ARG:HG3	2.02	0.42
2:B:264:PHE:CZ	2:B:274:GLY:HA3	2.55	0.42
3:C:148:MET:HE1	3:C:229:TYR:HD2	1.84	0.42
12:L:76:SER:HB2	39:6:179:ILE:HG21	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:e:9:LYS:HD2	27:e:12:GLY:HA3	2.00	0.42
34:1:106:ILE:HA	34:1:109:SER:HB3	2.02	0.42
35:2:395:TYR:HB3	35:2:398:ILE:HB	2.01	0.42
38:5:157:TRP:HZ3	38:5:243:PRO:HD3	1.85	0.42
1:A:83:CYS:SG	1:A:96:SER:N	2.92	0.42
2:B:219:GLU:HA	2:B:238:PHE:HE1	1.85	0.42
5:E:93:LEU:HD13	5:E:93:LEU:HA	1.86	0.42
11:K:97:ARG:HH11	30:h:56:LEU:HD11	1.84	0.42
12:L:50:ILE:HG13	41:9:6:ILE:HD13	2.02	0.42
14:O:35:ARG:HD2	14:O:80:PHE:HE1	1.85	0.42
16:Q:88:ASP:H	16:Q:91:ASP:HB2	1.85	0.42
25:c:26:ARG:NH2	38:5:440:ASN:OD1	2.53	0.42
38:5:240:MET:N	38:5:240:MET:SD	2.93	0.42
1:A:83:CYS:HB2	1:A:96:SER:HB3	2.02	0.41
4:D:26:GLN:HG2	34:1:271:PHE:O	2.20	0.41
5:E:107:MET:HE3	5:E:107:MET:HB2	1.76	0.41
5:E:247:ARG:NH1	5:E:334:ASP:O	2.53	0.41
16:Q:90:LEU:HB3	17:R:44:ARG:NH1	2.34	0.41
20:W:66:ARG:NH2	39:6:141:ILE:O	2.47	0.41
23:a:90:ASN:ND2	38:5:558:GLN:HE21	2.17	0.41
24:b:33:PRO:HA	24:b:36:TYR:HD2	1.85	0.41
26:d:20:HIS:HB2	33:n:70:VAL:HG11	2.01	0.41
37:4:274:THR:HA	37:4:277:ILE:HD12	2.02	0.41
41:9:31:ALA:HA	41:9:34:ARG:HG2	2.02	0.41
3:C:134:GLN:HE21	9:I:139:ILE:HA	1.84	0.41
6:F:98:GLY:HA2	9:I:51:PRO:HD3	2.01	0.41
8:H:109:THR:HA	8:H:116:ARG:NH2	2.34	0.41
13:M:34:GLU:HA	13:M:37:LYS:HE3	2.01	0.41
35:2:110:ASN:HD22	35:2:235:TYR:HE2	1.68	0.41
40:8:43:MET:HA	40:8:44:PRO:HD3	1.89	0.41
1:A:424:MET:O	1:A:428:ILE:HG12	2.20	0.41
5:E:117:GLU:OE2	13:M:66:GLN:N	2.48	0.41
5:E:177:SER:O	5:E:181:HIS:N	2.45	0.41
6:F:121:LYS:HG3	6:F:123:TRP:CZ2	2.55	0.41
26:d:20:HIS:CE1	26:d:24:ARG:HE	2.38	0.41
34:1:81:LEU:HA	34:1:230:ALA:HB2	2.02	0.41
38:5:310:MET:HA	38:5:313:LEU:HB2	2.02	0.41
40:8:37:ARG:HB3	40:8:42:TYR:CE1	2.56	0.41
3:C:435:LEU:HD13	3:C:459:LEU:HD13	2.03	0.41
3:C:459:LEU:HD23	3:C:459:LEU:HA	1.87	0.41
5:E:69:LEU:HA	5:E:69:LEU:HD12	1.87	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:PRO:HA	5:E:105:LEU:O	2.20	0.41
7:G:113:ARG:HE	7:G:171:LEU:HD13	1.84	0.41
13:M:39:ALA:HB3	13:M:42:ARG:H	1.86	0.41
22:Z:20:ILE:HD12	22:Z:20:ILE:HA	1.90	0.41
35:2:386:ILE:O	35:2:390:ILE:HG12	2.21	0.41
37:4:84:LEU:HB2	37:4:478:THR:HG21	2.02	0.41
37:4:93:VAL:HA	37:4:96:ILE:HG22	2.02	0.41
1:A:137:ASP:O	1:A:248:ARG:NH1	2.53	0.41
1:A:401:ILE:O	1:A:427:ARG:NH1	2.54	0.41
1:A:442:VAL:HG11	1:A:462:LEU:HD13	2.03	0.41
2:B:43:ASN:HB3	2:B:136:ASP:HB2	2.03	0.41
2:B:285:ASN:HB3	2:B:308:GLY:H	1.85	0.41
6:F:44:PRO:HA	6:F:47:ILE:HG22	2.02	0.41
10:J:142:ASP:OD1	10:J:143:ARG:N	2.53	0.41
23:a:130:LEU:HB3	23:a:133:GLU:HB2	2.02	0.41
30:h:23:GLN:HE22	30:h:31:LYS:H	1.68	0.41
32:j:15:LEU:HD13	35:2:427:ILE:HG21	2.02	0.41
34:1:323:ILE:HA	34:1:326:ILE:HG22	2.02	0.41
37:4:97:PRO:HA	37:4:100:LEU:HB3	2.02	0.41
1:A:228:ASN:HB3	1:A:292:TRP:CZ3	2.55	0.41
1:A:569:VAL:HG11	30:h:137:ARG:HH12	1.85	0.41
3:C:263:GLU:OE2	22:Z:34:ARG:NH2	2.53	0.41
3:C:400:TYR:HD1	3:C:413:TYR:HB2	1.85	0.41
11:K:83:LEU:HD12	11:K:84:ALA:HB2	2.02	0.41
12:L:15:PHE:CE2	35:2:163:ILE:HD11	2.55	0.41
17:R:59:LEU:O	17:R:63:LEU:HB2	2.20	0.41
23:a:29:PHE:HA	23:a:32:ALA:HB3	2.02	0.41
23:a:58:ASP:H	23:a:65:ASN:HA	1.86	0.41
30:h:79:PHE:CE2	30:h:85:VAL:HB	2.55	0.41
37:4:84:LEU:HG	37:4:256:TYR:HE1	1.85	0.41
38:5:521:VAL:O	38:5:525:ILE:HG12	2.21	0.41
38:5:526:VAL:HA	38:5:529:ASN:HD22	1.85	0.41
38:5:600:SER:HA	38:5:603:VAL:HG22	2.01	0.41
2:B:96:LEU:O	2:B:99:SER:OG	2.28	0.41
44:B:502:FMN:O4'	44:B:502:FMN:O2'	2.27	0.41
6:F:73:ASN:ND2	22:Z:149:GLY:O	2.54	0.41
11:K:202:LYS:HB3	11:K:205:ARG:NH2	2.36	0.41
18:S:108:ILE:HB	37:4:20:TRP:CD1	2.55	0.41
35:2:326:ILE:HD13	35:2:364:MET:HA	2.02	0.41
37:4:3:LEU:HA	37:4:6:ILE:HD12	2.01	0.41
38:5:8:ILE:HG21	38:5:89:LEU:HD21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:5:512:LEU:HG	38:5:516:ILE:HG13	2.03	0.41
1:A:131:LEU:HB2	13:M:113:ILE:HG22	2.03	0.41
1:A:496:ALA:HA	1:A:499:ASN:HB2	2.02	0.41
3:C:162:LEU:HD21	3:C:394:VAL:HG22	2.03	0.41
7:G:105:VAL:HG22	7:G:157:THR:HG21	2.03	0.41
9:I:99:TYR:HE2	34:1:35:ARG:HE	1.67	0.41
9:I:218:LEU:HD23	9:I:218:LEU:HA	1.89	0.41
11:K:73:GLN:HE22	11:K:199:ARG:HH11	1.68	0.41
34:1:191:ILE:HD12	34:1:311:PHE:HZ	1.85	0.41
1:A:282:PRO:HB3	1:A:293:ILE:HB	2.03	0.41
1:A:412:LEU:HG	1:A:441:SER:HA	2.02	0.41
2:B:62:TYR:CD2	2:B:63:LYS:HG2	2.56	0.41
2:B:134:ARG:NH2	8:H:217:ASP:OD2	2.54	0.41
2:B:210:GLU:CD	2:B:212:THR:H	2.29	0.41
3:C:295:MET:HE3	3:C:295:MET:HB2	1.99	0.41
3:C:341:ARG:NH2	20:W:21:ARG:HG2	2.35	0.41
3:C:400:TYR:HB2	3:C:413:TYR:HD1	1.86	0.41
3:C:402:ALA:HA	3:C:411:GLY:HA2	2.03	0.41
5:E:26:ASN:HB2	5:E:76:HIS:CD2	2.56	0.41
5:E:108:ASP:OD1	5:E:109:LEU:N	2.54	0.41
5:E:135:THR:OG1	5:E:138:PHE:N	2.54	0.41
7:G:139:GLU:HA	7:G:158:TYR:HA	2.03	0.41
21:X:152:ILE:HD11	35:2:119:HIS:CD2	2.55	0.41
22:Z:121:ILE:HG12	22:Z:126:VAL:HG22	2.03	0.41
36:3:102:PHE:O	36:3:105:GLU:HG3	2.21	0.41
37:4:133:ASP:H	37:4:136:SER:HG	1.67	0.41
37:4:266:LEU:HA	37:4:266:LEU:HD13	1.77	0.41
38:5:61:ASN:HB3	38:5:80:GLU:HG3	2.03	0.41
1:A:157:ARG:HH11	1:A:157:ARG:HD2	1.73	0.41
1:A:481:LEU:HD13	1:A:520:ASN:HD22	1.85	0.41
1:A:720:ASP:O	1:A:724:ASN:N	2.53	0.41
8:H:216:ARG:HB2	8:H:219:GLU:CD	2.45	0.41
10:J:101:ALA:HB2	10:J:129:CYS:HB2	2.03	0.41
12:L:62:LEU:HD23	12:L:62:LEU:HA	1.89	0.41
16:Q:105:LEU:HA	17:R:84:PHE:HE2	1.86	0.41
35:2:117:ILE:HG22	35:2:247:TYR:HB2	2.02	0.41
37:4:296:ILE:H	37:4:296:ILE:HG13	1.77	0.41
39:6:64:ILE:HA	39:6:68:ALA:HB3	2.02	0.41
40:8:20:LEU:HD13	40:8:23:ARG:HH21	1.86	0.41
1:A:81:ARG:NH2	2:B:426:ILE:HG13	2.35	0.40
1:A:457:ASN:OD1	1:A:690:LEU:N	2.49	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:ILE:HG23	2:B:356:VAL:HB	2.03	0.40
13:M:20:SER:HA	13:M:29:ILE:O	2.21	0.40
15:P:68:ASP:OD1	15:P:69:LEU:N	2.54	0.40
26:d:69:GLN:HG2	26:d:73:MET:HE2	2.03	0.40
2:B:141:VAL:HG22	2:B:175:ILE:HG12	2.02	0.40
3:C:432:PHE:HE1	7:G:200:MET:HE1	1.86	0.40
5:E:69:LEU:HD11	5:E:245:LEU:HD22	2.03	0.40
10:J:168:HIS:HB3	26:d:17:TYR:HD2	1.85	0.40
10:J:170:ARG:HG3	37:4:201:VAL:HG11	2.03	0.40
18:S:152:TRP:HD1	18:S:155:LYS:HG3	1.85	0.40
27:e:57:PRO:HD3	40:8:63:GLN:HG2	2.03	0.40
35:2:156:LEU:HD21	35:2:220:TRP:HB2	2.03	0.40
35:2:297:MET:HE2	35:2:297:MET:HB3	1.91	0.40
7:G:258:GLY:O	22:Z:85:GLN:NE2	2.54	0.40
9:I:183:ALA:HB3	42:I:302:SF4:S4	2.62	0.40
11:K:99:ASP:OD1	11:K:100:GLN:N	2.55	0.40
15:P:51:THR:HA	15:P:54:THR:HG22	2.03	0.40
17:R:102:MET:N	37:4:442:ARG:O	2.46	0.40
22:Z:131:ALA:O	22:Z:135:SER:N	2.55	0.40
34:1:231:GLU:O	34:1:235:ILE:HG12	2.21	0.40
35:2:265:ILE:HG23	35:2:401:VAL:HG21	2.04	0.40
35:2:292:ASN:HA	35:2:295:TYR:HD2	1.86	0.40
38:5:83:ALA:HA	38:5:86:ILE:HG22	2.03	0.40
39:6:61:MET:O	39:6:65:GLY:HA3	2.22	0.40
3:C:144:TYR:CD2	11:K:85:CYS:HA	2.55	0.40
3:C:356:ALA:HB2	20:W:8:LEU:HD11	2.03	0.40
11:K:150:CYS:HA	11:K:155:GLY:HA3	2.02	0.40
12:L:24:LEU:HA	12:L:27:ILE:HG12	2.03	0.40
19:U:95:ARG:O	19:U:99:GLN:HG2	2.21	0.40
28:f:55:PHE:HE1	28:f:65:LYS:HE2	1.87	0.40
37:4:84:LEU:HG	37:4:256:TYR:CE1	2.57	0.40
37:4:85:SER:OG	37:4:129:PHE:O	2.39	0.40
37:4:193:ASN:ND2	37:4:195:ILE:HB	2.37	0.40
37:4:193:ASN:HD22	37:4:196:ASN:ND2	2.20	0.40
38:5:267:ALA:HA	38:5:270:LEU:HD12	2.03	0.40
1:A:346:PHE:CE2	1:A:366:THR:HG22	2.57	0.40
2:B:454:LYS:O	2:B:458:GLU:HG2	2.20	0.40
3:C:136:LEU:HD22	3:C:232:PRO:HD3	2.02	0.40
5:E:67:SER:HA	5:E:93:LEU:HD11	2.03	0.40
7:G:51:ASP:OD1	7:G:52:GLU:N	2.55	0.40
7:G:72:HIS:CE1	7:G:263:PRO:HD3	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:111:GLN:HA	15:P:112:PRO:HD3	1.94	0.40
17:R:105:ASN:ND2	17:R:108:GLU:H	2.20	0.40
35:2:36:LEU:HA	35:2:36:LEU:HD23	1.90	0.40
37:4:469:GLN:HE21	38:5:69:ASN:H	1.70	0.40
38:5:382:LEU:HD22	38:5:387:MET:HG3	2.03	0.40
38:5:481:LEU:HA	38:5:481:LEU:HD23	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	690/728 (95%)	628 (91%)	61 (9%)	1 (0%)	48	80
2	B	454/488 (93%)	414 (91%)	40 (9%)	0	100	100
3	C	385/466 (83%)	347 (90%)	35 (9%)	3 (1%)	16	51
4	D	84/87 (97%)	74 (88%)	10 (12%)	0	100	100
5	E	329/375 (88%)	307 (93%)	22 (7%)	0	100	100
6	F	119/144 (83%)	108 (91%)	11 (9%)	0	100	100
7	G	237/281 (84%)	221 (93%)	16 (7%)	0	100	100
8	H	211/243 (87%)	184 (87%)	26 (12%)	1 (0%)	24	60
9	I	188/229 (82%)	171 (91%)	17 (9%)	0	100	100
10	J	110/198 (56%)	99 (90%)	11 (10%)	0	100	100
11	K	168/210 (80%)	149 (89%)	19 (11%)	0	100	100
12	L	81/89 (91%)	80 (99%)	1 (1%)	0	100	100
13	M	115/136 (85%)	97 (84%)	18 (16%)	0	100	100
14	O	75/109 (69%)	70 (93%)	5 (7%)	0	100	100
15	P	121/124 (98%)	114 (94%)	7 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	Q	83/132 (63%)	78 (94%)	5 (6%)	0	100	100
17	R	104/109 (95%)	92 (88%)	12 (12%)	0	100	100
18	S	168/249 (68%)	155 (92%)	12 (7%)	1 (1%)	21	57
19	U	169/172 (98%)	151 (89%)	17 (10%)	1 (1%)	21	57
20	W	119/123 (97%)	115 (97%)	4 (3%)	0	100	100
21	X	165/169 (98%)	155 (94%)	10 (6%)	0	100	100
22	Z	179/182 (98%)	160 (89%)	19 (11%)	0	100	100
23	a	122/149 (82%)	108 (88%)	14 (12%)	0	100	100
24	b	62/74 (84%)	61 (98%)	1 (2%)	0	100	100
25	c	42/60 (70%)	36 (86%)	6 (14%)	0	100	100
26	d	88/92 (96%)	82 (93%)	5 (6%)	1 (1%)	11	43
27	e	50/67 (75%)	46 (92%)	4 (8%)	0	100	100
28	f	78/87 (90%)	69 (88%)	9 (12%)	0	100	100
29	g	74/78 (95%)	61 (82%)	13 (18%)	0	100	100
30	h	134/138 (97%)	124 (92%)	9 (7%)	1 (1%)	18	54
31	i	81/90 (90%)	78 (96%)	3 (4%)	0	100	100
32	j	88/93 (95%)	79 (90%)	9 (10%)	0	100	100
33	n	111/120 (92%)	99 (89%)	12 (11%)	0	100	100
34	1	338/341 (99%)	303 (90%)	35 (10%)	0	100	100
35	2	467/469 (100%)	429 (92%)	37 (8%)	1 (0%)	43	75
36	3	112/128 (88%)	97 (87%)	14 (12%)	1 (1%)	14	48
37	4	484/486 (100%)	460 (95%)	23 (5%)	1 (0%)	43	75
38	5	626/655 (96%)	587 (94%)	37 (6%)	2 (0%)	36	69
39	6	134/185 (72%)	123 (92%)	11 (8%)	0	100	100
40	8	78/99 (79%)	72 (92%)	6 (8%)	0	100	100
41	9	64/89 (72%)	60 (94%)	4 (6%)	0	100	100
All	All	7587/8543 (89%)	6943 (92%)	630 (8%)	14 (0%)	44	75

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	3	30	PRO
38	5	555	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	660	ASP
18	S	161	LYS
3	C	92	PRO
35	2	188	ASP
38	5	556	SER
3	C	223	ALA
8	H	216	ARG
26	d	17	TYR
30	h	108	PRO
19	U	19	PRO
3	C	230	VAL
37	4	83	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	565/595 (95%)	565 (100%)	0	100	100
2	B	364/389 (94%)	364 (100%)	0	100	100
3	C	321/394 (82%)	321 (100%)	0	100	100
4	D	68/69 (99%)	68 (100%)	0	100	100
5	E	287/329 (87%)	286 (100%)	1 (0%)	86	85
6	F	109/129 (84%)	109 (100%)	0	100	100
7	G	216/245 (88%)	216 (100%)	0	100	100
8	H	188/212 (89%)	188 (100%)	0	100	100
9	I	156/187 (83%)	156 (100%)	0	100	100
10	J	62/147 (42%)	61 (98%)	1 (2%)	55	69
11	K	147/180 (82%)	146 (99%)	1 (1%)	76	79
12	L	72/77 (94%)	72 (100%)	0	100	100
13	M	97/115 (84%)	97 (100%)	0	100	100
14	O	65/91 (71%)	65 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	P	109/110 (99%)	109 (100%)	0	100	100
16	Q	72/111 (65%)	72 (100%)	0	100	100
17	R	97/100 (97%)	97 (100%)	0	100	100
18	S	149/211 (71%)	148 (99%)	1 (1%)	76	79
19	U	147/148 (99%)	147 (100%)	0	100	100
20	W	100/102 (98%)	100 (100%)	0	100	100
21	X	131/133 (98%)	131 (100%)	0	100	100
22	Z	147/148 (99%)	147 (100%)	0	100	100
23	a	108/129 (84%)	108 (100%)	0	100	100
24	b	50/59 (85%)	50 (100%)	0	100	100
25	c	30/45 (67%)	30 (100%)	0	100	100
26	d	83/85 (98%)	83 (100%)	0	100	100
27	e	44/55 (80%)	44 (100%)	0	100	100
28	f	69/73 (94%)	69 (100%)	0	100	100
29	g	62/64 (97%)	62 (100%)	0	100	100
30	h	121/123 (98%)	121 (100%)	0	100	100
31	i	64/68 (94%)	64 (100%)	0	100	100
32	j	71/73 (97%)	71 (100%)	0	100	100
33	n	97/102 (95%)	97 (100%)	0	100	100
34	1	292/302 (97%)	290 (99%)	2 (1%)	76	79
35	2	433/433 (100%)	431 (100%)	2 (0%)	81	82
36	3	98/114 (86%)	98 (100%)	0	100	100
37	4	434/434 (100%)	432 (100%)	2 (0%)	81	82
38	5	530/580 (91%)	530 (100%)	0	100	100
39	6	122/167 (73%)	122 (100%)	0	100	100
40	8	69/76 (91%)	69 (100%)	0	100	100
41	9	57/76 (75%)	57 (100%)	0	100	100
All	All	6503/7280 (89%)	6493 (100%)	10 (0%)	85	87

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	223	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	147	LEU
11	K	85	CYS
18	S	234	LEU
34	1	134	LEU
34	1	286	LEU
35	2	231	LEU
35	2	266	LEU
37	4	86	LEU
37	4	168	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	212	GLN
1	A	222	ASN
1	A	267	ASN
1	A	337	GLN
1	A	398	ASN
1	A	575	ASN
2	B	43	ASN
2	B	305	HIS
3	C	134	GLN
3	C	163	ASN
3	C	237	GLN
3	C	268	ASN
3	C	284	GLN
3	C	440	HIS
5	E	29	GLN
5	E	32	ASN
5	E	76	HIS
5	E	103	ASN
5	E	121	HIS
5	E	144	HIS
5	E	170	ASN
5	E	295	GLN
5	E	317	GLN
5	E	321	GLN
6	F	19	GLN
6	F	108	HIS
7	G	49	HIS
7	G	67	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	136	ASN
7	G	143	ASN
7	G	149	HIS
7	G	240	GLN
8	H	39	ASN
8	H	125	GLN
8	H	133	GLN
8	H	174	ASN
10	J	149	GLN
11	K	73	GLN
11	K	100	GLN
13	M	93	ASN
14	O	105	GLN
15	P	72	GLN
15	P	110	HIS
16	Q	120	GLN
17	R	75	HIS
18	S	201	GLN
18	S	238	GLN
19	U	87	ASN
19	U	97	HIS
19	U	106	HIS
20	W	6	GLN
21	X	13	ASN
21	X	145	HIS
22	Z	38	ASN
22	Z	161	GLN
23	a	61	GLN
23	a	87	HIS
23	a	90	ASN
23	a	146	GLN
24	b	51	HIS
24	b	52	ASN
26	d	34	GLN
27	e	23	HIS
28	f	14	GLN
28	f	28	ASN
28	f	62	HIS
30	h	23	GLN
30	h	55	HIS
30	h	78	HIS
32	j	27	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1	173	GLN
35	2	21	ASN
35	2	173	ASN
35	2	180	ASN
35	2	320	HIS
35	2	340	GLN
35	2	385	ASN
35	2	393	ASN
35	2	422	GLN
36	3	22	ASN
36	3	107	ASN
37	4	23	ASN
37	4	26	HIS
37	4	112	ASN
37	4	153	HIS
37	4	335	HIS
37	4	424	GLN
37	4	441	HIS
37	4	480	ASN
38	5	58	ASN
38	5	76	ASN
38	5	113	GLN
38	5	335	HIS
38	5	351	HIS
38	5	355	ASN
38	5	529	ASN
38	5	574	ASN
38	5	578	HIS
39	6	136	GLN
39	6	157	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z > 2$
43	FES	H	301	8	0,4,4	-	-	-		
45	NDP	E	401	-	51,52,52	3.59	22 (43%)	71,80,80	2.14	15 (21%)
42	SF4	I	301	9	0,12,12	-	-	-		
42	SF4	I	302	9	0,12,12	-	-	-		
43	FES	A	803	1	0,4,4	-	-	-		
44	FMN	B	502	-	33,33,33	2.86	12 (36%)	48,50,50	1.61	11 (22%)
42	SF4	A	801	1	0,12,12	-	-	-		
42	SF4	B	501	2	0,12,12	-	-	-		
42	SF4	A	802	1	0,12,12	-	-	-		
47	ZMP	O	201	14	24,29,36	1.84	6 (25%)	28,36,45	2.08	8 (28%)
42	SF4	K	301	11	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	FES	H	301	8	-	-	0/1/1/1
45	NDP	E	401	-	-	14/34/77/77	0/5/5/5
42	SF4	I	301	9	-	-	0/6/5/5
42	SF4	I	302	9	-	-	0/6/5/5
43	FES	A	803	1	-	-	0/1/1/1
44	FMN	B	502	-	-	7/18/18/18	0/3/3/3
42	SF4	A	801	1	-	-	0/6/5/5
42	SF4	B	501	2	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	SF4	A	802	1	-	-	0/6/5/5
47	ZMP	O	201	14	-	17/34/36/43	-
42	SF4	K	301	11	-	-	0/6/5/5

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	E	401	NDP	C2B-C1B	-8.26	1.32	1.53
45	E	401	NDP	O4B-C1B	7.68	1.59	1.42
45	E	401	NDP	O4D-C1D	7.62	1.59	1.42
45	E	401	NDP	C2D-C1D	-7.43	1.30	1.53
45	E	401	NDP	PN-O3	7.37	1.67	1.59
45	E	401	NDP	C6N-C5N	7.26	1.55	1.33
45	E	401	NDP	O4D-C4D	-6.97	1.29	1.45
44	B	502	FMN	C4A-N5	6.89	1.45	1.30
44	B	502	FMN	C10-N1	6.77	1.46	1.33
45	E	401	NDP	O4B-C4B	-6.47	1.30	1.45
44	B	502	FMN	C5A-N5	5.63	1.49	1.39
45	E	401	NDP	PA-O3	5.30	1.65	1.59
47	O	201	ZMP	C13-N1	5.20	1.45	1.33
44	B	502	FMN	C2-N1	5.18	1.48	1.36
47	O	201	ZMP	C16-N2	4.94	1.45	1.33
45	E	401	NDP	C2N-C3N	4.92	1.48	1.35
44	B	502	FMN	C2-N3	4.76	1.49	1.39
44	B	502	FMN	C9A-N10	4.52	1.49	1.41
45	E	401	NDP	C6A-N6A	4.51	1.45	1.34
45	E	401	NDP	P2B-O2B	4.24	1.67	1.59
45	E	401	NDP	O2D-C2D	4.02	1.52	1.43
45	E	401	NDP	C4N-C3N	3.86	1.57	1.50
44	B	502	FMN	C10-N10	3.85	1.45	1.37
44	B	502	FMN	C4-N3	3.80	1.46	1.38
45	E	401	NDP	C5A-C4A	-3.23	1.33	1.39
45	E	401	NDP	C7N-N7N	3.17	1.42	1.33
45	E	401	NDP	C6N-N1N	3.09	1.44	1.37
45	E	401	NDP	C4N-C5N	2.71	1.56	1.49
44	B	502	FMN	O2-C2	-2.66	1.19	1.24
45	E	401	NDP	C5D-C4D	2.61	1.59	1.51
44	B	502	FMN	O4-C4	-2.57	1.18	1.23
47	O	201	ZMP	C10-S1	2.53	1.82	1.76
45	E	401	NDP	C5A-N7A	-2.45	1.34	1.39
44	B	502	FMN	C7M-C7	2.41	1.55	1.51
47	O	201	ZMP	C9-C10	2.40	1.53	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	E	401	NDP	C8A-N9A	-2.32	1.33	1.37
47	O	201	ZMP	O3-C16	-2.31	1.19	1.23
47	O	201	ZMP	O2-C13	-2.25	1.18	1.23
44	B	502	FMN	C8M-C8	2.15	1.55	1.51
45	E	401	NDP	O3B-C3B	-2.06	1.37	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	O	201	ZMP	C9-C10-S1	6.89	121.61	113.40
45	E	401	NDP	C4A-N9A-C1B	-6.65	111.09	126.63
45	E	401	NDP	N6A-C6A-N1A	-6.38	104.18	118.38
45	E	401	NDP	C1B-N9A-C8A	5.94	140.28	127.09
45	E	401	NDP	N3A-C2A-N1A	-5.82	119.77	128.58
45	E	401	NDP	C5A-C6A-N6A	4.94	135.52	123.29
44	B	502	FMN	C7M-C7-C6	-4.72	111.25	119.57
45	E	401	NDP	C2B-C1B-N9A	-4.68	106.05	113.75
45	E	401	NDP	N9A-C8A-N7A	-4.57	107.45	113.94
45	E	401	NDP	C5A-C4A-N3A	-4.53	120.48	126.72
47	O	201	ZMP	O1-C10-C9	-4.06	119.29	123.98
44	B	502	FMN	C7M-C7-C8	3.62	128.16	120.76
44	B	502	FMN	C4-N3-C2	-3.50	119.43	125.64
45	E	401	NDP	C2A-N3A-C4A	3.41	120.15	111.83
47	O	201	ZMP	C11-S1-C10	3.39	111.86	101.84
45	E	401	NDP	C5A-N7A-C8A	2.98	108.14	103.45
47	O	201	ZMP	O1-C10-S1	-2.82	119.10	122.68
45	E	401	NDP	C4A-N9A-C8A	2.74	108.61	105.74
45	E	401	NDP	N3A-C4A-N9A	2.63	131.64	127.17
44	B	502	FMN	O4-C4-C4A	-2.62	119.60	126.53
44	B	502	FMN	C4A-C4-N3	2.48	119.55	113.25
44	B	502	FMN	C5A-C9A-N10	2.47	120.20	117.97
45	E	401	NDP	P2B-O2B-C2B	-2.42	116.96	123.43
45	E	401	NDP	C4A-C5A-N7A	-2.34	107.91	110.58
44	B	502	FMN	C9A-C5A-N5	-2.33	119.98	122.45
47	O	201	ZMP	C14-C13-N1	2.31	120.55	116.34
47	O	201	ZMP	C15-C14-C13	-2.27	108.61	112.39
47	O	201	ZMP	C17-C16-N2	2.20	120.67	116.48
44	B	502	FMN	C4-C4A-C10	2.17	120.66	116.93
45	E	401	NDP	C5B-C4B-C3B	-2.17	107.40	115.21
44	B	502	FMN	C4A-C10-N10	2.09	119.48	116.48
44	B	502	FMN	C5'-C4'-C3'	-2.06	108.33	112.22
44	B	502	FMN	C10-C4A-N5	-2.06	120.60	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	O	201	ZMP	C12-N1-C13	-2.01	119.08	122.82

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	B	502	FMN	N10-C1'-C2'-O2'
44	B	502	FMN	N10-C1'-C2'-C3'
44	B	502	FMN	C1'-C2'-C3'-O3'
44	B	502	FMN	C1'-C2'-C3'-C4'
44	B	502	FMN	O2'-C2'-C3'-O3'
44	B	502	FMN	O2'-C2'-C3'-C4'
45	E	401	NDP	C4B-C5B-O5B-PA
47	O	201	ZMP	O4-C17-C18-C21
47	O	201	ZMP	C16-C17-C18-C21
47	O	201	ZMP	O4-C17-C18-C19
47	O	201	ZMP	C16-C17-C18-C19
47	O	201	ZMP	C16-C17-C18-C20
47	O	201	ZMP	O3-C16-C17-C18
47	O	201	ZMP	C13-C14-C15-N2
47	O	201	ZMP	C12-C11-S1-C10
47	O	201	ZMP	O1-C10-S1-C11
47	O	201	ZMP	C9-C10-S1-C11
45	E	401	NDP	C3B-C2B-O2B-P2B
45	E	401	NDP	C3B-C4B-C5B-O5B
45	E	401	NDP	O4B-C4B-C5B-O5B
45	E	401	NDP	O4D-C4D-C5D-O5D
45	E	401	NDP	C2D-C1D-N1N-C6N
47	O	201	ZMP	O4-C17-C18-C20
47	O	201	ZMP	C5-C6-C7-C8
47	O	201	ZMP	N2-C16-C17-C18
47	O	201	ZMP	N2-C16-C17-O4
45	E	401	NDP	C2D-C1D-N1N-C2N
45	E	401	NDP	C5D-O5D-PN-O1N
45	E	401	NDP	O4D-C1D-N1N-C6N
45	E	401	NDP	C2B-O2B-P2B-O3X
45	E	401	NDP	O4D-C1D-N1N-C2N
47	O	201	ZMP	N1-C13-C14-C15
45	E	401	NDP	C2B-O2B-P2B-O1X
47	O	201	ZMP	O1-C10-C9-C8
47	O	201	ZMP	O2-C13-C14-C15
45	E	401	NDP	PA-O3-PN-O2N

Continued on next page...

Continued from previous page...

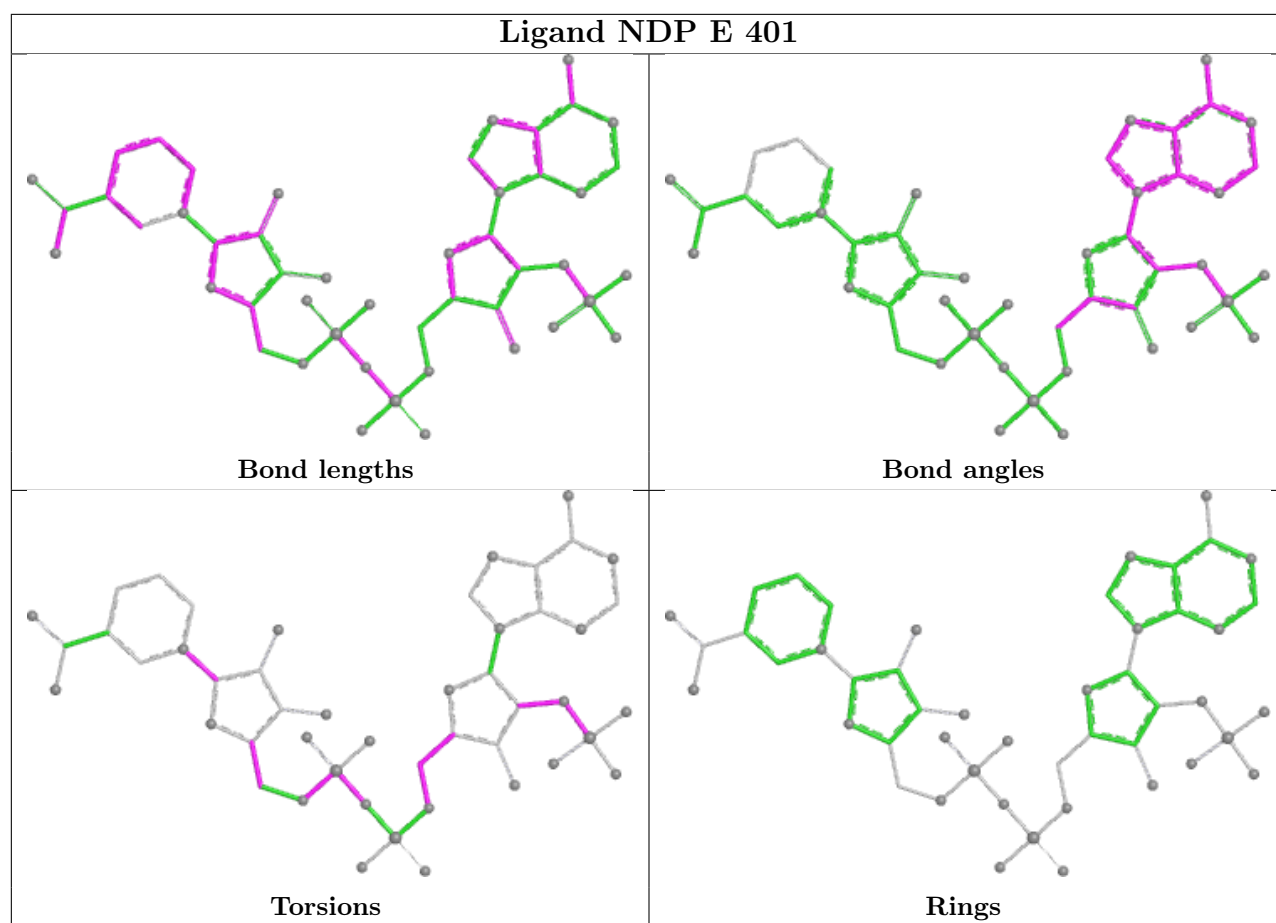
Mol	Chain	Res	Type	Atoms
44	B	502	FMN	O3'-C3'-C4'-C5'
45	E	401	NDP	C3D-C4D-C5D-O5D

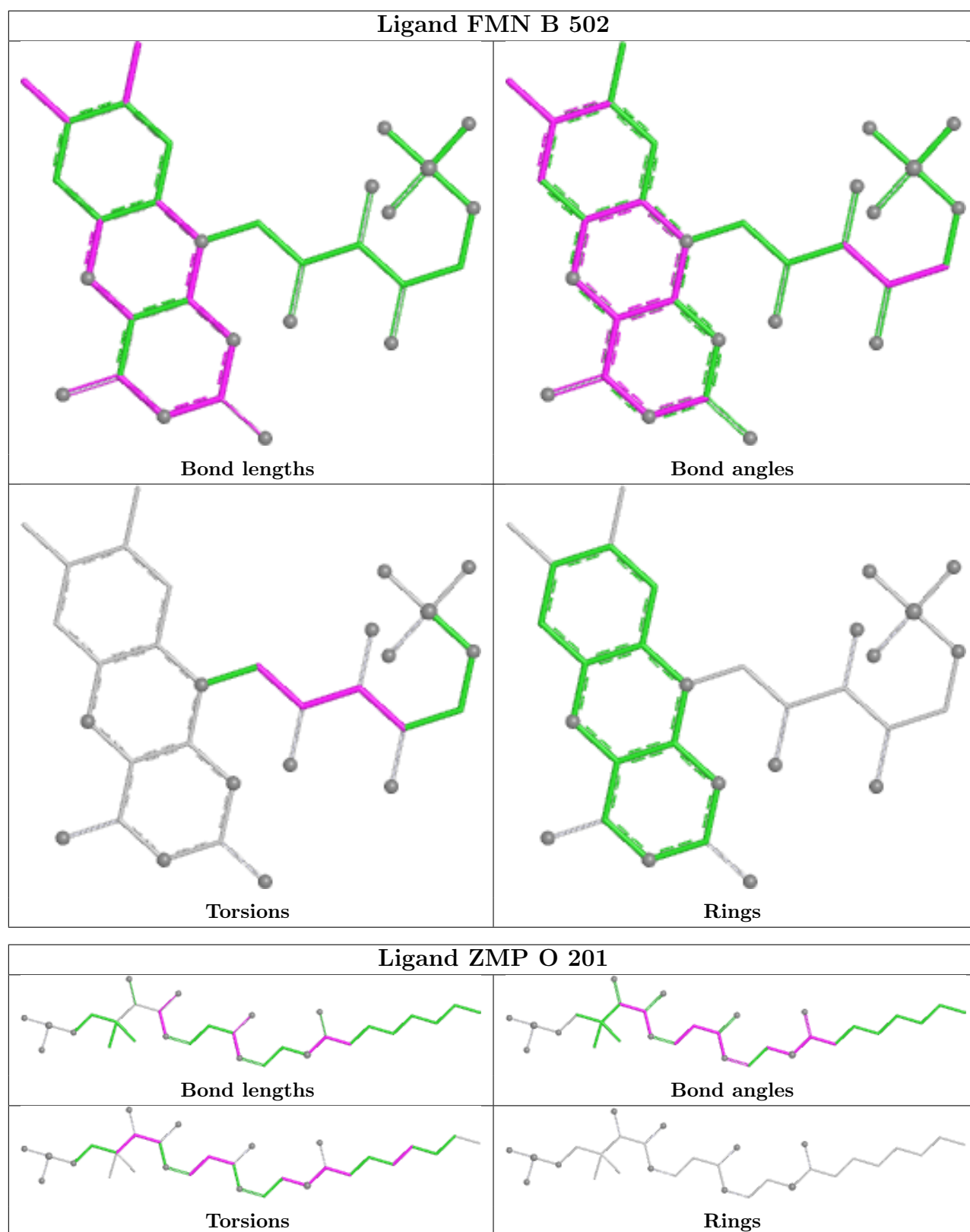
There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	H	301	FES	2	0
45	E	401	NDP	2	0
42	I	301	SF4	2	0
42	I	302	SF4	3	0
44	B	502	FMN	2	0
42	B	501	SF4	2	0
42	A	802	SF4	5	0
47	O	201	ZMP	1	0
42	K	301	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
38	5	2
10	J	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	623:ASN	C	637:SER	N	19.55
1	J	110:VAL	C	116:PRO	N	11.30
1	J	82:MET	C	94:TRP	N	10.82
1	5	606:LEU	C	613:SER	N	9.79

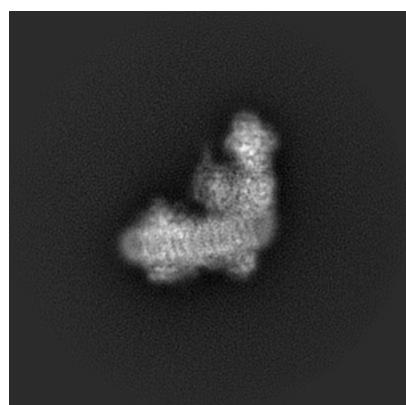
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4874. These allow visual inspection of the internal detail of the map and identification of artifacts.

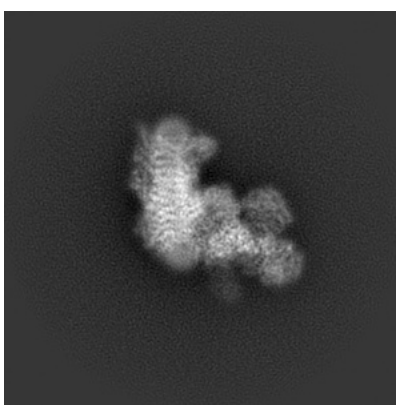
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

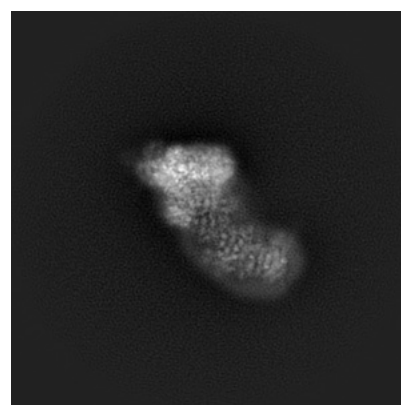
6.1.1 Primary map



X



Y

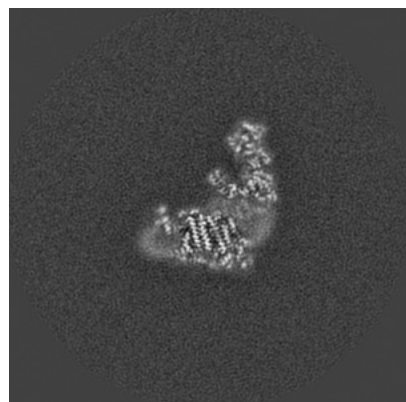


Z

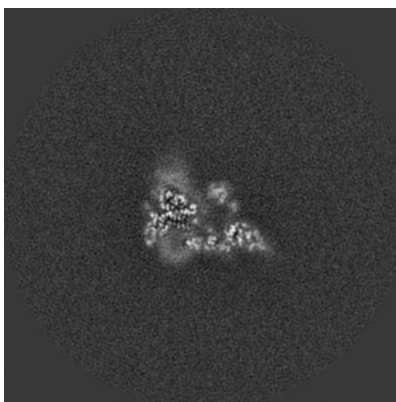
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

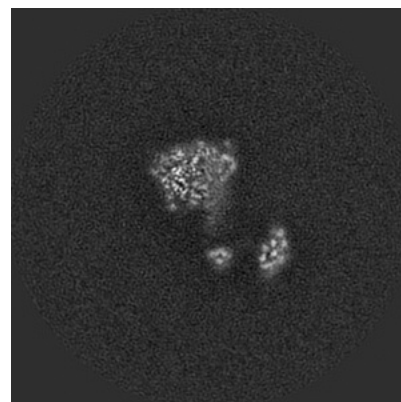
6.2.1 Primary map



X Index: 228



Y Index: 228

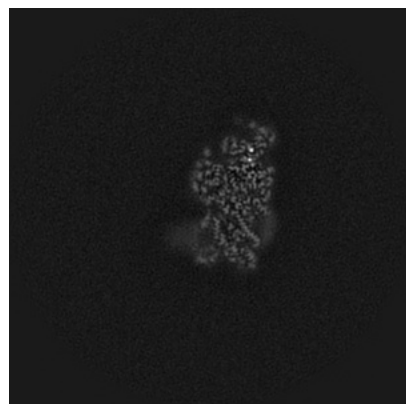


Z Index: 228

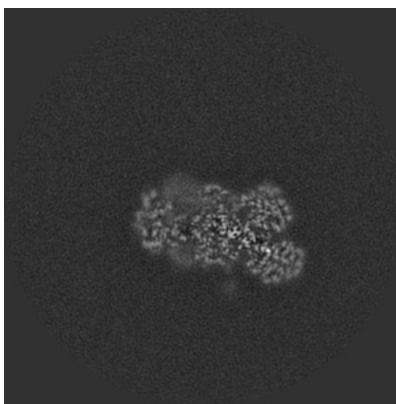
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

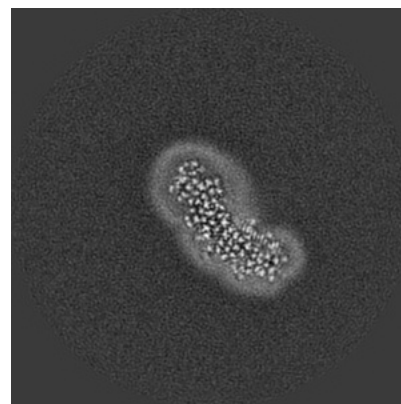
6.3.1 Primary map



X Index: 193



Y Index: 270

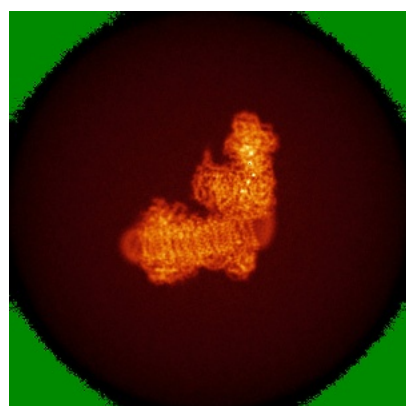


Z Index: 201

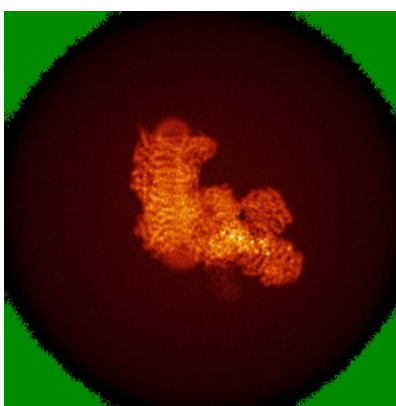
The images above show the largest variance slices of the map in three orthogonal directions.

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

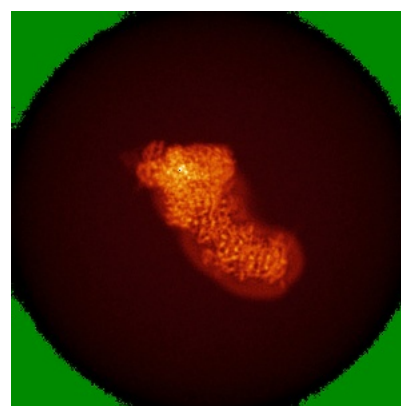
6.4.1 Primary map



X



Y

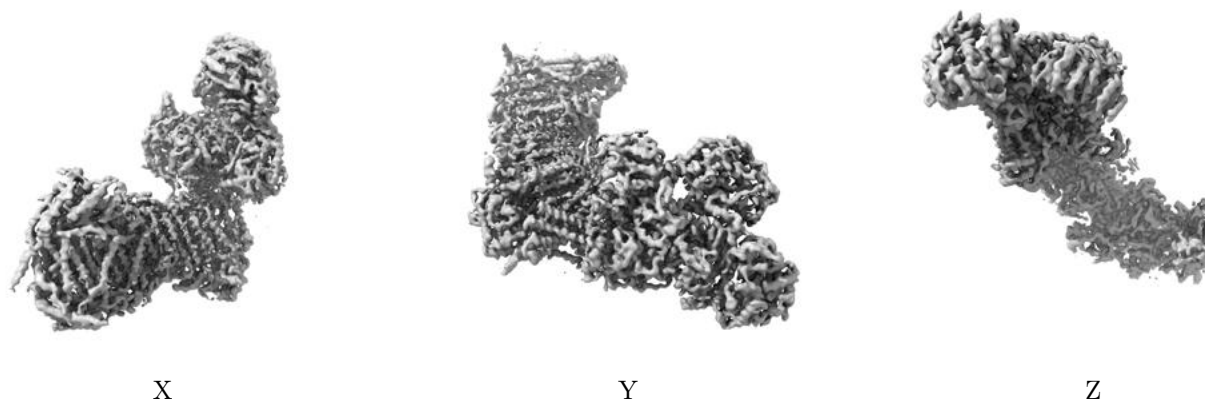


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

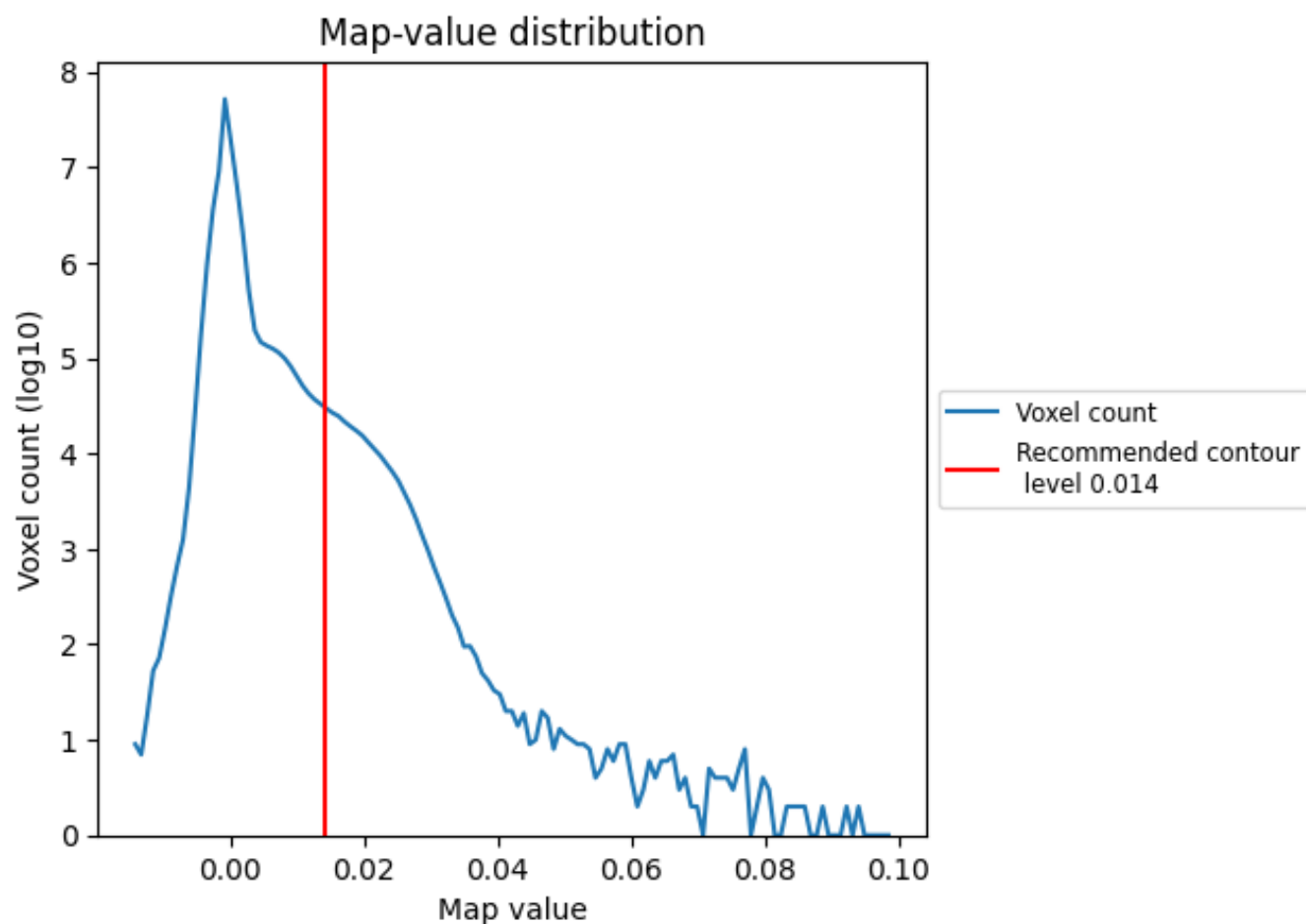
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

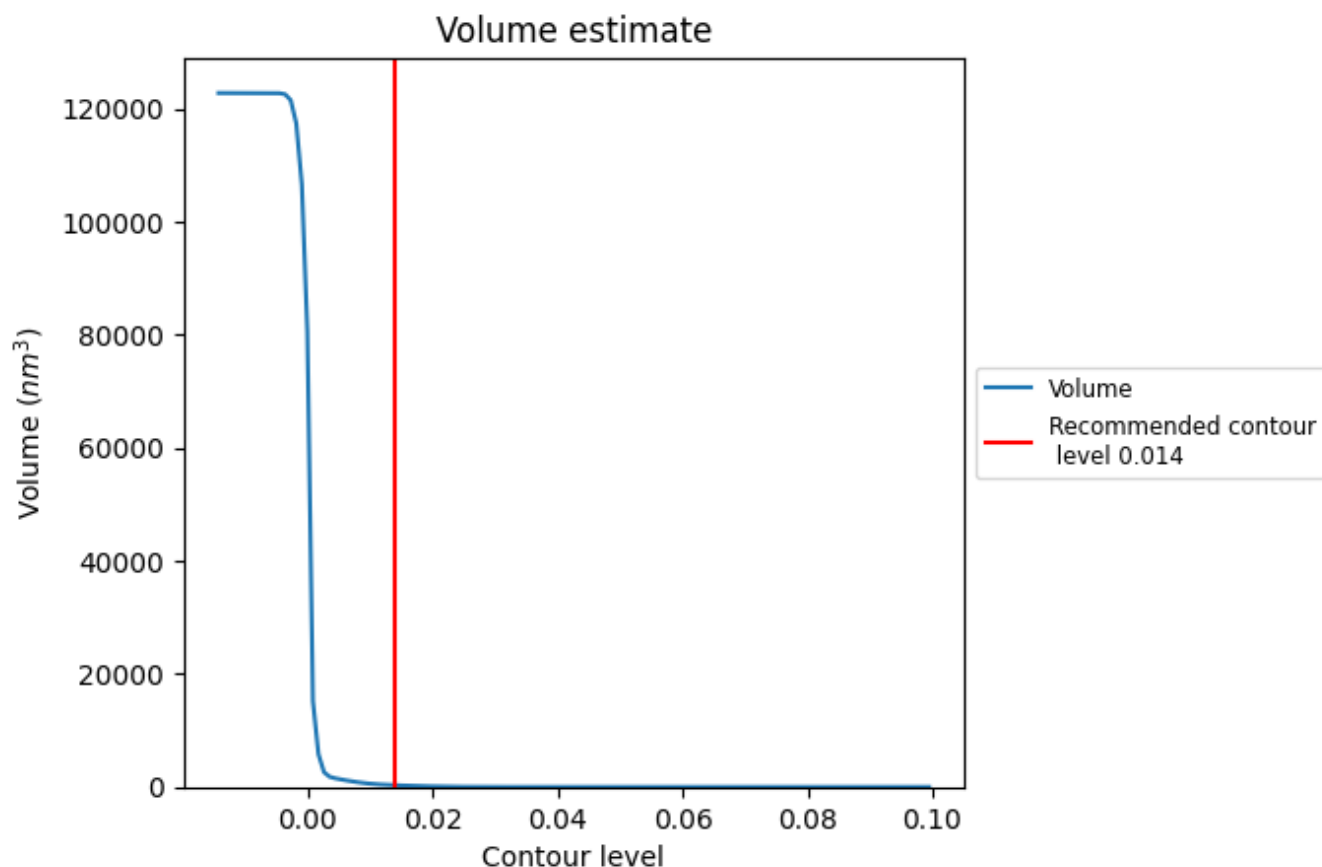
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

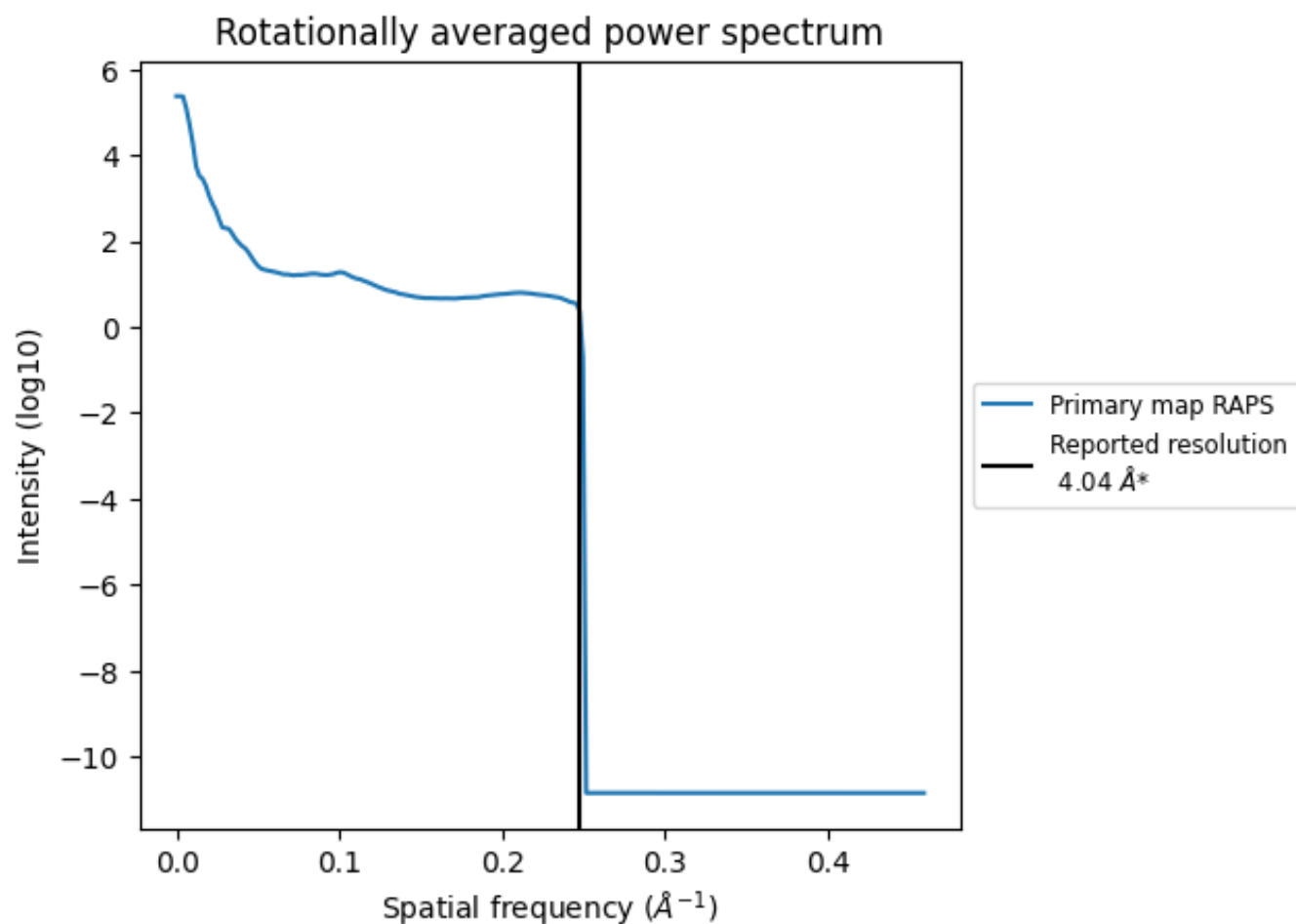
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm³; this corresponds to an approximate mass of 275 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 ⓘ

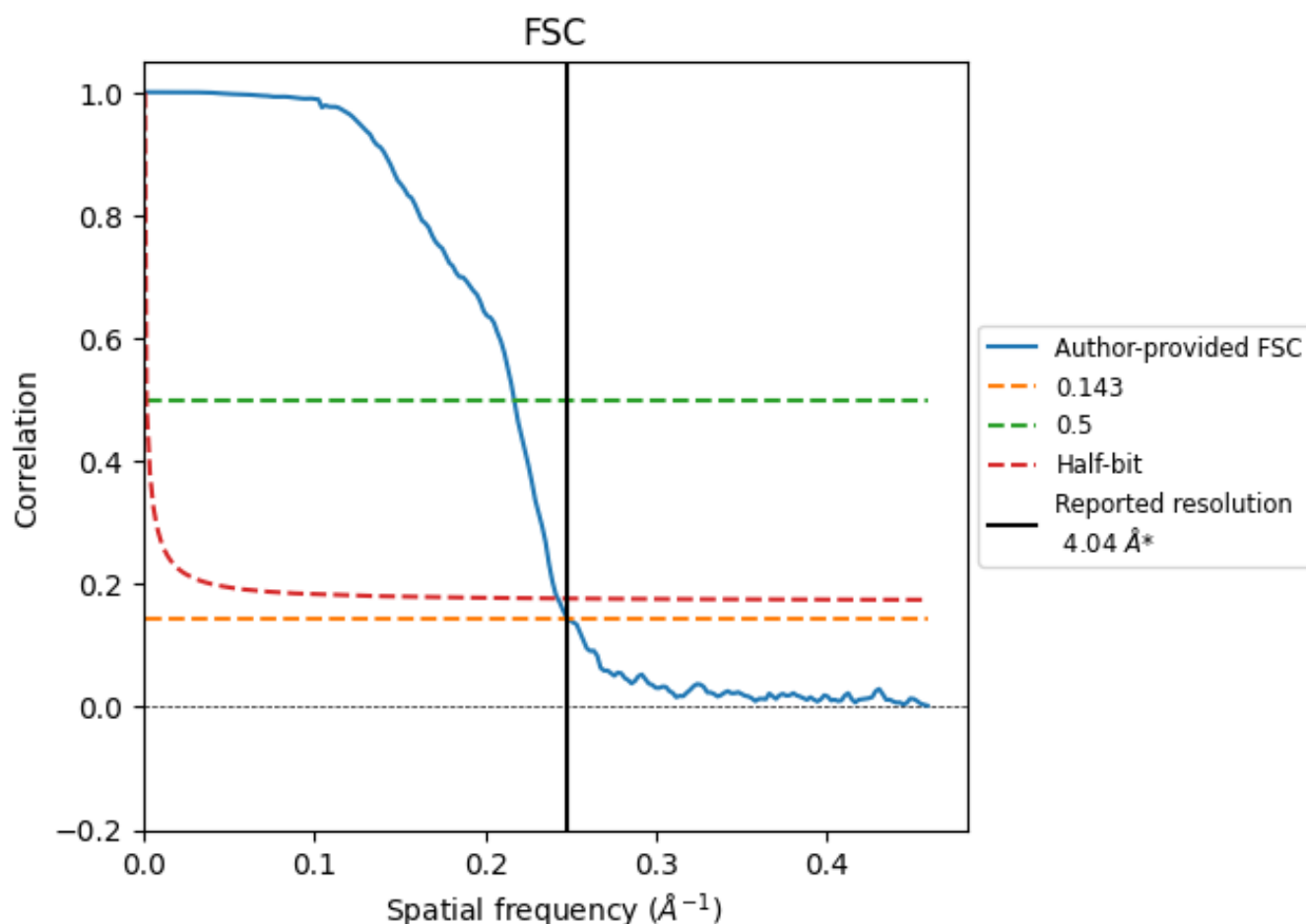


*Reported resolution corresponds to spatial frequency of 0.248 Å⁻¹

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 0.248 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

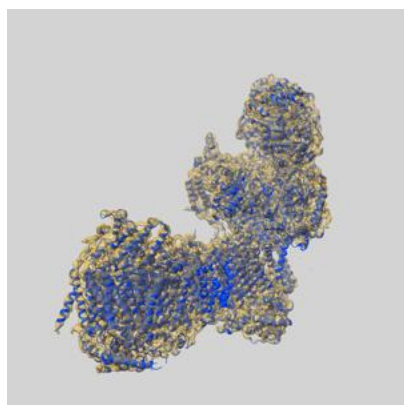
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.04	-	-
Author-provided FSC curve	4.02	4.61	4.12
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

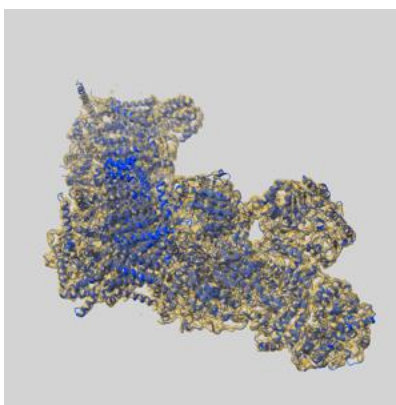
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4874 and PDB model 6RFS. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

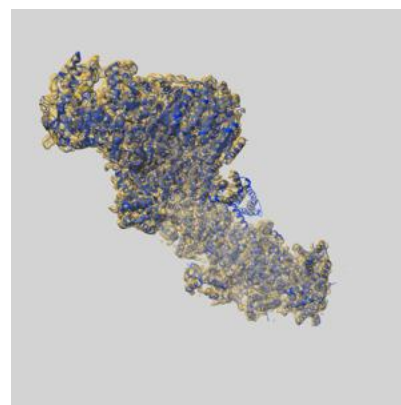
9.1 Map-model overlay [i](#)



X



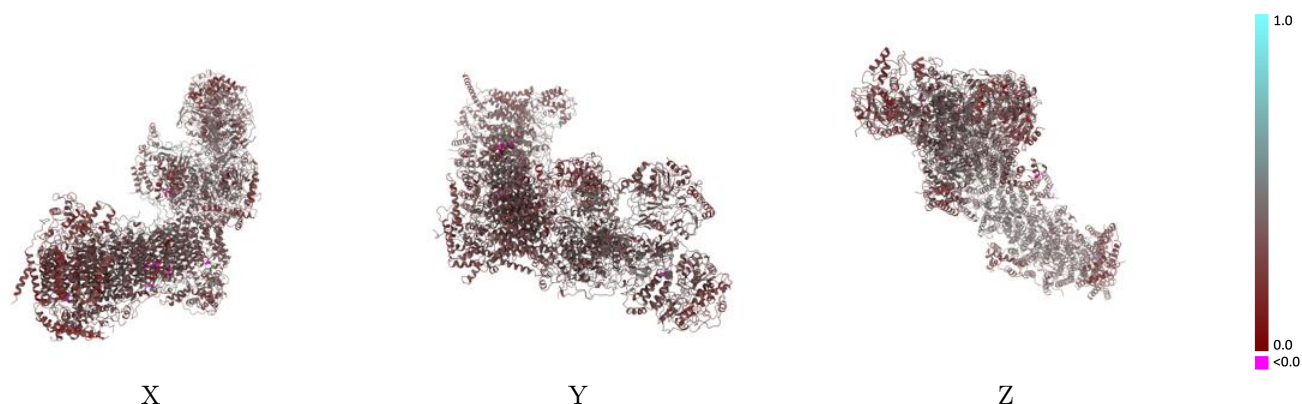
Y



Z

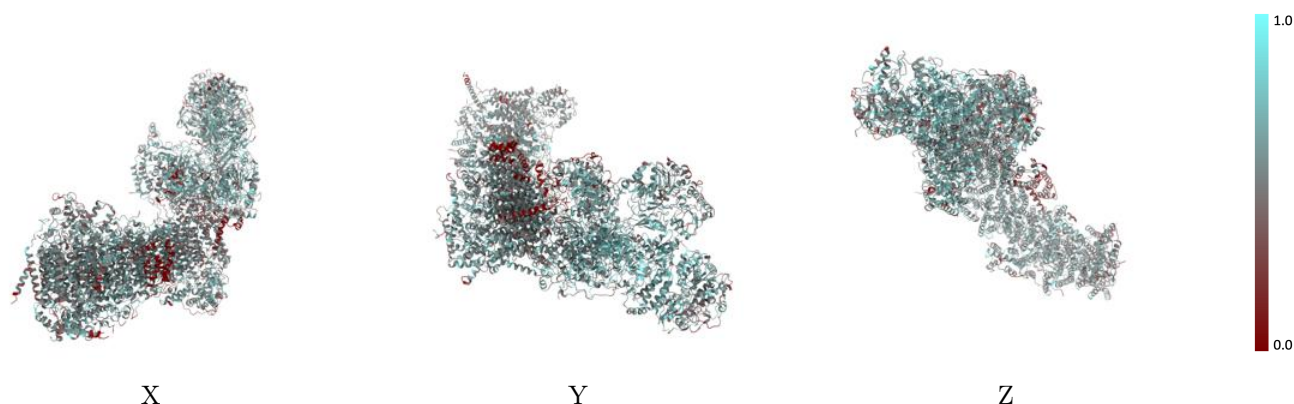
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



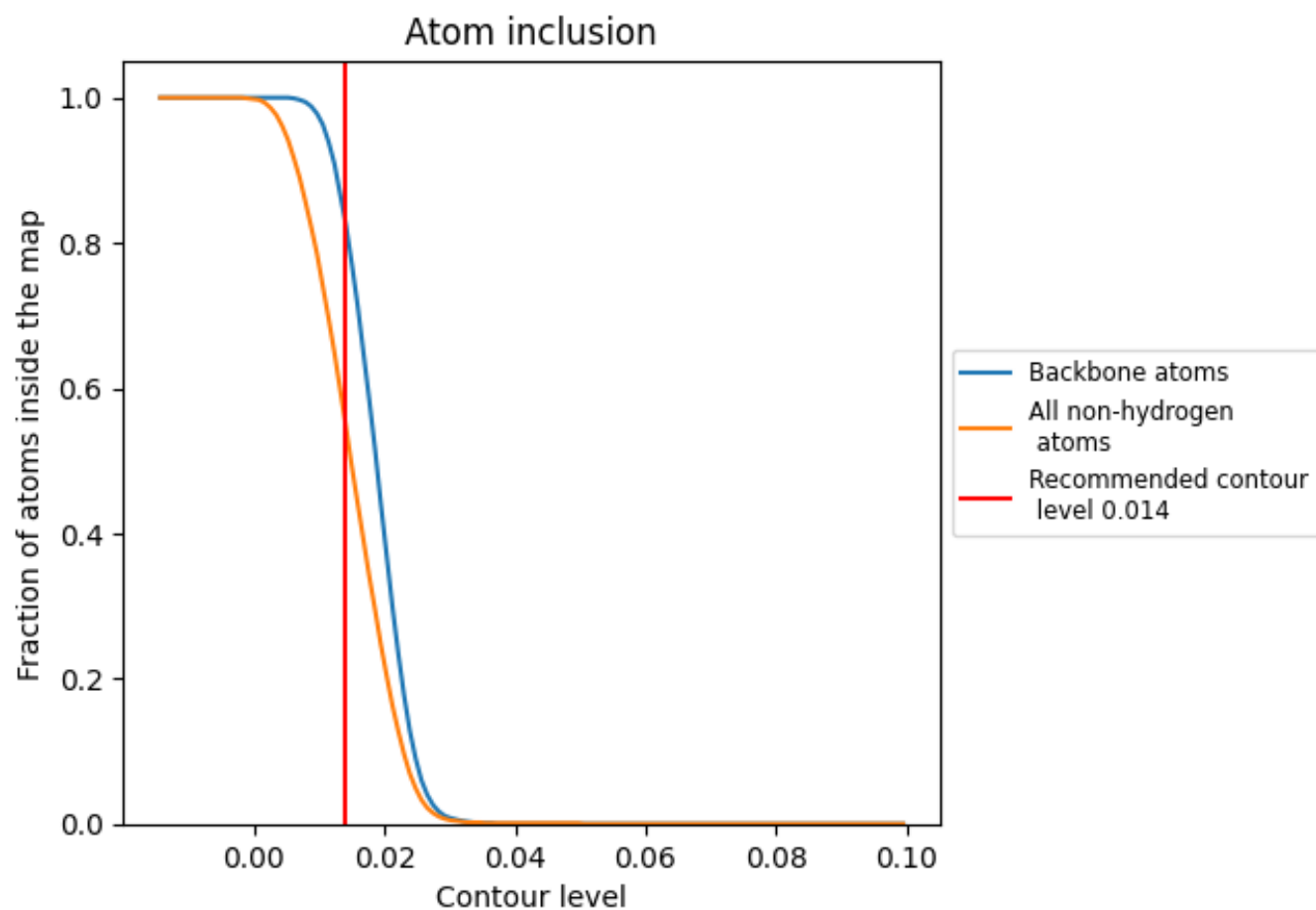
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 55% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5540	 0.3420
1	 0.5010	 0.3370
2	 0.5930	 0.3710
3	 0.3790	 0.3330
4	 0.5700	 0.3560
5	 0.5090	 0.3130
6	 0.4980	 0.3420
8	 0.4850	 0.2730
9	 0.5620	 0.3300
A	 0.5960	 0.3520
B	 0.5750	 0.3170
C	 0.6110	 0.3760
D	 0.5410	 0.3360
E	 0.4980	 0.3230
F	 0.5970	 0.3390
G	 0.6100	 0.3890
H	 0.5580	 0.3250
I	 0.6390	 0.3740
J	 0.3550	 0.3110
K	 0.6280	 0.3780
L	 0.5260	 0.3380
M	 0.6550	 0.3920
O	 0.3830	 0.2810
P	 0.5550	 0.3370
Q	 0.4260	 0.2770
R	 0.5310	 0.3110
S	 0.5080	 0.3010
U	 0.5390	 0.3260
W	 0.5900	 0.3420
X	 0.5630	 0.3500
Z	 0.5930	 0.3710
a	 0.5040	 0.3220
b	 0.5930	 0.3470
c	 0.4780	 0.2980
d	 0.5870	 0.3230



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.4730	 0.2970
f	 0.5220	 0.3010
g	 0.5700	 0.3620
h	 0.6140	 0.3780
i	 0.5670	 0.3340
j	 0.5460	 0.3780
n	 0.5640	 0.3390