Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 08:23 PM JST

PDB ID	:	7DH0
EMDB ID	:	EMD-30677
Title	:	Activity optimized complex I (open form)
Authors	:	Jeon, T.J.; Lee, S.G.; Yoo, S.H.; Ryu, J.H.; Kim, D.S.; Hyun, J.K.; Kim, H.M.; Ryu, S.E.
Deposited on	:	2020-11-12
Resolution	:	4.20 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:

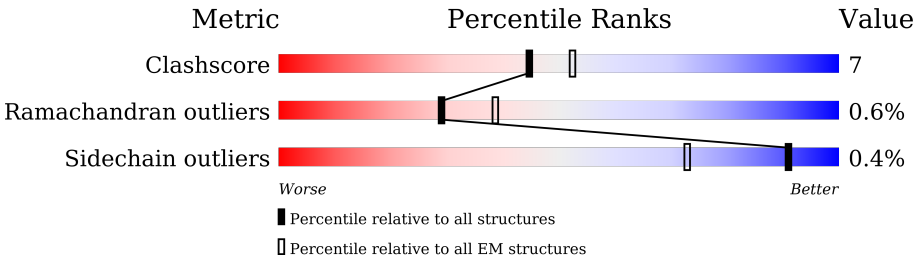
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	347	14% 86% 14%
2	3	115	25% 66% 15% 19%
3	4	459	29% 86% 14%
4	5	98	21% 81% 17%
5	7	175	38% 89% 7%
6	8	444	82% 14%
7	9	217	71% 24% 5%
8	A	704	80% 17%

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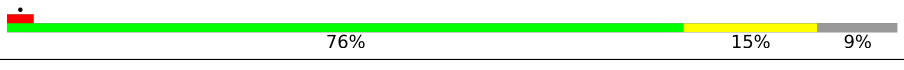
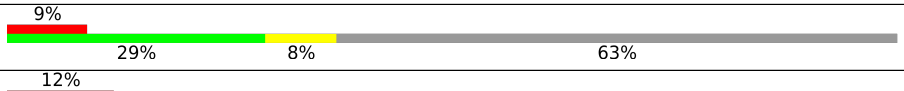
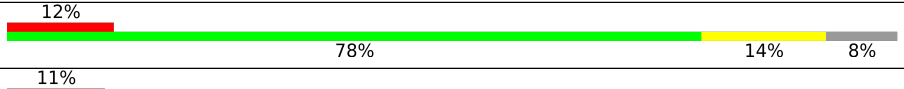
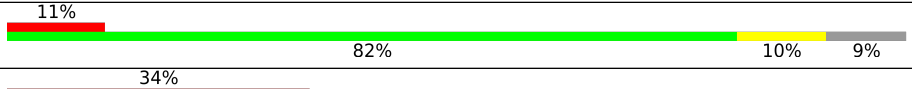
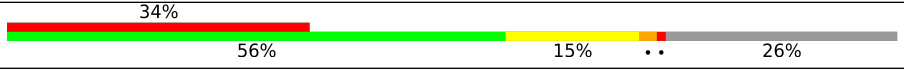
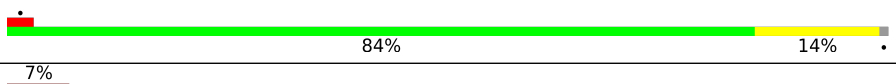
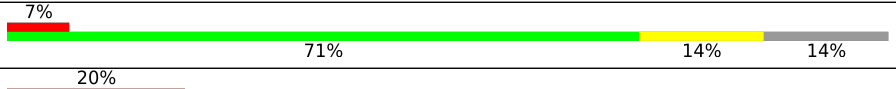
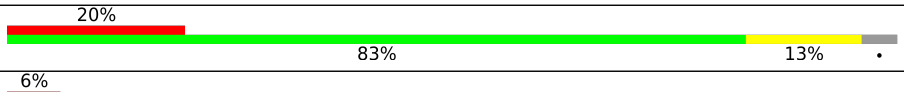
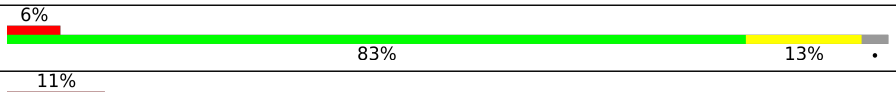
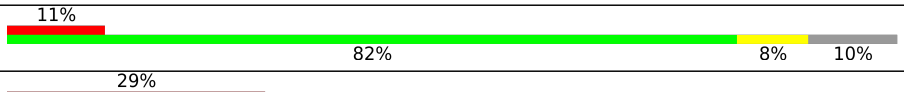
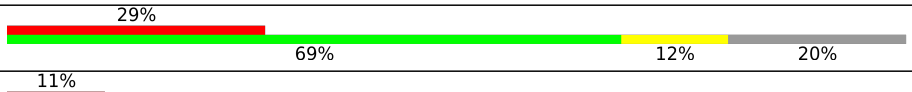
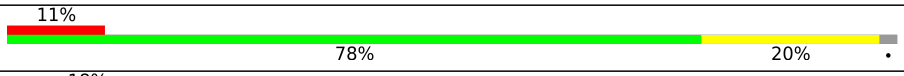
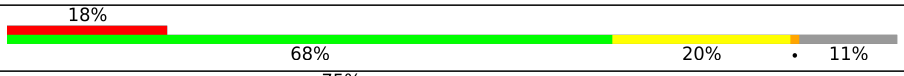
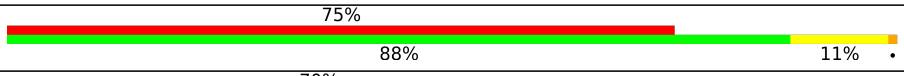
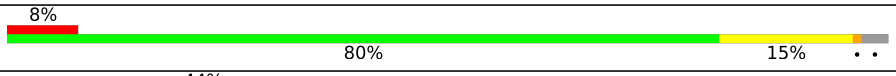
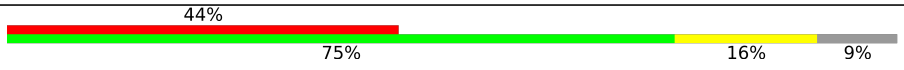
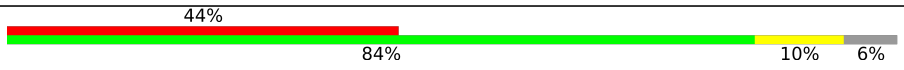
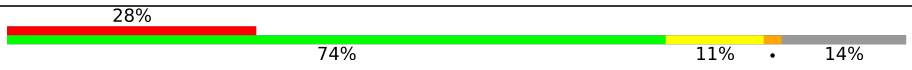
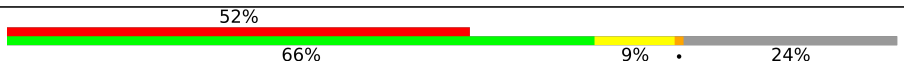
Mol	Chain	Length	Quality of chain
9	B	430	
10	C	228	
11	D	179	
12	E	176	
13	F	75	
14	G	133	
15	H	105	
16	I	96	
17	J	70	
18	K	98	
19	L	83	
20	N	115	
21	O	127	
22	P	112	
23	Q	171	
24	R	345	
25	S	320	
26	T	140	
27	U	145	
28	V	143	
29	M	88	
29	W	88	
30	X	57	
31	Y	72	
32	Z	97	

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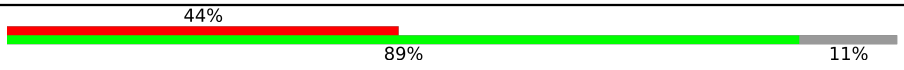
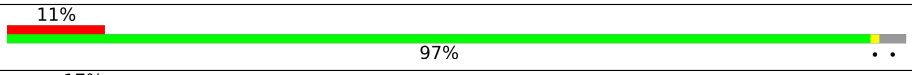
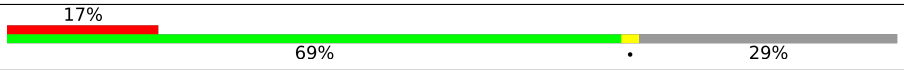
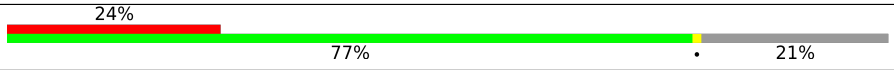
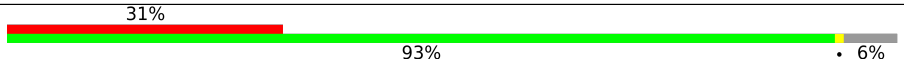
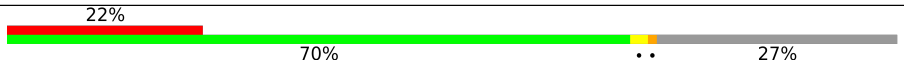
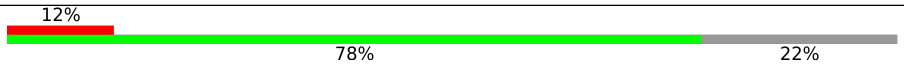
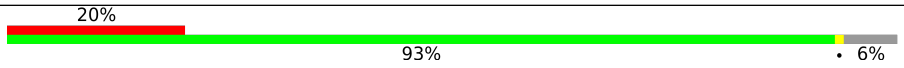
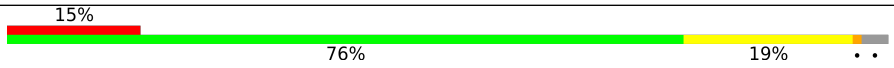
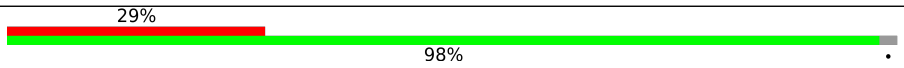
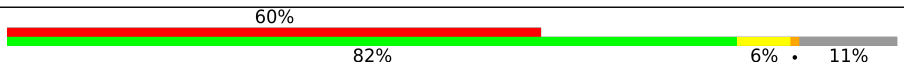
Mol	Chain	Length	Quality of chain
33	a	128	
34	b	143	
35	c	127	
36	d	136	
37	f	178	
38	h	125	
39	i	49	
40	j	120	
41	1	318	
42	6	606	
43	g	176	
44	e	158	

2 Entry composition (i)

There are 52 unique types of molecules in this entry. The entry contains 60091 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	344	2582	1707	404	437	34	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	93	719	492	104	120	3	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	458	3447	2293	548	574	32	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	96	697	454	109	124	10	0	0

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	7	172	1186	798	179	202	7	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	8	427	2965	1864	552	534	15	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	207	Total	C	N	O	S	0	0
			1535	978	261	286	10		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	688	Total	C	N	O	S	0	0
			5183	3254	915	978	36		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	385	Total	C	N	O	S	0	0
			3076	1963	530	559	24		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	208	Total	C	N	O	S	0	0
			1705	1102	294	306	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	152	Total	C	N	O	S	0	0
			1200	769	209	208	14		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	176	Total	C	N	O	S	0	0
			1388	874	239	264	11		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	F	28	Total	C	N	O	0	0
			183	116	32	35		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	123	Total	C	N	O	S	0	0
			981	619	177	182	3		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	96	Total	C	N	O	S	0	0
			780	494	147	134	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	71	Total	C	N	O	S	0	0
			532	332	99	98	3		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	69	Total	C	N	O	S	0	0
			530	344	96	88	2		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	K	84	Total	C	N	O	0	0
			652	409	125	118		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	80	Total	C	N	O	S	0	0
			602	398	97	105	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	111	Total	C	N	O	S	0	0
			862	559	149	152	2		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	114	Total	C	N	O	S	0	0
			925	595	170	156	4		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	90	Total	C	N	O	S	0	0
			698	442	128	126	2		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	168	Total	C	N	O	S	0	0
			1345	851	242	243	9		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	306	Total	C	N	O	S	0	0
			2334	1505	417	409	3		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	319	Total	C	N	O	S	0	0
			2299	1457	395	438	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	138	Total	C	N	O	S	0	0
			942	599	165	172	6		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	132	Total	C	N	O	S	0	0
			1019	659	179	178	3		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	138	Total	C	N	O	S	0	0
			1093	702	189	193	9		

- Molecule 29 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	83	Total	C	N	O	S	0	0
			596	386	95	111	4		
29	M	80	Total	C	N	O	S	0	0
			642	413	96	128	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	X	49	Total	C	N	O	0	0
			372	243	64	65		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	57	Total	C	N	O	S	0	0
			409	277	65	66	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	74	Total	C	N	O	S	0	0
			493	320	89	82	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	a	114	Total	C	N	O	0	0
			857	550	159	148		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	139	Total	C	N	O	S	0	0
			1032	672	190	168	2		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	c	90	Total	C	N	O	0	0
			617	391	119	107		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	107	Total	C	N	O	S	0	0
			708	445	134	125	4		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	167	Total	C	N	O	S	0	0
			1156	739	205	208	4		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	91	Total	C	N	O	S	0	0
			721	461	123	135	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	i	38	Total	C	N	O	0	0
			277	185	46	46		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	113	Total	C	N	O	S	0	0
			892	587	149	153	3		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1	309	Total	C	N	O	S	0	0
			2442	1642	376	401	23		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	6	606	Total	C	N	O	S	0	0
			4765	3172	732	819	42		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

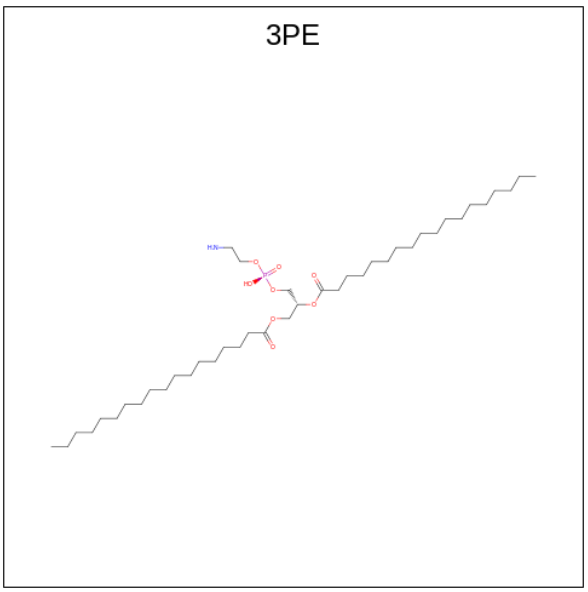
Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	173	Total	C	N	O	S	0	0
			1351	849	246	248	8		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	e	141	Total	C	N	O	S	0	0
			864	539	161	160	4		

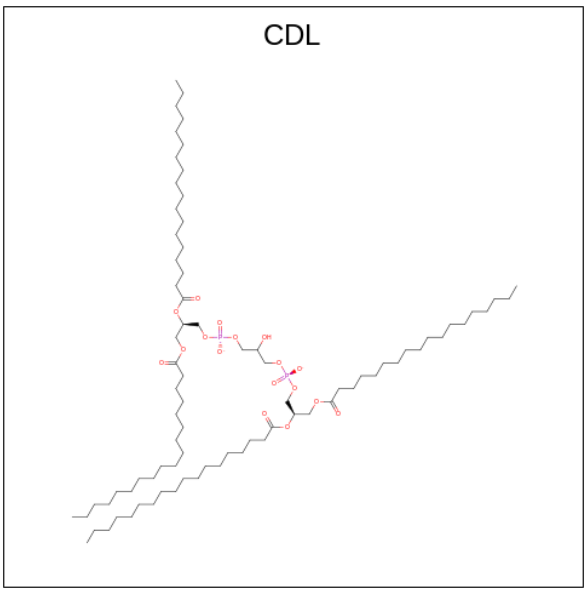
- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE)

(formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



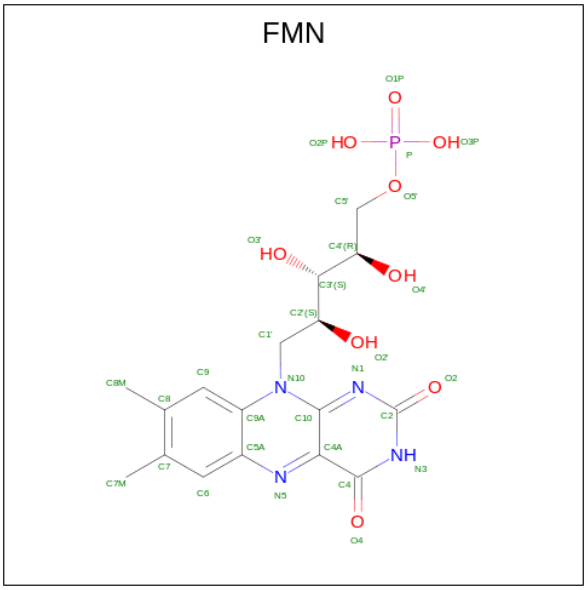
Mol	Chain	Residues	Atoms					AltConf
45	2	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	B	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 46 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



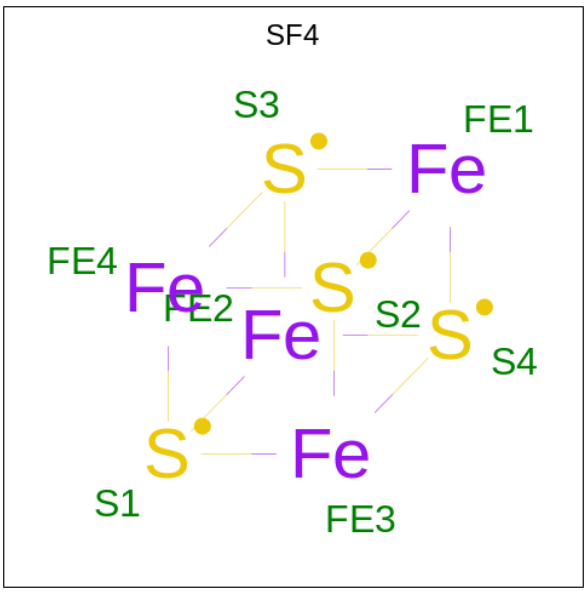
Mol	Chain	Residues	Atoms				AltConf
46	4	1	Total	C	O	P	0
			82	63	17	2	

- Molecule 47 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



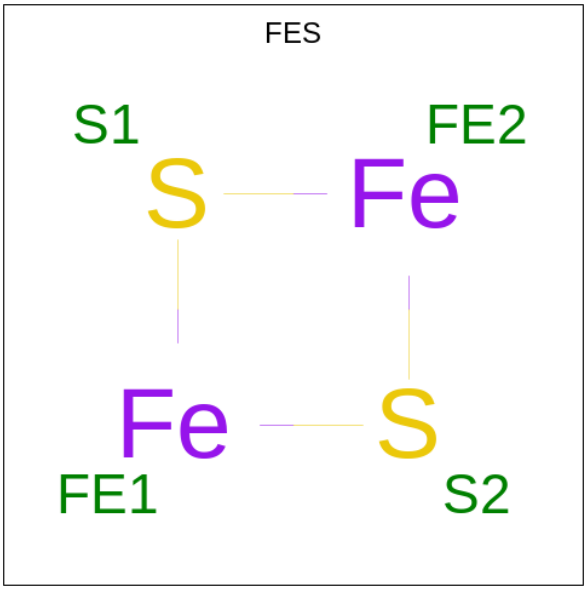
Mol	Chain	Residues	Atoms					AltConf
47	8	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 48 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
48	8	1	Total Fe S 8 4 4	0
48	A	1	Total Fe S 16 8 8	0
48	A	1	Total Fe S 16 8 8	0
48	D	1	Total Fe S 8 4 4	0
48	E	1	Total Fe S 16 8 8	0
48	E	1	Total Fe S 16 8 8	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



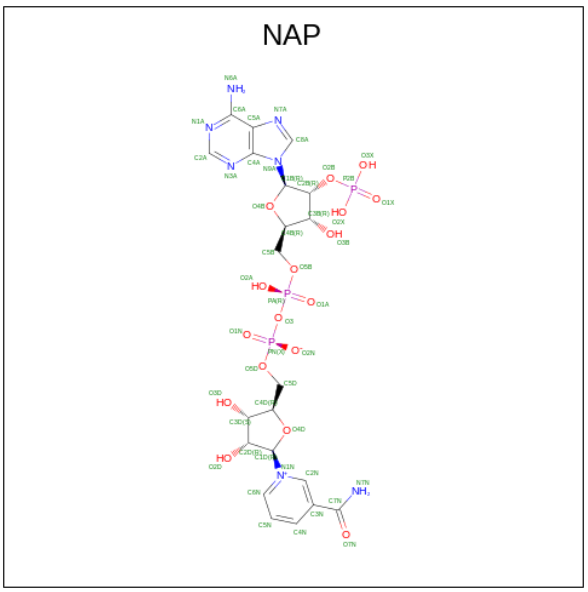
Mol	Chain	Residues	Atoms	AltConf
49	9	1	Total Fe S 4 2 2	0
49	A	1	Total Fe S 4 2 2	0

- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
50	I	1	Total Zn 1 1	0

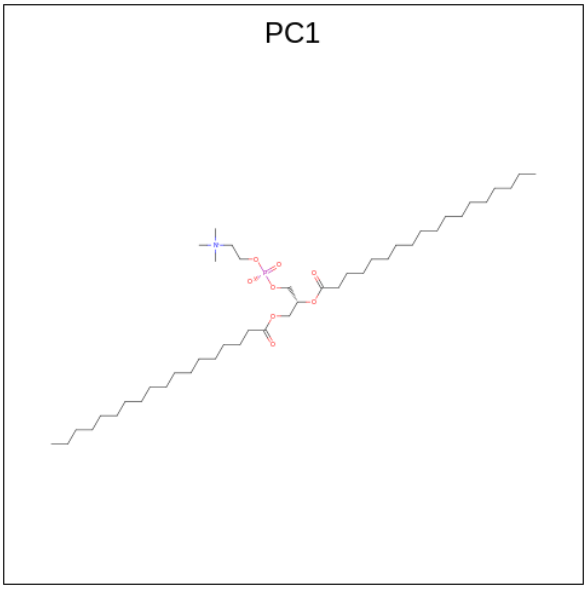
- Molecule 51 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE

(three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

- Molecule 52 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
52	S	1	Total	C	N	O	P	0
			47	37	1	8	1	

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Continued from previous page...

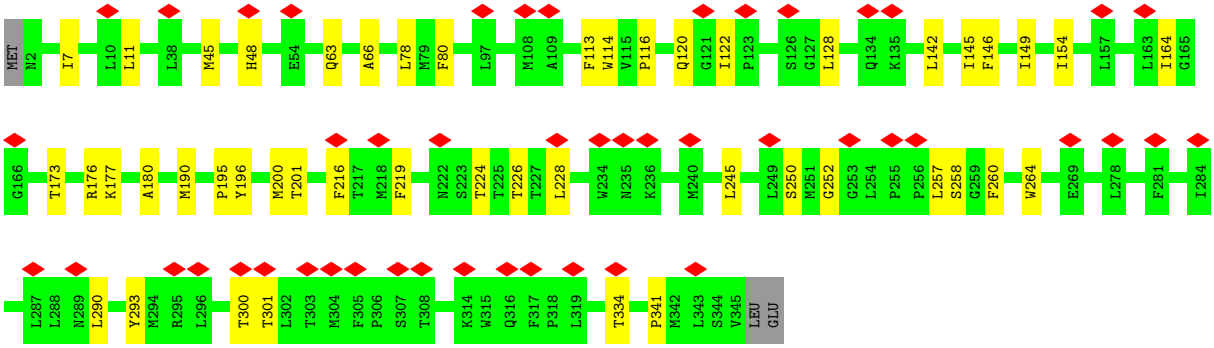
Mol	Chain	Residues	Atoms					AltConf
52	j	1	Total	C	N	O	P	0
			39	29	1	8	1	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

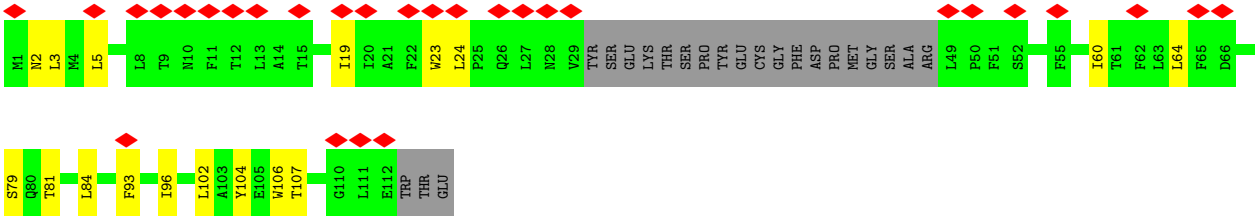
• Molecule 1: NADH-ubiquinone oxidoreductase chain 2

Chain 2:



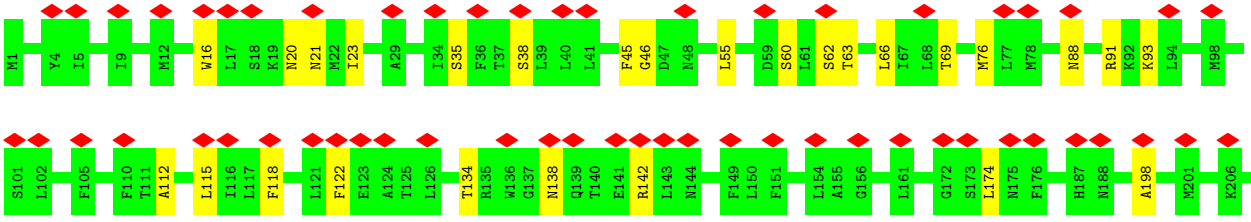
• Molecule 2: NADH-ubiquinone oxidoreductase chain 3

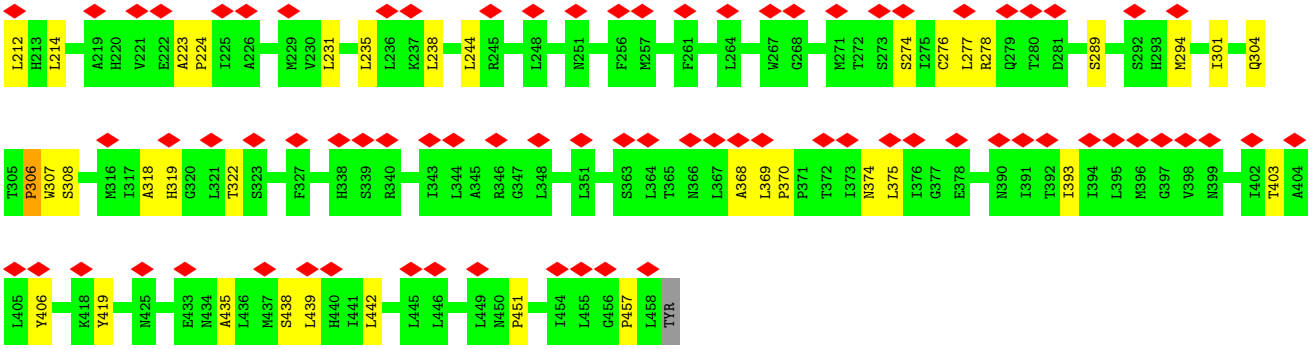
Chain 3:



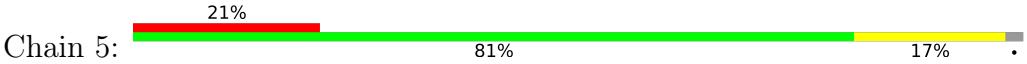
• Molecule 3: NADH-ubiquinone oxidoreductase chain 4

Chain 4:

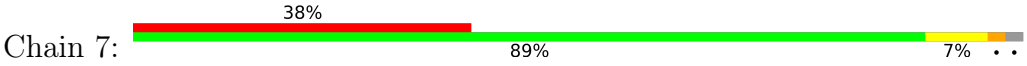


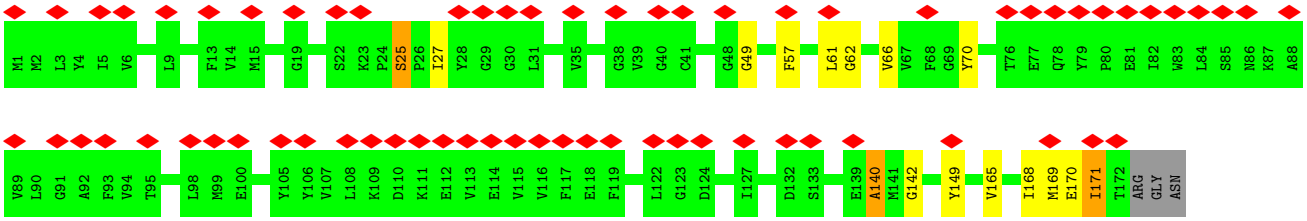


• Molecule 4: NADH-ubiquinone oxidoreductase chain 4L

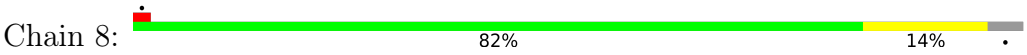


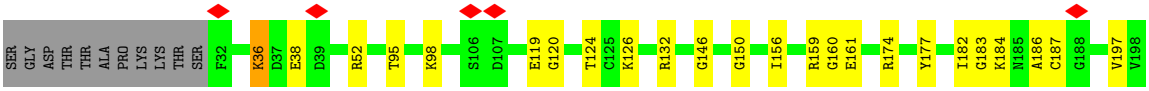
• Molecule 5: NADH-ubiquinone oxidoreductase chain 6

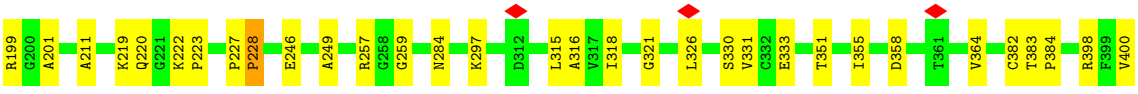


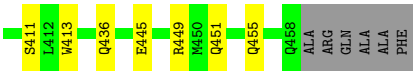


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

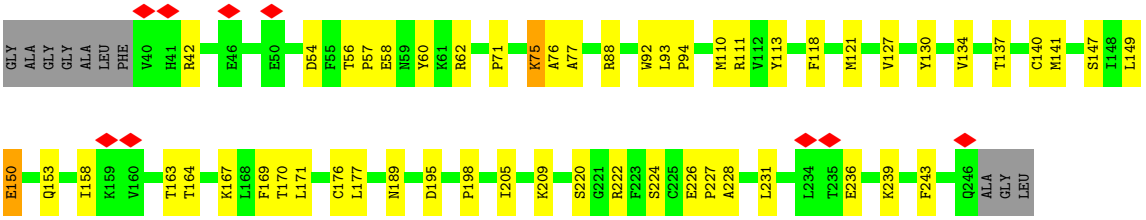






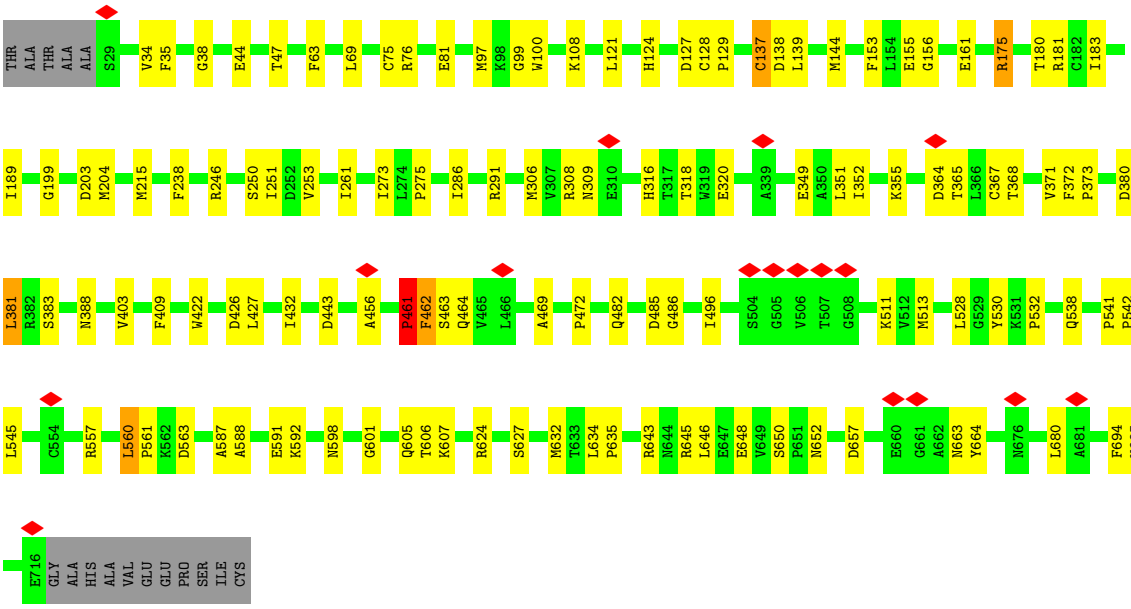


• Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



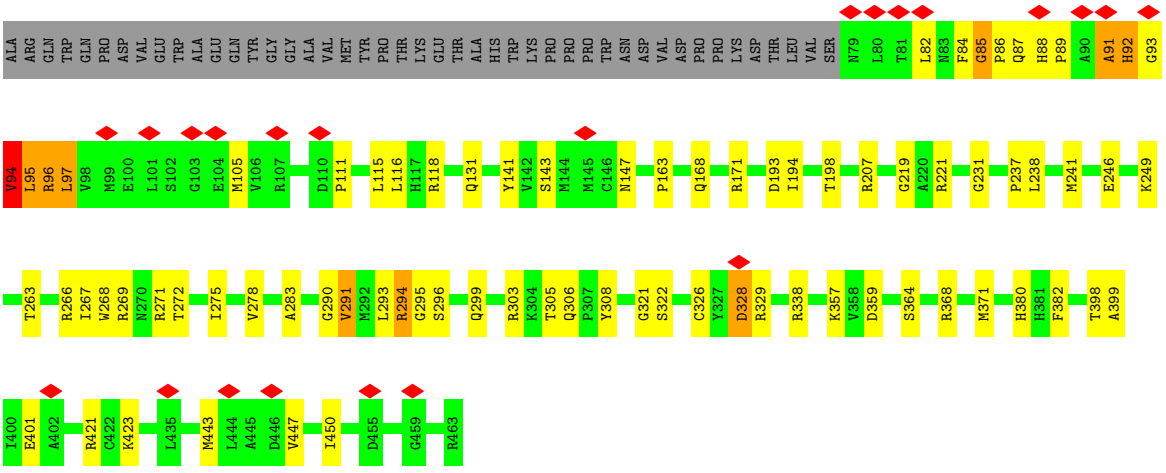
• Molecule 8: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain A:



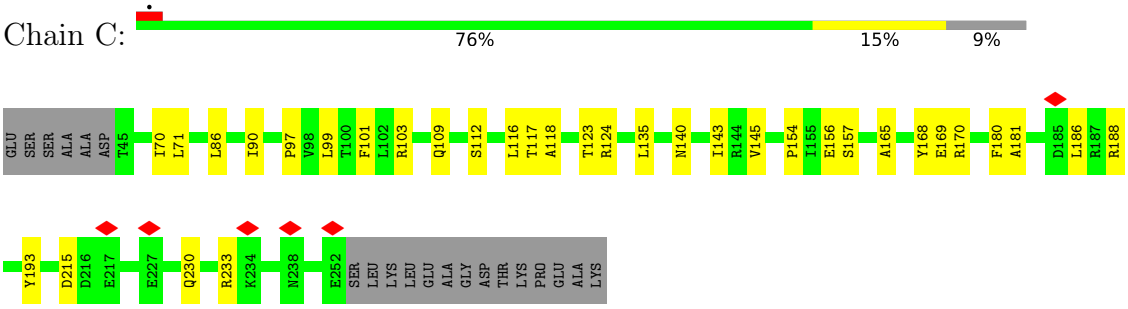
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain B:



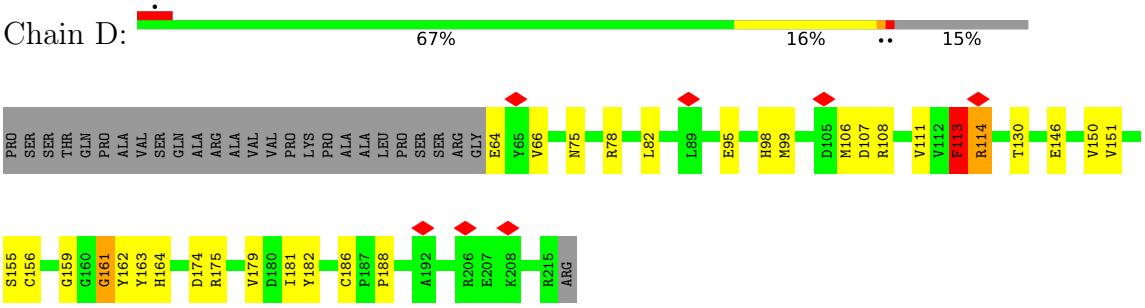
• Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:



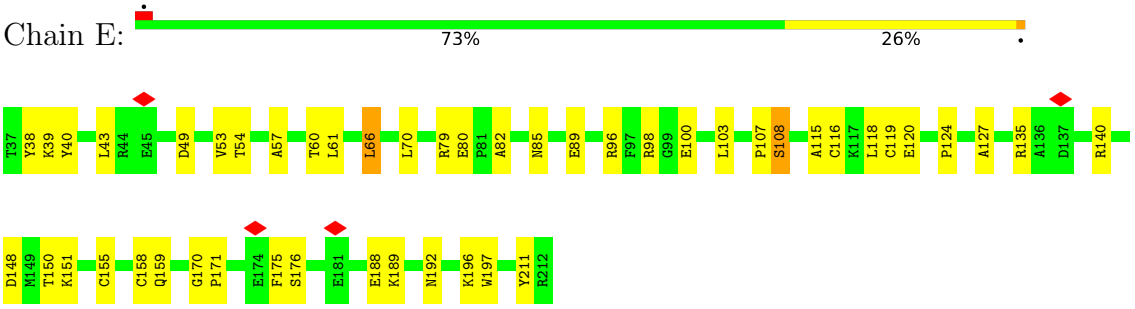
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain D:



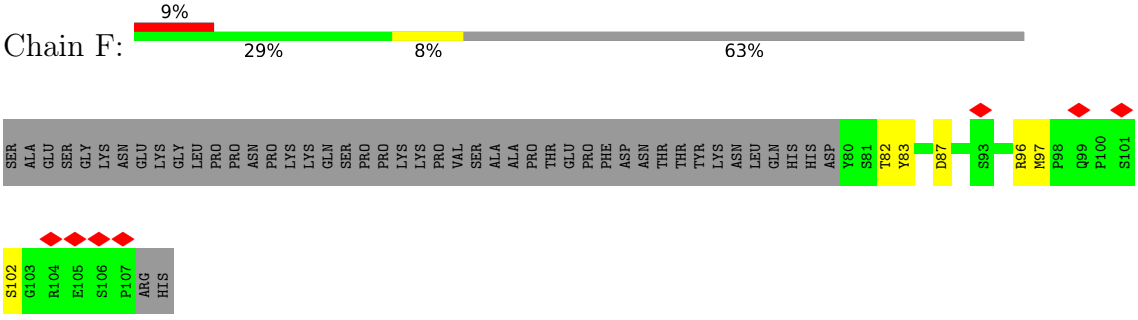
• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain E:



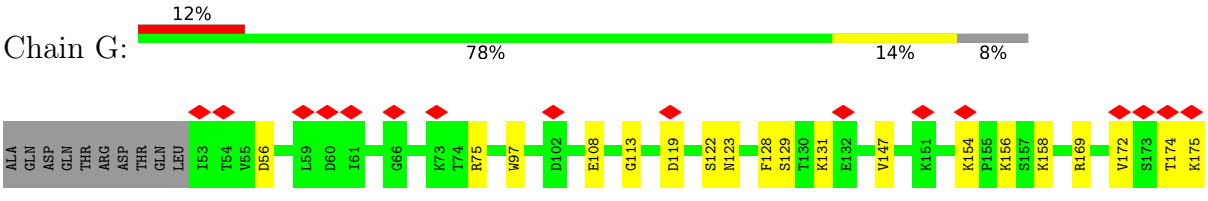
• Molecule 13: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain F:



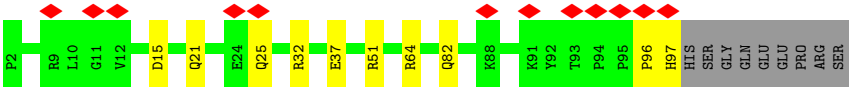
• Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain G:



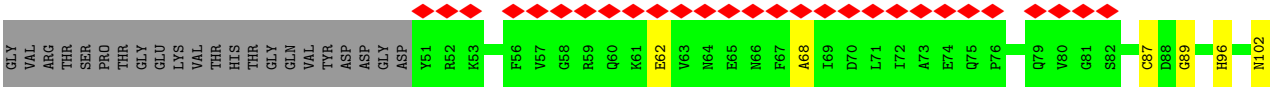
• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

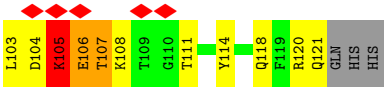
Chain H:



• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

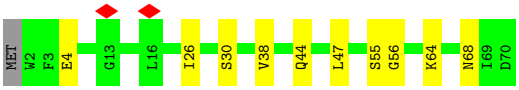
Chain I:





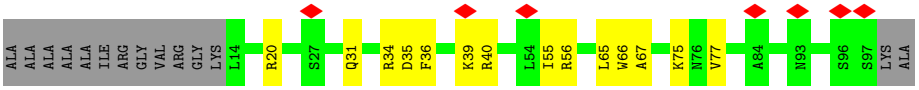
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain J:



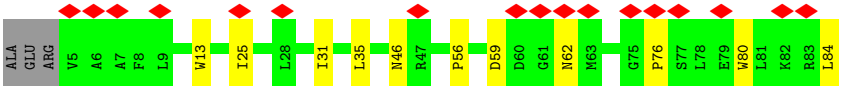
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain K:



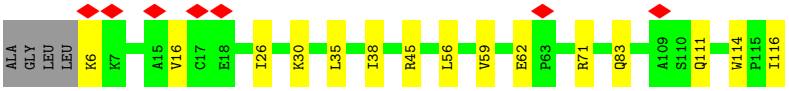
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain L:



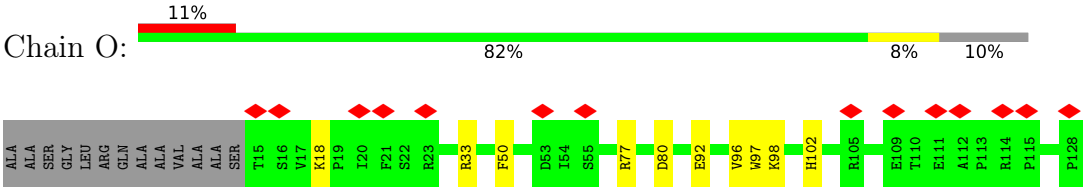
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain N:



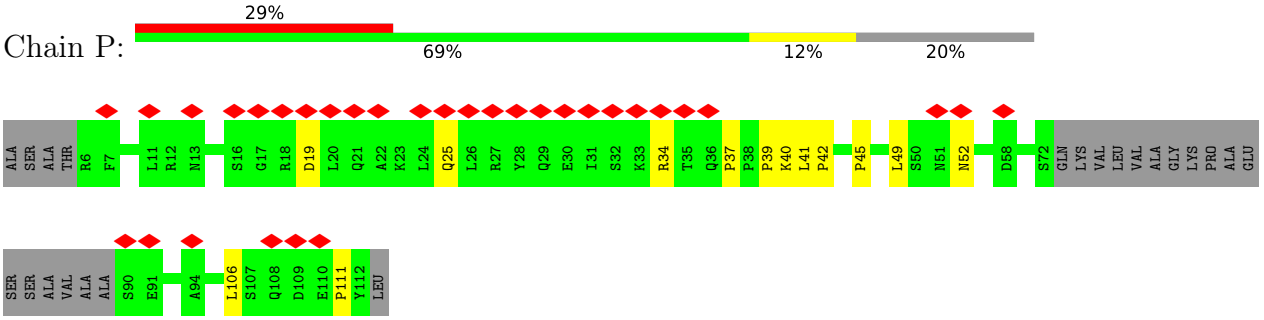
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain O:



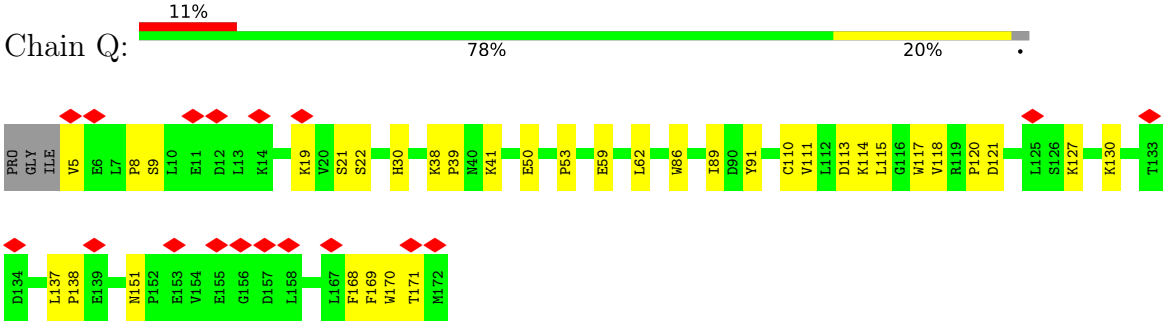
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain P:



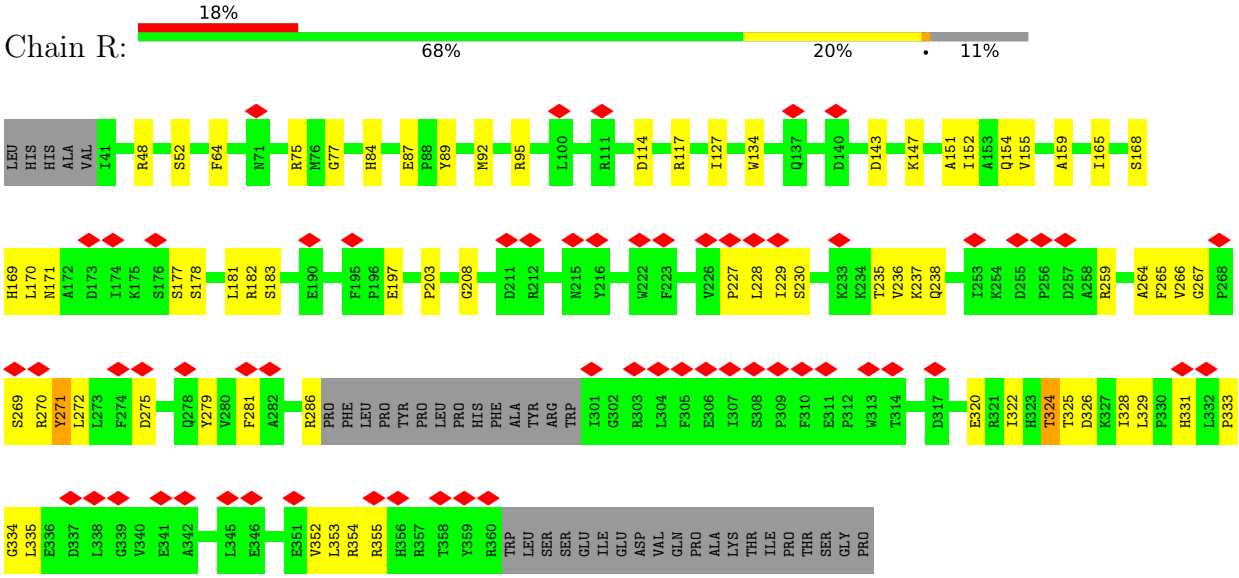
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Q:



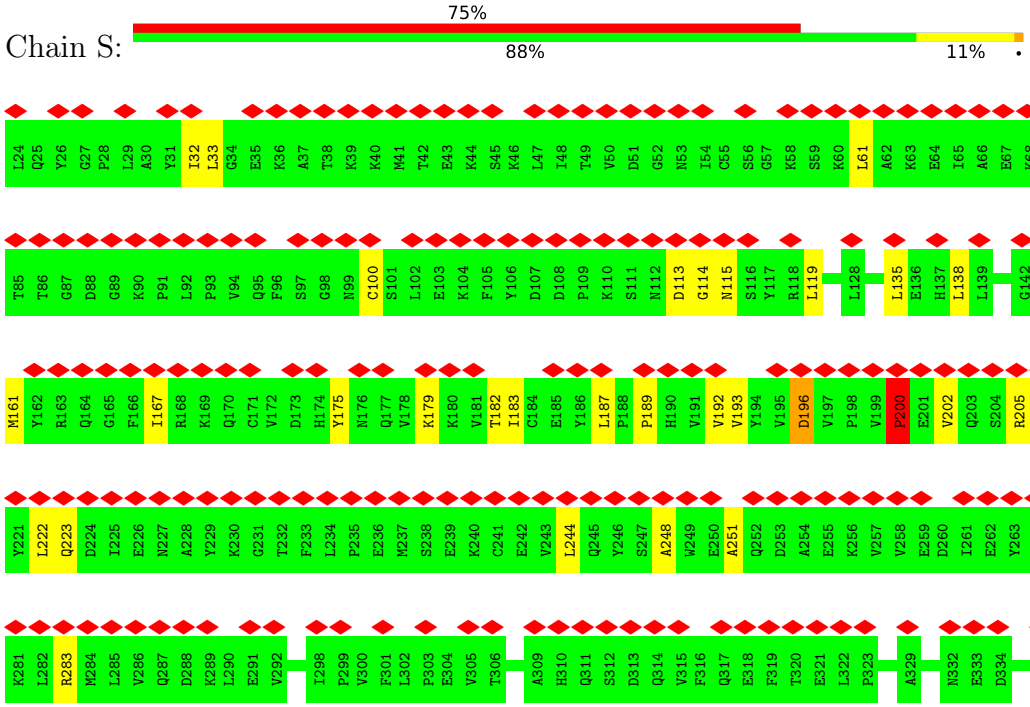
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain R:



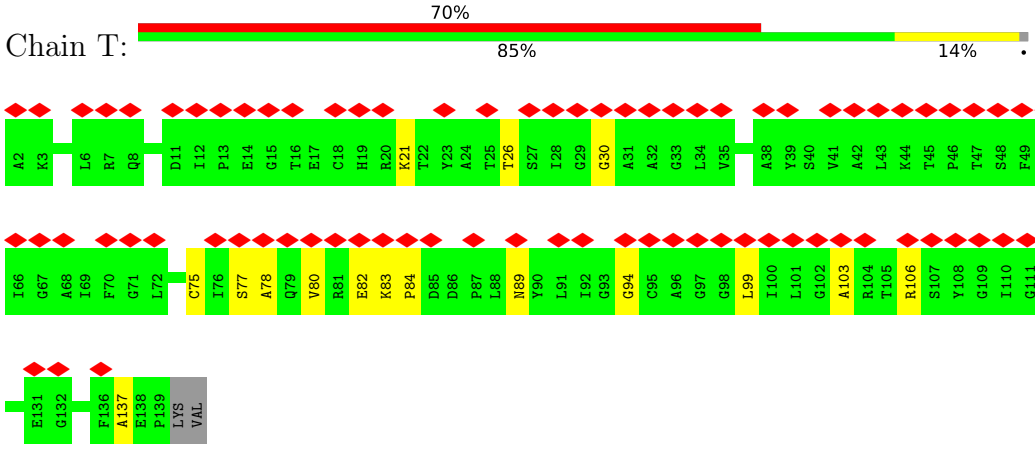
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain S:



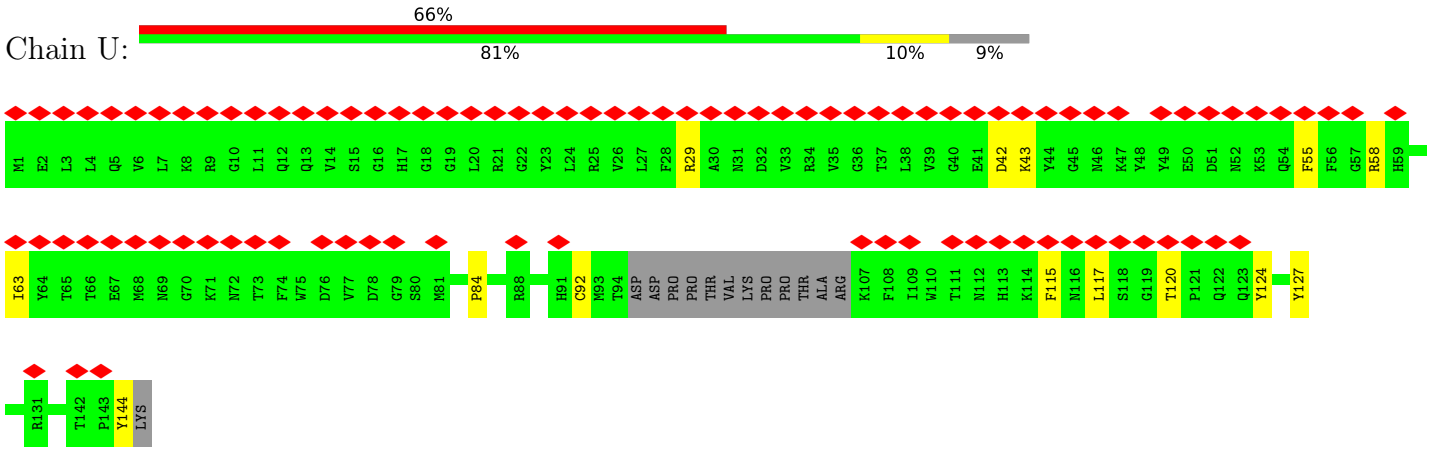
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain T:



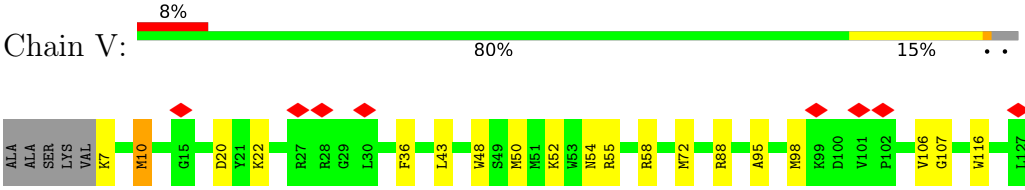
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain U:



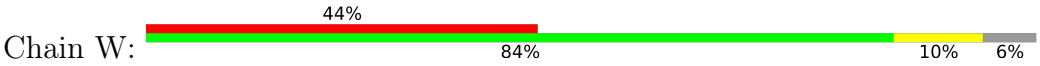
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

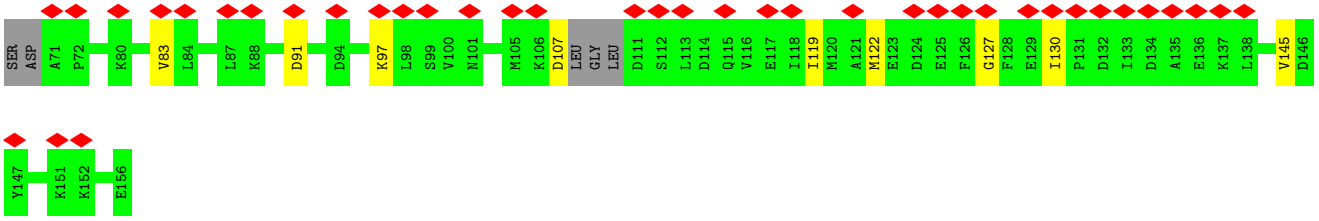
Chain V:



• Molecule 29: Acyl carrier protein, mitochondrial

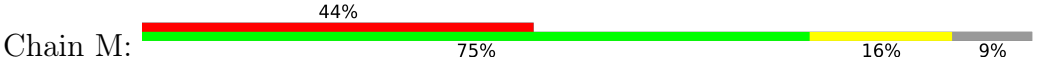
Chain W:

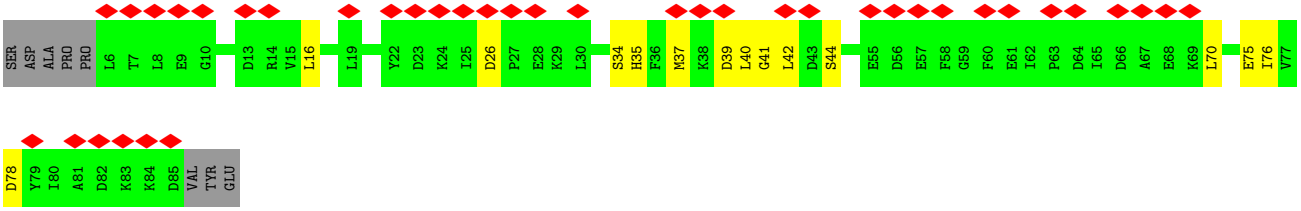




• Molecule 29: Acyl carrier protein, mitochondrial

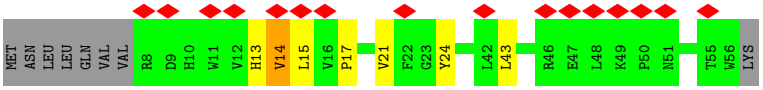
Chain M:





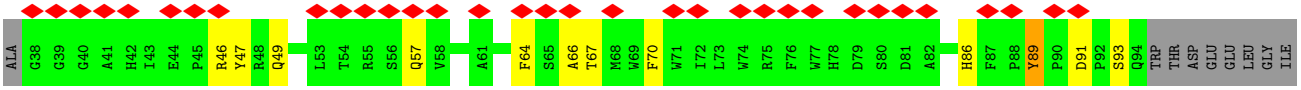
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain X:



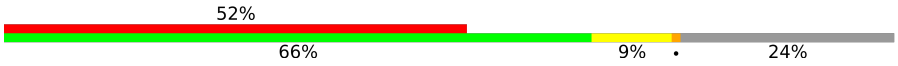
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

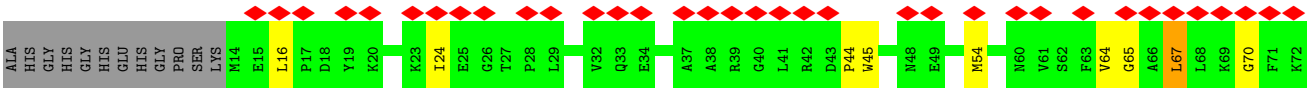
Chain Y:

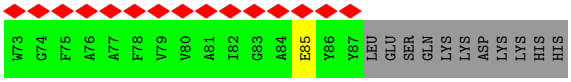


• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:

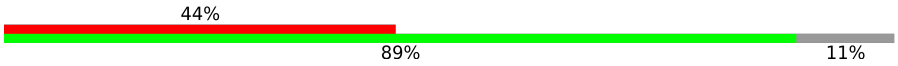


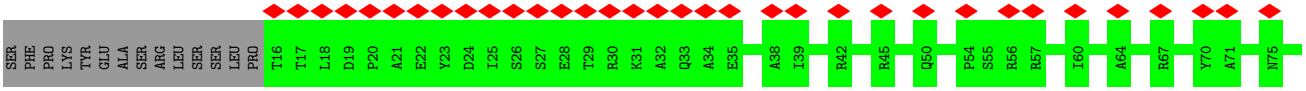


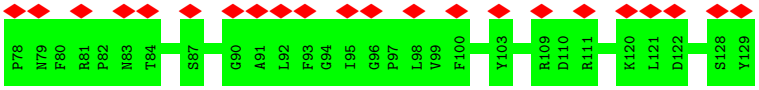


• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain a:

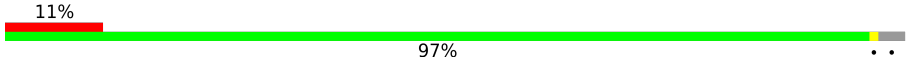


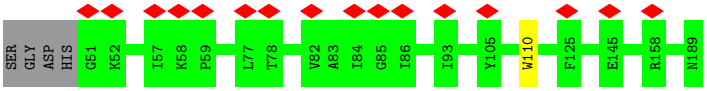




• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

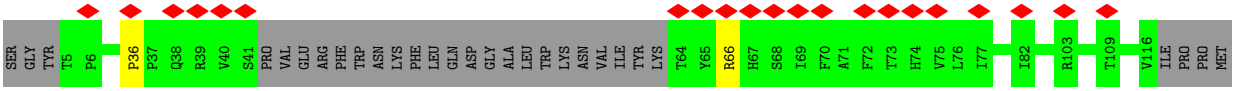
Chain b:





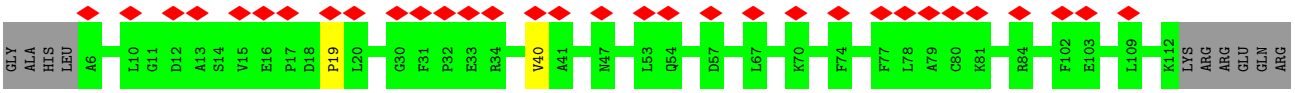
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain c:



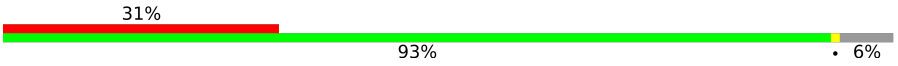
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

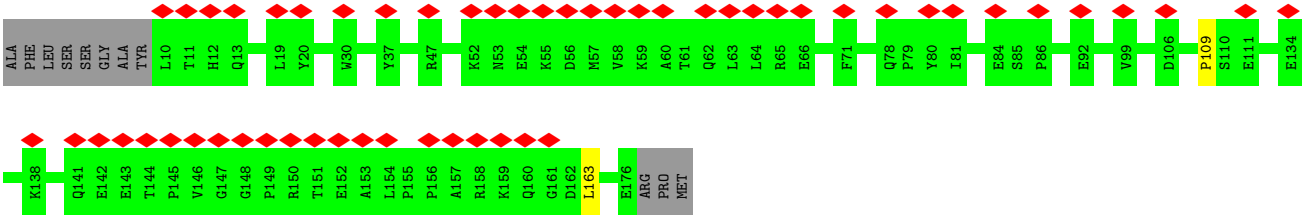
Chain d:



• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

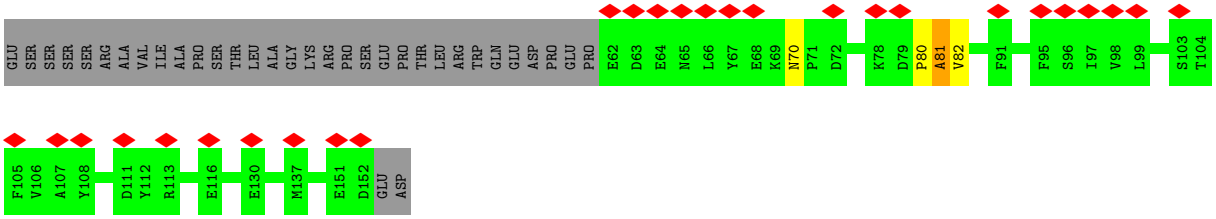
Chain f:





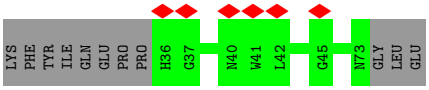
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain h:



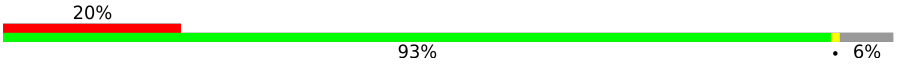
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

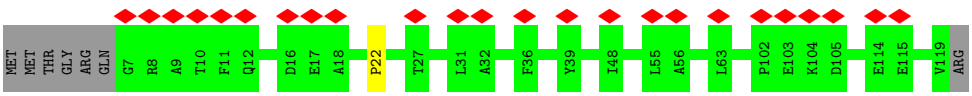
Chain i:



• Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2

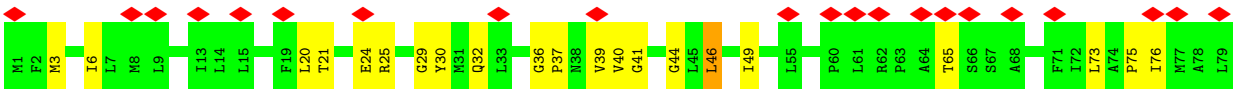
Chain j:

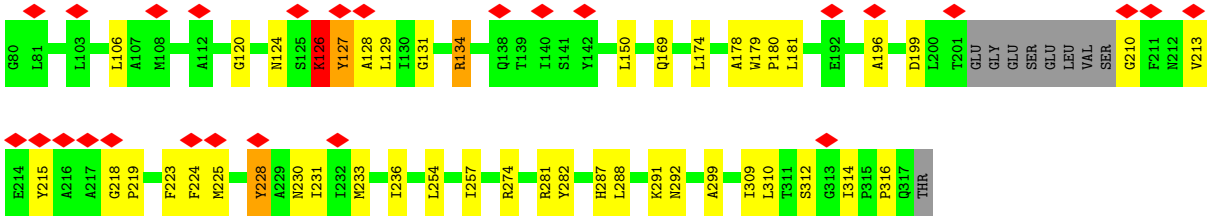




• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

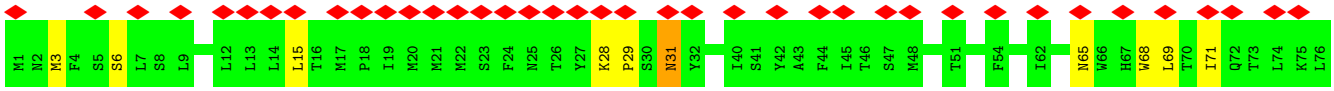
Chain 1:

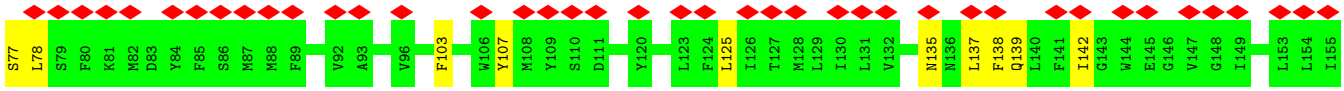


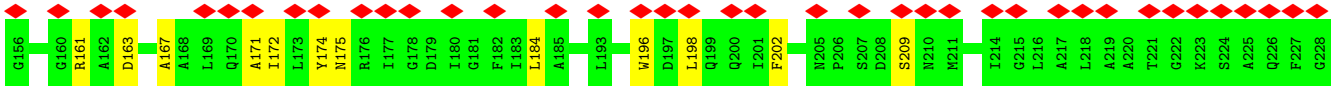


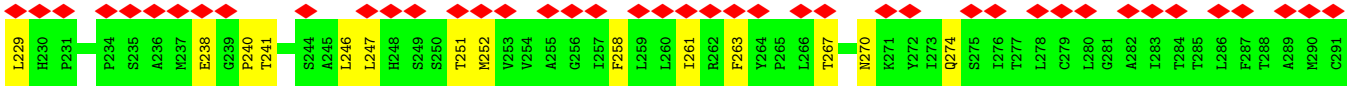
• Molecule 42: NADH-ubiquinone oxidoreductase chain 5

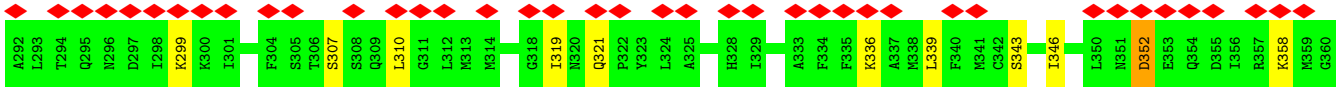
Chain 6:

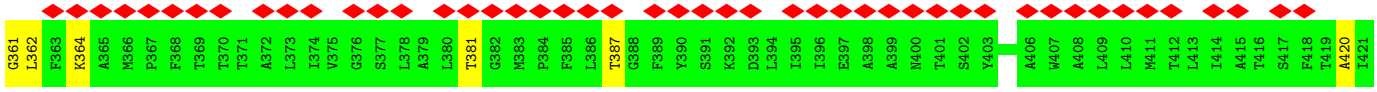


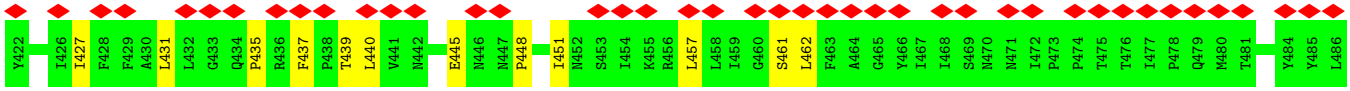


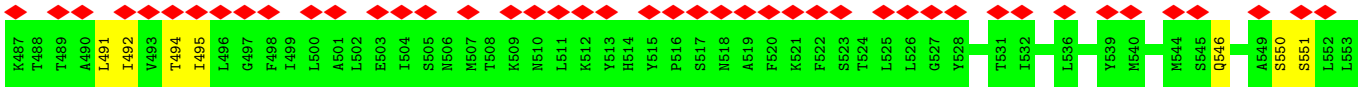


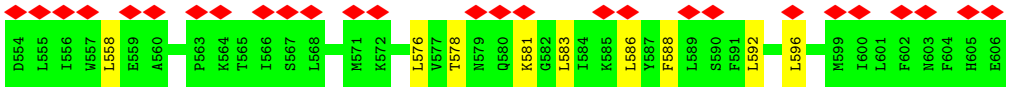






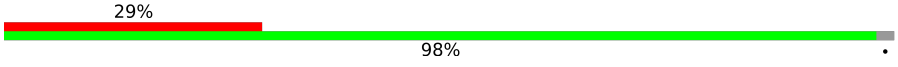


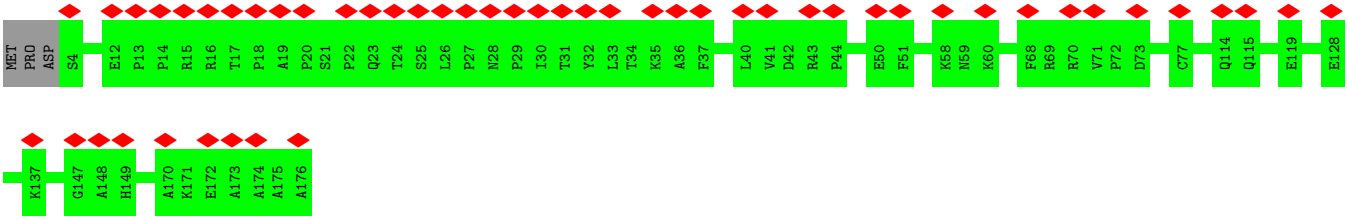




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain g:





• Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain e:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	72302	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.925	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.107	Depositor
Map size (Å)	391.244, 391.244, 391.244	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3973, 1.3973, 1.3973	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	2	0.37	0/2646	0.65	0/3618
2	3	0.34	0/736	0.73	2/1011 (0.2%)
3	4	0.34	0/3538	0.67	1/4845 (0.0%)
4	5	0.34	0/706	0.66	0/960
5	7	0.34	0/1213	0.63	0/1659
6	8	0.34	0/3035	0.60	3/4130 (0.1%)
7	9	0.34	0/1572	0.64	1/2150 (0.0%)
8	A	0.37	0/5269	0.63	5/7152 (0.1%)
9	B	0.43	0/3150	0.65	0/4260
10	C	0.40	0/1756	0.61	0/2394
11	D	0.42	0/1231	0.58	0/1669
12	E	0.43	0/1418	0.65	1/1922 (0.1%)
13	F	0.37	0/188	1.05	1/259 (0.4%)
14	G	0.37	0/1004	0.66	1/1359 (0.1%)
15	H	0.33	0/800	0.58	0/1076
16	I	0.34	0/540	0.68	0/725
17	J	0.33	0/545	0.51	0/740
18	K	0.31	0/663	0.60	0/896
19	L	0.33	0/623	0.66	1/862 (0.1%)
20	N	0.31	0/882	0.59	0/1203
21	O	0.31	0/948	0.55	0/1279
22	P	0.33	0/719	0.66	0/981
23	Q	0.33	0/1381	0.62	0/1869
24	R	0.32	0/2392	0.64	0/3248
25	S	0.31	0/2348	0.64	2/3198 (0.1%)
26	T	0.31	0/959	0.59	0/1305
27	U	0.32	0/1053	0.64	1/1439 (0.1%)
28	V	0.35	0/1121	0.60	0/1515
29	M	0.29	0/651	0.65	0/876
29	W	0.30	0/603	0.63	0/817
30	X	0.30	0/383	0.63	1/523 (0.2%)
31	Y	0.35	0/428	0.61	1/592 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Z	0.31	0/506	0.66	2/688 (0.3%)
33	a	0.31	0/878	0.59	0/1195
34	b	0.31	0/1058	0.60	0/1434
35	c	0.32	0/632	0.69	2/871 (0.2%)
36	d	0.32	0/724	0.53	0/989
37	f	0.29	0/1191	0.55	1/1639 (0.1%)
38	h	0.33	0/743	0.58	0/1013
39	i	0.27	0/286	0.42	0/392
40	j	0.35	0/922	0.66	1/1254 (0.1%)
41	1	0.37	0/2513	0.65	1/3432 (0.0%)
42	6	0.30	0/4892	0.59	0/6660
43	g	0.30	0/1380	0.52	0/1872
44	e	0.33	0/888	0.73	2/1234 (0.2%)
All	All	0.34	0/61114	0.63	30/83205 (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	2	0	2
3	4	0	3
4	5	0	1
5	7	0	3
6	8	0	1
7	9	0	3
8	A	0	6
9	B	0	3
11	D	0	4
12	E	0	2
22	P	0	1
23	Q	0	2
24	R	0	3
25	S	0	1
26	T	0	1
28	V	0	3
29	M	0	1
31	Y	0	1
34	b	0	1
37	f	0	1
38	h	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
41	1	0	1
42	6	0	2
44	e	0	4
All	All	0	52

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	F	97	MET	C-N-CD	-6.83	105.58	120.60
7	9	177	LEU	CA-CB-CG	6.69	130.69	115.30
31	Y	86	HIS	C-N-CA	6.54	138.06	121.70
3	4	212	LEU	CA-CB-CG	6.52	130.29	115.30
2	3	3	LEU	C-N-CA	6.36	137.60	121.70
27	U	120	THR	C-N-CD	-6.34	106.65	120.60
37	f	163	LEU	C-N-CA	6.22	148.13	122.00
2	3	5	LEU	CA-CB-CG	5.99	129.06	115.30
41	1	46	LEU	CA-CB-CG	5.82	128.69	115.30
8	A	381	LEU	CA-CB-CG	5.68	128.37	115.30
8	A	560	LEU	CA-CB-CG	5.68	128.37	115.30
44	e	75	TYR	C-N-CD	-5.67	108.13	120.60
14	G	56	ASP	CB-CG-OD1	5.60	123.34	118.30
12	E	66	LEU	CA-CB-CG	5.53	128.02	115.30
40	j	22	PRO	C-N-CD	-5.52	108.45	120.60
35	c	36	PRO	C-N-CD	-5.44	108.62	120.60
30	X	43	LEU	C-N-CA	5.41	135.22	121.70
35	c	66	ARG	C-N-CA	5.22	134.74	121.70
25	S	196	ASP	CB-CG-OD2	5.19	122.97	118.30
6	8	36	LYS	C-N-CA	5.18	134.66	121.70
19	L	62	ASN	C-N-CA	5.16	134.59	121.70
6	8	228	PRO	C-N-CA	5.15	134.58	121.70
8	A	461	PRO	C-N-CA	5.11	134.46	121.70
6	8	259	GLY	C-N-CA	5.09	134.43	121.70
25	S	113	ASP	C-N-CA	5.08	132.98	122.30
32	Z	85	GLU	C-N-CA	5.05	134.33	121.70
8	A	137	CYS	CA-CB-SG	-5.05	104.91	114.00
44	e	77	LYS	N-CA-C	-5.02	97.44	111.00
8	A	657	ASP	CB-CG-OD1	5.02	122.82	118.30
32	Z	67	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	1	199	ASP	Peptide
1	2	293	TYR	Peptide
1	2	45	MET	Peptide
3	4	224	PRO	Peptide
3	4	306	PRO	Peptide
3	4	369	LEU	Peptide
4	5	24	SER	Peptide
42	6	29	PRO	Peptide
42	6	352	ASP	Peptide
5	7	140	ALA	Peptide
5	7	170	GLU	Peptide
5	7	25	SER	Peptide
6	8	228	PRO	Peptide
7	9	150	GLU	Peptide
7	9	167	LYS	Peptide
7	9	75	LYS	Peptide
8	A	128	CYS	Peptide
8	A	175	ARG	Peptide
8	A	308	ARG	Peptide
8	A	309	ASN	Peptide
8	A	461	PRO	Peptide
8	A	462	PHE	Peptide
9	B	290	GLY	Peptide
9	B	291	VAL	Peptide
9	B	328	ASP	Peptide
11	D	161	GLY	Peptide
11	D	162	TYR	Peptide
11	D	186	CYS	Peptide
11	D	188	PRO	Peptide
12	E	107	PRO	Peptide
12	E	108	SER	Peptide
29	M	16	LEU	Peptide
22	P	52	ASN	Peptide
23	Q	169	PHE	Peptide
23	Q	91	TYR	Peptide
24	R	271	TYR	Peptide
24	R	324	THR	Peptide
24	R	333	PRO	Peptide
25	S	275	ASN	Peptide
26	T	83	LYS	Peptide
28	V	10	MET	Peptide
28	V	142	TRP	Peptide

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Mol	Chain	Res	Type	Group
28	V	72	MET	Peptide
31	Y	89	TYR	Peptide
34	b	110	TRP	Peptide
44	e	115	ASN	Mainchain
44	e	81	ARG	Peptide
44	e	87	ASP	Peptide
44	e	97	LEU	Peptide
37	f	109	PRO	Peptide
38	h	80	PRO	Peptide
38	h	81	ALA	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	2	2582	0	2612	26	0
2	3	719	0	741	10	0
3	4	3447	0	3442	37	0
4	5	697	0	708	13	0
5	7	1186	0	1123	11	0
6	8	2965	0	2596	38	0
7	9	1535	0	1491	34	0
8	A	5183	0	5179	72	0
9	B	3076	0	3041	76	0
10	C	1705	0	1645	21	0
11	D	1200	0	1195	28	0
12	E	1388	0	1340	37	0
13	F	183	0	132	5	0
14	G	981	0	965	13	0
15	H	780	0	753	8	0
16	I	532	0	513	22	0
17	J	530	0	503	7	0
18	K	652	0	636	10	0
19	L	602	0	592	9	0
20	N	862	0	868	9	0
21	O	925	0	907	6	0
22	P	698	0	659	12	0
23	Q	1345	0	1282	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	R	2334	0	2258	51	0
25	S	2299	0	2028	21	0
26	T	942	0	890	10	0
27	U	1019	0	900	10	0
28	V	1093	0	1048	18	0
29	M	642	0	642	8	0
29	W	596	0	553	6	0
30	X	372	0	314	3	0
31	Y	409	0	318	7	0
32	Z	493	0	395	6	0
33	a	857	0	765	0	0
34	b	1032	0	954	0	0
35	c	617	0	492	0	0
36	d	708	0	514	0	0
37	f	1156	0	892	0	0
38	h	721	0	632	0	0
39	i	277	0	240	0	0
40	j	892	0	835	0	0
41	1	2442	0	2563	70	0
42	6	4765	0	4894	54	0
43	g	1351	0	1262	0	0
44	e	864	0	567	0	0
45	2	41	0	59	3	0
45	4	41	0	59	1	0
45	B	51	0	82	2	0
46	4	82	0	114	1	0
47	8	31	0	19	2	0
48	8	8	0	0	0	0
48	A	16	0	0	1	0
48	D	8	0	0	0	0
48	E	16	0	0	0	0
49	9	4	0	0	0	0
49	A	4	0	0	0	0
50	I	1	0	0	1	0
51	R	48	0	23	3	0
52	S	47	0	71	1	0
52	j	39	0	55	0	0
All	All	60091	0	57361	686	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (686) 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)
41:1:126:LYS:HD3	41:1:127:TYR:N	1.31	1.38
24:R:170:LEU:O	24:R:328:ILE:CD1	1.78	1.30
24:R:170:LEU:O	24:R:328:ILE:HD11	1.21	1.29
51:R:601:NAP:O4D	51:R:601:NAP:C1D	1.63	1.27
41:1:75:PRO:HG3	41:1:223:PHE:CZ	1.75	1.21
24:R:328:ILE:HG22	24:R:329:LEU:H	1.09	1.15
9:B:94:VAL:HG12	9:B:115:LEU:HD22	1.28	1.10
25:S:200:PRO:HG3	25:S:223:GLN:HE22	1.18	1.07
9:B:82:LEU:HD21	41:1:126:LYS:HG3	1.04	1.02
41:1:75:PRO:CG	41:1:223:PHE:CZ	2.42	1.02
41:1:126:LYS:CD	41:1:127:TYR:N	2.23	1.01
41:1:75:PRO:HA	41:1:223:PHE:HE1	1.26	1.00
9:B:82:LEU:CD2	41:1:126:LYS:HG3	1.93	0.98
9:B:82:LEU:HD21	41:1:126:LYS:CG	1.93	0.98
24:R:328:ILE:HG22	24:R:329:LEU:N	1.80	0.96
16:I:104:ASP:O	16:I:105:LYS:HB3	1.63	0.95
24:R:328:ILE:CG2	24:R:329:LEU:H	1.80	0.95
9:B:94:VAL:HG12	9:B:115:LEU:CD2	1.96	0.95
9:B:97:LEU:HD12	9:B:97:LEU:H	1.31	0.94
41:1:75:PRO:HA	41:1:223:PHE:CE1	2.02	0.94
41:1:25:ARG:HH11	41:1:25:ARG:HG2	1.36	0.89
41:1:75:PRO:CD	41:1:223:PHE:HZ	1.85	0.89
41:1:126:LYS:HD3	41:1:127:TYR:H	1.11	0.89
11:D:114:ARG:HG3	11:D:114:ARG:HH21	1.38	0.88
9:B:91:ALA:HB2	9:B:193:ASP:OD2	1.73	0.87
24:R:170:LEU:O	24:R:328:ILE:HD12	1.73	0.85
7:9:224:SER:OG	7:9:226:GLU:HG2	1.75	0.85
41:1:126:LYS:HD3	41:1:127:TYR:CA	2.07	0.85
41:1:75:PRO:N	41:1:223:PHE:HZ	1.79	0.81
25:S:200:PRO:CG	25:S:223:GLN:HE22	1.94	0.80
16:I:104:ASP:O	16:I:105:LYS:CB	2.30	0.79
41:1:126:LYS:O	41:1:129:LEU:N	2.15	0.79
9:B:94:VAL:CG1	9:B:115:LEU:HD22	2.12	0.79
11:D:107:ASP:OD2	11:D:113:PHE:CE1	2.37	0.77
16:I:106:GLU:O	16:I:108:LYS:NZ	2.18	0.75
41:1:75:PRO:CD	41:1:223:PHE:CZ	2.67	0.75
11:D:107:ASP:OD2	11:D:113:PHE:HE1	1.70	0.74
41:1:75:PRO:CA	41:1:223:PHE:CE1	2.70	0.73
9:B:82:LEU:HD11	41:1:126:LYS:CE	2.19	0.73
26:T:82:GLU:HG3	26:T:84:PRO:HD2	1.72	0.71
11:D:113:PHE:HB2	11:D:114:ARG:HE	1.54	0.70
9:B:92:HIS:CE1	9:B:141:TYR:HE2	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:367:CYS:SG	8:A:368:THR:N	2.66	0.69
25:S:200:PRO:HG3	25:S:223:GLN:NE2	2.01	0.68
41:1:120:GLY:O	41:1:128:ALA:O	2.12	0.68
6:8:211:ALA:HB2	6:8:223:PRO:HB3	1.76	0.67
16:I:106:GLU:N	16:I:106:GLU:OE1	2.27	0.67
7:9:224:SER:OG	7:9:226:GLU:CG	2.42	0.67
9:B:163:PRO:HG2	9:B:168:GLN:HE21	1.59	0.67
18:K:20:ARG:HB2	18:K:66:TRP:HB2	1.77	0.67
41:1:75:PRO:N	41:1:223:PHE:CZ	2.64	0.66
16:I:105:LYS:O	16:I:105:LYS:HG3	1.96	0.66
41:1:75:PRO:CA	41:1:223:PHE:CZ	2.79	0.65
10:C:123:THR:HG21	14:G:129:SER:H	1.62	0.65
7:9:137:THR:H	7:9:140:CYS:HB2	1.60	0.64
17:J:47:LEU:HD23	23:Q:22:SER:HB2	1.80	0.64
42:6:138:PHE:HB2	42:6:196:TRP:HE1	1.62	0.64
9:B:82:LEU:HD11	41:1:126:LYS:HE3	1.80	0.64
42:6:28:LYS:HE3	42:6:31:ASN:HD21	1.63	0.64
8:A:124:HIS:NE2	48:A:801:SF4:S3	2.71	0.63
16:I:96:HIS:HB2	16:I:114:TYR:HB3	1.81	0.63
41:1:288:LEU:HA	41:1:292:ASN:HD22	1.63	0.63
42:6:578:THR:HA	42:6:581:LYS:HE2	1.79	0.63
23:Q:50:GLU:HB3	23:Q:138:PRO:HG3	1.80	0.63
8:A:34:VAL:HG22	8:A:99:GLY:HA2	1.81	0.62
6:8:52:ARG:HH21	6:8:132:ARG:HG3	1.63	0.62
29:M:70:LEU:HD13	29:M:76:ILE:HG12	1.82	0.62
7:9:130:TYR:HA	7:9:189:ASN:HD21	1.65	0.62
9:B:82:LEU:HD11	41:1:126:LYS:CD	2.30	0.61
28:V:58:ARG:HE	41:1:316:PRO:HB3	1.63	0.61
9:B:87:GLN:OE1	9:B:87:GLN:HA	2.01	0.61
11:D:99:MET:HG2	11:D:106:MET:HB2	1.83	0.61
41:1:25:ARG:HG2	41:1:25:ARG:NH1	2.10	0.61
14:G:75:ARG:NH2	14:G:119:ASP:OD1	2.34	0.61
9:B:95:LEU:O	9:B:95:LEU:HD23	2.01	0.61
41:1:25:ARG:O	41:1:29:GLY:N	2.34	0.61
11:D:114:ARG:HH21	11:D:114:ARG:CG	2.13	0.60
8:A:69:LEU:O	14:G:158:LYS:NZ	2.34	0.60
8:A:273:ILE:HD11	8:A:291:ARG:HA	1.83	0.60
9:B:171:ARG:HH21	9:B:231:GLY:HA2	1.66	0.60
41:1:75:PRO:HG3	41:1:223:PHE:CE2	2.32	0.60
42:6:209:SER:OG	42:6:270:ASN:ND2	2.34	0.60
8:A:75:CYS:SG	8:A:76:ARG:N	2.75	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:97:LEU:HD12	9:B:97:LEU:N	2.01	0.60
10:C:215:ASP:OD2	24:R:75:ARG:NH2	2.34	0.60
9:B:443:MET:SD	41:1:281:ARG:NH1	2.75	0.60
7:9:236:GLU:OE1	7:9:239:LYS:NZ	2.35	0.60
9:B:92:HIS:O	9:B:94:VAL:N	2.35	0.60
25:S:219:SER:HA	25:S:222:LEU:HB2	1.83	0.60
3:4:294:MET:SD	3:4:319:HIS:NE2	2.70	0.59
7:9:71:PRO:HA	13:F:102:SER:HB3	1.85	0.59
11:D:64:GLU:HG2	11:D:66:VAL:H	1.67	0.59
7:9:149:LEU:HD23	7:9:150:GLU:H	1.67	0.59
28:V:50:MET:SD	28:V:54:ASN:ND2	2.75	0.59
4:5:49:LEU:HD21	5:7:49:GLY:H	1.68	0.59
21:O:33:ARG:NH1	29:M:44:SER:O	2.34	0.59
20:N:38:ILE:O	20:N:45:ARG:NH2	2.36	0.59
41:1:126:LYS:CD	41:1:127:TYR:H	1.98	0.59
14:G:131:LYS:HE3	14:G:147:VAL:HG11	1.85	0.59
12:E:188:GLU:O	12:E:192:ASN:ND2	2.36	0.59
10:C:109:GLN:HE21	20:N:83:GLN:HE22	1.50	0.59
8:A:127:ASP:OD2	8:A:175:ARG:NH1	2.36	0.58
8:A:381:LEU:HD12	18:K:55:ILE:HG21	1.85	0.58
8:A:469:ALA:HB3	8:A:472:PRO:HG3	1.84	0.58
8:A:557:ARG:NE	27:U:144:TYR:OH	2.34	0.58
9:B:305:THR:HG23	9:B:306:GLN:HG2	1.85	0.58
16:I:107:THR:HB	16:I:121:GLN:O	2.03	0.58
25:S:193:VAL:HG22	25:S:244:LEU:HB3	1.85	0.58
8:A:246:ARG:NH1	14:G:123:ASN:OD1	2.37	0.58
2:3:64:LEU:HD13	5:7:165:VAL:HG22	1.85	0.58
9:B:338:ARG:NH1	28:V:22:LYS:O	2.37	0.58
3:4:60:SER:OG	3:4:63:THR:O	2.20	0.58
14:G:154:LYS:HB2	14:G:156:LYS:HE2	1.85	0.58
5:7:57:PHE:O	5:7:62:GLY:N	2.37	0.58
41:1:228:TYR:O	41:1:231:ILE:HG22	2.03	0.58
3:4:115:LEU:HB2	3:4:174:LEU:HD13	1.85	0.57
41:1:41:GLY:HA3	41:1:44:GLY:H	1.69	0.57
29:M:37:MET:HG2	29:M:42:LEU:H	1.67	0.57
9:B:263:THR:O	9:B:269:ARG:NH2	2.37	0.57
12:E:66:LEU:HD12	12:E:70:LEU:HD12	1.87	0.57
23:Q:168:PHE:H	23:Q:170:TRP:HD1	1.52	0.57
26:T:103:ALA:O	26:T:106:ARG:NH1	2.37	0.57
4:5:96:LEU:HD13	42:6:581:LYS:HB3	1.86	0.57
9:B:97:LEU:CB	9:B:111:PRO:HA	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:230:GLN:HE21	10:C:233:ARG:HH12	1.53	0.57
22:P:40:LYS:O	28:V:7:LYS:N	2.37	0.57
2:3:102:LEU:O	2:3:106:TRP:N	2.38	0.57
42:6:247:LEU:HD12	42:6:252:MET:HG3	1.87	0.57
15:H:21:GLN:HB3	15:H:37:GLU:HG3	1.85	0.57
24:R:238:GLN:HB3	24:R:267:GLY:HA3	1.87	0.57
42:6:174:TYR:HB3	42:6:229:LEU:HD23	1.87	0.57
5:7:57:PHE:HA	5:7:61:LEU:HB3	1.87	0.57
8:A:380:ASP:OD1	8:A:380:ASP:N	2.38	0.56
6:8:411:SER:HB3	22:P:49:LEU:HD13	1.86	0.56
7:9:56:THR:HG22	7:9:58:GLU:H	1.70	0.56
9:B:116:LEU:HD23	9:B:118:ARG:HE	1.70	0.56
9:B:198:THR:HG22	41:1:32:GLN:HE22	1.70	0.56
42:6:267:THR:O	42:6:274:GLN:NE2	2.38	0.56
6:8:315:LEU:H	6:8:358:ASP:HA	1.69	0.56
6:8:382:CYS:HB3	6:8:384:PRO:HD2	1.88	0.56
8:A:456:ALA:HA	8:A:496:ILE:HD13	1.86	0.56
9:B:237:PRO:HD3	12:E:96:ARG:HH22	1.70	0.56
8:A:624:ARG:NH1	8:A:634:LEU:O	2.37	0.56
24:R:328:ILE:CG2	24:R:329:LEU:N	2.49	0.56
1:2:176:ARG:O	1:2:180:ALA:N	2.37	0.56
8:A:121:LEU:HD21	8:A:139:LEU:HD22	1.87	0.56
24:R:354:ARG:O	24:R:355:ARG:NH2	2.36	0.56
9:B:357:LYS:HD3	9:B:364:SER:HB2	1.87	0.56
3:4:278:ARG:H	42:6:546:GLN:HE22	1.54	0.56
8:A:645:ARG:NH1	8:A:648:GLU:OE1	2.39	0.56
9:B:92:HIS:HE1	9:B:141:TYR:HE2	1.54	0.56
26:T:78:ALA:HA	26:T:89:ASN:HD21	1.71	0.56
8:A:381:LEU:HD21	8:A:664:TYR:HB2	1.87	0.56
9:B:305:THR:OG1	10:C:140:ASN:ND2	2.39	0.56
3:4:451:PRO:HG2	42:6:69:LEU:HD23	1.88	0.55
7:9:88:ARG:NH1	13:F:82:THR:O	2.39	0.55
24:R:84:HIS:HD2	24:R:87:GLU:H	1.53	0.55
6:8:159:ARG:HG2	6:8:161:GLU:H	1.71	0.55
8:A:180:THR:HA	8:A:183:ILE:HD12	1.89	0.55
9:B:295:GLY:HA2	9:B:321:GLY:H	1.72	0.55
24:R:92:MET:HG3	24:R:95:ARG:HH21	1.71	0.55
2:3:81:THR:H	19:L:46:ASN:HD21	1.53	0.55
20:N:35:LEU:O	20:N:45:ARG:NH2	2.40	0.55
29:W:91:ASP:H	32:Z:45:TRP:HB3	1.71	0.55
8:A:588:ALA:O	8:A:592:LYS:NZ	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:159:ARG:NH1	7:9:176:CYS:O	2.38	0.55
21:O:92:GLU:HG3	21:O:97:TRP:HE3	1.72	0.55
23:Q:110:CYS:HA	23:Q:113:ASP:HB3	1.88	0.55
6:8:222:LYS:O	14:G:175:LYS:NZ	2.40	0.55
16:I:106:GLU:O	16:I:108:LYS:HG3	2.07	0.55
3:4:289:SER:HB3	3:4:406:TYR:HE2	1.71	0.55
24:R:203:PRO:HA	24:R:265:PHE:HB2	1.88	0.55
1:2:224:THR:H	1:2:228:LEU:HD23	1.71	0.54
6:8:156:ILE:HD11	6:8:197:VAL:HG22	1.88	0.54
6:8:174:ARG:NH2	13:F:87:ASP:O	2.41	0.54
12:E:39:LYS:HG3	22:P:111:PRO:HA	1.88	0.54
29:M:35:HIS:H	29:M:39:ASP:HB3	1.72	0.54
6:8:220:GLN:HE21	7:9:118:PHE:HB2	1.72	0.54
5:7:66:VAL:O	5:7:70:TYR:N	2.39	0.54
15:H:51:ARG:NH1	23:Q:151:ASN:OD1	2.40	0.54
3:4:319:HIS:HA	3:4:322:THR:HB	1.90	0.54
7:9:62:ARG:NH2	13:F:83:TYR:OH	2.40	0.54
8:A:349:GLU:HG2	8:A:646:LEU:HD11	1.88	0.54
19:L:59:ASP:HB3	23:Q:130:LYS:HD2	1.90	0.54
23:Q:30:HIS:NE2	23:Q:120:PRO:O	2.41	0.54
3:4:403:THR:HA	3:4:406:TYR:HB3	1.90	0.54
3:4:23:ILE:HG21	3:4:93:LYS:HE3	1.89	0.54
8:A:137:CYS:SG	8:A:138:ASP:N	2.80	0.53
6:8:201:ALA:HB1	7:9:121:MET:HB2	1.90	0.53
16:I:106:GLU:HB3	16:I:108:LYS:NZ	2.23	0.53
23:Q:9:SER:HA	28:V:88:ARG:HH12	1.73	0.53
41:1:37:PRO:HB2	41:1:44:GLY:HA2	1.90	0.53
11:D:82:LEU:HB2	11:D:111:VAL:HG22	1.90	0.53
28:V:48:TRP:O	28:V:52:LYS:NZ	2.39	0.53
12:E:82:ALA:HB2	22:P:25:GLN:HE21	1.73	0.53
9:B:97:LEU:HB3	9:B:111:PRO:HB3	1.90	0.53
42:6:361:GLY:O	42:6:364:LYS:NZ	2.40	0.53
1:2:142:LEU:HD23	1:2:145:ILE:HD12	1.91	0.53
4:5:17:VAL:HG12	42:6:588:PHE:HB3	1.91	0.53
10:C:170:ARG:HG3	10:C:186:LEU:HD12	1.91	0.53
11:D:113:PHE:N	11:D:113:PHE:CD1	2.73	0.53
25:S:275:ASN:O	25:S:277:ARG:N	2.41	0.53
9:B:91:ALA:CB	9:B:193:ASP:OD2	2.50	0.53
17:J:64:LYS:H	23:Q:21:SER:HB3	1.74	0.53
4:5:93:LEU:HD22	42:6:583:LEU:H	1.73	0.53
9:B:86:PRO:HG3	9:B:96:ARG:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:118:PHE:O	3:4:122:PHE:N	2.39	0.52
10:C:70:ILE:HG13	10:C:71:LEU:HD12	1.90	0.52
19:L:76:PRO:HD2	23:Q:127:LYS:HG2	1.91	0.52
1:2:164:ILE:HG13	42:6:576:LEU:HD11	1.89	0.52
3:4:439:LEU:H	3:4:442:LEU:HD13	1.74	0.52
8:A:388:ASN:ND2	8:A:513:MET:O	2.36	0.52
8:A:557:ARG:HG3	8:A:560:LEU:HD23	1.91	0.52
25:S:32:ILE:HG13	25:S:33:LEU:HD12	1.91	0.52
7:9:111:ARG:NE	14:G:174:THR:OG1	2.42	0.52
9:B:87:GLN:CB	9:B:89:PRO:HD3	2.32	0.52
1:2:196:TYR:OH	26:T:137:ALA:O	2.26	0.52
12:E:116:CYS:HA	12:E:140:ARG:HH22	1.74	0.52
41:1:210:GLY:HA2	41:1:213:VAL:HG12	1.91	0.52
8:A:161:GLU:OE1	16:I:102:ASN:ND2	2.42	0.52
24:R:281:PHE:HB3	24:R:286:ARG:HD3	1.91	0.52
29:W:83:VAL:HG21	29:W:145:VAL:HG22	1.91	0.52
9:B:303:ARG:HD3	9:B:401:GLU:HG2	1.92	0.52
18:K:65:LEU:HB3	18:K:77:VAL:HG23	1.92	0.52
24:R:264:ALA:H	24:R:334:GLY:HA3	1.75	0.52
9:B:299:GLN:HG2	12:E:38:TYR:HE1	1.75	0.52
24:R:127:ILE:HG22	24:R:165:ILE:HB	1.91	0.52
41:1:46:LEU:HG	41:1:49:ILE:HD11	1.91	0.52
42:6:550:SER:OG	42:6:551:SER:N	2.42	0.52
9:B:97:LEU:HB3	9:B:111:PRO:CB	2.41	0.51
11:D:75:ASN:OD1	11:D:78:ARG:NH2	2.43	0.51
5:7:165:VAL:O	5:7:169:MET:N	2.42	0.51
7:9:222:ARG:HD3	7:9:228:ALA:HB2	1.92	0.51
42:6:427:ILE:HG13	42:6:431:LEU:HD12	1.91	0.51
3:4:214:LEU:HD11	42:6:558:LEU:HB3	1.92	0.51
42:6:439:THR:OG1	42:6:440:LEU:N	2.42	0.51
3:4:301:ILE:O	3:4:304:GLN:NE2	2.43	0.51
28:V:55:ARG:NH2	41:1:312:SER:OG	2.32	0.51
42:6:103:PHE:O	42:6:107:TYR:N	2.40	0.51
10:C:124:ARG:NH1	20:N:111:GLN:O	2.43	0.51
7:9:54:ASP:OD1	7:9:60:TYR:OH	2.29	0.51
8:A:199:GLY:HA3	8:A:204:MET:HA	1.93	0.51
1:2:300:THR:HG23	1:2:301:THR:HG23	1.93	0.51
11:D:114:ARG:HG3	11:D:114:ARG:NH2	2.15	0.51
24:R:171:ASN:HD21	24:R:324:THR:HB	1.76	0.51
41:1:25:ARG:NH1	41:1:25:ARG:CG	2.73	0.51
8:A:587:ALA:HB1	8:A:591:GLU:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:6:241:THR:HG23	42:6:299:LYS:HZ1	1.76	0.51
15:H:21:GLN:O	15:H:25:GLN:NE2	2.43	0.51
24:R:168:SER:OG	24:R:169:HIS:N	2.44	0.51
24:R:197:GLU:HB2	24:R:259:ARG:HE	1.75	0.51
8:A:403:VAL:HG12	8:A:432:ILE:HB	1.92	0.50
24:R:326:ASP:O	24:R:328:ILE:HG13	2.10	0.50
24:R:329:LEU:HG	24:R:331:HIS:H	1.76	0.50
42:6:258:PHE:HA	42:6:261:ILE:HD12	1.92	0.50
23:Q:111:VAL:HG12	23:Q:117:TRP:HB2	1.93	0.50
41:1:230:ASN:HA	41:1:233:MET:HE2	1.93	0.50
42:6:172:ILE:HA	42:6:175:ASN:HD22	1.76	0.50
24:R:281:PHE:HD1	24:R:286:ARG:HA	1.75	0.50
1:2:63:GLN:HE21	1:2:114:TRP:HZ2	1.59	0.50
3:4:134:THR:O	3:4:142:ARG:NH1	2.44	0.50
1:2:78:LEU:HD11	4:5:48:ILE:HD11	1.93	0.50
3:4:276:CYS:SG	3:4:406:TYR:OH	2.65	0.50
22:P:41:LEU:HD12	22:P:42:PRO:HD2	1.94	0.50
7:9:227:PRO:HD2	7:9:231:LEU:HA	1.93	0.50
8:A:371:VAL:HB	8:A:482:GLN:HG3	1.94	0.50
25:S:182:THR:HG23	25:S:183:ILE:HG13	1.92	0.50
1:2:245:LEU:HD22	1:2:301:THR:HG21	1.94	0.50
12:E:189:LYS:HB2	27:U:124:TYR:CZ	2.46	0.50
9:B:86:PRO:HD3	9:B:96:ARG:HA	1.94	0.50
24:R:329:LEU:HD11	24:R:331:HIS:HD2	1.77	0.50
41:1:127:TYR:C	41:1:127:TYR:CD1	2.86	0.50
8:A:352:ILE:HD11	8:A:528:LEU:HD22	1.94	0.49
9:B:272:THR:HA	9:B:275:ILE:HD12	1.93	0.49
25:S:189:PRO:HB2	25:S:192:VAL:HG22	1.94	0.49
16:I:106:GLU:HB3	16:I:108:LYS:HZ1	1.77	0.49
24:R:143:ASP:O	24:R:147:LYS:N	2.43	0.49
31:Y:46:ARG:HA	31:Y:49:GLN:HE22	1.76	0.49
6:8:321:GLY:N	6:8:351:THR:OG1	2.44	0.49
9:B:326:CYS:HA	9:B:329:ARG:HG2	1.94	0.49
11:D:155:SER:OG	12:E:150:THR:O	2.30	0.49
12:E:61:LEU:HD23	28:V:36:PHE:HE1	1.77	0.49
24:R:178:SER:H	24:R:181:LEU:HB3	1.77	0.49
41:1:131:GLY:HA2	41:1:134:ARG:HE	1.76	0.49
1:2:122:ILE:HD13	1:2:128:LEU:HD11	1.95	0.49
6:8:119:GLU:O	6:8:159:ARG:NH2	2.45	0.49
2:3:93:PHE:HA	2:3:96:ILE:HD12	1.95	0.49
11:D:159:GLY:O	11:D:164:HIS:ND1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:E:188:GLU:OE1	27:U:127:TYR:OH	2.30	0.49
24:R:84:HIS:CD2	24:R:87:GLU:H	2.30	0.49
26:T:21:LYS:HG2	26:T:75:CYS:HB3	1.94	0.49
6:8:95:THR:HA	6:8:98:LYS:HG2	1.95	0.49
8:A:443:ASP:N	8:A:443:ASP:OD1	2.45	0.49
9:B:266:ARG:HH22	12:E:60:THR:HA	1.76	0.49
10:C:188:ARG:NH1	10:C:193:TYR:O	2.45	0.49
11:D:114:ARG:CG	11:D:114:ARG:NH2	2.73	0.49
21:O:50:PHE:HE1	21:O:96:VAL:HG12	1.77	0.49
29:M:34:SER:HB3	29:M:40:LEU:HD22	1.95	0.49
7:9:228:ALA:HA	7:9:231:LEU:HD23	1.94	0.49
11:D:151:VAL:HG22	11:D:181:ILE:HB	1.95	0.49
20:N:6:LYS:HE2	20:N:16:VAL:HG11	1.95	0.49
24:R:182:ARG:O	24:R:183:SER:OG	2.29	0.49
28:V:95:ALA:HB2	28:V:106:VAL:HG11	1.95	0.49
8:A:542:PRO:HG2	8:A:545:LEU:HD11	1.95	0.49
9:B:97:LEU:N	9:B:97:LEU:CD1	2.73	0.49
9:B:241:MET:HG3	28:V:10:MET:HB3	1.95	0.49
41:1:73:LEU:HA	41:1:76:ILE:HD12	1.94	0.49
7:9:163:THR:HA	7:9:170:THR:HA	1.94	0.49
18:K:55:ILE:O	18:K:56:ARG:NH1	2.43	0.49
42:6:491:LEU:O	42:6:494:THR:OG1	2.26	0.49
9:B:131:GLN:HE21	12:E:124:PRO:HA	1.77	0.48
23:Q:38:LYS:HG3	23:Q:39:PRO:HD3	1.95	0.48
24:R:178:SER:H	24:R:182:ARG:H	1.61	0.48
24:R:238:GLN:HE22	24:R:271:TYR:HA	1.78	0.48
29:W:119:ILE:HD12	29:W:130:ILE:HG21	1.95	0.48
42:6:381:THR:HA	42:6:420:ALA:HA	1.95	0.48
17:J:26:ILE:O	17:J:30:SER:N	2.42	0.48
6:8:364:VAL:HG12	6:8:400:VAL:HG22	1.95	0.48
12:E:80:GLU:O	22:P:25:GLN:NE2	2.47	0.48
41:1:169:GLN:HE21	41:1:174:LEU:HD13	1.78	0.48
8:A:355:LYS:HD2	8:A:530:TYR:HE1	1.77	0.48
9:B:322:SER:OG	9:B:328:ASP:OD2	2.31	0.48
28:V:134:LEU:HG	28:V:138:TYR:HD2	1.78	0.48
4:5:36:MET:O	4:5:39:SER:OG	2.31	0.48
9:B:86:PRO:HG3	9:B:96:ARG:CB	2.44	0.48
9:B:207:ARG:HD3	11:D:98:HIS:HE1	1.79	0.48
10:C:112:SER:HB2	10:C:135:LEU:HB3	1.96	0.48
12:E:40:TYR:HB3	12:E:43:LEU:HD13	1.95	0.48
24:R:170:LEU:HD12	24:R:328:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:W:122:MET:O	29:W:127:GLY:N	2.43	0.48
1:2:252:GLY:HA3	1:2:290:LEU:HD13	1.96	0.48
9:B:143:SER:OG	9:B:147:ASN:OD1	2.30	0.48
18:K:67:ALA:O	18:K:75:LYS:N	2.45	0.48
27:U:29:ARG:HH12	27:U:63:ILE:HG23	1.79	0.48
25:S:61:LEU:HD22	25:S:251:ALA:HB2	1.96	0.48
3:4:66:LEU:O	3:4:69:THR:OG1	2.28	0.48
8:A:318:THR:HG22	8:A:320:GLU:H	1.79	0.48
8:A:373:PRO:HG3	8:A:486:GLY:HA3	1.96	0.48
18:K:31:GLN:HA	18:K:34:ARG:HE	1.79	0.48
24:R:147:LYS:O	24:R:151:ALA:N	2.47	0.48
6:8:257:ARG:HA	7:9:243:PHE:HB2	1.96	0.47
9:B:82:LEU:HD11	41:1:126:LYS:CG	2.44	0.47
26:T:94:GLY:HA3	26:T:119:GLY:HA2	1.96	0.47
41:1:21:THR:O	41:1:25:ARG:HG3	2.14	0.47
42:6:362:LEU:HB3	42:6:431:LEU:HB3	1.96	0.47
4:5:79:VAL:O	4:5:83:ASN:N	2.48	0.47
9:B:293:LEU:O	9:B:296:SER:N	2.35	0.47
23:Q:5:VAL:N	28:V:107:GLY:O	2.47	0.47
41:1:287:HIS:CE1	41:1:291:LYS:HG3	2.49	0.47
1:2:120:GLN:HG2	1:2:177:LYS:HE3	1.97	0.47
2:3:19:ILE:HA	2:3:23:TRP:HB2	1.95	0.47
7:9:137:THR:O	7:9:141:MET:N	2.43	0.47
8:A:409:PHE:HD1	8:A:694:PHE:HB2	1.80	0.47
8:A:426:ASP:HA	14:G:169:ARG:HH12	1.79	0.47
23:Q:8:PRO:O	28:V:88:ARG:NH2	2.47	0.47
24:R:237:LYS:HA	24:R:325:THR:HG23	1.96	0.47
25:S:100:CYS:HB3	25:S:119:LEU:HB2	1.97	0.47
1:2:149:ILE:HD12	1:2:154:ILE:HG21	1.95	0.47
28:V:58:ARG:NH2	41:1:314:ILE:O	2.47	0.47
3:4:306:PRO:HA	3:4:308:SER:H	1.80	0.47
7:9:57:PRO:HA	7:9:60:TYR:HD2	1.79	0.47
8:A:261:ILE:HG22	8:A:286:ILE:HD11	1.97	0.47
10:C:154:PRO:HG2	21:O:18:LYS:HE2	1.97	0.47
12:E:100:GLU:O	12:E:170:GLY:N	2.46	0.47
24:R:114:ASP:HA	24:R:117:ARG:HB2	1.95	0.47
25:S:114:GLY:HA3	25:S:115:ASN:HA	1.62	0.47
31:Y:64:PHE:HA	31:Y:67:THR:HG22	1.97	0.47
42:6:592:LEU:HD23	42:6:596:LEU:HD23	1.97	0.47
1:2:113:PHE:HA	1:2:116:PRO:HD2	1.97	0.47
1:2:260:PHE:HE2	1:2:264:TRP:HE3	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:235:LEU:HA	3:4:238:LEU:HG	1.97	0.47
8:A:650:SER:OG	8:A:652:ASN:OD1	2.30	0.47
23:Q:110:CYS:O	23:Q:114:LYS:N	2.42	0.47
7:9:75:LYS:O	7:9:77:ALA:N	2.45	0.47
24:R:352:VAL:HG13	24:R:353:LEU:HD12	1.96	0.47
29:M:75:GLU:HA	29:M:78:ASP:HB2	1.97	0.47
8:A:97:MET:HB2	8:A:100:TRP:HE1	1.79	0.47
10:C:156:GLU:HA	10:C:181:ALA:HB3	1.96	0.47
23:Q:111:VAL:O	23:Q:117:TRP:N	2.44	0.47
23:Q:118:VAL:HG13	23:Q:120:PRO:HD3	1.96	0.47
41:1:233:MET:HA	41:1:236:ILE:HG22	1.97	0.47
5:7:140:ALA:HA	5:7:142:GLY:H	1.80	0.46
8:A:485:ASP:HB3	8:A:680:LEU:HG	1.97	0.46
16:I:111:THR:HG22	16:I:118:GLN:HA	1.97	0.46
21:O:98:LYS:HB3	21:O:102:HIS:HB2	1.95	0.46
42:6:246:LEU:O	42:6:251:THR:OG1	2.31	0.46
3:4:88:ASN:HB2	3:4:91:ARG:HE	1.80	0.46
26:T:99:LEU:O	26:T:103:ALA:N	2.47	0.46
6:8:219:LYS:NZ	14:G:172:VAL:O	2.42	0.46
6:8:451:GLN:O	6:8:455:GLN:N	2.44	0.46
9:B:293:LEU:HD23	9:B:293:LEU:HA	1.81	0.46
16:I:62:GLU:HB3	27:U:124:TYR:HA	1.97	0.46
42:6:202:PHE:HZ	42:6:263:PHE:HA	1.78	0.46
29:M:37:MET:H	29:M:41:GLY:H	1.61	0.46
2:3:60:ILE:HG21	5:7:168:ILE:HG21	1.97	0.46
8:A:306:MET:HA	8:A:316:HIS:HA	1.98	0.46
12:E:150:THR:OG1	12:E:151:LYS:N	2.48	0.46
25:S:175:TYR:O	25:S:179:LYS:N	2.45	0.46
42:6:457:LEU:O	42:6:461:SER:N	2.46	0.46
3:4:138:ASN:ND2	3:4:223:ALA:O	2.48	0.46
6:8:398:ARG:NH2	8:A:155:GLU:OE2	2.48	0.46
24:R:275:ASP:O	24:R:279:TYR:N	2.48	0.46
7:9:110:MET:HA	7:9:113:TYR:HD2	1.81	0.46
16:I:103:LEU:HD13	16:I:121:GLN:HB3	1.98	0.46
24:R:154:GLN:HG3	24:R:155:VAL:H	1.81	0.46
24:R:269:SER:HA	24:R:270:ARG:HA	1.64	0.46
25:S:161:MET:HG2	25:S:167:ILE:HB	1.98	0.46
45:2:401:3PE:H2C2	3:4:16:TRP:HE1	1.80	0.46
6:8:330:SER:OG	6:8:331:VAL:N	2.46	0.46
8:A:215:MET:SD	8:A:695:TYR:OH	2.73	0.46
24:R:52:SER:OG	24:R:77:GLY:O	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:20:ASP:HB2	28:V:22:LYS:H	1.81	0.46
29:W:97:LYS:NZ	29:W:107:ASP:CB	2.79	0.46
12:E:158:CYS:SG	12:E:159:GLN:N	2.89	0.46
20:N:114:TRP:O	20:N:116:ILE:N	2.46	0.46
3:4:45:PHE:HA	3:4:46:GLY:HA3	1.68	0.46
8:A:238:PHE:CD2	12:E:140:ARG:HB3	2.51	0.46
23:Q:86:TRP:HA	23:Q:89:ILE:HG22	1.98	0.46
1:2:173:THR:O	1:2:226:THR:OG1	2.27	0.46
6:8:146:GLY:O	6:8:150:GLY:N	2.48	0.46
41:1:21:THR:CG2	41:1:25:ARG:NH2	2.79	0.46
7:9:42:ARG:NH2	8:A:203:ASP:O	2.49	0.45
8:A:364:ASP:OD1	8:A:364:ASP:N	2.48	0.45
14:G:97:TRP:HB2	14:G:128:PHE:HB2	1.98	0.45
42:6:343:SER:HA	42:6:346:ILE:HD12	1.97	0.45
1:2:258:SER:HA	1:2:334:THR:HB	1.99	0.45
42:6:161:ARG:NH2	42:6:238:GLU:OE1	2.49	0.45
45:2:401:3PE:H292	45:2:401:3PE:H2E1	1.98	0.45
4:5:17:VAL:HA	4:5:20:LEU:HB3	1.98	0.45
7:9:164:THR:HB	7:9:169:PHE:HB2	1.98	0.45
9:B:85:GLY:C	9:B:87:GLN:N	2.70	0.45
42:6:139:GLN:HA	42:6:142:ILE:HD12	1.98	0.45
3:4:115:LEU:HD12	3:4:174:LEU:HB2	1.99	0.45
8:A:381:LEU:HD11	8:A:664:TYR:HD2	1.81	0.45
9:B:368:ARG:HA	9:B:371:MET:HG2	1.98	0.45
25:S:196:ASP:HB3	25:S:248:ALA:H	1.81	0.45
3:4:55:LEU:HD22	23:Q:171:THR:HG22	1.99	0.45
6:8:318:ILE:HD13	6:8:355:ILE:HG13	1.99	0.45
24:R:177:SER:HA	24:R:178:SER:HA	1.68	0.45
45:2:401:3PE:H331	45:2:401:3PE:H362	1.82	0.45
3:4:318:ALA:HB1	3:4:374:ASN:HD22	1.82	0.45
6:8:413:TRP:HE1	6:8:436:GLN:HG3	1.82	0.45
20:N:56:LEU:HA	20:N:59:VAL:HB	1.99	0.45
42:6:352:ASP:N	42:6:352:ASP:OD1	2.49	0.45
1:2:146:PHE:HE1	1:2:195:PRO:HA	1.82	0.45
8:A:627:SER:OG	8:A:632:MET:O	2.31	0.45
15:H:96:PRO:HA	15:H:97:HIS:HA	1.65	0.45
20:N:62:GLU:OE2	20:N:71:ARG:NH1	2.37	0.45
42:6:171:ALA:O	42:6:175:ASN:ND2	2.50	0.45
3:4:393:ILE:HG21	42:6:184:LEU:HD13	1.98	0.45
6:8:177:TYR:HD1	6:8:182:ILE:HB	1.82	0.45
11:D:174:ASP:OD1	11:D:182:TYR:OH	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Z:44:PRO:HA	32:Z:45:TRP:HA	1.81	0.45
3:4:368:ALA:HB1	3:4:374:ASN:HB2	1.99	0.45
5:7:25:SER:O	5:7:27:ILE:N	2.47	0.45
8:A:153:PHE:HE2	8:A:156:GLY:HA3	1.81	0.45
8:A:161:GLU:HG3	16:I:105:LYS:HE3	1.99	0.45
12:E:196:LYS:HD2	12:E:197:TRP:CZ3	2.52	0.45
14:G:108:GLU:HG2	14:G:113:GLY:HA2	1.99	0.45
16:I:89:GLY:H	16:I:96:HIS:CE1	2.34	0.45
51:R:601:NAP:O4D	51:R:601:NAP:C2N	2.65	0.45
45:B:501:3PE:H382	41:1:180:PRO:HB3	1.99	0.44
32:Z:65:GLY:O	32:Z:70:GLY:N	2.48	0.44
41:1:65:THR:OG1	41:1:124:ASN:ND2	2.49	0.44
42:6:15:LEU:HD21	42:6:125:LEU:HD22	1.99	0.44
3:4:16:TRP:HA	3:4:93:LYS:HD3	1.99	0.44
3:4:76:MET:HG2	3:4:231:LEU:HD12	1.99	0.44
3:4:307:TRP:HE1	42:6:71:ILE:HD12	1.81	0.44
8:A:81:GLU:HG3	8:A:108:LYS:HD2	1.99	0.44
9:B:382:PHE:HD1	12:E:118:LEU:HD11	1.81	0.44
42:6:137:LEU:HB3	42:6:196:TRP:HD1	1.81	0.44
6:8:246:GLU:HA	6:8:249:ALA:HB3	1.98	0.44
11:D:150:VAL:HG12	11:D:179:VAL:HG13	1.99	0.44
9:B:97:LEU:CD1	9:B:97:LEU:C	2.85	0.44
19:L:56:PRO:HG3	23:Q:41:LYS:HB3	2.00	0.44
24:R:155:VAL:O	24:R:159:ALA:N	2.49	0.44
31:Y:47:TYR:HD2	32:Z:16:LEU:HD12	1.82	0.44
42:6:135:ASN:HA	42:6:198:LEU:HD12	1.99	0.44
4:5:51:SER:HA	15:H:32:ARG:HE	1.83	0.44
9:B:359:ASP:HB2	22:P:45:PRO:HG2	2.00	0.44
41:1:126:LYS:HD3	41:1:126:LYS:C	2.22	0.44
41:1:254:LEU:HA	41:1:257:ILE:HD12	1.99	0.44
42:6:307:SER:HA	42:6:310:LEU:HD12	1.99	0.44
6:8:445:GLU:O	6:8:449:ARG:NH1	2.51	0.44
11:D:175:ARG:HG2	24:R:48:ARG:HH21	1.83	0.44
23:Q:121:ASP:OD1	23:Q:121:ASP:N	2.49	0.44
24:R:64:PHE:HZ	24:R:208:GLY:HA3	1.81	0.44
41:1:39:VAL:HG13	41:1:40:VAL:HG13	1.99	0.44
3:4:62:SER:HB2	3:4:457:PRO:HD3	2.00	0.44
9:B:308:TYR:OH	9:B:401:GLU:N	2.47	0.44
12:E:79:ARG:NH2	22:P:19:ASP:OD2	2.50	0.44
41:1:3:MET:HA	41:1:6:ILE:HD12	2.00	0.44
3:4:198:ALA:HB2	45:4:502:3PE:H271	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:8:124:THR:HG22	6:8:126:LYS:H	1.82	0.44
7:9:195:ASP:OD2	7:9:220:SER:OG	2.34	0.44
8:A:35:PHE:HB3	8:A:38:GLY:HA2	2.00	0.44
8:A:275:PRO:HB3	8:A:286:ILE:HB	1.99	0.44
31:Y:66:ALA:O	31:Y:70:PHE:N	2.50	0.44
7:9:153:GLN:HG3	7:9:158:ILE:HG13	2.00	0.44
17:J:68:ASN:ND2	23:Q:19:LYS:O	2.51	0.44
1:2:48:HIS:HD2	5:7:171:ILE:HG23	1.83	0.43
12:E:197:TRP:HB3	27:U:84:PRO:HB2	2.00	0.43
31:Y:57:GLN:HE22	42:6:445:GLU:HB3	1.83	0.43
6:8:284:ASN:HD22	7:9:228:ALA:HB3	1.83	0.43
25:S:280:HIS:O	25:S:283:ARG:N	2.51	0.43
42:6:448:PRO:HA	42:6:451:ILE:HB	2.00	0.43
8:A:63:PHE:O	8:A:181:ARG:NH2	2.51	0.43
8:A:422:TRP:HA	8:A:427:LEU:HB3	1.99	0.43
9:B:118:ARG:HD3	11:D:163:TYR:CZ	2.54	0.43
10:C:117:THR:OG1	10:C:118:ALA:N	2.50	0.43
6:8:177:TYR:O	13:F:96:ARG:NH1	2.52	0.43
9:B:97:LEU:HB3	9:B:111:PRO:HA	1.98	0.43
9:B:221:ARG:NH1	11:D:95:GLU:OE2	2.51	0.43
10:C:165:ALA:HB1	10:C:169:GLU:HG3	2.00	0.43
12:E:175:PHE:HB3	12:E:176:SER:H	1.63	0.43
24:R:235:THR:HA	24:R:236:VAL:HA	1.57	0.43
25:S:150:SER:OG	25:S:151:ILE:N	2.51	0.43
7:9:92:TRP:HB3	7:9:127:VAL:HG22	2.00	0.43
29:W:97:LYS:HZ3	29:W:107:ASP:CB	2.32	0.43
41:1:75:PRO:CB	41:1:223:PHE:CE1	3.02	0.43
41:1:178:ALA:HB1	41:1:181:LEU:HB2	2.01	0.43
1:2:80:PHE:HB3	15:H:64:ARG:HH12	1.82	0.43
8:A:250:SER:OG	8:A:251:ILE:N	2.51	0.43
9:B:92:HIS:HE1	9:B:141:TYR:CE2	2.34	0.43
10:C:157:SER:HB3	10:C:180:PHE:HB3	2.01	0.43
23:Q:59:GLU:HA	23:Q:62:LEU:HD13	2.00	0.43
23:Q:137:LEU:HD12	23:Q:138:PRO:HD2	2.01	0.43
24:R:152:ILE:H	24:R:152:ILE:HG13	1.72	0.43
30:X:21:VAL:HA	30:X:24:TYR:HB3	1.99	0.43
12:E:119:CYS:SG	12:E:120:GLU:N	2.92	0.43
22:P:34:ARG:NH2	27:U:92:CYS:O	2.46	0.43
27:U:42:ASP:HA	27:U:43:LYS:HA	1.75	0.43
41:1:75:PRO:CB	41:1:223:PHE:CZ	2.99	0.43
1:2:63:GLN:HA	1:2:66:ALA:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:370:PRO:HA	3:4:375:LEU:HB2	1.99	0.43
9:B:398:THR:OG1	9:B:399:ALA:N	2.52	0.43
25:S:202:VAL:HA	25:S:205:ARG:HB2	2.01	0.43
32:Z:24:ILE:HG12	32:Z:54:MET:HE1	2.00	0.43
47:8:501:FMN:H1'1	47:8:501:FMN:H9	1.68	0.43
9:B:267:ILE:O	9:B:271:ARG:N	2.49	0.43
11:D:113:PHE:HB2	11:D:114:ARG:H	1.62	0.43
12:E:85:ASN:O	12:E:89:GLU:N	2.42	0.43
16:I:108:LYS:HA	16:I:120:ARG:HA	2.01	0.43
30:X:14:VAL:HA	30:X:17:PRO:HD2	2.01	0.43
1:2:200:MET:HG2	1:2:341:PRO:HB3	2.01	0.42
7:9:134:VAL:HG23	7:9:171:LEU:HD11	2.01	0.42
12:E:38:TYR:HB2	22:P:106:LEU:HA	2.01	0.42
42:6:336:LYS:HA	42:6:339:LEU:HB3	2.01	0.42
9:B:278:VAL:HG12	9:B:283:ALA:HB2	2.00	0.42
8:A:251:ILE:HB	8:A:606:THR:HG22	2.01	0.42
9:B:238:LEU:HD13	22:P:37:PRO:HD2	2.02	0.42
10:C:116:LEU:HD23	10:C:168:TYR:HB3	2.02	0.42
42:6:358:LYS:HB3	42:6:437:PHE:HA	2.02	0.42
6:8:183:GLY:HA2	6:8:184:LYS:HA	1.67	0.42
8:A:144:MET:HA	9:B:380:HIS:HE2	1.84	0.42
8:A:351:LEU:O	8:A:530:TYR:OH	2.34	0.42
9:B:293:LEU:HB3	9:B:294:ARG:H	1.51	0.42
41:1:20:LEU:O	41:1:24:GLU:N	2.49	0.42
2:3:2:ASN:OD1	2:3:2:ASN:N	2.52	0.42
6:8:120:GLY:N	47:8:501:FMN:O4	2.41	0.42
6:8:160:GLY:HA2	6:8:199:ARG:HD2	2.00	0.42
8:A:560:LEU:HD12	8:A:561:PRO:HD2	1.99	0.42
9:B:94:VAL:HB	9:B:95:LEU:H	1.64	0.42
10:C:86:LEU:HB2	10:C:143:ILE:HG13	2.01	0.42
16:I:87:CYS:O	16:I:96:HIS:NE2	2.53	0.42
52:S:401:PC1:H262	52:S:401:PC1:H292	1.84	0.42
42:6:319:ILE:HG22	42:6:321:GLN:HG2	1.99	0.42
6:8:383:THR:OG1	8:A:75:CYS:O	2.30	0.42
12:E:103:LEU:HD23	12:E:103:LEU:HA	1.92	0.42
18:K:56:ARG:HA	18:K:56:ARG:HD3	1.86	0.42
19:L:25:ILE:HB	41:1:299:ALA:HB1	2.00	0.42
11:D:114:ARG:HD2	11:D:114:ARG:O	2.20	0.42
25:S:187:LEU:HD13	25:S:277:ARG:HB2	2.01	0.42
41:1:196:ALA:HB2	41:1:274:ARG:HH21	1.83	0.42
42:6:364:LYS:HD3	42:6:435:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:35:SER:O	3:4:38:SER:OG	2.35	0.42
4:5:32:CYS:O	4:5:36:MET:N	2.53	0.42
8:A:34:VAL:HG13	8:A:100:TRP:H	1.84	0.42
8:A:634:LEU:HA	8:A:635:PRO:HD3	1.81	0.42
9:B:91:ALA:HB2	9:B:193:ASP:CG	2.39	0.42
9:B:194:ILE:HD13	9:B:268:TRP:HE1	1.85	0.42
10:C:97:PRO:O	10:C:101:PHE:N	2.50	0.42
21:O:77:ARG:HA	21:O:80:ASP:HB3	2.01	0.42
23:Q:30:HIS:CD2	23:Q:120:PRO:HG2	2.55	0.42
25:S:135:LEU:HA	25:S:138:LEU:HD13	2.02	0.42
7:9:147:SER:HB2	7:9:198:PRO:HG3	2.01	0.42
10:C:99:LEU:O	10:C:103:ARG:N	2.52	0.42
12:E:54:THR:HG22	19:L:13:TRP:HH2	1.85	0.42
17:J:55:SER:OG	17:J:56:GLY:N	2.52	0.42
32:Z:64:VAL:HA	32:Z:67:LEU:HG	2.02	0.42
12:E:211:TYR:CZ	22:P:39:PRO:HG3	2.55	0.42
17:J:38:VAL:O	17:J:44:GLN:NE2	2.53	0.42
42:6:3:MET:HA	42:6:6:SER:HB2	2.02	0.42
42:6:583:LEU:HD23	42:6:586:LEU:HD13	2.02	0.42
3:4:435:ALA:O	3:4:438:SER:OG	2.31	0.41
8:A:598:ASN:OD1	8:A:601:GLY:N	2.53	0.41
9:B:447:VAL:HA	9:B:450:ILE:HD12	2.02	0.41
24:R:154:GLN:HG3	24:R:155:VAL:HG23	2.02	0.41
24:R:322:ILE:H	24:R:322:ILE:HG13	1.73	0.41
26:T:26:THR:O	26:T:30:GLY:N	2.52	0.41
26:T:77:SER:HA	26:T:80:VAL:HG22	2.02	0.41
42:6:492:ILE:HA	42:6:495:ILE:HD12	2.02	0.41
8:A:372:PHE:HB3	8:A:532:PRO:HB2	2.02	0.41
8:A:511:LYS:HD3	8:A:663:ASN:HB3	2.02	0.41
9:B:116:LEU:HA	11:D:130:THR:HG21	2.02	0.41
42:6:68:TRP:H	42:6:77:SER:HA	1.84	0.41
9:B:421:ARG:HH21	9:B:423:LYS:HB2	1.86	0.41
11:D:108:ARG:HD3	41:1:36:GLY:HA2	2.01	0.41
11:D:146:GLU:O	24:R:89:TYR:OH	2.35	0.41
11:D:150:VAL:HB	11:D:179:VAL:HA	2.02	0.41
12:E:170:GLY:HA2	12:E:171:PRO:HD3	1.78	0.41
16:I:106:GLU:N	16:I:106:GLU:CD	2.73	0.41
2:3:79:SER:O	19:L:46:ASN:ND2	2.50	0.41
8:A:189:ILE:H	8:A:189:ILE:HG13	1.66	0.41
16:I:87:CYS:HB3	50:I:300:ZN:ZN	1.52	0.41
17:J:4:GLU:OE1	41:1:30:TYR:OH	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:6:163:ASP:O	42:6:167:ALA:N	2.51	0.41
12:E:53:VAL:O	12:E:57:ALA:N	2.53	0.41
12:E:98:ARG:NH2	12:E:155:CYS:O	2.53	0.41
12:E:127:ALA:HB1	12:E:148:ASP:H	1.86	0.41
27:U:55:PHE:HB3	27:U:58:ARG:HG3	2.02	0.41
28:V:43:LEU:HB2	41:1:179:TRP:HE1	1.86	0.41
1:2:250:SER:HB2	1:2:257:LEU:HD13	2.03	0.41
6:8:36:LYS:HB2	6:8:38:GLU:HG3	2.01	0.41
6:8:316:ALA:HB1	6:8:326:LEU:HD22	2.02	0.41
7:9:93:LEU:HA	7:9:94:PRO:HD3	1.94	0.41
8:A:422:TRP:O	14:G:169:ARG:NH1	2.53	0.41
8:A:605:GLN:HG3	8:A:607:LYS:HZ2	1.85	0.41
9:B:326:CYS:SG	9:B:329:ARG:NH1	2.94	0.41
10:C:230:GLN:HE21	10:C:233:ARG:NH1	2.16	0.41
12:E:115:ALA:O	12:E:140:ARG:NH1	2.40	0.41
1:2:7:ILE:O	1:2:11:LEU:N	2.53	0.41
3:4:274:SER:HA	3:4:277:LEU:HD13	2.03	0.41
12:E:135:ARG:NH1	16:I:68:ALA:O	2.54	0.41
15:H:15:ASP:OD1	15:H:15:ASP:N	2.52	0.41
5:7:140:ALA:HA	5:7:142:GLY:N	2.36	0.41
7:9:205:ILE:HG22	7:9:209:LYS:HE2	2.03	0.41
30:X:13:HIS:O	30:X:15:LEU:N	2.54	0.41
31:Y:89:TYR:O	31:Y:91:ASP:N	2.53	0.41
42:6:65:ASN:HB2	42:6:78:LEU:HD11	2.01	0.41
1:2:216:PHE:HA	1:2:219:PHE:HB2	2.02	0.41
2:3:84:LEU:HD21	41:1:309:ILE:HD13	2.03	0.41
24:R:228:LEU:HA	24:R:229:ILE:HA	1.78	0.41
24:R:266:VAL:HG23	24:R:335:LEU:HB3	2.02	0.41
51:R:601:NAP:H3B	51:R:601:NAP:PA	2.61	0.41
25:S:73:HIS:NE2	25:S:148:GLU:OE2	2.41	0.41
27:U:115:PHE:HB3	27:U:117:LEU:HG	2.02	0.41
41:1:24:GLU:OE1	41:1:228:TYR:OH	2.35	0.41
41:1:127:TYR:C	41:1:127:TYR:HD1	2.23	0.41
29:M:26:ASP:N	29:M:26:ASP:OD1	2.54	0.41
4:5:88:ASP:N	4:5:88:ASP:OD1	2.50	0.41
6:8:186:ALA:HA	6:8:187:CYS:HA	1.57	0.41
8:A:44:GLU:HB3	8:A:47:THR:HG23	2.03	0.41
8:A:643:ARG:HA	8:A:646:LEU:HB2	2.03	0.41
10:C:90:ILE:HD12	10:C:145:VAL:HG13	2.03	0.41
12:E:49:ASP:N	12:E:49:ASP:OD1	2.53	0.41
18:K:35:ASP:OD1	18:K:39:LYS:NZ	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:6:387:THR:HG22	42:6:462:LEU:HA	2.03	0.41
11:D:156:CYS:HA	11:D:161:GLY:N	2.36	0.40
18:K:31:GLN:HB3	18:K:34:ARG:HH21	1.86	0.40
18:K:36:PHE:O	18:K:40:ARG:N	2.50	0.40
19:L:31:ILE:HG22	19:L:35:LEU:HD11	2.03	0.40
31:Y:91:ASP:O	31:Y:93:SER:N	2.54	0.40
41:1:106:LEU:HD11	41:1:150:LEU:HD13	2.03	0.40
1:2:190:MET:HB2	1:2:201:THR:HG23	2.02	0.40
2:3:104:TYR:O	2:3:107:THR:OG1	2.31	0.40
3:4:244:LEU:HD21	3:4:301:ILE:HD12	2.03	0.40
4:5:7:ASN:HA	4:5:8:ILE:HA	1.72	0.40
23:Q:53:PRO:HD2	28:V:116:TRP:CD1	2.55	0.40
41:1:218:GLY:HA3	41:1:219:PRO:HD3	1.92	0.40
42:6:107:TYR:HE2	42:6:240:PRO:HB3	1.87	0.40
4:5:26:LEU:HB3	4:5:88:ASP:HB2	2.04	0.40
45:B:501:3PE:H3H2	45:B:501:3PE:H3E2	1.96	0.40
16:I:105:LYS:HB3	16:I:105:LYS:HE2	1.82	0.40
19:L:80:TRP:O	19:L:84:LEU:N	2.54	0.40
24:R:227:PRO:HG2	24:R:230:SER:HA	2.02	0.40
26:T:124:LEU:O	26:T:128:GLY:N	2.55	0.40
41:1:215:TYR:HD1	41:1:219:PRO:HB2	1.86	0.40
6:8:297:LYS:N	6:8:333:GLU:O	2.45	0.40
8:A:462:PHE:O	8:A:464:GLN:N	2.39	0.40
9:B:246:GLU:HA	9:B:249:LYS:HE3	2.02	0.40
20:N:26:ILE:O	20:N:30:LYS:N	2.48	0.40
46:4:501:CDL:H742	46:4:501:CDL:H712	1.80	0.40
9:B:271:ARG:HD2	9:B:271:ARG:HA	1.95	0.40
15:H:82:GLN:HE21	28:V:98:MET:HB2	1.86	0.40
24:R:320:GLU:O	24:R:324:THR:OG1	2.38	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	2	342/347 (99%)	295 (86%)	47 (14%)	0	100	100
2	3	89/115 (77%)	74 (83%)	14 (16%)	1 (1%)	14	52
3	4	457/459 (100%)	383 (84%)	70 (15%)	4 (1%)	17	56
4	5	94/98 (96%)	82 (87%)	12 (13%)	0	100	100
5	7	170/175 (97%)	140 (82%)	28 (16%)	2 (1%)	13	50
6	8	425/444 (96%)	346 (81%)	78 (18%)	1 (0%)	47	80
7	9	205/217 (94%)	169 (82%)	35 (17%)	1 (0%)	29	68
8	A	686/704 (97%)	572 (83%)	107 (16%)	7 (1%)	15	54
9	B	383/430 (89%)	334 (87%)	40 (10%)	9 (2%)	6	37
10	C	206/228 (90%)	177 (86%)	29 (14%)	0	100	100
11	D	150/179 (84%)	130 (87%)	19 (13%)	1 (1%)	22	62
12	E	174/176 (99%)	158 (91%)	15 (9%)	1 (1%)	25	64
13	F	26/75 (35%)	19 (73%)	7 (27%)	0	100	100
14	G	121/133 (91%)	99 (82%)	21 (17%)	1 (1%)	19	60
15	H	94/105 (90%)	73 (78%)	21 (22%)	0	100	100
16	I	69/96 (72%)	53 (77%)	14 (20%)	2 (3%)	4	32
17	J	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
18	K	82/98 (84%)	63 (77%)	19 (23%)	0	100	100
19	L	78/83 (94%)	66 (85%)	12 (15%)	0	100	100
20	N	109/115 (95%)	93 (85%)	16 (15%)	0	100	100
21	O	112/127 (88%)	97 (87%)	15 (13%)	0	100	100
22	P	86/112 (77%)	63 (73%)	23 (27%)	0	100	100
23	Q	166/171 (97%)	126 (76%)	40 (24%)	0	100	100
24	R	302/345 (88%)	241 (80%)	59 (20%)	2 (1%)	22	62
25	S	317/320 (99%)	247 (78%)	68 (22%)	2 (1%)	25	64
26	T	136/140 (97%)	116 (85%)	20 (15%)	0	100	100
27	U	128/145 (88%)	103 (80%)	25 (20%)	0	100	100
28	V	136/143 (95%)	121 (89%)	14 (10%)	1 (1%)	22	62
29	M	78/88 (89%)	62 (80%)	16 (20%)	0	100	100
29	W	79/88 (90%)	68 (86%)	11 (14%)	0	100	100
30	X	47/57 (82%)	38 (81%)	8 (17%)	1 (2%)	7	39
31	Y	55/72 (76%)	46 (84%)	9 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	Z	72/97 (74%)	57 (79%)	15 (21%)	0	100 100
33	a	112/128 (88%)	95 (85%)	17 (15%)	0	100 100
34	b	137/143 (96%)	113 (82%)	24 (18%)	0	100 100
35	c	86/127 (68%)	68 (79%)	18 (21%)	0	100 100
36	d	105/136 (77%)	82 (78%)	21 (20%)	2 (2%)	8 41
37	f	165/178 (93%)	135 (82%)	30 (18%)	0	100 100
38	h	89/125 (71%)	62 (70%)	25 (28%)	2 (2%)	6 38
39	i	36/49 (74%)	35 (97%)	1 (3%)	0	100 100
40	j	111/120 (92%)	92 (83%)	19 (17%)	0	100 100
41	1	305/318 (96%)	269 (88%)	34 (11%)	2 (1%)	22 62
42	6	604/606 (100%)	536 (89%)	67 (11%)	1 (0%)	47 80
43	g	171/176 (97%)	139 (81%)	32 (19%)	0	100 100
44	e	139/158 (88%)	82 (59%)	50 (36%)	7 (5%)	2 23
All	All	7801/8516 (92%)	6480 (83%)	1271 (16%)	50 (1%)	29 64

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	A	463	SER
9	B	88	HIS
9	B	294	ARG
16	I	105	LYS
25	S	200	PRO
25	S	276	ASP
36	d	40	VAL
38	h	81	ALA
38	h	82	VAL
41	1	126	LYS
44	e	68	ASP
44	e	71	GLY
44	e	81	ARG
44	e	82	SER
5	7	171	ILE
9	B	84	PHE
9	B	91	ALA
9	B	93	GLY
9	B	94	VAL

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Mol	Chain	Res	Type
11	D	113	PHE
16	I	107	THR
30	X	14	VAL
41	1	282	TYR
44	e	74	ASP
44	e	76	PRO
3	4	20	ASN
3	4	21	ASN
3	4	419	TYR
5	7	149	TYR
8	A	365	THR
8	A	383	SER
9	B	85	GLY
14	G	122	SER
24	R	134	TRP
24	R	272	LEU
6	8	227	PRO
7	9	76	ALA
8	A	563	ASP
28	V	143	TYR
36	d	19	PRO
3	4	112	ALA
8	A	541	PRO
9	B	291	VAL
12	E	108	SER
42	6	31	ASN
9	B	219	GLY
2	3	24	LEU
8	A	461	PRO
8	A	129	PRO
44	e	78	LEU

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	2	274/316 (87%)	274 (100%)	0	100 100
2	3	75/101 (74%)	75 (100%)	0	100 100
3	4	351/413 (85%)	351 (100%)	0	100 100
4	5	75/86 (87%)	75 (100%)	0	100 100
5	7	104/142 (73%)	104 (100%)	0	100 100
6	8	236/353 (67%)	236 (100%)	0	100 100
7	9	160/183 (87%)	160 (100%)	0	100 100
8	A	551/588 (94%)	549 (100%)	2 (0%)	91 94
9	B	330/371 (89%)	324 (98%)	6 (2%)	59 76
10	C	183/204 (90%)	183 (100%)	0	100 100
11	D	126/150 (84%)	124 (98%)	2 (2%)	62 79
12	E	145/151 (96%)	145 (100%)	0	100 100
13	F	13/69 (19%)	13 (100%)	0	100 100
14	G	105/119 (88%)	105 (100%)	0	100 100
15	H	80/95 (84%)	80 (100%)	0	100 100
16	I	53/79 (67%)	51 (96%)	2 (4%)	33 58
17	J	50/59 (85%)	50 (100%)	0	100 100
18	K	66/81 (82%)	66 (100%)	0	100 100
19	L	63/71 (89%)	63 (100%)	0	100 100
20	N	88/101 (87%)	88 (100%)	0	100 100
21	O	95/113 (84%)	95 (100%)	0	100 100
22	P	72/96 (75%)	72 (100%)	0	100 100
23	Q	142/154 (92%)	141 (99%)	1 (1%)	84 90
24	R	230/298 (77%)	230 (100%)	0	100 100
25	S	205/283 (72%)	204 (100%)	1 (0%)	88 93
26	T	79/101 (78%)	79 (100%)	0	100 100
27	U	95/131 (72%)	95 (100%)	0	100 100
28	V	107/120 (89%)	107 (100%)	0	100 100
29	M	73/81 (90%)	73 (100%)	0	100 100
29	W	55/81 (68%)	55 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	X	32/54 (59%)	32 (100%)	0	100 100
31	Y	29/62 (47%)	29 (100%)	0	100 100
32	Z	28/75 (37%)	28 (100%)	0	100 100
33	a	70/114 (61%)	70 (100%)	0	100 100
34	b	85/124 (68%)	85 (100%)	0	100 100
35	c	45/121 (37%)	45 (100%)	0	100 100
36	d	42/119 (35%)	42 (100%)	0	100 100
37	f	80/160 (50%)	80 (100%)	0	100 100
38	h	70/112 (62%)	69 (99%)	1 (1%)	67 80
39	i	23/45 (51%)	23 (100%)	0	100 100
40	j	88/106 (83%)	88 (100%)	0	100 100
41	1	267/275 (97%)	260 (97%)	7 (3%)	46 67
42	6	523/534 (98%)	523 (100%)	0	100 100
43	g	130/157 (83%)	130 (100%)	0	100 100
44	e	44/141 (31%)	43 (98%)	1 (2%)	50 70
All	All	5837/7389 (79%)	5814 (100%)	23 (0%)	91 94

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	A	253	VAL
8	A	538	GLN
9	B	92	HIS
9	B	94	VAL
9	B	95	LEU
9	B	96	ARG
9	B	97	LEU
9	B	105	MET
11	D	113	PHE
11	D	114	ARG
16	I	105	LYS
16	I	106	GLU
23	Q	115	LEU
25	S	200	PRO
38	h	70	ASN
41	1	126	LYS
41	1	127	TYR

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Mol	Chain	Res	Type
41	1	134	ARG
41	1	224	PHE
41	1	225	MET
41	1	228	TYR
41	1	310	LEU
44	e	75	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	48	HIS
1	2	63	GLN
2	3	80	GLN
3	4	138	ASN
3	4	374	ASN
3	4	440	HIS
6	8	220	GLN
6	8	393	ASN
8	A	142	GLN
8	A	309	ASN
8	A	359	ASN
8	A	571	HIS
8	A	572	HIS
8	A	666	GLN
9	B	92	HIS
9	B	131	GLN
9	B	168	GLN
9	B	182	ASN
9	B	250	ASN
10	C	140	ASN
10	C	230	GLN
11	D	98	HIS
12	E	204	ASN
15	H	21	GLN
15	H	27	HIS
15	H	45	HIS
18	K	22	HIS
20	N	83	GLN
23	Q	35	GLN
24	R	43	HIS
24	R	84	HIS
24	R	169	HIS

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Mol	Chain	Res	Type
24	R	171	ASN
24	R	331	HIS
25	S	223	GLN
25	S	278	ASN
27	U	13	GLN
30	X	13	HIS
33	a	33	GLN
33	a	79	ASN
35	c	14	GLN
37	f	12	HIS
37	f	14	GLN
38	h	70	ASN
41	1	47	GLN
41	1	235	ASN
41	1	292	ASN
41	1	317	GLN
42	6	175	ASN
42	6	226	GLN
42	6	270	ASN
42	6	332	HIS
42	6	446	ASN
42	6	471	ASN
42	6	546	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\#\|Z\| > 2$
49	FES	9	301	7	0,4,4	-	-	-		
46	CDL	4	501	-	81,81,99	0.96	6 (7%)	87,93,111	1.10	5 (5%)
45	3PE	2	401	-	40,40,50	0.94	2 (5%)	43,45,55	1.13	2 (4%)
48	SF4	A	801	-	0,12,12	-	-	-		
48	SF4	E	301	12	0,12,12	-	-	-		
48	SF4	8	502	-	0,12,12	-	-	-		
47	FMN	8	501	-	33,33,33	1.06	2 (6%)	48,50,50	1.43	10 (20%)
48	SF4	E	302	12	0,12,12	-	-	-		
49	FES	A	803	8	0,4,4	-	-	-		
52	PC1	S	401	-	46,46,53	0.99	4 (8%)	52,54,61	1.03	2 (3%)
45	3PE	4	502	-	40,40,50	0.94	3 (7%)	43,45,55	1.19	2 (4%)
51	NAP	R	601	-	45,52,52	4.68	20 (44%)	56,80,80	1.84	8 (14%)
52	PC1	j	201	-	38,38,53	1.09	4 (10%)	44,46,61	1.03	2 (4%)
45	3PE	B	501	9	50,50,50	0.87	4 (8%)	53,55,55	1.11	2 (3%)
48	SF4	A	802	-	0,12,12	-	-	-		
48	SF4	D	301	-	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
49	FES	9	301	7	-	-	0/1/1/1
46	CDL	4	501	-	-	42/92/92/110	-
45	3PE	2	401	-	-	20/44/44/54	-
48	SF4	A	801	-	-	-	0/6/5/5
48	SF4	E	301	12	-	-	0/6/5/5
48	SF4	8	502	-	-	-	0/6/5/5
47	FMN	8	501	-	-	7/18/18/18	0/3/3/3
52	PC1	S	401	-	-	21/50/50/57	-
48	SF4	E	302	12	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	FES	A	803	8	-	-	0/1/1/1
45	3PE	4	502	-	-	25/44/44/54	-
51	NAP	R	601	-	-	17/31/67/67	0/5/5/5
52	PC1	j	201	-	-	21/42/42/57	-
45	3PE	B	501	9	-	26/54/54/54	-
48	SF4	A	802	-	-	-	0/6/5/5
48	SF4	D	301	-	-	-	0/6/5/5

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	R	601	NAP	O4D-C1D	16.06	1.63	1.41
51	R	601	NAP	O4B-C1B	14.96	1.61	1.41
51	R	601	NAP	C2D-C1D	-14.74	1.31	1.53
51	R	601	NAP	C7N-N7N	7.23	1.46	1.33
51	R	601	NAP	O4D-C4D	-6.60	1.30	1.45
51	R	601	NAP	O4B-C4B	-5.75	1.32	1.45
51	R	601	NAP	C3N-C7N	5.37	1.58	1.50
51	R	601	NAP	O3D-C3D	-4.22	1.33	1.43
51	R	601	NAP	O2D-C2D	3.51	1.51	1.43
51	R	601	NAP	O7N-C7N	-3.38	1.17	1.24
47	8	501	FMN	C4A-N5	3.26	1.37	1.30
51	R	601	NAP	C6A-N6A	2.99	1.44	1.34
51	R	601	NAP	O3B-C3B	-2.76	1.36	1.43
45	B	501	3PE	O21-C2	-2.72	1.39	1.46
46	4	501	CDL	OA6-CA4	-2.68	1.39	1.46
51	R	601	NAP	PA-O5B	2.65	1.70	1.59
52	j	201	PC1	O21-C2	-2.59	1.40	1.46
46	4	501	CDL	OB6-CB5	2.58	1.41	1.34
51	R	601	NAP	C2A-N3A	2.54	1.36	1.32
51	R	601	NAP	P2B-O2B	2.53	1.64	1.59
52	S	401	PC1	O21-C2	-2.49	1.40	1.46
45	4	502	3PE	O21-C21	2.45	1.41	1.34
45	2	401	3PE	O31-C31	2.44	1.40	1.33
45	2	401	3PE	O21-C21	2.43	1.41	1.34
46	4	501	CDL	OA8-CA7	2.42	1.40	1.33
52	S	401	PC1	O31-C31	2.41	1.40	1.33
51	R	601	NAP	C5A-N7A	-2.38	1.31	1.39
46	4	501	CDL	OB8-CB7	2.38	1.40	1.33
51	R	601	NAP	C5A-C4A	-2.32	1.34	1.40
45	B	501	3PE	O31-C31	2.29	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B	501	3PE	O31-C3	-2.28	1.40	1.45
45	4	502	3PE	O31-C3	-2.27	1.40	1.45
51	R	601	NAP	PN-O5D	2.27	1.68	1.59
52	j	201	PC1	O31-C31	2.26	1.39	1.33
47	8	501	FMN	C10-N1	2.26	1.37	1.33
45	4	502	3PE	O31-C31	2.24	1.39	1.33
45	B	501	3PE	O21-C21	2.24	1.40	1.34
46	4	501	CDL	OB8-CB6	-2.22	1.40	1.45
52	j	201	PC1	O31-C3	-2.20	1.40	1.45
52	S	401	PC1	O21-C21	2.08	1.40	1.34
52	j	201	PC1	O21-C21	2.07	1.40	1.34
51	R	601	NAP	C4N-C3N	-2.07	1.35	1.39
46	4	501	CDL	OA8-CA6	-2.03	1.40	1.45
52	S	401	PC1	O31-C3	-2.02	1.40	1.45
51	R	601	NAP	O2B-C2B	2.02	1.51	1.44

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
51	R	601	NAP	C5A-C6A-N6A	7.56	131.84	120.35
51	R	601	NAP	N3A-C2A-N1A	-5.82	119.59	128.68
51	R	601	NAP	N6A-C6A-N1A	-5.18	107.83	118.57
45	2	401	3PE	O21-C21-C22	4.34	120.86	111.50
45	4	502	3PE	O21-C21-C22	4.22	120.60	111.50
46	4	501	CDL	OA6-CA5-C11	4.17	120.49	111.50
52	S	401	PC1	O21-C21-C22	4.17	120.48	111.50
45	B	501	3PE	O21-C21-C22	3.92	119.96	111.50
46	4	501	CDL	OB6-CB5-C51	3.78	119.64	111.50
47	8	501	FMN	C4-N3-C2	-3.58	119.02	125.64
51	R	601	NAP	C1B-N9A-C4A	-3.49	120.52	126.64
52	j	201	PC1	O21-C21-C22	3.45	120.43	110.80
51	R	601	NAP	PN-O3-PA	-3.31	121.45	132.83
47	8	501	FMN	O4-C4-C4A	-3.10	118.36	126.60
47	8	501	FMN	C4A-C10-N1	-2.98	117.82	124.73
47	8	501	FMN	C4A-C4-N3	2.90	120.54	113.19
47	8	501	FMN	C5'-C4'-C3'	-2.67	107.05	112.20
46	4	501	CDL	OA8-CA7-C31	2.59	120.04	111.91
46	4	501	CDL	OB8-CB7-C71	2.57	119.98	111.91
45	B	501	3PE	O31-C31-C32	2.54	119.89	111.91
45	2	401	3PE	O31-C31-C32	2.52	119.83	111.91
47	8	501	FMN	C5A-C9A-N10	2.52	120.56	117.95
52	S	401	PC1	O31-C31-C32	2.52	119.82	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	j	201	PC1	O31-C31-C32	2.48	119.69	111.91
45	4	502	3PE	O31-C31-C32	2.41	119.47	111.91
47	8	501	FMN	C10-N1-C2	2.40	121.69	116.90
51	R	601	NAP	C6N-N1N-C2N	-2.36	119.82	121.97
51	R	601	NAP	C3D-C2D-C1D	2.35	104.52	100.98
47	8	501	FMN	C4-C4A-C10	2.35	120.74	116.79
51	R	601	NAP	C3N-C7N-N7N	2.18	120.36	117.75
47	8	501	FMN	C4A-C10-N10	2.14	119.61	116.48
47	8	501	FMN	C9A-C5A-N5	-2.13	120.12	122.43
46	4	501	CDL	CA4-OA6-CA5	-2.02	112.83	117.79

There are no chirality outliers.

All (179) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	2	401	3PE	C1-O11-P-O14
45	2	401	3PE	C22-C21-O21-C2
45	4	502	3PE	C11-O13-P-O12
45	4	502	3PE	C11-O13-P-O14
45	4	502	3PE	C2-C1-O11-P
45	4	502	3PE	O13-C11-C12-N
45	4	502	3PE	C22-C21-O21-C2
45	B	501	3PE	C1-O11-P-O13
45	B	501	3PE	O11-C1-C2-O21
45	B	501	3PE	O22-C21-O21-C2
45	B	501	3PE	C22-C21-O21-C2
46	4	501	CDL	CA2-OA2-PA1-OA4
46	4	501	CDL	OA6-CA4-CA6-OA8
46	4	501	CDL	OA7-CA5-OA6-CA4
46	4	501	CDL	C11-CA5-OA6-CA4
47	8	501	FMN	N10-C1'-C2'-O2'
47	8	501	FMN	N10-C1'-C2'-C3'
47	8	501	FMN	C5'-O5'-P-O2P
47	8	501	FMN	C5'-O5'-P-O3P
51	R	601	NAP	C5B-O5B-PA-O1A
51	R	601	NAP	C5B-O5B-PA-O2A
51	R	601	NAP	C1B-C2B-O2B-P2B
51	R	601	NAP	C2B-O2B-P2B-O3X
51	R	601	NAP	PA-O3-PN-O5D
51	R	601	NAP	C5D-O5D-PN-O3
51	R	601	NAP	C5D-O5D-PN-O2N
51	R	601	NAP	C2D-C1D-N1N-C2N

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Mol	Chain	Res	Type	Atoms
51	R	601	NAP	C2D-C1D-N1N-C6N
52	j	201	PC1	C11-O13-P-O12
52	j	201	PC1	C11-O13-P-O14
52	j	201	PC1	C11-O13-P-O11
52	j	201	PC1	O22-C21-O21-C2
45	4	502	3PE	O32-C31-O31-C3
45	2	401	3PE	O22-C21-O21-C2
45	4	502	3PE	O22-C21-O21-C2
45	4	502	3PE	C32-C31-O31-C3
52	j	201	PC1	C22-C21-O21-C2
46	4	501	CDL	C71-CB7-OB8-CB6
52	S	401	PC1	O22-C21-O21-C2
46	4	501	CDL	OB9-CB7-OB8-CB6
52	S	401	PC1	C22-C21-O21-C2
51	R	601	NAP	O4B-C4B-C5B-O5B
51	R	601	NAP	O4D-C4D-C5D-O5D
46	4	501	CDL	C31-CA7-OA8-CA6
46	4	501	CDL	CB5-C51-C52-C53
45	B	501	3PE	C21-C22-C23-C24
46	4	501	CDL	CA5-C11-C12-C13
46	4	501	CDL	OA9-CA7-OA8-CA6
45	4	502	3PE	C1-O11-P-O13
45	4	502	3PE	C11-O13-P-O11
46	4	501	CDL	CA2-OA2-PA1-OA5
46	4	501	CDL	CB2-OB2-PB2-OB5
52	S	401	PC1	C11-O13-P-O11
46	4	501	CDL	C51-CB5-OB6-CB4
45	2	401	3PE	C2C-C2D-C2E-C2F
46	4	501	CDL	C78-C79-C80-C81
46	4	501	CDL	OB7-CB5-OB6-CB4
45	2	401	3PE	C21-C22-C23-C24
45	B	501	3PE	C23-C24-C25-C26
46	4	501	CDL	C1-CA2-OA2-PA1
46	4	501	CDL	C13-C14-C15-C16
46	4	501	CDL	CA7-C31-C32-C33
52	S	401	PC1	C25-C26-C27-C28
45	B	501	3PE	C37-C38-C39-C3A
46	4	501	CDL	C73-C74-C75-C76
45	4	502	3PE	C28-C29-C2A-C2B
46	4	501	CDL	C72-C73-C74-C75
52	S	401	PC1	C33-C34-C35-C36
45	2	401	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
46	4	501	CDL	C74-C75-C76-C77
46	4	501	CDL	C77-C78-C79-C80
45	2	401	3PE	C32-C31-O31-C3
45	B	501	3PE	C31-C32-C33-C34
45	4	502	3PE	C34-C35-C36-C37
45	B	501	3PE	C2E-C2F-C2G-C2H
46	4	501	CDL	C75-C76-C77-C78
45	2	401	3PE	O32-C31-O31-C3
46	4	501	CDL	C83-C84-C85-C86
52	S	401	PC1	O11-C1-C2-C3
45	4	502	3PE	C23-C24-C25-C26
45	B	501	3PE	C35-C36-C37-C38
45	2	401	3PE	C1-C2-C3-O31
52	j	201	PC1	C1-C2-C3-O31
46	4	501	CDL	C80-C81-C82-C83
45	B	501	3PE	C2F-C2G-C2H-C2I
45	B	501	3PE	C3C-C3D-C3E-C3F
45	2	401	3PE	C28-C29-C2A-C2B
45	B	501	3PE	C27-C28-C29-C2A
45	2	401	3PE	C3-C2-O21-C21
46	4	501	CDL	C51-C52-C53-C54
52	j	201	PC1	C34-C35-C36-C37
47	8	501	FMN	C5'-O5'-P-O1P
51	R	601	NAP	PN-O3-PA-O1A
52	j	201	PC1	C32-C31-O31-C3
45	4	502	3PE	C24-C25-C26-C27
45	4	502	3PE	C26-C27-C28-C29
45	2	401	3PE	O11-C1-C2-C3
45	B	501	3PE	O11-C1-C2-C3
46	4	501	CDL	OB5-CB3-CB4-CB6
45	4	502	3PE	C29-C2A-C2B-C2C
52	S	401	PC1	C32-C31-O31-C3
52	S	401	PC1	C21-C22-C23-C24
45	2	401	3PE	C22-C23-C24-C25
46	4	501	CDL	CA3-CA4-CA6-OA8
45	2	401	3PE	C2A-C2B-C2C-C2D
45	2	401	3PE	C25-C26-C27-C28
52	S	401	PC1	C3B-C3C-C3D-C3E
46	4	501	CDL	OA5-CA3-CA4-OA6
52	S	401	PC1	C32-C33-C34-C35
45	B	501	3PE	C2-C1-O11-P
46	4	501	CDL	CA4-CA3-OA5-PA1

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Mol	Chain	Res	Type	Atoms
51	R	601	NAP	PN-O3-PA-O5B
51	R	601	NAP	C3B-C4B-C5B-O5B
45	4	502	3PE	C3-C2-O21-C21
46	4	501	CDL	CB3-CB4-OB6-CB5
52	j	201	PC1	O32-C31-O31-C3
46	4	501	CDL	OB5-CB3-CB4-OB6
52	S	401	PC1	O11-C1-C2-O21
52	S	401	PC1	O32-C31-O31-C3
52	j	201	PC1	O21-C2-C3-O31
45	2	401	3PE	C1-O11-P-O13
45	2	401	3PE	C1-O11-P-O12
45	4	502	3PE	C1-O11-P-O12
45	4	502	3PE	C1-O11-P-O14
46	4	501	CDL	CB2-OB2-PB2-OB4
52	S	401	PC1	C11-O13-P-O12
52	S	401	PC1	C1-O11-P-O12
45	B	501	3PE	C32-C31-O31-C3
46	4	501	CDL	OA5-CA3-CA4-CA6
45	4	502	3PE	C12-C11-O13-P
47	8	501	FMN	C1'-C2'-C3'-O3'
45	2	401	3PE	O11-C1-C2-O21
45	4	502	3PE	C27-C28-C29-C2A
52	S	401	PC1	O13-C11-C12-N
52	j	201	PC1	O13-C11-C12-N
45	2	401	3PE	O21-C2-C3-O31
45	4	502	3PE	O21-C2-C3-O31
47	8	501	FMN	O2'-C2'-C3'-C4'
45	B	501	3PE	O32-C31-O31-C3
46	4	501	CDL	C52-C53-C54-C55
45	B	501	3PE	C24-C25-C26-C27
52	j	201	PC1	O11-C1-C2-O21
52	j	201	PC1	C1-O11-P-O13
46	4	501	CDL	CB4-CB3-OB5-PB2
51	R	601	NAP	C4B-C5B-O5B-PA
46	4	501	CDL	C14-C15-C16-C17
45	2	401	3PE	C26-C27-C28-C29
52	S	401	PC1	C2-C1-O11-P
51	R	601	NAP	C3D-C4D-C5D-O5D
45	B	501	3PE	C2D-C2E-C2F-C2G
45	B	501	3PE	C32-C33-C34-C35
46	4	501	CDL	C58-C59-C60-C61
45	4	502	3PE	C2E-C2F-C2G-C2H

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Mol	Chain	Res	Type	Atoms
46	4	501	CDL	CA2-C1-CB2-OB2
45	4	502	3PE	C1-C2-C3-O31
45	B	501	3PE	C26-C27-C28-C29
45	B	501	3PE	C38-C39-C3A-C3B
52	j	201	PC1	O21-C21-C22-C23
45	B	501	3PE	C25-C26-C27-C28
46	4	501	CDL	C71-C72-C73-C74
45	B	501	3PE	C1-C2-C3-O31
45	B	501	3PE	O21-C2-C3-O31
52	j	201	PC1	O22-C21-C22-C23
52	S	401	PC1	C23-C24-C25-C26
52	S	401	PC1	C26-C27-C28-C29
51	R	601	NAP	C5B-O5B-PA-O3
45	B	501	3PE	C3B-C3C-C3D-C3E
45	4	502	3PE	C2B-C2C-C2D-C2E
46	4	501	CDL	C76-C77-C78-C79
46	4	501	CDL	CB2-OB2-PB2-OB3
52	S	401	PC1	C11-O13-P-O14
52	j	201	PC1	C1-O11-P-O14
52	j	201	PC1	O11-C1-C2-C3
52	S	401	PC1	O21-C21-C22-C23
52	j	201	PC1	C12-C11-O13-P
52	j	201	PC1	O31-C31-C32-C33
52	j	201	PC1	O32-C31-C32-C33
52	S	401	PC1	O22-C21-C22-C23
52	j	201	PC1	C3A-C3B-C3C-C3D

There are no ring outliers.

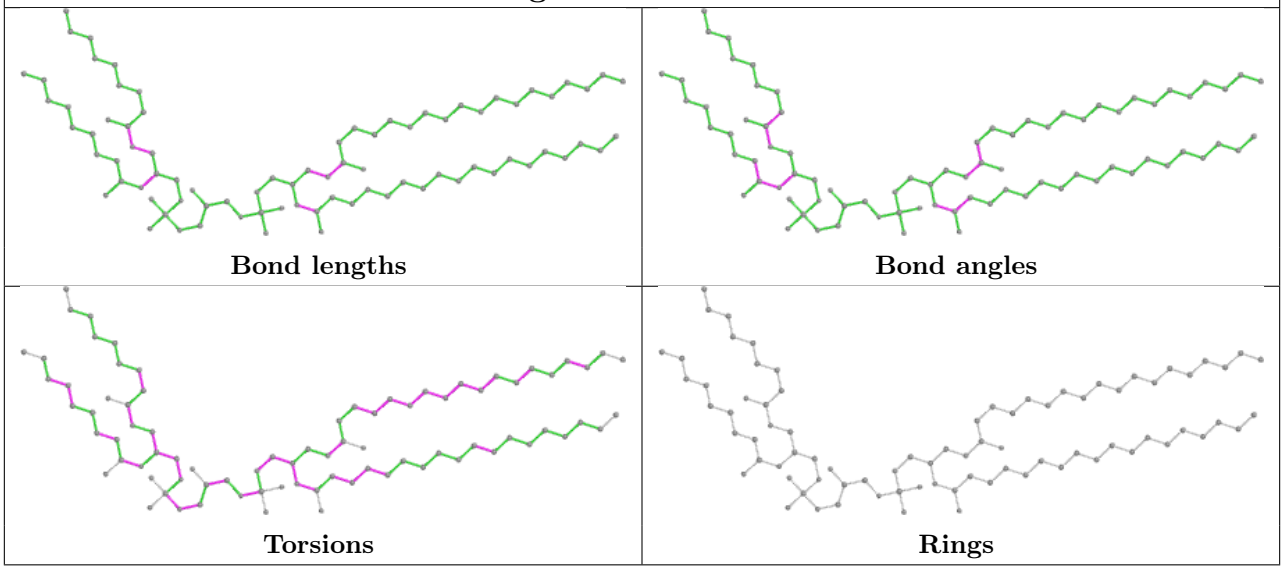
8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	4	501	CDL	1	0
45	2	401	3PE	3	0
48	A	801	SF4	1	0
47	8	501	FMN	2	0
52	S	401	PC1	1	0
45	4	502	3PE	1	0
51	R	601	NAP	3	0
45	B	501	3PE	2	0

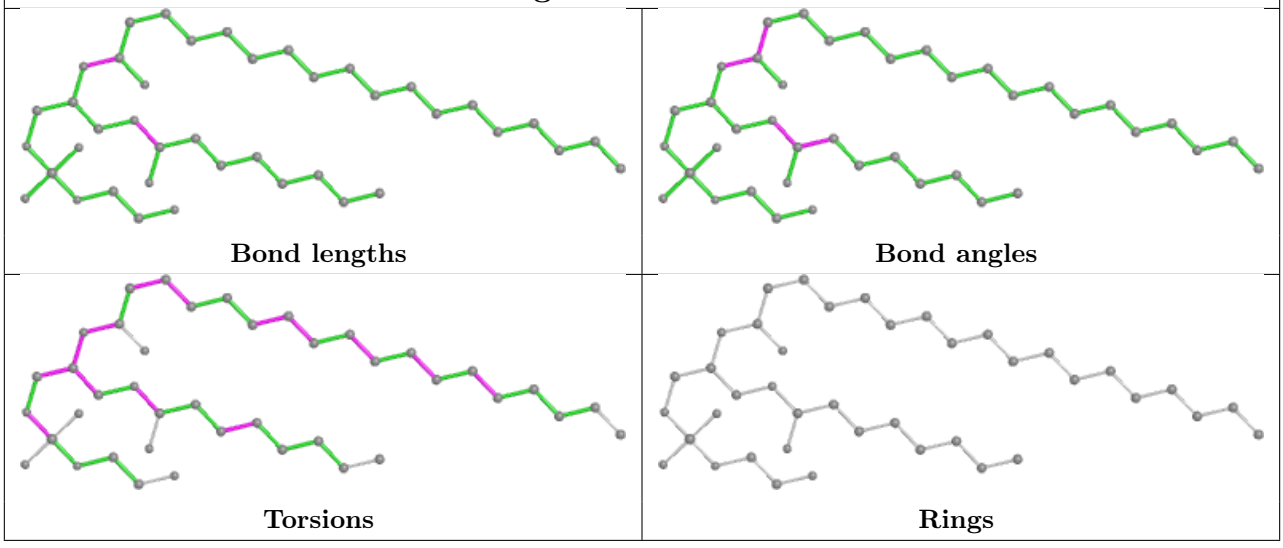
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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

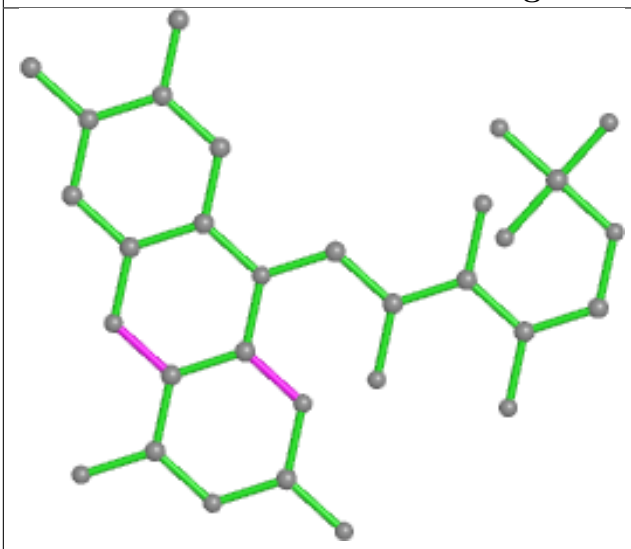
Ligand CDL 4 501



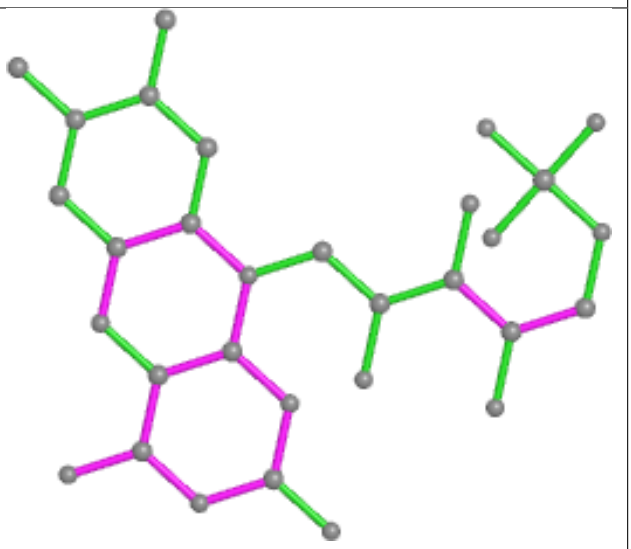
Ligand 3PE 2 401



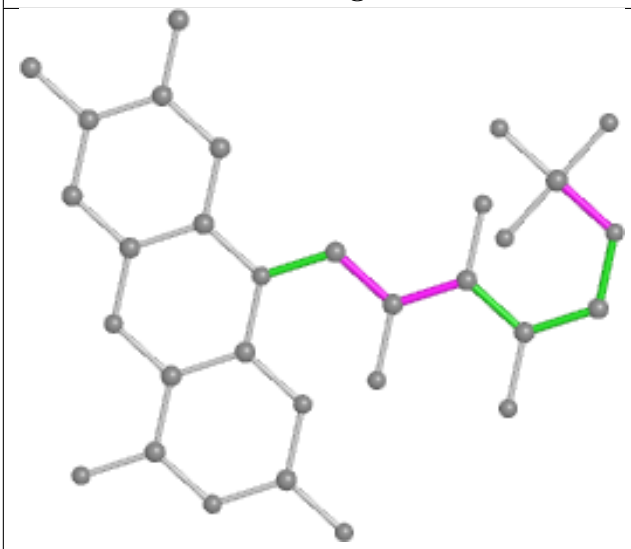
Ligand FMN 8 501



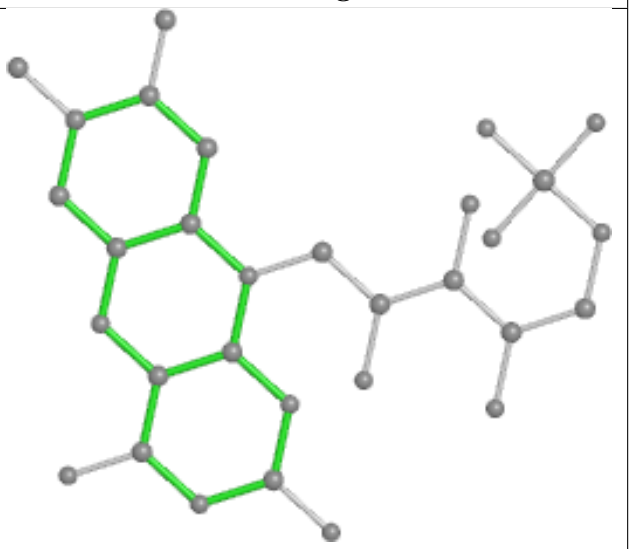
Bond lengths



Bond angles

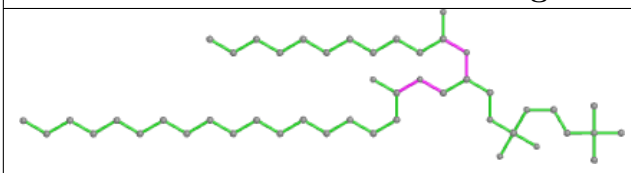


Torsions

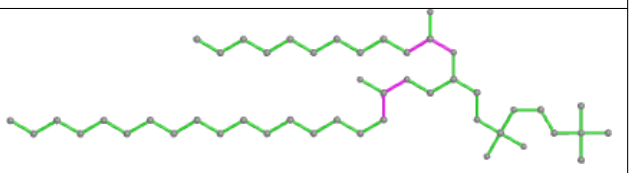


Rings

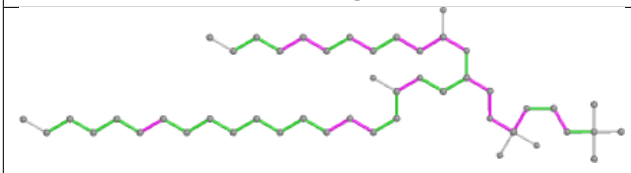
Ligand PC1 S 401



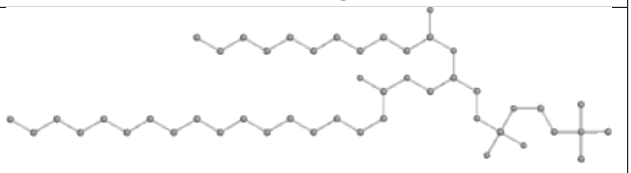
Bond lengths



Bond angles

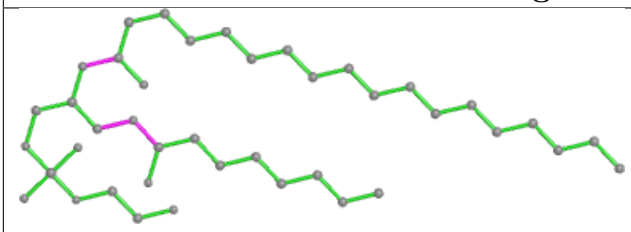


Torsions

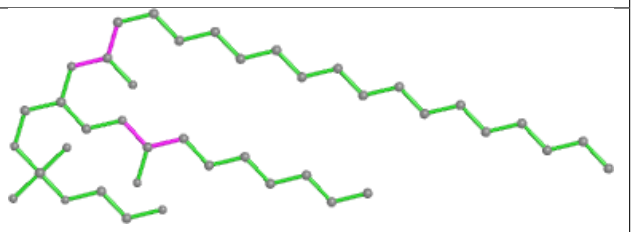


Rings

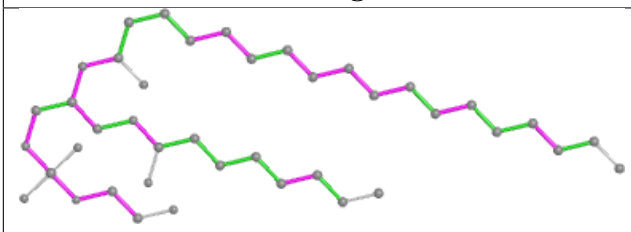
Ligand 3PE 4 502



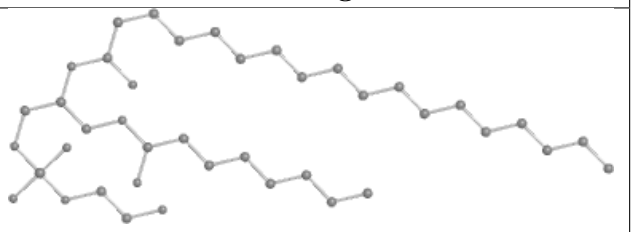
Bond lengths



Bond angles

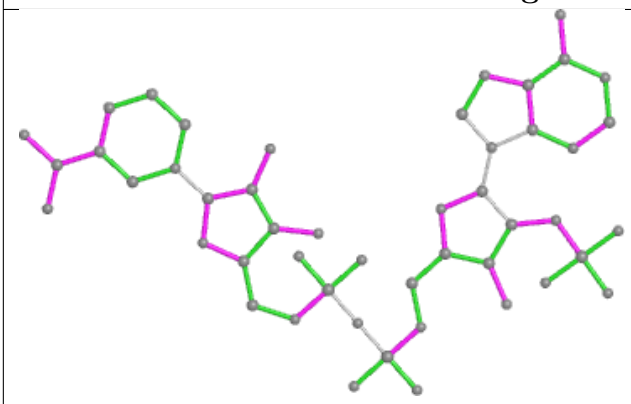


Torsions

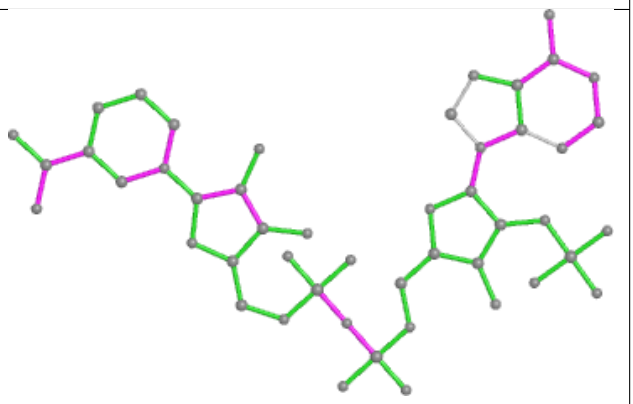


Rings

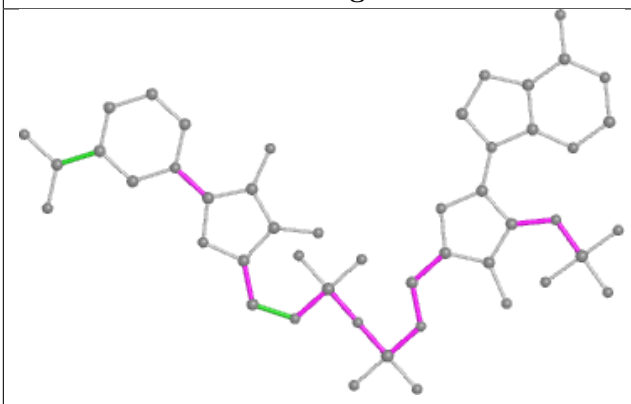
Ligand NAP R 601



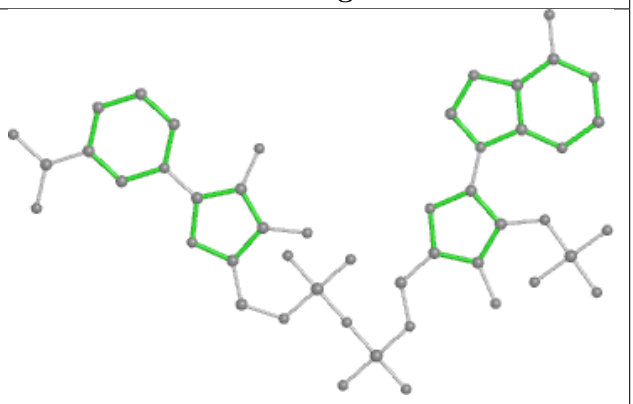
Bond lengths



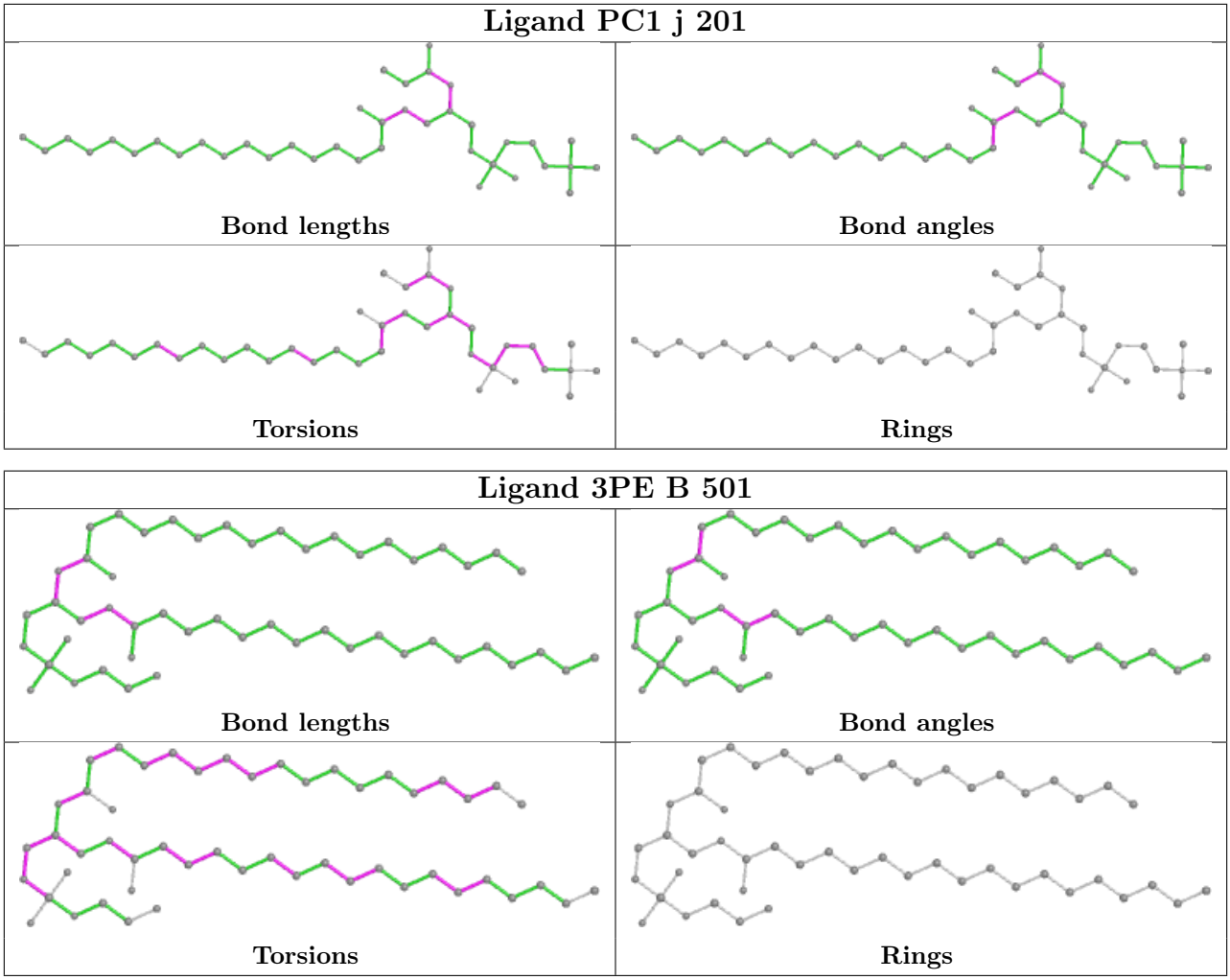
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

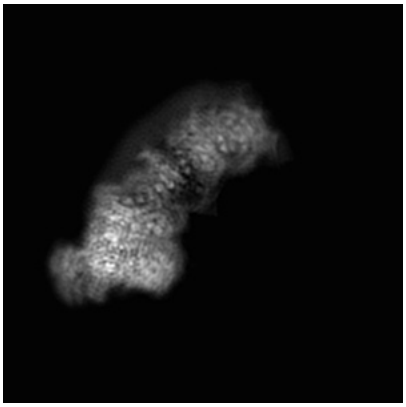
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30677. These allow visual inspection of the internal detail of the map and identification of artifacts.

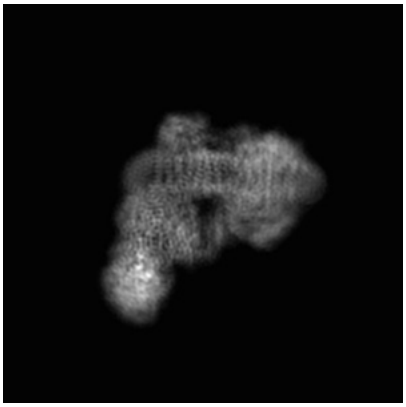
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

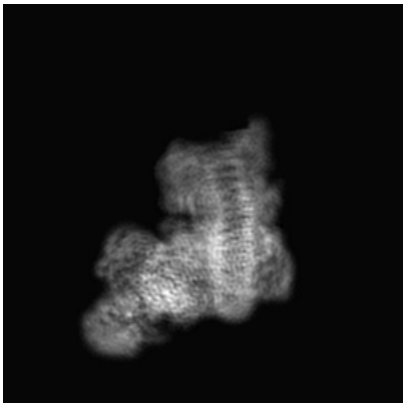
6.1.1 Primary map



X



Y

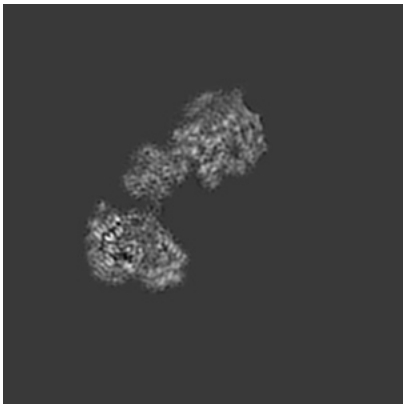


Z

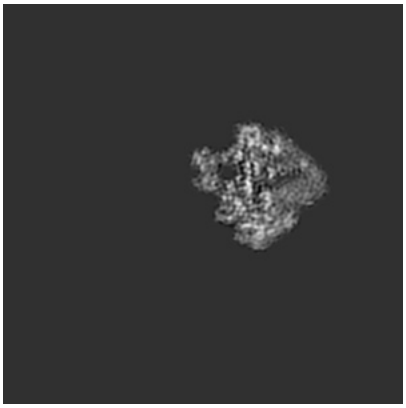
The images above show the map projected in three orthogonal directions.

6.2 Central slices

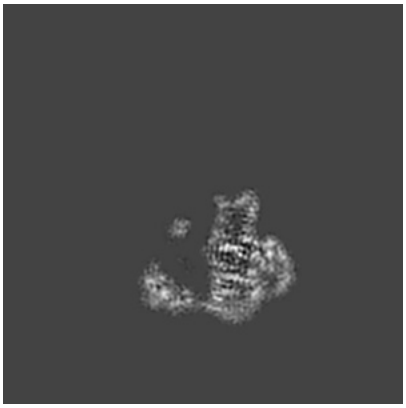
6.2.1 Primary map



X Index: 140



Y Index: 140

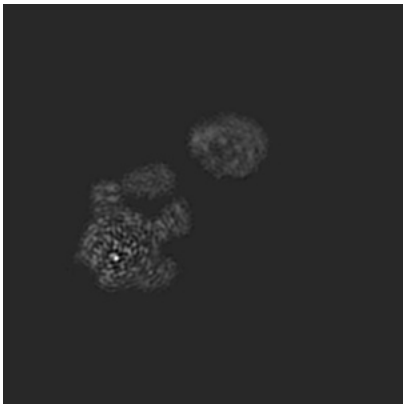


Z Index: 140

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

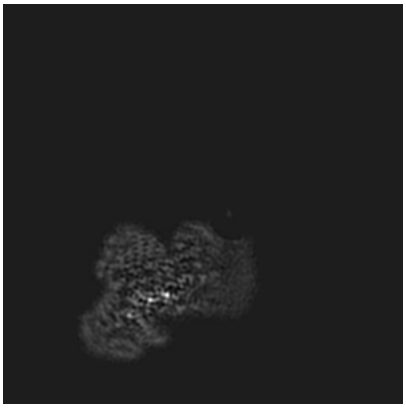
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 120

Y Index: 73



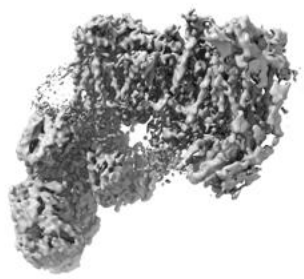
Z Index: 96

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

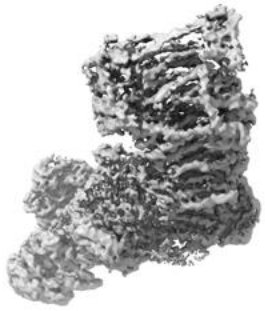
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.107. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

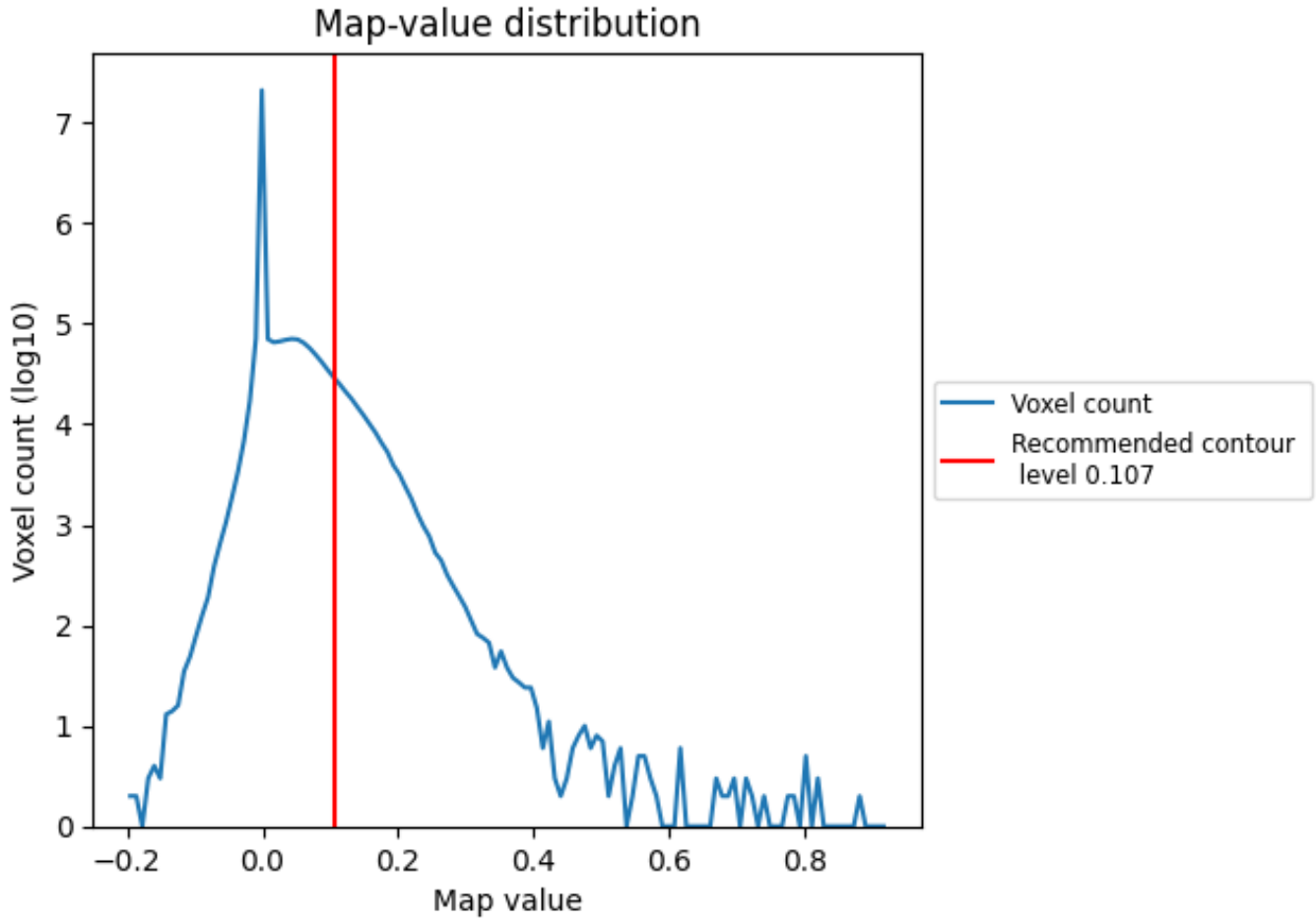
6.5 Mask visualisation (i)

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

7 Map analysis

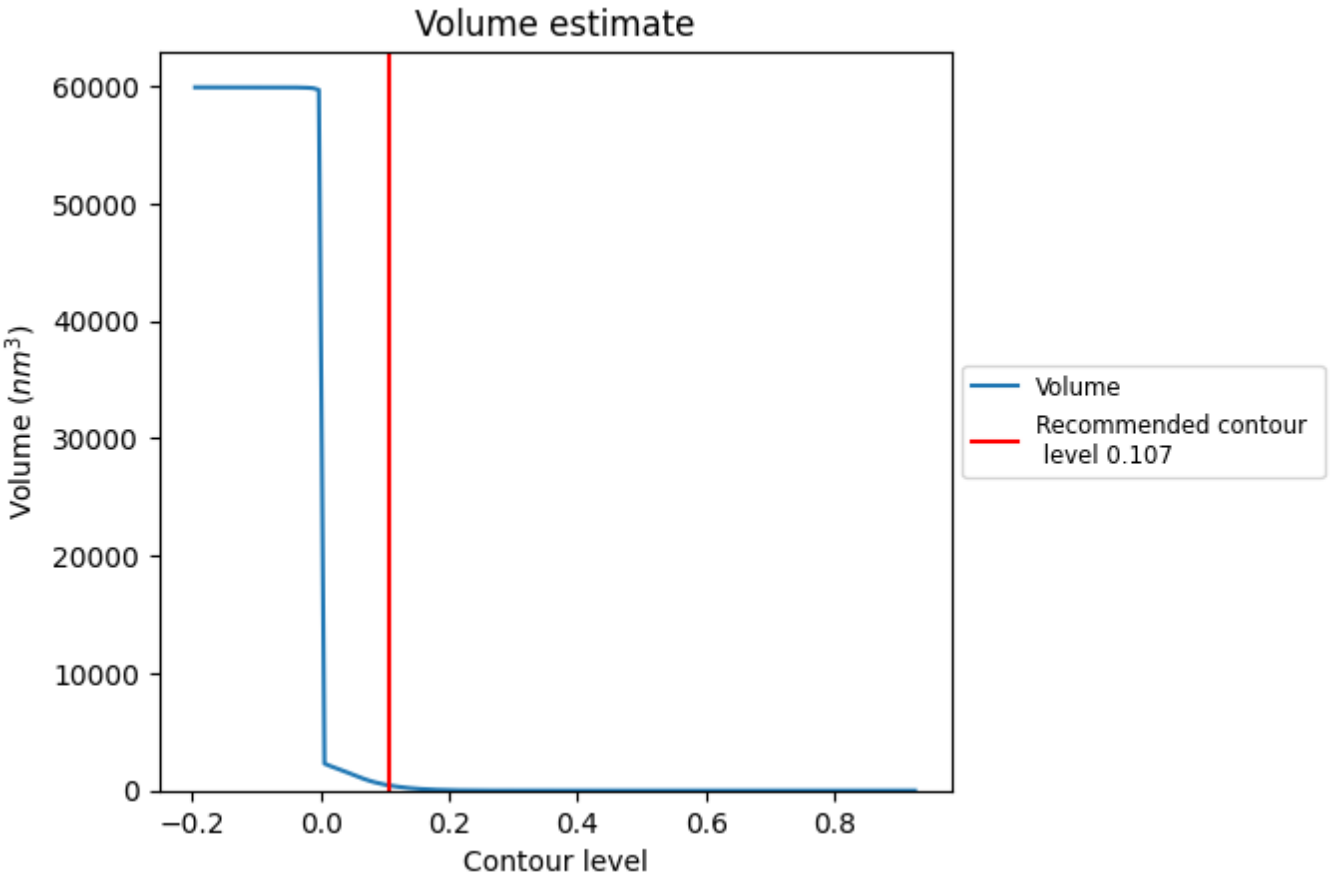
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

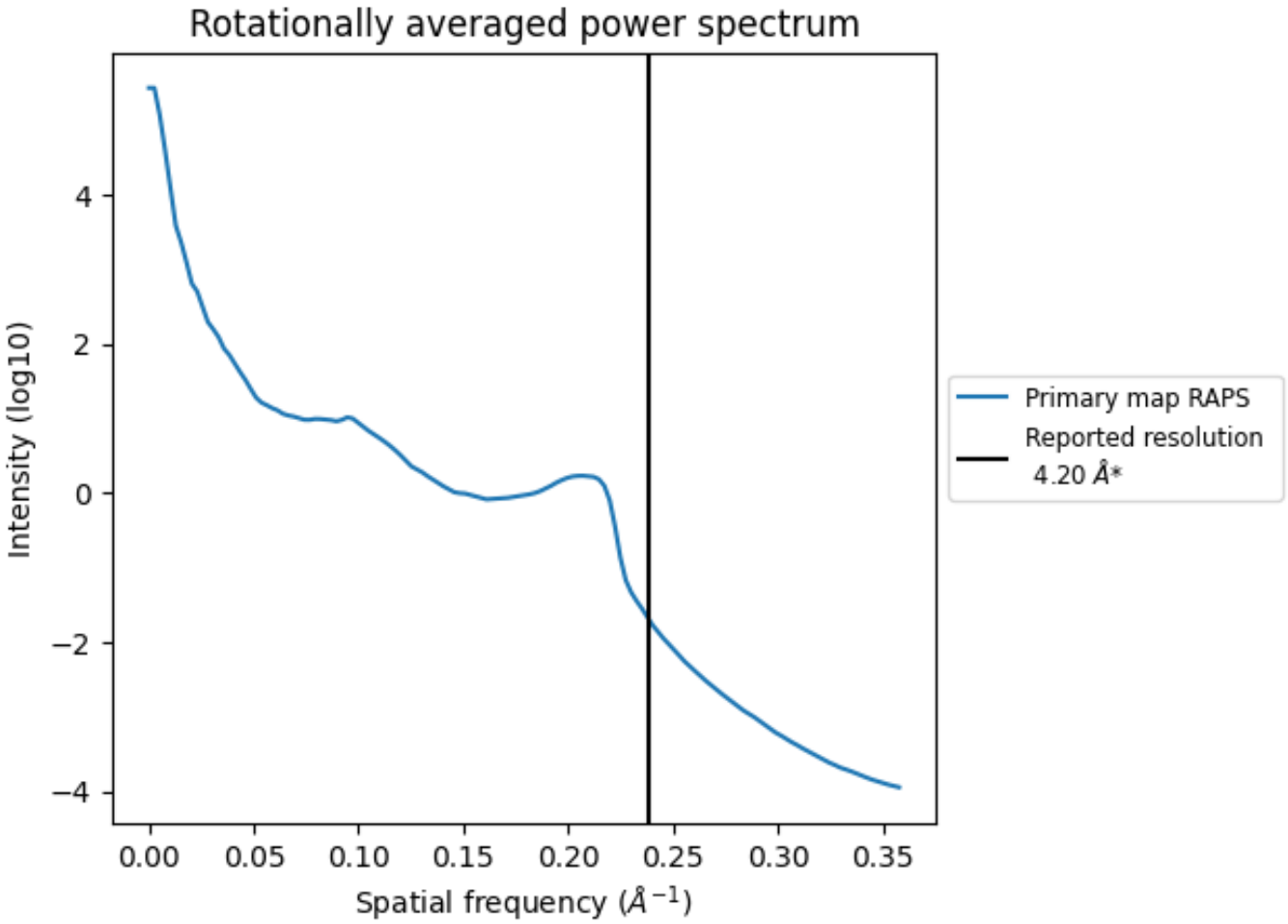
7.2 Volume estimate



The volume at the recommended contour level is 438 nm^3; this corresponds to an approximate mass of 396 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.238 Å^{-1}

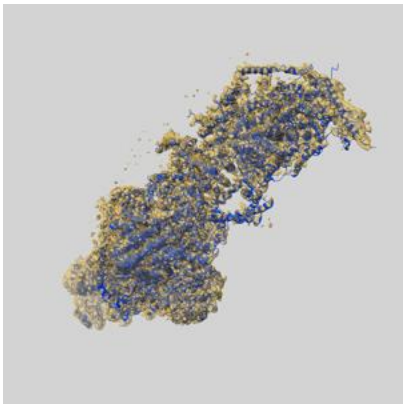
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

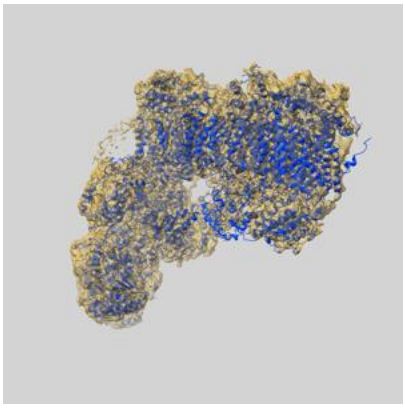
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30677 and PDB model 7DH0. Per-residue inclusion information can be found in section 3 on page 17.

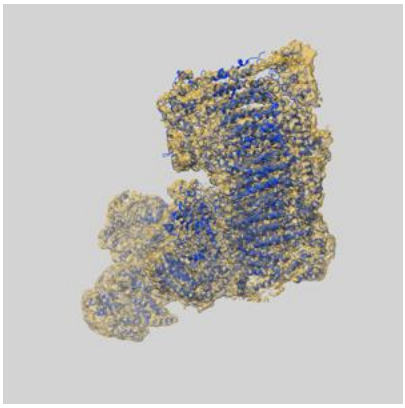
9.1 Map-model overlay



X



Y



Z

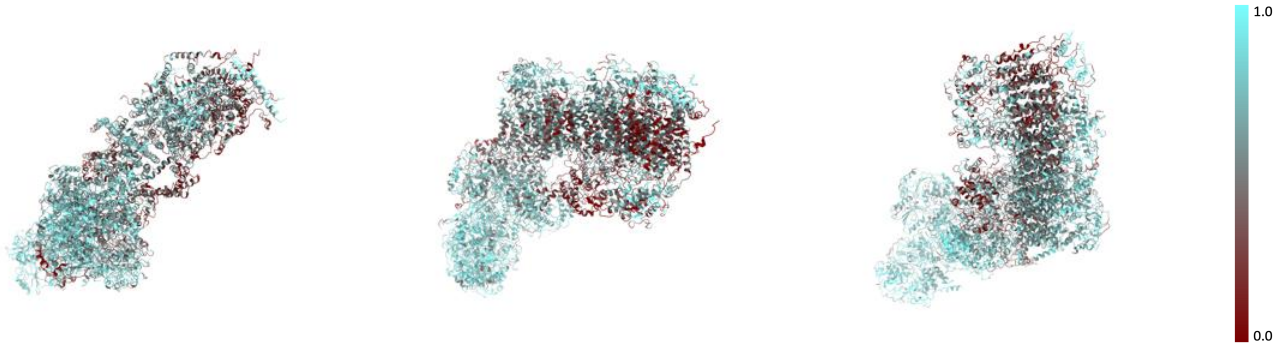
The images above show the 3D surface view of the map at the recommended contour level 0.107 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

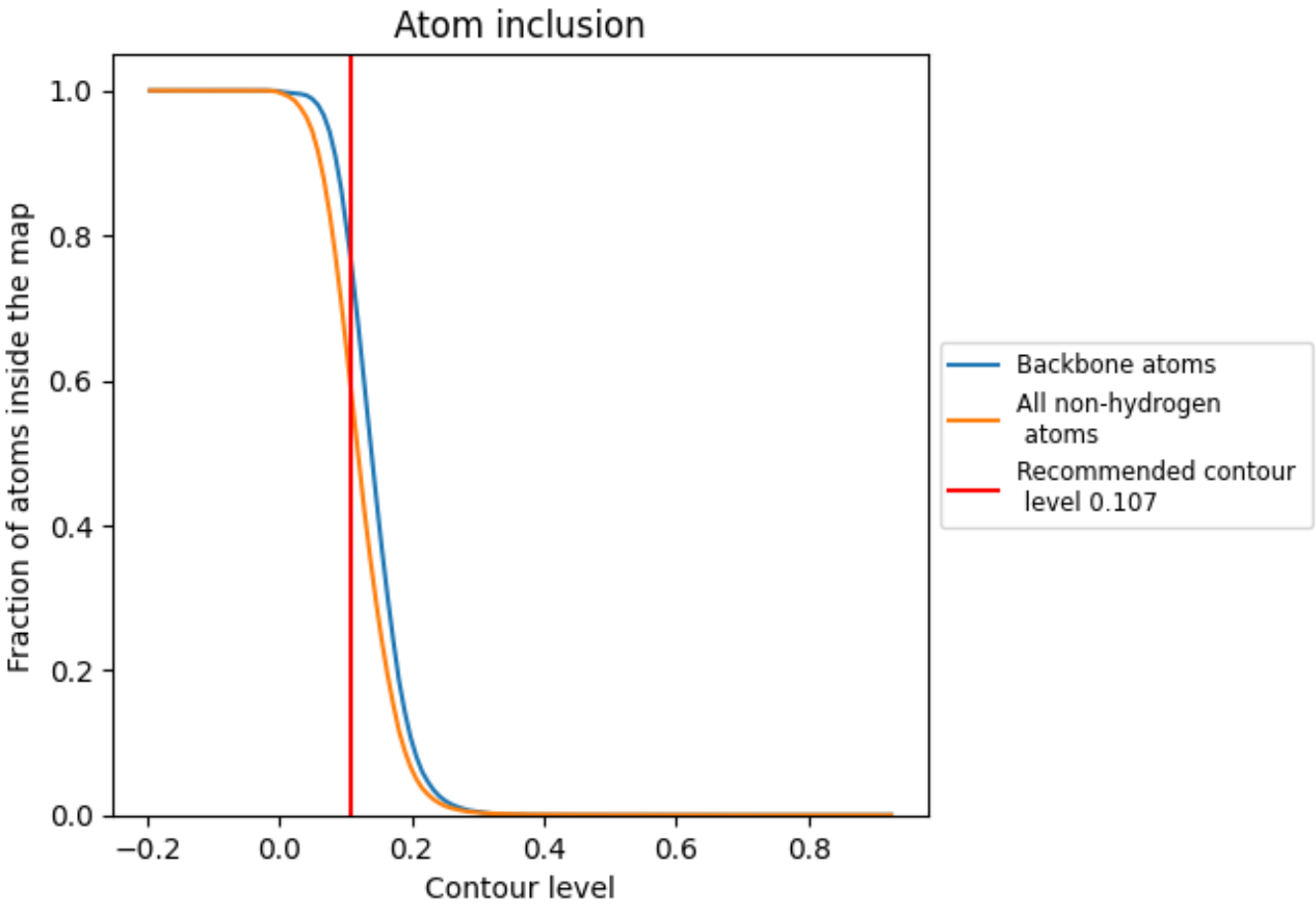
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.107).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 60% 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 (0.107) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6002	0.3110
1	0.5985	0.3370
2	0.6133	0.3580
3	0.4993	0.2980
4	0.5161	0.3230
5	0.5650	0.3360
6	0.3524	0.2320
7	0.4804	0.3140
8	0.8418	0.3100
9	0.8088	0.2930
A	0.7921	0.3570
B	0.7570	0.3930
C	0.7898	0.3860
D	0.7410	0.3910
E	0.8120	0.3870
F	0.5866	0.2090
G	0.7171	0.3930
H	0.6719	0.3350
I	0.4942	0.3290
J	0.7121	0.3290
K	0.7678	0.2920
L	0.5912	0.3300
M	0.4160	0.2360
N	0.7438	0.3060
O	0.6611	0.3280
P	0.5510	0.3400
Q	0.7129	0.2990
R	0.6272	0.3060
S	0.2349	0.2690
T	0.2900	0.2870
U	0.2918	0.2980
V	0.7007	0.3140
W	0.4595	0.1800
X	0.5000	0.2820
Y	0.4268	0.2160

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Chain	Atom inclusion	Q-score
Z	0.3264	0.2070
a	0.4322	0.2820
b	0.6650	0.3220
c	0.5662	0.2450
d	0.6282	0.2080
e	0.3318	0.2770
f	0.5626	0.2310
g	0.5559	0.2410
h	0.5556	0.2640
i	0.5641	0.2730
j	0.6156	0.3190