



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:41 PM UTC

PDB ID : 7PSA / pdb_00007psa
EMDB ID : EMD-13611
Title : The acetogenin-bound complex I of *Mus musculus* resolved to 3.4 angstroms
Authors : Grba, D.; Hirst, J.
Deposited on : 2021-09-22
Resolution : 3.40 Å (reported)
Based on initial model : 6ZR2

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

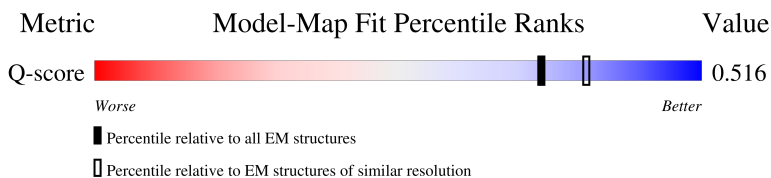
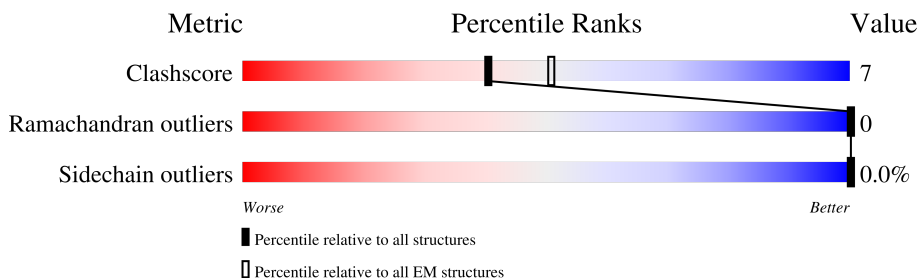
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

Mol	Chain	Length	Quality of chain
1	A	115	 80% 20%
2	B	224	 54% 16% 30%
3	C	263	 62% 17% 21%
4	D	463	 5% 75% 18% 7%

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Mol	Chain	Length	Quality of chain
5	E	248	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	172	
11	K	98	
12	L	607	
13	M	459	
14	N	345	
15	O	355	
16	P	377	
17	Q	175	
18	R	116	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	131	
23	X	172	
24	Y	143	
25	Z	144	
26	a	70	
27	b	84	
28	c	76	

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Mol	Chain	Length	Quality of chain
29	d	120	
30	e	106	
31	f	57	
32	g	151	
33	h	189	
34	i	128	
35	j	105	
36	k	104	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	104	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
55	EHZ	T	201	X	-	-	-
55	EHZ	U	201	X	-	-	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 134755 atoms, of which 67673 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 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	115	1902	633	969	133	160	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	156	2502	796	1255	223	214	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	207	3402	1111	1681	296	311	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	430	6878	2215	3414	595	630	24	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	212	3287	1048	1639	277	312	11	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	F	428	6559	2080	3259	589	609	22	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
7	G	688	10618	3321	5322	919	1015	41	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
8	H	318	5166	1706	2626	384	428	22	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	I	178	2812	898	1381	245	276	12	0	0

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
10	J	171	2615	874	1315	185	226	15	0	0

- Molecule 11 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
11	K	98	1505	477	768	112	137	11	0	0

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	L	606	9785	3182	4985	746	827	45	0	0

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
13	M	459	7485	2408	3853	567	617	40	0	0

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
14	N	344	5591	1791	2895	416	452	37	0	0

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
15	O	320	5171	1674	2564	431	492	10	0	0

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
16	P	342	5514	1777	2766	483	481	7	0	0

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
17	Q	125	2031	642	1016	179	190	4	0	0

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
18	R	94	1453	458	715	135	142	3	0	0

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
19	S	83	1353	419	686	126	119	3	0	0

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
20	T	76	1213	392	602	90	124	5	0	0
20	U	86	1378	446	686	102	139	5	0	0

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
21	V	114	1895	604	968	154	166	3	0	0

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
22	W	114	1961	619	991	180	165	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
23	X	171	2773	889	1377	250	247	10	0	0

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
24	Y	140	2062	662	1025	175	192	8	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-2	MET	-	variant	UNP Q9D8B4
Y	-1	ALA	-	variant	UNP Q9D8B4
Y	39	SER	ARG	conflict	UNP Q9D8B4

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
25	Z	141	2333	750	1166	207	202	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
26	a	68	1124	360	568	99	93	4	0	0

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
27	b	80	1256	414	628	99	111	4	0	0

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
28	c	48	797	261	399	69	67	1	0	0

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
29	d	120	1997	651	1001	171	165	9	0	0

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
30	e	105	1746	555	869	162	152	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
31	f	53	908	295	452	82	77	2	0	0

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
32	g	101	1633	549	783	136	161	4	0	0

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
33	h	138	2325	762	1163	194	203	3	0	0

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
34	i	94	1578	513	794	134	134	3	0	0

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
35	j	62	1033	355	496	88	93	1	0	0

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
36	k	75	1213	404	604	103	100	2	0	0

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
37	l	154	2481	834	1187	215	234	11	0	0

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
38	m	126	2111	676	1061	189	185	0	0

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
39	n	177	2998	981	1464	275	267	11	0	0

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
40	o	111	1894	605	937	176	168	8	0	0

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
41	p	169	2832	901	1399	257	267	8	0	0

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
42	q	144	2361	773	1158	213	212	5	0	0

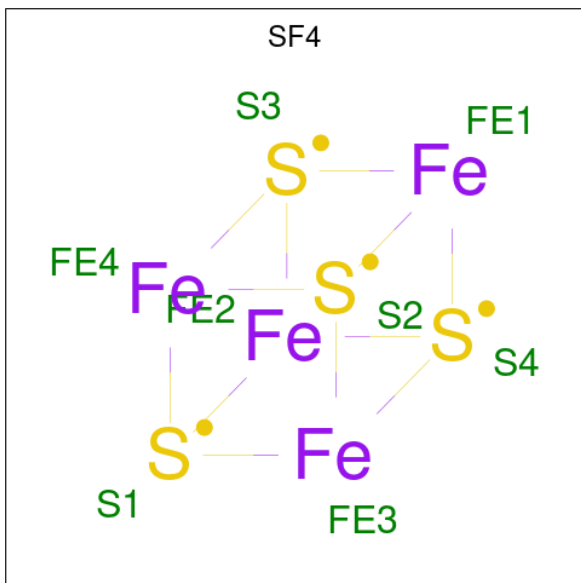
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
43	r	100	1638	507	836	149	143	3	0	0

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

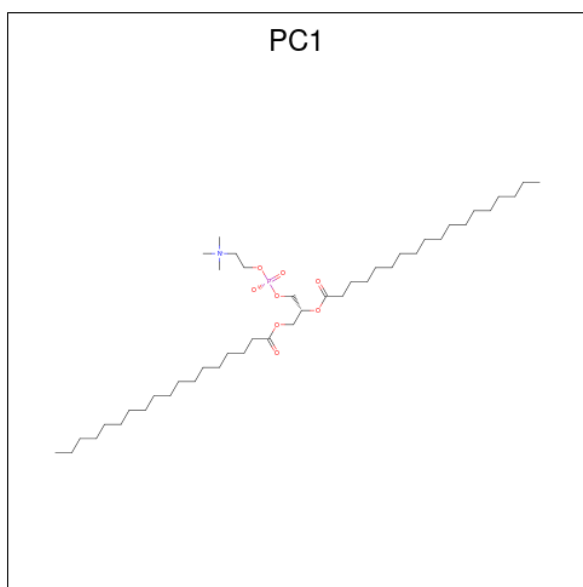
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
44	s	41	668	215	324	61	68	0	0

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



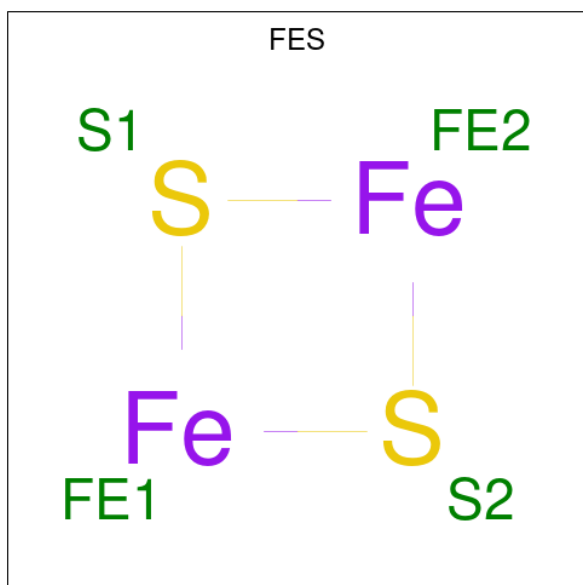
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
45	B	1	8	4	4	0
45	F	1	8	4	4	0
45	G	1	8	4	4	0
45	G	1	8	4	4	0
45	I	1	8	4	4	0
45	I	1	8	4	4	0

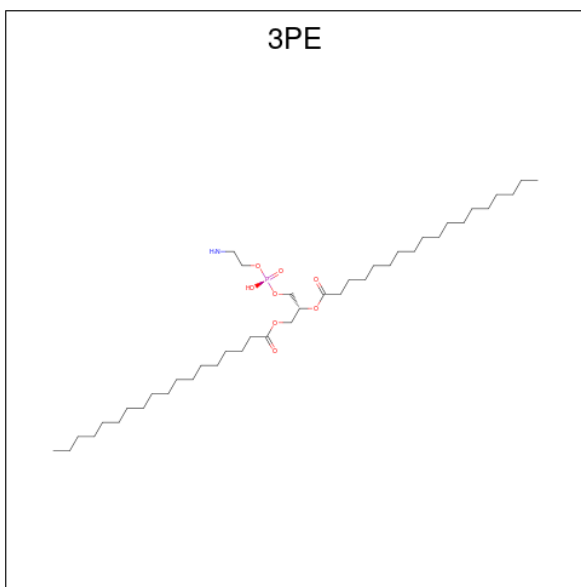
- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
46	B	1	83	25	48	1	8	1	0
46	B	1	108	33	65	1	8	1	0
46	J	1	104	32	62	1	8	1	0
46	Z	1	113	35	68	1	8	1	0

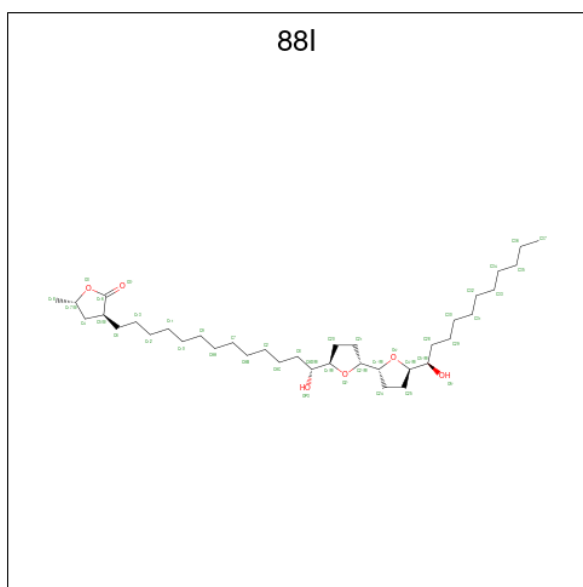
- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).





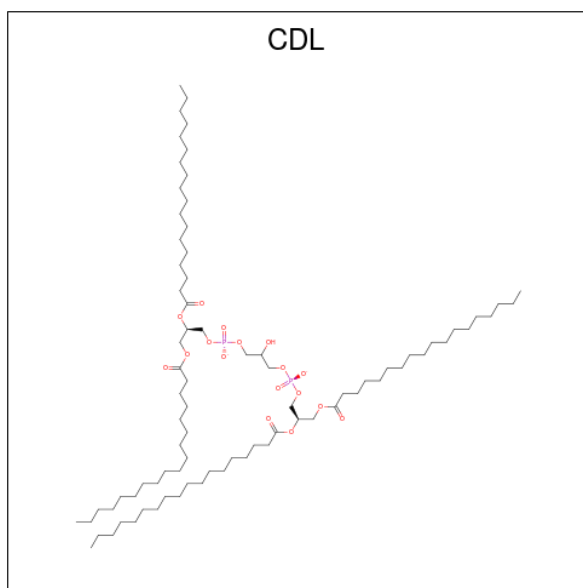
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
49	H	1	Total 133	C 41	H 82	N 1	O 8	P 1	0
49	H	1	Total 111	C 34	H 67	N 1	O 8	P 1	0
49	K	1	Total 77	C 23	H 44	N 1	O 8	P 1	0
49	L	1	Total 126	C 39	H 77	N 1	O 8	P 1	0
49	L	1	Total 105	C 32	H 63	N 1	O 8	P 1	0
49	L	1	Total 126	C 39	H 77	N 1	O 8	P 1	0
49	M	1	Total 89	C 27	H 52	N 1	O 8	P 1	0
49	M	1	Total 105	C 32	H 63	N 1	O 8	P 1	0
49	Y	1	Total 101	C 31	H 60	N 1	O 8	P 1	0

- Molecule 50 is (3 {S},5 {S})-5-methyl-3-[(13 {R})-13-oxidanyl-13-[(2 {R},5 {R})-5-[(2 {R},5 {R})-5-[(1 {R})-1-oxidanylundecyl]oxolan-2-yl]oxolan-2-yl]tridecyl]oxolan-2-one (CCD ID: 88I) (formula: C₃₇H₆₈O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
50	H	1	109	37	66	6	0

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



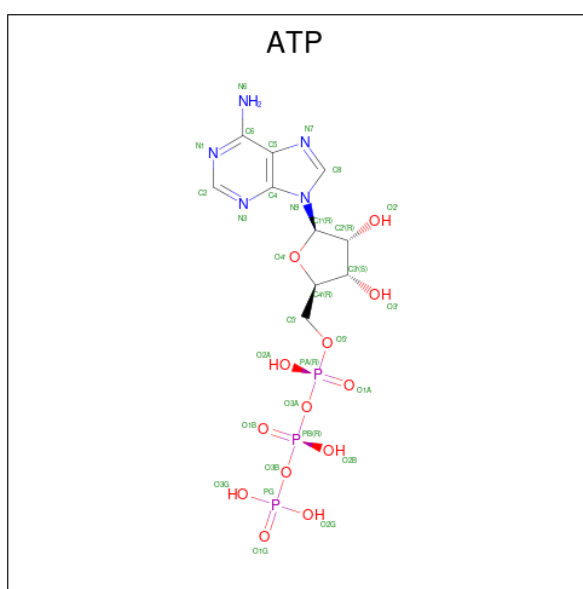
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
51	L	1	174	55	100	17	2	0
51	N	1	148	46	83	17	2	0
51	X	1	154	48	87	17	2	0

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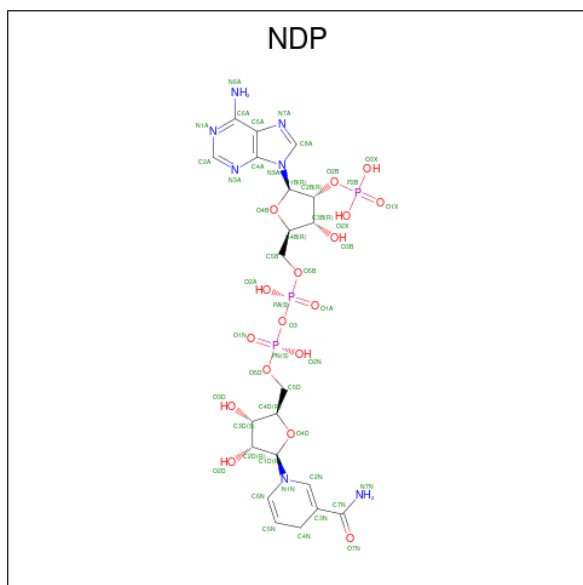
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
51	d	1	Total	C	H	O	P	0
			133	41	74	16	2	
51	d	1	Total	C	H	O	P	0
			141	44	78	17	2	
51	i	1	Total	C	H	O	P	0
			163	51	93	17	2	
51	r	1	Total	C	H	O	P	0
			123	38	66	17	2	

- Molecule 52 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
52	O	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

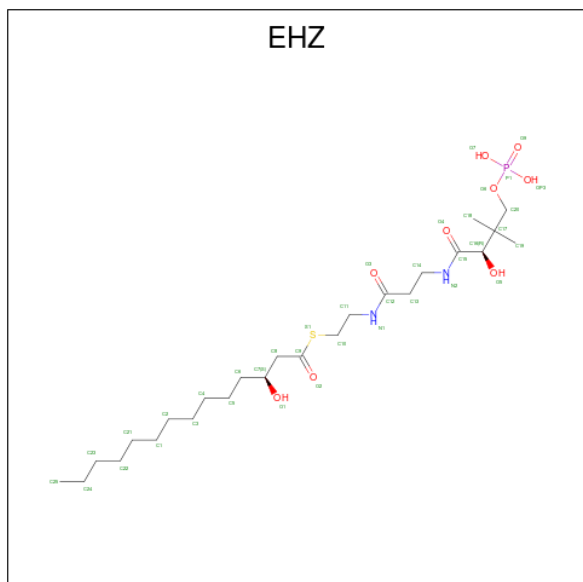


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
53	P	1	74	21	26	7	17	3	0

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
54	R	1	1	1	0

- Molecule 55 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonoxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).

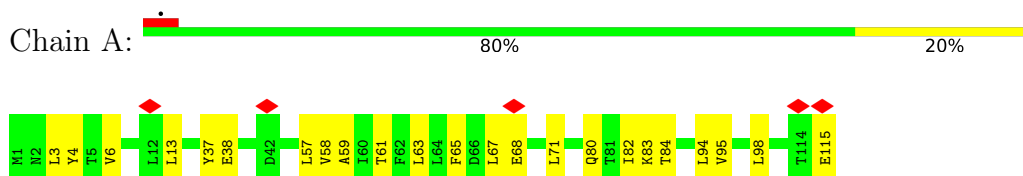


Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	S	
55	T	1	84	25	47	2	8	1	1	0
55	U	1	84	25	47	2	8	1	1	0

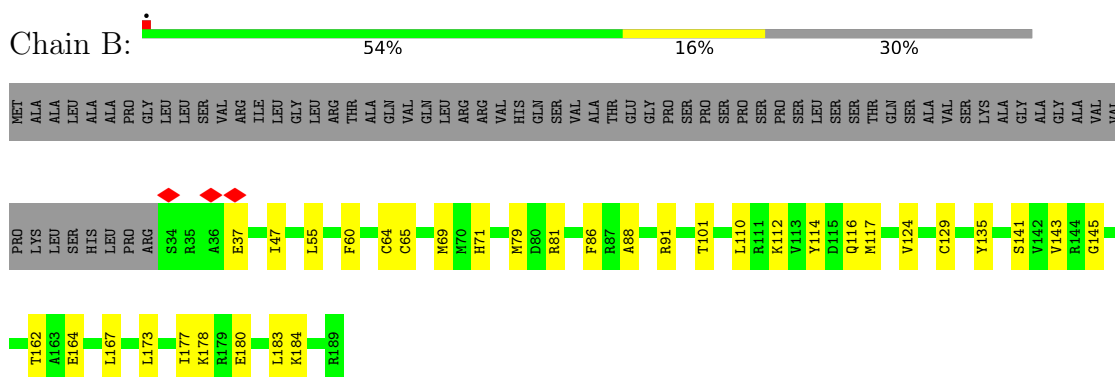
3 Residue-property plots [i](#)

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.

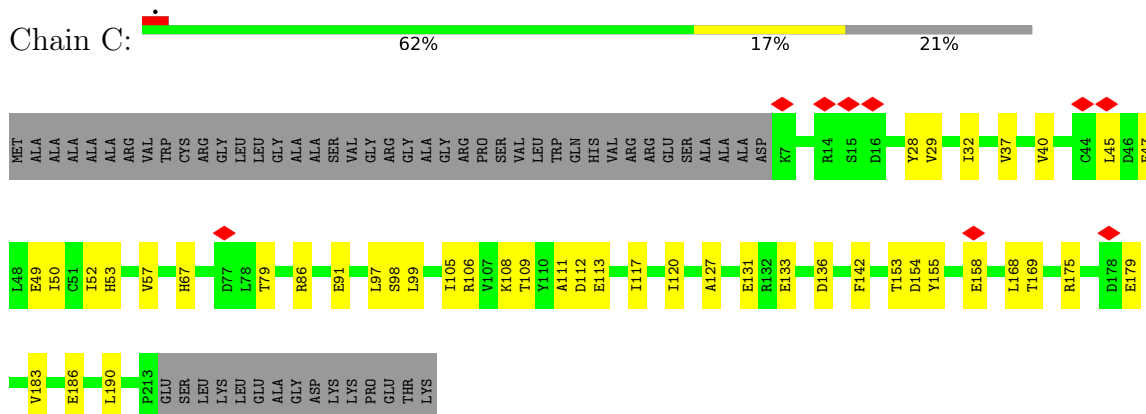
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



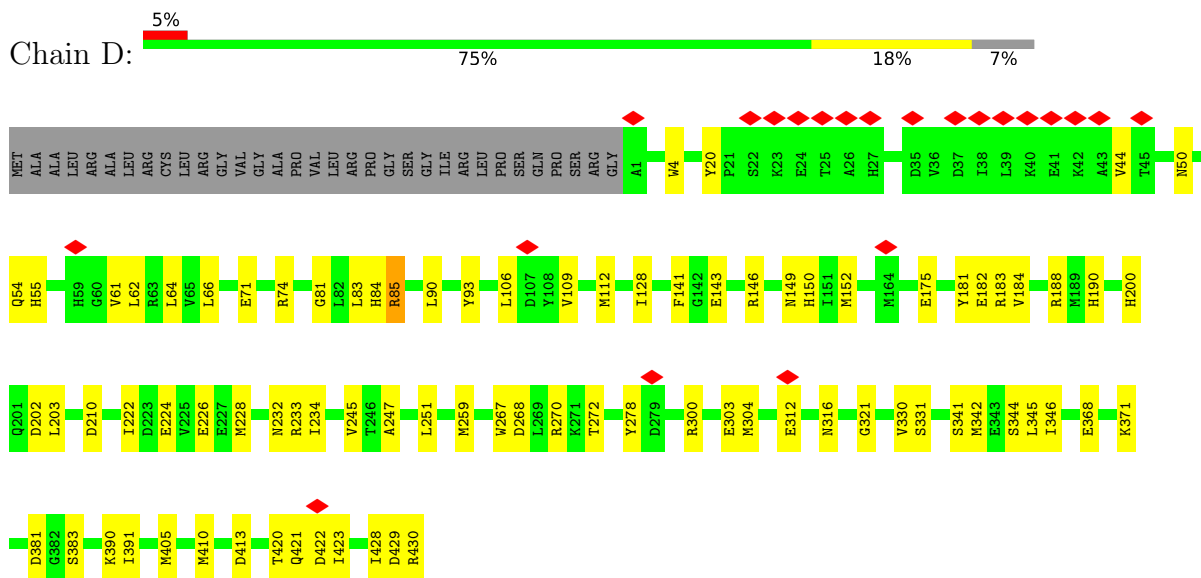
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



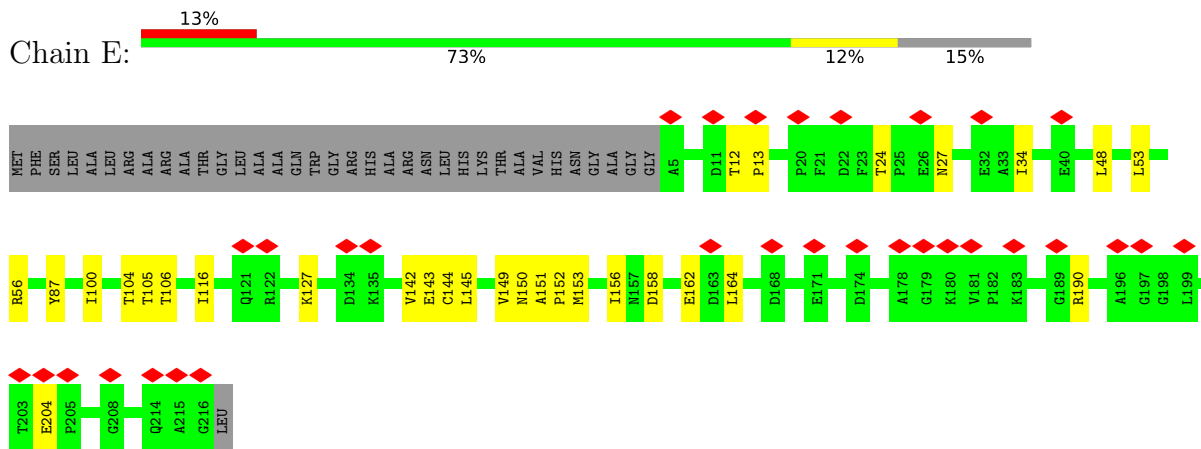
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



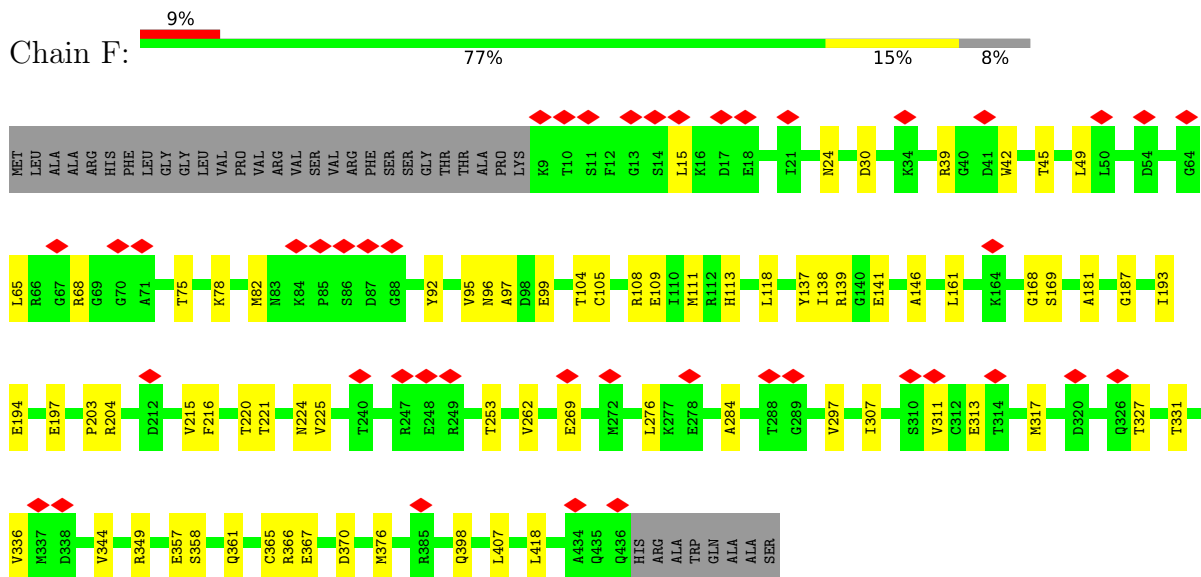
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

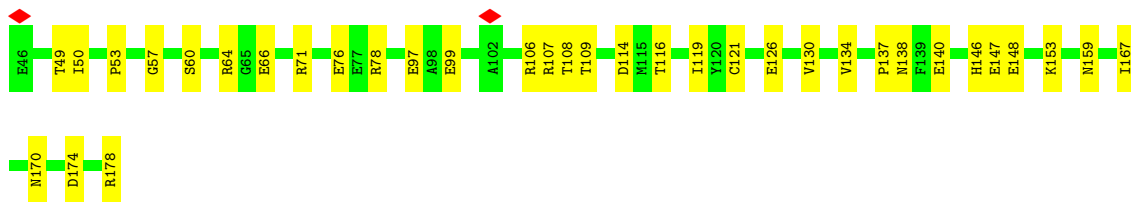


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

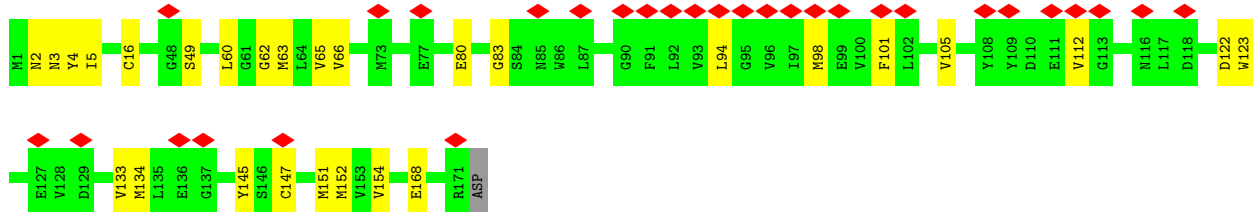
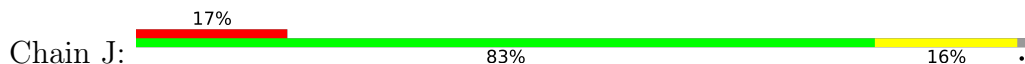


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

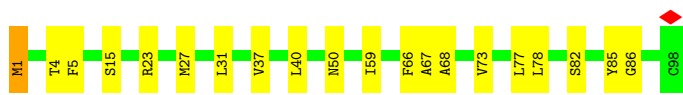
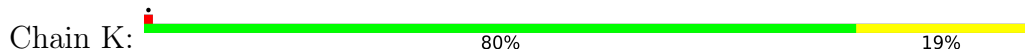




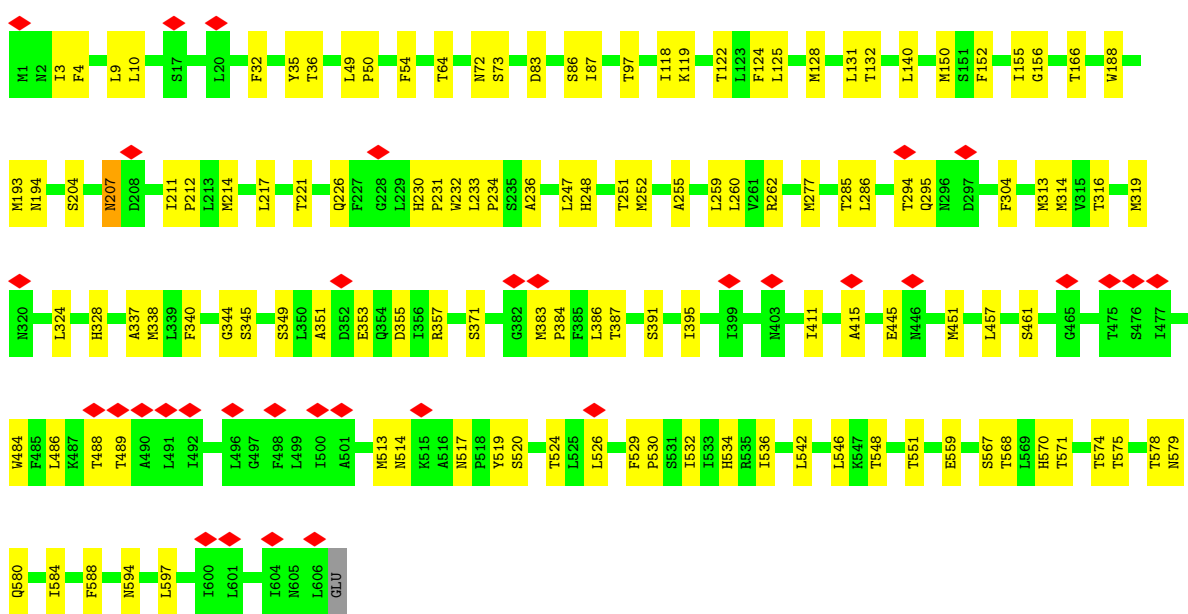
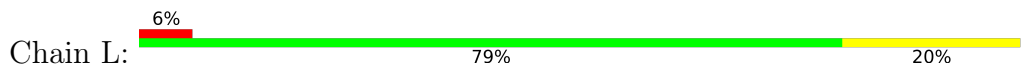
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



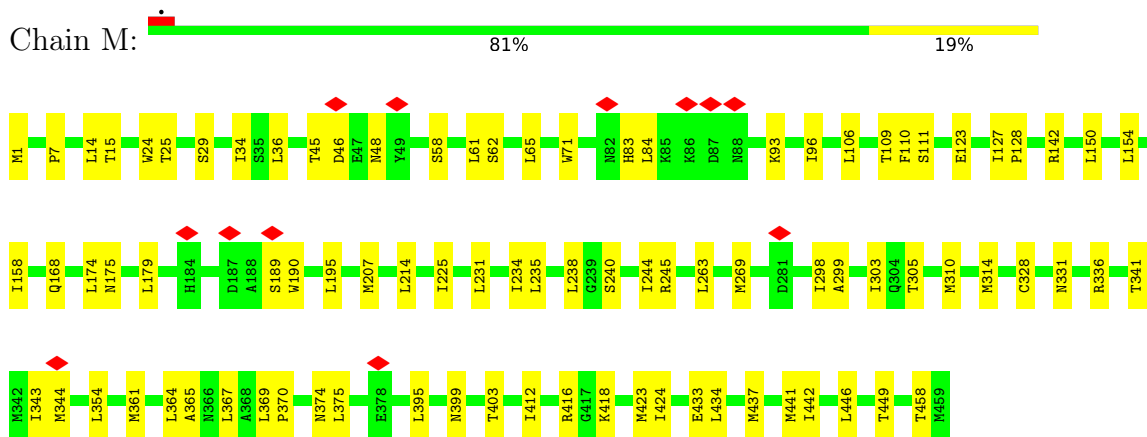
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



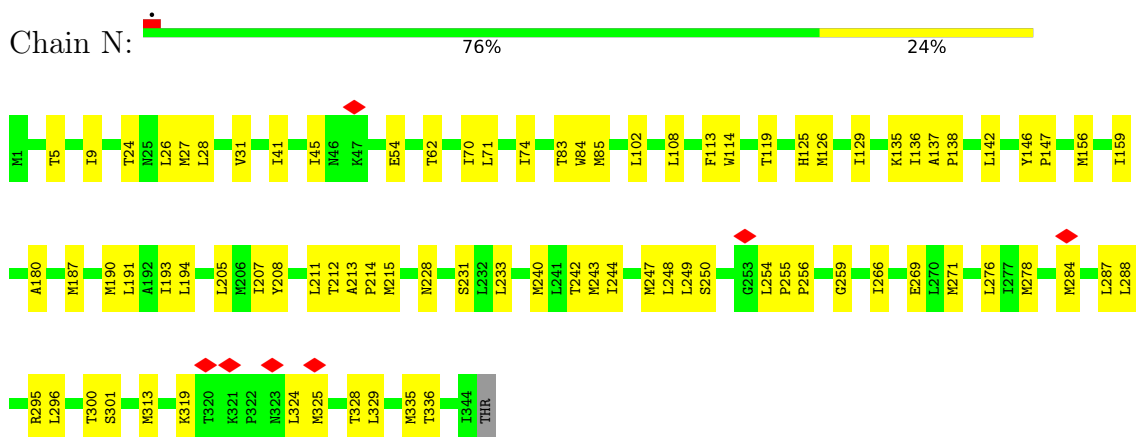
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



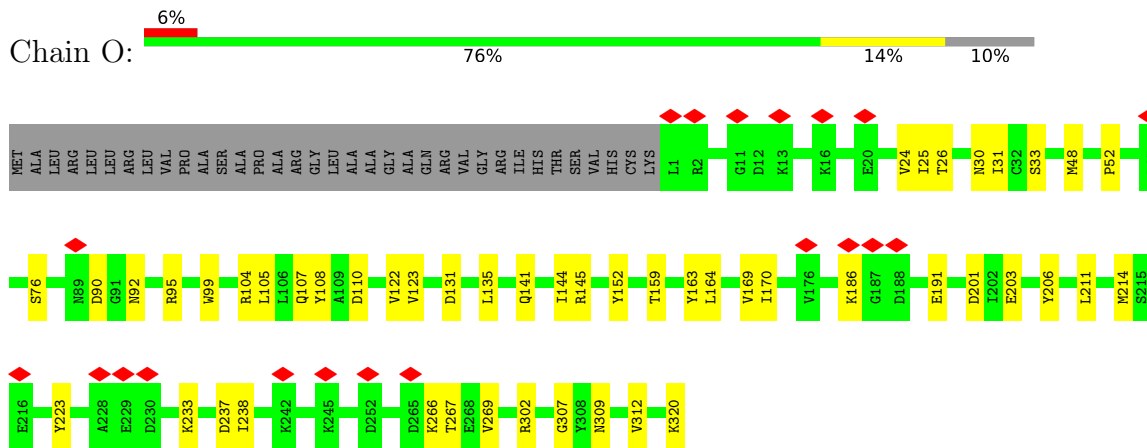
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

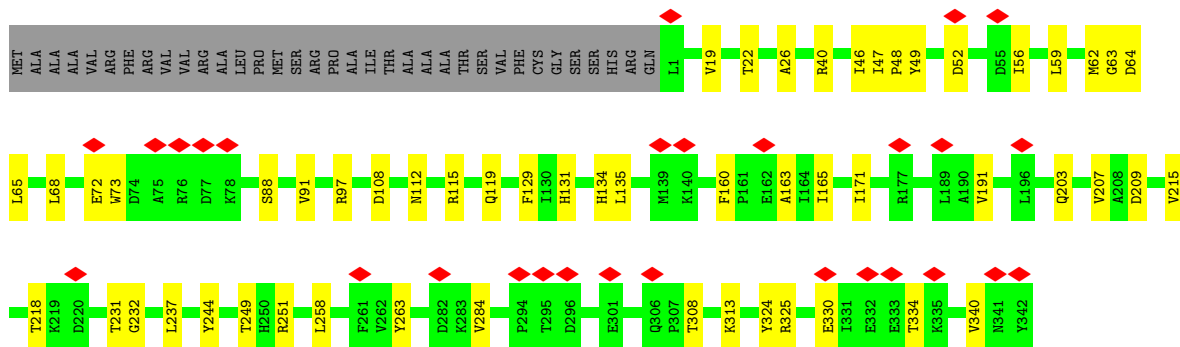


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

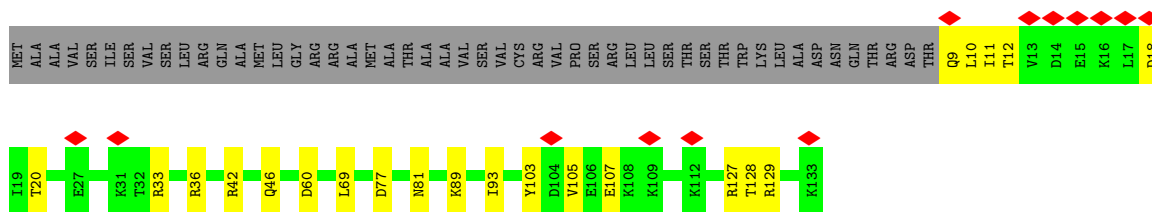


• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

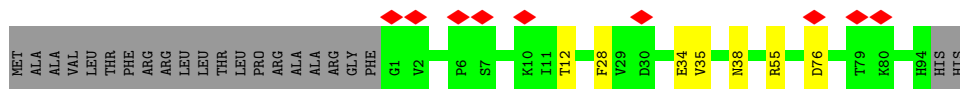
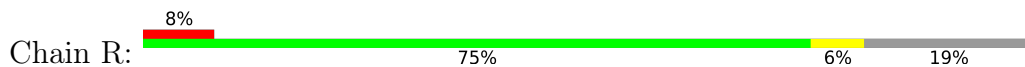




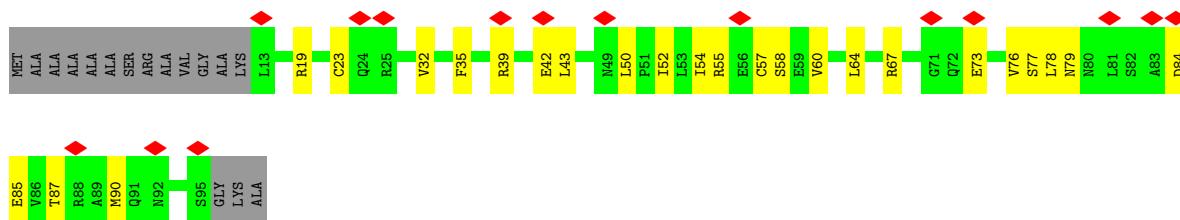
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



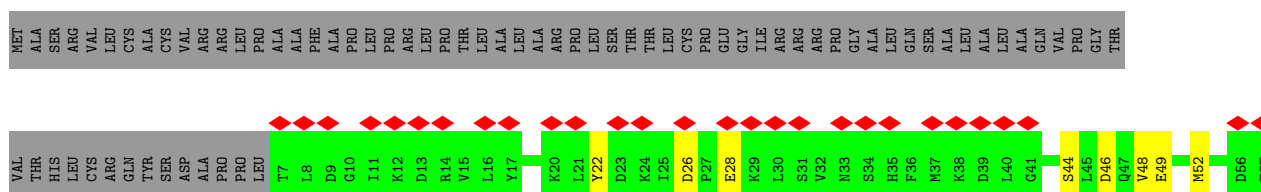
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

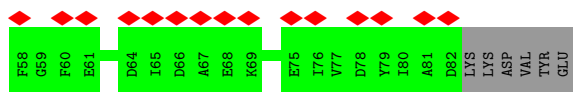


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

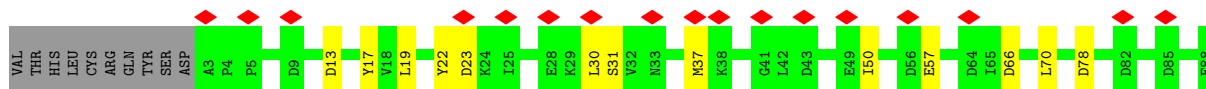


• Molecule 20: Acyl carrier protein, mitochondrial

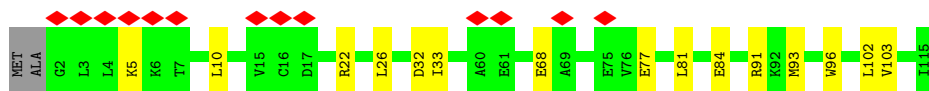
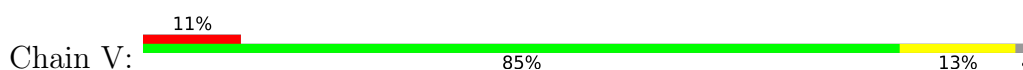




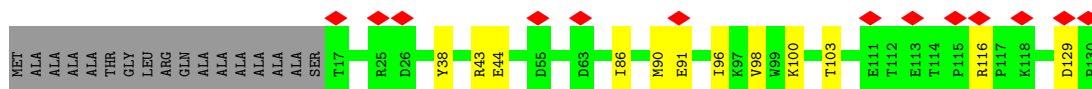
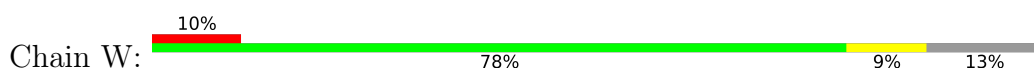
• Molecule 20: Acyl carrier protein, mitochondrial



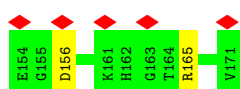
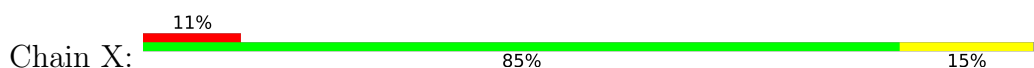
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



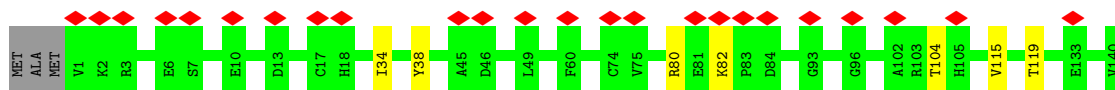
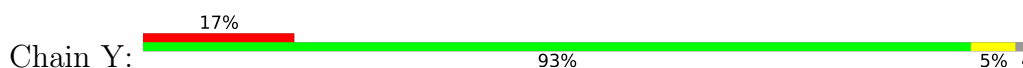
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



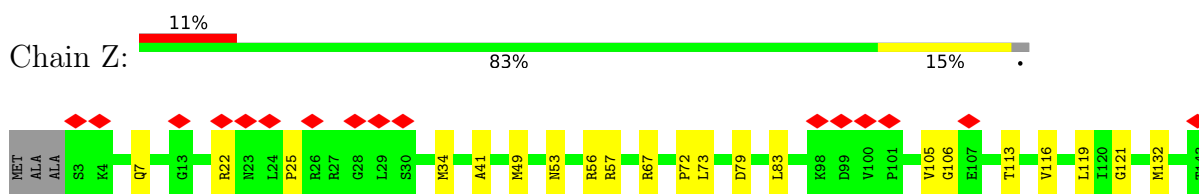
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



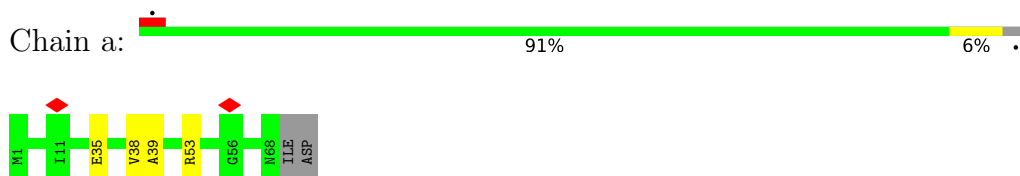
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



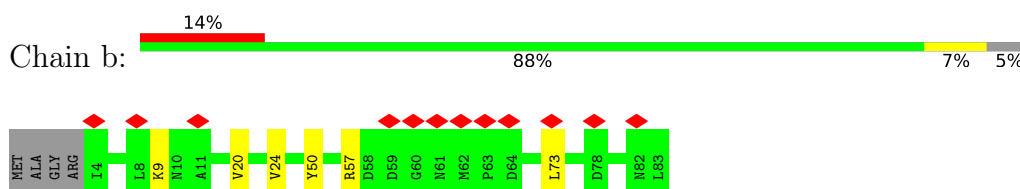
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



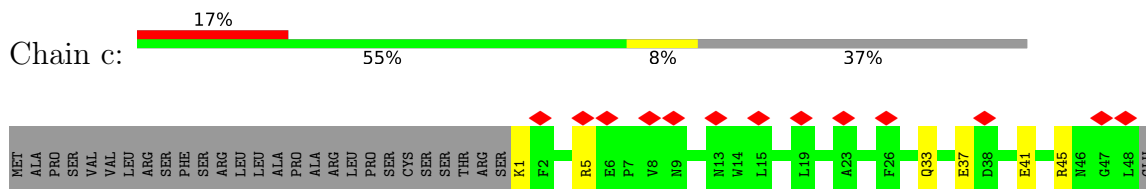
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



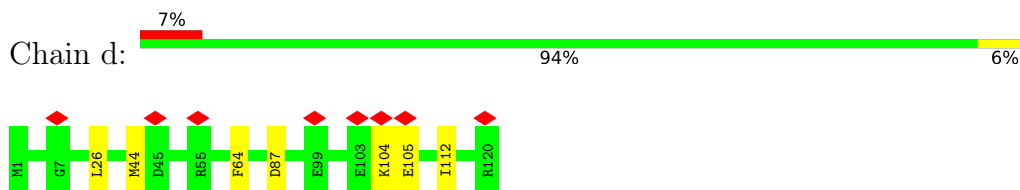
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



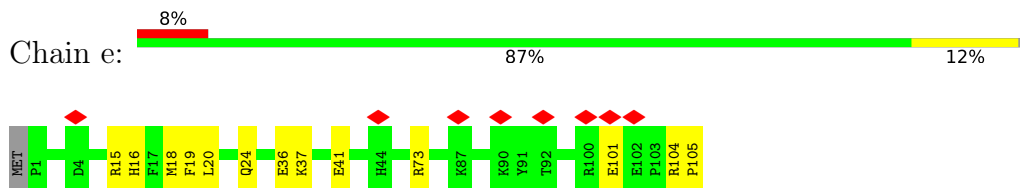
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



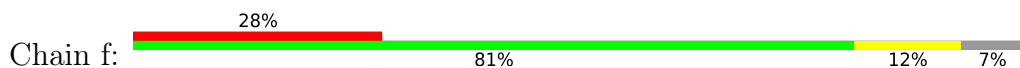
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

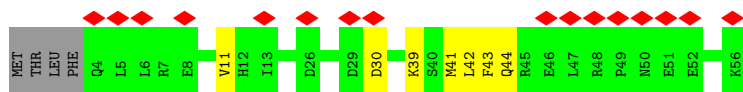


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

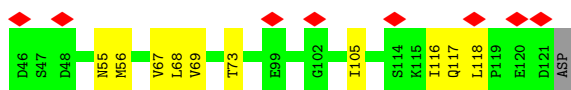


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

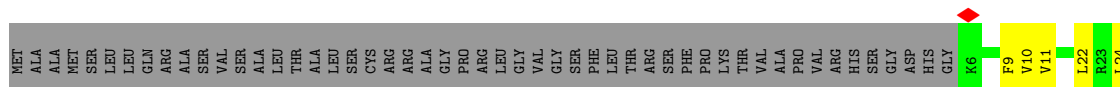




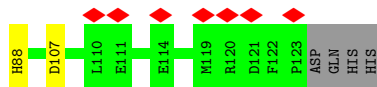
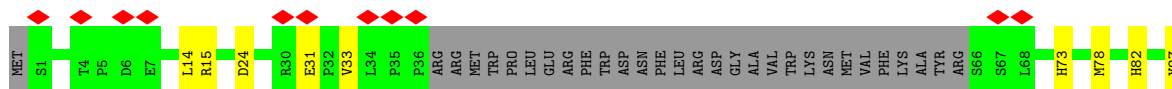
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



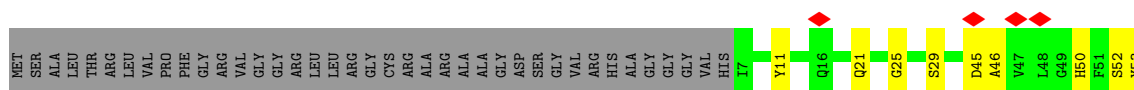
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

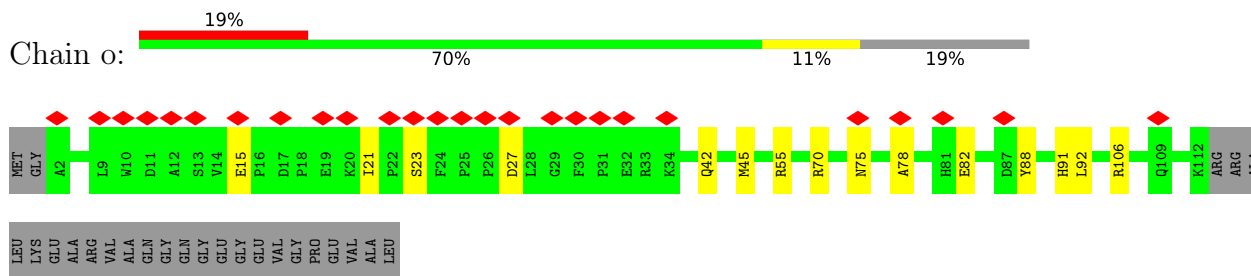


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

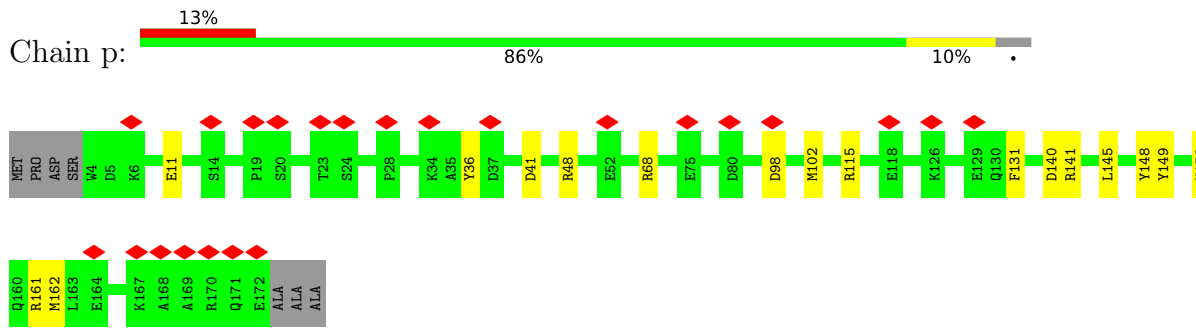


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

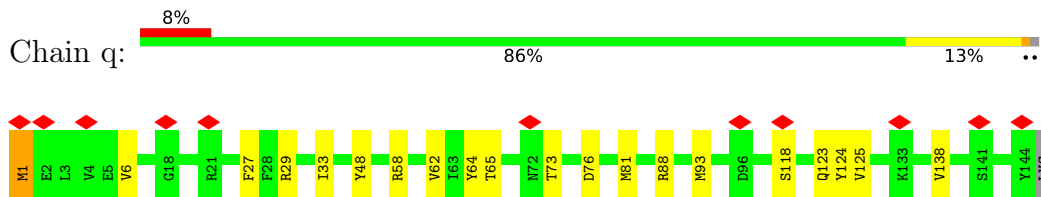




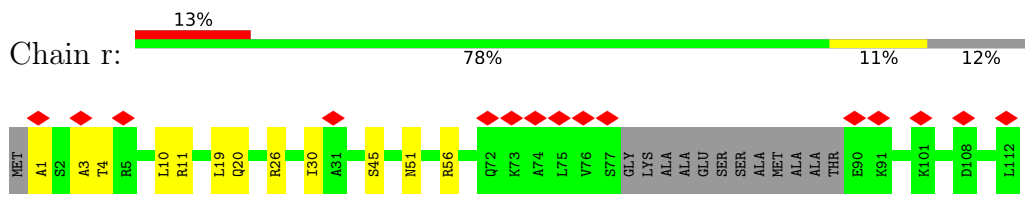
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



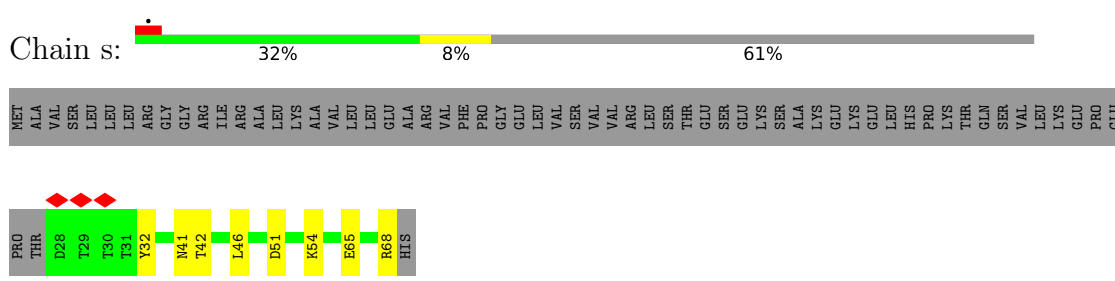
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.265	Depositor
Minimum map value	-0.084	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	469.35, 469.35, 469.35	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.043, 1.043, 1.043	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: PC1, ATP, 88I, 3PE, FES, CDL, ZN, AME, AYA, EHZ, FME, SF4, NDP, FMN, 2MR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.22	0/949	0.33	0/1297
2	B	0.32	0/1278	0.38	1/1730 (0.1%)
3	C	0.28	0/1771	0.37	0/2412
4	D	0.28	0/3540	0.35	0/4795
5	E	0.20	0/1688	0.36	0/2300
6	F	0.23	0/3374	0.35	0/4557
7	G	0.24	0/5383	0.34	0/7293
8	H	0.24	0/2607	0.38	0/3564
9	I	0.31	0/1461	0.40	0/1974
10	J	0.21	0/1322	0.34	0/1799
11	K	0.22	0/738	0.34	0/1002
12	L	0.23	0/4913	0.36	0/6686
13	M	0.24	0/3709	0.35	0/5052
14	N	0.24	0/2748	0.40	0/3741
15	O	0.21	0/2674	0.29	0/3626
16	P	0.23	0/2823	0.36	0/3828
17	Q	0.23	0/1038	0.30	0/1401
18	R	0.26	0/751	0.38	0/1011
19	S	0.18	0/678	0.34	0/915
20	T	0.14	0/620	0.32	0/836
20	U	0.20	0/704	0.36	0/951
21	V	0.20	0/949	0.35	0/1286
22	W	0.21	0/993	0.34	0/1335
23	X	0.21	0/1434	0.37	0/1937
24	Y	0.17	0/1061	0.26	0/1439
25	Z	0.21	0/1198	0.35	0/1616
26	a	0.21	0/569	0.32	0/766
27	b	0.18	0/651	0.30	0/895
28	c	0.17	0/409	0.25	0/555
29	d	0.22	0/1028	0.30	0/1387
30	e	0.21	0/900	0.32	0/1199
31	f	0.17	0/468	0.30	0/630

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.21	0/878	0.33	0/1196
33	h	0.22	0/1197	0.30	0/1621
34	i	0.21	0/810	0.35	0/1102
35	j	0.23	0/561	0.38	1/768 (0.1%)
36	k	0.16	0/629	0.31	0/851
37	l	0.21	0/1348	0.35	0/1840
38	m	0.19	0/1079	0.32	0/1463
39	n	0.19	0/1589	0.29	0/2152
40	o	0.18	0/982	0.37	0/1320
41	p	0.20	0/1466	0.32	0/1981
42	q	0.25	0/1234	0.34	0/1681
43	r	0.23	0/812	0.45	0/1098
44	s	0.19	0/353	0.31	0/479
All	All	0.23	0/67367	0.35	2/91367 (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
42	q	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	j	56	PRO	CA-N-CD	-5.61	104.15	112.00
2	B	65	CYS	CA-CB-SG	5.13	126.19	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
42	q	1	AME	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	933	969	969	26	0
2	B	1247	1255	1255	30	0
3	C	1721	1681	1680	38	0
4	D	3464	3414	3417	73	0
5	E	1648	1639	1639	25	0
6	F	3300	3259	3258	53	0
7	G	5296	5322	5322	103	0
8	H	2540	2626	2626	60	0
9	I	1431	1381	1383	38	0
10	J	1300	1315	1315	29	0
11	K	737	768	768	18	0
12	L	4800	4985	4985	100	0
13	M	3632	3853	3853	75	0
14	N	2696	2895	2895	74	0
15	O	2607	2564	2566	35	0
16	P	2748	2766	2768	38	0
17	Q	1015	1016	1016	17	0
18	R	738	715	717	5	0
19	S	667	686	685	17	0
20	T	611	602	602	5	0
20	U	692	686	686	9	0
21	V	927	968	968	12	0
22	W	970	991	991	8	0
23	X	1396	1377	1381	19	0
24	Y	1037	1025	1027	5	0
25	Z	1167	1166	1166	19	0
26	a	556	568	568	4	0
27	b	628	628	628	6	0
28	c	398	399	401	4	0
29	d	996	1001	1001	8	0
30	e	877	869	871	12	0
31	f	456	452	452	5	0
32	g	850	783	783	13	0
33	h	1162	1163	1163	16	0
34	i	784	794	796	10	0
35	j	537	496	495	12	0
36	k	609	604	603	5	0
37	l	1294	1187	1186	21	0
38	m	1050	1061	1061	18	0
39	n	1534	1464	1466	16	0
40	o	957	937	937	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	p	1433	1399	1399	17	0
42	q	1203	1158	1158	19	0
43	r	802	836	836	8	0
44	s	344	324	324	6	0
45	B	8	0	0	0	0
45	F	8	0	0	0	0
45	G	16	0	0	0	0
45	I	16	0	0	0	0
46	B	78	113	107	0	0
46	J	42	62	58	2	0
46	Z	45	68	64	0	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	19	19	4	0
49	H	95	149	147	3	0
49	K	33	44	40	0	0
49	L	140	217	211	2	0
49	M	79	115	109	0	0
49	Y	41	60	56	0	0
50	H	43	66	0	0	0
51	L	74	100	92	0	0
51	N	65	83	77	1	0
51	X	67	87	81	0	0
51	d	122	152	138	1	0
51	i	70	93	87	1	0
51	r	57	66	58	0	0
52	O	31	12	12	1	0
53	P	48	26	26	2	0
54	R	1	0	0	0	0
55	T	37	47	0	2	0
55	U	37	47	0	1	0
All	All	67082	67673	67448	936	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 (936) 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)
12:L:316:THR:HG22	12:L:395:ILE:HD12	1.48	0.94
14:N:243:MET:HE3	29:d:44:MET:HE3	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:LEU:HD11	4:D:90:LEU:HD12	1.56	0.88
12:L:128:MET:HE3	12:L:251:THR:HG22	1.55	0.87
7:G:258:ILE:HG22	7:G:368:ILE:HD12	1.57	0.87
13:M:269:MET:SD	13:M:399:ASN:ND2	2.47	0.87
22:W:91:GLU:OE2	22:W:100:LYS:NZ	2.07	0.87
13:M:175:ASN:ND2	33:h:97:GLU:OE1	2.08	0.86
11:K:1:FME:SD	11:K:50:ASN:ND2	2.49	0.86
7:G:324:ASP:OD1	7:G:569:LYS:NZ	2.08	0.85
12:L:313:MET:O	12:L:316:THR:OG1	1.95	0.85
7:G:331:LEU:HD22	7:G:525:LEU:HD22	1.58	0.85
1:A:71:LEU:O	10:J:145:TYR:OH	1.94	0.84
26:a:53:ARG:NH1	30:e:105:PRO:O	2.09	0.84
12:L:36:THR:HG21	12:L:118:ILE:HG21	1.61	0.83
34:i:14:LEU:HD21	39:n:169:ILE:HG21	1.60	0.82
15:O:170:ILE:HD11	15:O:238:ILE:HD11	1.61	0.82
7:G:45:ARG:NH2	7:G:256:GLU:OE2	2.13	0.81
4:D:109:VAL:HG11	4:D:152:MET:HE1	1.62	0.81
3:C:28:TYR:HH	3:C:67:HIS:HE2	1.25	0.81
14:N:249:LEU:HD22	14:N:254:LEU:HD12	1.61	0.81
21:V:22:ARG:NH2	21:V:84:GLU:OE2	2.14	0.81
7:G:118:ASP:OD2	17:Q:46:GLN:NE2	2.14	0.81
20:U:57:GLU:OE2	35:j:11:TYR:OH	1.97	0.80
22:W:116:ARG:NH2	22:W:129:ASP:OD2	2.15	0.80
37:l:41:MET:SD	38:m:85:ASN:ND2	2.55	0.80
13:M:106:LEU:HD13	13:M:234:ILE:HG21	1.62	0.80
13:M:46:ASP:OD2	13:M:48:ASN:ND2	2.15	0.80
7:G:140:LYS:O	7:G:148:THR:OG1	2.01	0.78
21:V:5:LYS:NZ	21:V:68:GLU:OE2	2.17	0.78
19:S:39:ARG:NH1	19:S:42:GLU:OE1	2.17	0.78
6:F:108:ARG:NH1	6:F:109:GLU:OE2	2.17	0.78
3:C:175:ARG:NH1	3:C:186:GLU:OE2	2.16	0.78
11:K:85:TYR:OH	14:N:54:GLU:OE2	2.00	0.77
6:F:24:ASN:ND2	6:F:30:ASP:O	2.17	0.77
15:O:302:ARG:O	15:O:309:ASN:ND2	2.18	0.77
9:I:170:ASN:OD1	42:q:88:ARG:NH1	2.18	0.77
41:p:98:ASP:OD2	41:p:141:ARG:NH2	2.17	0.76
15:O:233:LYS:NZ	21:V:32:ASP:OD2	2.18	0.76
19:S:84:ASP:O	19:S:87:THR:OG1	2.03	0.76
4:D:4:TRP:O	13:M:142:ARG:NH2	2.19	0.76
15:O:76:SER:O	15:O:95:ARG:NH1	2.18	0.76
38:m:23:ASP:O	38:m:29:ARG:NH1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:365:ALA:O	13:M:374:ASN:ND2	2.19	0.76
36:k:25:ARG:O	36:k:28:LYS:NZ	2.19	0.75
4:D:228:MET:O	4:D:232:ASN:ND2	2.18	0.75
20:U:78:ASP:OD2	34:i:15:ARG:NH1	2.19	0.75
4:D:428:ILE:O	4:D:430:ARG:NH1	2.20	0.75
8:H:93:HIS:NE2	26:a:35:GLU:OE2	2.19	0.75
3:C:179:GLU:OE1	16:P:40:ARG:NH2	2.19	0.75
9:I:14:VAL:O	27:b:9:LYS:NZ	2.19	0.75
4:D:413:ASP:OD1	8:H:281:ARG:NH1	2.19	0.74
1:A:37:TYR:OH	4:D:54:GLN:OE1	2.03	0.74
10:J:16:CYS:SG	11:K:15:SER:OG	2.44	0.74
44:s:65:GLU:OE1	44:s:68:ARG:NH2	2.20	0.74
7:G:403:ASP:OD1	17:Q:127:ARG:NH2	2.20	0.74
7:G:341:ASP:OD2	19:S:67:ARG:NH2	2.21	0.73
11:K:77:LEU:HD21	14:N:41:ILE:HG21	1.70	0.73
8:H:114:TYR:OH	10:J:60:LEU:O	2.05	0.73
37:l:61:TYR:OH	38:m:43:LYS:NZ	2.22	0.73
13:M:446:LEU:O	13:M:449:THR:OG1	2.07	0.73
48:F:502:FMN:O3'	48:F:502:FMN:N1	2.22	0.73
14:N:108:LEU:CD1	14:N:191:LEU:HD22	2.19	0.73
5:E:48:LEU:HD22	6:F:181:ALA:HB2	1.69	0.73
14:N:119:THR:HG21	14:N:180:ALA:HB2	1.71	0.72
7:G:53:ARG:O	7:G:93:VAL:HG21	1.89	0.72
5:E:56:ARG:NH2	5:E:158:ASP:OD2	2.22	0.72
2:B:37:GLU:OE2	2:B:184:LYS:NZ	2.23	0.71
9:I:53:PRO:O	42:q:64:TYR:OH	2.05	0.71
7:G:383:ASN:ND2	7:G:665:GLN:O	2.22	0.71
6:F:97:ALA:HB1	6:F:111:MET:HE1	1.70	0.71
41:p:11:GLU:OE2	41:p:115:ARG:NH2	2.23	0.71
5:E:24:THR:OG1	5:E:27:ASN:OD1	2.09	0.70
7:G:620:ARG:NH1	7:G:633:TYR:OH	2.24	0.70
8:H:192:GLU:O	8:H:193:THR:OG1	2.08	0.70
44:s:51:ASP:OD1	44:s:54:LYS:NZ	2.24	0.70
42:q:27:PHE:CD1	42:q:33:ILE:HD11	2.26	0.70
6:F:168:GLY:O	6:F:169:SER:OG	2.08	0.70
28:c:41:GLU:OE2	28:c:45:ARG:NH1	2.25	0.70
14:N:324:LEU:HD11	29:d:64:PHE:HZ	1.57	0.70
13:M:15:THR:O	13:M:93:LYS:NZ	2.22	0.70
37:l:76:ILE:HG23	37:l:80:LEU:HD22	1.73	0.70
6:F:313:GLU:OE1	6:F:313:GLU:N	2.25	0.69
29:d:104:LYS:NZ	29:d:105:GLU:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:109:VAL:HG11	4:D:152:MET:CE	2.21	0.69
7:G:231:MET:HE1	7:G:677:ILE:HG21	1.74	0.69
4:D:200:HIS:NE2	9:I:126:GLU:OE1	2.25	0.69
8:H:81:LEU:HD21	8:H:111:LEU:HD23	1.73	0.69
6:F:99:GLU:O	6:F:139:ARG:NH1	2.25	0.69
7:G:443:LEU:HD21	7:G:477:ILE:HD12	1.72	0.69
4:D:146:ARG:NH2	4:D:368:GLU:O	2.25	0.69
30:e:37:LYS:NZ	30:e:41:GLU:OE2	2.25	0.69
3:C:112:ASP:OD2	3:C:113:GLU:N	2.26	0.69
6:F:358:SER:OG	6:F:365:CYS:SG	2.47	0.69
11:K:37:VAL:HG21	11:K:67:ALA:HB1	1.74	0.69
2:B:91:ARG:NH1	2:B:116:GLN:OE1	2.26	0.68
7:G:261:GLU:OE2	17:Q:42:ARG:NH2	2.26	0.68
5:E:151:ALA:HB3	5:E:152:PRO:HD3	1.75	0.68
19:S:78:LEU:O	19:S:78:LEU:HD12	1.94	0.68
9:I:34:ARG:NH2	25:Z:25:PRO:O	2.25	0.68
9:I:64:ARG:NH1	9:I:121:CYS:O	2.26	0.68
12:L:328:HIS:ND1	12:L:391:SER:OG	2.22	0.67
10:J:83:GLY:N	46:J:201:PC1:O32	2.27	0.67
15:O:30:ASN:ND2	15:O:203:GLU:OE2	2.28	0.67
15:O:186:LYS:NZ	15:O:191:GLU:OE1	2.26	0.67
15:O:108:TYR:OH	15:O:164:LEU:O	2.13	0.66
23:X:44:LEU:HD22	23:X:130:VAL:HG13	1.76	0.66
2:B:71:HIS:ND1	4:D:175:GLU:OE2	2.29	0.66
15:O:141:GLN:NE2	15:O:201:ASP:OD2	2.29	0.66
12:L:517:ASN:OD1	12:L:519:TYR:N	2.29	0.66
7:G:321:GLY:O	7:G:498:SER:OG	2.07	0.66
5:E:104:THR:O	6:F:349:ARG:NE	2.29	0.66
12:L:131:LEU:HD21	12:L:255:ALA:HB1	1.77	0.66
9:I:66:GLU:OE2	9:I:159:ASN:ND2	2.29	0.66
6:F:366:ARG:NE	6:F:367:GLU:OE2	2.27	0.65
13:M:310:MET:SD	13:M:314:MET:HE3	2.36	0.65
14:N:296:LEU:O	14:N:300:THR:HG22	1.96	0.65
3:C:111:ALA:CB	3:C:117:ILE:HD11	2.25	0.65
3:C:49:GLU:OE2	3:C:108:LYS:NZ	2.30	0.65
6:F:141:GLU:OE1	6:F:141:GLU:N	2.29	0.65
8:H:24:GLU:OE2	8:H:228:TYR:OH	2.06	0.65
7:G:35:MET:SD	7:G:81:THR:OG1	2.53	0.65
12:L:4:PHE:HZ	12:L:87:ILE:HD11	1.61	0.65
12:L:580:GLN:HE22	14:N:113:PHE:HE1	1.45	0.65
12:L:207:ASN:O	12:L:207:ASN:ND2	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:25:ILE:HD12	15:O:48:MET:HE1	1.79	0.65
43:r:3:ALA:O	43:r:4:THR:OG1	2.12	0.65
7:G:231:MET:HE3	7:G:270:ALA:HB3	1.78	0.64
12:L:36:THR:HG21	12:L:118:ILE:CG2	2.27	0.64
6:F:370:ASP:OD2	7:G:179:ASN:ND2	2.31	0.64
8:H:138:GLN:OE1	8:H:285:LEU:HD21	1.96	0.64
7:G:303:VAL:HG11	7:G:603:LEU:HD11	1.77	0.64
37:l:98:ASP:OD1	37:l:99:VAL:N	2.30	0.64
3:C:111:ALA:HB1	3:C:117:ILE:HD11	1.80	0.64
8:H:283:ASP:OD1	8:H:284:GLN:N	2.30	0.64
19:S:19:ARG:NH2	19:S:73:GLU:OE1	2.31	0.64
23:X:44:LEU:HD21	27:b:57:ARG:HD3	1.80	0.64
29:d:112:ILE:O	41:p:159:LYS:NZ	2.31	0.64
3:C:154:ASP:OD1	3:C:155:TYR:N	2.29	0.64
18:R:55:ARG:NH1	18:R:76:ASP:OD2	2.31	0.64
7:G:364:LEU:HD23	7:G:491:ASN:HB3	1.79	0.64
34:i:24:ASP:OD2	39:n:124:TRP:NE1	2.29	0.64
4:D:150:HIS:NE2	4:D:303:GLU:OE1	2.31	0.64
13:M:1:FME:HE2	13:M:111:SER:CB	2.28	0.64
16:P:308:THR:HG21	16:P:313:LYS:HD2	1.81	0.63
4:D:312:GLU:O	4:D:316:ASN:ND2	2.30	0.63
5:E:204:GLU:N	5:E:204:GLU:OE1	2.30	0.63
6:F:42:TRP:CD2	6:F:161:LEU:HD23	2.33	0.63
4:D:106:LEU:HD11	4:D:391:ILE:HD13	1.81	0.63
12:L:559:GLU:CD	13:M:214:LEU:HD23	2.23	0.63
55:U:201:EHZ:O3	55:U:201:EHZ:N2	2.31	0.63
16:P:49:TYR:OH	16:P:72:GLU:OE1	2.17	0.63
16:P:64:ASP:OD1	16:P:65:LEU:N	2.31	0.63
42:q:29:ARG:NH2	42:q:65:THR:O	2.32	0.63
2:B:178:LYS:NZ	42:q:76:ASP:OD1	2.32	0.62
8:H:28:LEU:HD23	8:H:275:ALA:HB2	1.80	0.62
3:C:40:VAL:HG12	3:C:50:ILE:HG12	1.82	0.62
9:I:174:ASP:OD2	9:I:178:ARG:NH2	2.33	0.62
12:L:574:THR:O	12:L:578:THR:HG22	1.99	0.62
34:i:107:ASP:OD2	40:o:70:ARG:NH2	2.32	0.62
13:M:244:ILE:O	41:p:148:TYR:OH	2.15	0.62
10:J:66:VAL:HG11	11:K:31:LEU:HD21	1.81	0.62
6:F:276:LEU:HD13	6:F:317:MET:HE3	1.80	0.62
1:A:83:LYS:O	1:A:84:THR:OG1	2.14	0.61
12:L:542:LEU:HD23	37:l:82:MET:HB3	1.81	0.61
39:n:170:VAL:O	39:n:171:THR:OG1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:THR:HG22	5:E:13:PRO:HD2	1.80	0.61
43:r:51:ASN:O	43:r:56:ARG:NH1	2.34	0.61
55:T:201:EHZ:S1	55:T:201:EHZ:O1	2.58	0.61
4:D:226:GLU:OE2	25:Z:22:ARG:NE	2.32	0.61
12:L:520:SER:O	12:L:524:THR:OG1	2.13	0.61
13:M:418:LYS:N	37:l:67:GLU:OE1	2.34	0.61
12:L:150:MET:HE3	12:L:150:MET:HA	1.83	0.60
14:N:45:ILE:O	14:N:45:ILE:HG22	2.00	0.60
7:G:43:HIS:NE2	7:G:261:GLU:OE1	2.33	0.60
7:G:104:ASP:OD2	7:G:152:ARG:NH2	2.34	0.60
7:G:194:GLU:N	7:G:194:GLU:OE1	2.34	0.60
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.66	0.60
16:P:97:ARG:NH2	53:P:501:NDP:O3X	2.33	0.60
6:F:82:MET:HE3	6:F:221:THR:HG23	1.83	0.60
23:X:15:GLU:O	23:X:67:LEU:HD11	2.00	0.60
2:B:79:MET:HE1	2:B:167:LEU:HD13	1.84	0.60
15:O:31:ILE:HD12	52:O:401:ATP:O2'	2.01	0.60
2:B:47:ILE:HG22	8:H:57:MET:SD	2.41	0.60
4:D:20:TYR:OH	14:N:295:ARG:NH2	2.34	0.60
40:o:75:ASN:O	40:o:78:ALA:N	2.35	0.60
6:F:224:ASN:OD1	6:F:225:VAL:N	2.34	0.60
7:G:604:SER:HB3	7:G:611:LEU:HD13	1.84	0.60
7:G:199:VAL:CG1	7:G:208:LEU:HD11	2.32	0.60
12:L:524:THR:HG21	39:n:76:PRO:HG2	1.84	0.60
15:O:24:VAL:HG22	15:O:122:VAL:CG2	2.32	0.60
7:G:27:LEU:HD13	7:G:69:CYS:HA	1.83	0.59
9:I:116:THR:HG21	9:I:146:HIS:NE2	2.16	0.59
6:F:344:VAL:HG12	6:F:418:LEU:HD21	1.83	0.59
1:A:4:TYR:OH	10:J:4:TYR:OH	2.19	0.59
6:F:97:ALA:HB1	6:F:111:MET:CE	2.33	0.59
7:G:239:VAL:HG23	7:G:253:ARG:HG3	1.85	0.59
12:L:32:PHE:O	12:L:36:THR:HG22	2.03	0.59
3:C:86:ARG:NH1	3:C:91:GLU:OE1	2.34	0.59
4:D:224:GLU:OE1	9:I:42:TYR:OH	2.17	0.59
12:L:152:PHE:HE1	13:M:412:ILE:HD11	1.67	0.59
14:N:142:LEU:HB3	14:N:194:LEU:HD21	1.84	0.59
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.84	0.59
4:D:81:GLY:N	4:D:429:ASP:OD1	2.36	0.59
7:G:514:ILE:HG21	7:G:532:ILE:CD1	2.33	0.59
23:X:12:LEU:O	30:e:104:ARG:NH2	2.34	0.59
32:g:55:ASN:C	32:g:55:ASN:HD22	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:217:LEU:O	12:L:221:THR:OG1	2.12	0.59
30:e:101:GLU:N	30:e:101:GLU:OE1	2.36	0.59
43:r:11:ARG:NH2	43:r:20:GLN:OE1	2.36	0.58
14:N:228:ASN:O	14:N:231:SER:OG	2.11	0.58
14:N:243:MET:HE3	29:d:44:MET:CE	2.32	0.58
37:l:138:TYR:OH	37:l:143:GLY:O	2.18	0.58
4:D:321:GLY:O	25:Z:7:GLN:NE2	2.37	0.58
6:F:357:GLU:OE2	7:G:177:ARG:NH2	2.36	0.58
9:I:66:GLU:OE1	9:I:138:ASN:ND2	2.36	0.58
14:N:244:ILE:HG22	14:N:248:LEU:HD12	1.85	0.58
20:U:37:MET:HE2	20:U:37:MET:N	2.19	0.58
16:P:330:GLU:N	16:P:330:GLU:OE1	2.37	0.58
4:D:233:ARG:NH2	9:I:25:ARG:O	2.36	0.58
8:H:181:MET:SD	8:H:300:LEU:HD13	2.43	0.58
15:O:307:GLY:O	15:O:320:LYS:NZ	2.28	0.58
7:G:632:ARG:NH1	19:S:57:CYS:SG	2.77	0.58
8:H:97:ASN:ND2	26:a:38:VAL:HG22	2.19	0.58
4:D:342:MET:HE2	7:G:101:HIS:HD2	1.69	0.58
8:H:81:LEU:CD2	8:H:111:LEU:HD23	2.34	0.58
8:H:176:LEU:HD12	25:Z:41:ALA:HB1	1.86	0.58
12:L:226:GLN:CD	12:L:314:MET:HE2	2.28	0.58
4:D:143:GLU:OE2	4:D:278:TYR:OH	2.22	0.58
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.38	0.58
9:I:116:THR:HG21	9:I:146:HIS:CD2	2.39	0.58
12:L:316:THR:CG2	12:L:395:ILE:HD12	2.29	0.58
7:G:379:LEU:HD23	7:G:452:VAL:CG2	2.34	0.57
10:J:80:GLU:OE2	11:K:23:ARG:NH2	2.36	0.57
17:Q:18:ASP:OD1	17:Q:20:THR:HG23	2.03	0.57
5:E:127:LYS:HE3	5:E:127:LYS:HA	1.85	0.57
7:G:258:ILE:CG2	7:G:368:ILE:HD12	2.32	0.57
12:L:152:PHE:CE1	13:M:412:ILE:HD11	2.39	0.57
7:G:443:LEU:CD2	7:G:477:ILE:HD12	2.34	0.57
12:L:445:GLU:OE1	35:j:21:GLN:NE2	2.38	0.57
14:N:335:MET:O	14:N:336:THR:OG1	2.19	0.57
14:N:249:LEU:HD22	14:N:254:LEU:CD1	2.32	0.57
44:s:41:ASN:OD1	44:s:42:THR:N	2.36	0.57
49:H:403:3PE:N	26:a:39:ALA:O	2.37	0.57
11:K:27:MET:HE2	11:K:78:LEU:HD13	1.87	0.57
11:K:59:ILE:HG23	14:N:27:MET:HG2	1.87	0.57
14:N:5:THR:HG22	14:N:9:ILE:HD12	1.86	0.57
3:C:127:ALA:O	3:C:131:GLU:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:351:ALA:N	12:L:353:GLU:OE1	2.38	0.57
23:X:36:ASP:OD1	23:X:37:LYS:N	2.37	0.57
13:M:354:LEU:HD22	13:M:434:LEU:HD11	1.86	0.57
16:P:131:HIS:HB3	16:P:165:ILE:HD13	1.86	0.57
5:E:105:THR:HG22	5:E:106:THR:H	1.70	0.57
31:f:42:LEU:O	41:p:68:ARG:NE	2.38	0.56
3:C:99:LEU:HD22	4:D:251:LEU:HD21	1.87	0.56
7:G:481:THR:O	7:G:483:VAL:HG13	2.05	0.56
13:M:370:PRO:HA	13:M:375:LEU:HD22	1.87	0.56
30:e:20:LEU:O	30:e:24:GLN:NE2	2.37	0.56
32:g:56:MET:SD	33:h:24:LEU:HD21	2.46	0.56
42:q:73:THR:OG1	42:q:81:MET:HE1	2.05	0.56
7:G:378:LEU:HD21	7:G:409:ILE:HD12	1.86	0.56
8:H:176:LEU:CD1	25:Z:41:ALA:HB1	2.36	0.56
42:q:48:TYR:CD1	42:q:62:VAL:HG22	2.41	0.56
7:G:54:MET:HE1	7:G:94:MET:HE2	1.87	0.56
14:N:126:MET:CE	14:N:129:ILE:HD12	2.35	0.56
4:D:106:LEU:CD1	4:D:391:ILE:HD13	2.35	0.56
4:D:259:MET:HE2	4:D:421:GLN:HG2	1.88	0.56
12:L:371:SER:OG	35:j:29:SER:OG	2.21	0.56
1:A:67:LEU:HD11	11:K:68:ALA:HB3	1.87	0.56
7:G:199:VAL:HG11	7:G:208:LEU:HD11	1.86	0.56
7:G:534:ARG:NH2	7:G:556:MET:O	2.38	0.56
7:G:601:ARG:O	7:G:604:SER:OG	2.21	0.56
12:L:338:MET:HE2	12:L:461:SER:HB3	1.88	0.56
33:h:9:PHE:HE2	39:n:103:LEU:HD21	1.71	0.56
39:n:34:ASP:OD1	39:n:35:LYS:N	2.38	0.56
3:C:136:ASP:OD1	3:C:153:THR:OG1	2.23	0.56
33:h:11:VAL:HG13	39:n:103:LEU:HD11	1.88	0.56
6:F:97:ALA:HB3	6:F:137:TYR:O	2.06	0.56
15:O:110:ASP:OD2	28:c:5:ARG:NH2	2.38	0.56
8:H:225:MET:O	8:H:229:THR:HG23	2.05	0.55
15:O:26:THR:HG22	15:O:169:VAL:HG12	1.89	0.55
20:U:17:TYR:OH	36:k:27:TRP:NE1	2.37	0.55
22:W:98:VAL:HG12	22:W:98:VAL:O	2.05	0.55
24:Y:115:VAL:O	24:Y:119:THR:OG1	2.10	0.55
37:l:140:GLU:OE2	40:o:42:GLN:NE2	2.37	0.55
12:L:324:LEU:HB3	12:L:395:ILE:HD11	1.87	0.55
38:m:114:LEU:HD22	38:m:119:LYS:HE3	1.88	0.55
3:C:158:GLU:N	3:C:158:GLU:OE1	2.39	0.55
14:N:187:MET:HG2	14:N:190:MET:HE3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:VAL:HA	3:C:32:ILE:HG22	1.88	0.55
4:D:55:HIS:NE2	8:H:205:SER:O	2.36	0.55
6:F:104:THR:OG1	6:F:331:THR:OG1	2.22	0.55
6:F:68:ARG:O	6:F:224:ASN:ND2	2.39	0.55
7:G:326:GLU:OE2	7:G:620:ARG:NE	2.32	0.55
11:K:37:VAL:HG21	11:K:67:ALA:CB	2.36	0.55
13:M:263:LEU:HD21	38:m:97:LEU:O	2.06	0.55
7:G:303:VAL:CG1	7:G:603:LEU:HD11	2.36	0.55
8:H:102:ILE:HD11	8:H:154:LEU:HD22	1.88	0.55
12:L:4:PHE:CZ	12:L:87:ILE:HD11	2.41	0.55
4:D:267:TRP:CZ3	4:D:272:THR:HG21	2.41	0.55
12:L:247:LEU:HD22	12:L:248:HIS:CD2	2.42	0.55
9:I:50:ILE:HG22	42:q:58:ARG:CG	2.37	0.55
17:Q:93:ILE:HD11	17:Q:105:VAL:HG21	1.87	0.55
3:C:50:ILE:HD12	3:C:105:ILE:HD11	1.89	0.54
16:P:171:ILE:CG2	16:P:207:VAL:HG22	2.37	0.54
23:X:146:ARG:NH2	30:e:41:GLU:OE1	2.39	0.54
38:m:128:TYR:OH	41:p:145:LEU:O	2.13	0.54
6:F:398:GLN:OE1	7:G:129:ARG:NH2	2.40	0.54
48:F:502:FMN:O4'	48:F:502:FMN:O2'	2.26	0.54
6:F:138:ILE:HG21	6:F:146:ALA:HB2	1.88	0.54
15:O:26:THR:CG2	15:O:169:VAL:HG12	2.36	0.54
13:M:354:LEU:HD22	13:M:434:LEU:CD1	2.37	0.54
16:P:22:THR:HG22	16:P:46:ILE:HB	1.89	0.54
16:P:56:ILE:HD12	16:P:59:LEU:HD12	1.89	0.54
20:T:22:TYR:OH	20:T:46:ASP:OD1	2.24	0.54
20:T:52:MET:HE3	22:W:43:ARG:CZ	2.38	0.54
23:X:19:VAL:HG22	23:X:23:VAL:HG11	1.89	0.54
6:F:197:GLU:OE2	17:Q:129:ARG:NH1	2.41	0.54
6:F:193:ILE:HG23	6:F:215:VAL:HA	1.90	0.54
7:G:281:GLU:HB2	7:G:592:LEU:HD12	1.90	0.54
13:M:14:LEU:HD12	31:f:11:VAL:HG22	1.89	0.54
7:G:200:ILE:HD13	7:G:210:SER:HB3	1.90	0.54
8:H:317:TYR:CD1	10:J:134:MET:HE1	2.42	0.54
6:F:311:VAL:O	6:F:311:VAL:HG13	2.08	0.54
7:G:113:GLU:OE2	7:G:249:ARG:NH2	2.40	0.54
7:G:317:ALA:HB1	7:G:331:LEU:HD21	1.90	0.54
16:P:209:ASP:OD2	16:P:308:THR:N	2.41	0.54
13:M:424:ILE:O	39:n:105:TYR:OH	2.17	0.53
15:O:135:LEU:HD13	15:O:152:TYR:CG	2.43	0.53
16:P:191:VAL:HG13	16:P:191:VAL:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:27:GLU:OE1	38:m:30:ARG:NE	2.37	0.53
41:p:140:ASP:O	41:p:161:ARG:NH1	2.41	0.53
5:E:144:CYS:O	6:F:139:ARG:NH2	2.37	0.53
14:N:70:ILE:HD12	14:N:102:LEU:HD21	1.91	0.53
30:e:15:ARG:NH1	33:h:129:GLU:OE2	2.42	0.53
8:H:102:ILE:HD11	8:H:160:TYR:HD1	1.72	0.53
14:N:213:ALA:HB3	14:N:214:PRO:HD3	1.91	0.53
23:X:25:LYS:NZ	23:X:94:GLN:O	2.38	0.53
12:L:155:ILE:HD11	12:L:248:HIS:NE2	2.23	0.53
55:T:201:EHZ:N2	55:T:201:EHZ:O3	2.42	0.53
2:B:114:TYR:HA	2:B:117:MET:HE2	1.90	0.53
8:H:233:LEU:O	8:H:236:ALA:N	2.42	0.53
9:I:28:MET:SD	25:Z:34:MET:HE2	2.49	0.53
12:L:3:ILE:HD13	41:p:36:TYR:CG	2.44	0.53
14:N:126:MET:HE1	14:N:129:ILE:HD12	1.90	0.53
16:P:258:LEU:HD23	16:P:263:TYR:CD1	2.44	0.53
34:i:31:GLU:O	34:i:33:VAL:N	2.41	0.53
9:I:78:ARG:NH1	9:I:130:VAL:O	2.42	0.53
9:I:116:THR:HG21	9:I:146:HIS:HE2	1.73	0.53
15:O:30:ASN:N	15:O:33:SER:OG	2.39	0.53
9:I:97:GLU:O	9:I:109:THR:OG1	2.27	0.53
12:L:9:LEU:HD12	49:L:702:3PE:H2D2	1.91	0.53
4:D:342:MET:HE2	7:G:101:HIS:CD2	2.44	0.52
7:G:415:LEU:O	7:G:416:THR:OG1	2.20	0.52
10:J:151:MET:SD	14:N:28:LEU:HD21	2.49	0.52
23:X:165:ARG:NH2	29:d:87:ASP:OD1	2.37	0.52
3:C:57:VAL:HG22	3:C:109:THR:HG21	1.91	0.52
7:G:514:ILE:HG21	7:G:532:ILE:HD11	1.91	0.52
43:r:45:SER:O	43:r:51:ASN:ND2	2.43	0.52
14:N:284:MET:HE3	14:N:284:MET:HA	1.91	0.52
2:B:60:PHE:CE2	2:B:110:LEU:HD13	2.44	0.52
7:G:9:ILE:HG23	7:G:75:LYS:HG2	1.91	0.52
3:C:47:GLU:OE2	3:C:106:ARG:NH1	2.42	0.52
12:L:594:ASN:OD1	24:Y:38:TYR:OH	2.20	0.52
19:S:54:ILE:O	19:S:55:ARG:NH1	2.41	0.52
6:F:95:VAL:HG11	6:F:118:LEU:HD11	1.92	0.52
8:H:299:ALA:HB1	27:b:24:VAL:HG13	1.91	0.52
12:L:559:GLU:OE2	13:M:214:LEU:HD23	2.09	0.52
14:N:26:LEU:HD23	14:N:85:MET:HA	1.91	0.52
8:H:63:PRO:O	8:H:66:THR:HG22	2.09	0.52
32:g:117:GLN:N	32:g:117:GLN:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:82:HIS:NE2	41:p:41:ASP:OD1	2.42	0.52
5:E:48:LEU:HD21	5:E:87:TYR:CE2	2.45	0.52
7:G:541:CYS:SG	7:G:542:PHE:N	2.82	0.52
16:P:19:VAL:HG12	16:P:19:VAL:O	2.10	0.52
3:C:131:GLU:OE2	3:C:142:PHE:CD1	2.63	0.52
6:F:65:LEU:O	6:F:75:THR:HG22	2.10	0.52
13:M:168:GLN:CG	13:M:174:LEU:HD11	2.39	0.52
14:N:159:ILE:HD11	14:N:278:MET:HE3	1.92	0.52
12:L:286:LEU:HB2	12:L:411:ILE:HG23	1.92	0.52
12:L:286:LEU:HD22	12:L:411:ILE:HD12	1.92	0.51
32:g:73:THR:HG21	33:h:36:VAL:HG11	1.91	0.51
3:C:79:THR:HG22	4:D:390:LYS:HG2	1.92	0.51
12:L:226:GLN:NE2	12:L:314:MET:HE2	2.24	0.51
12:L:513:MET:HE3	12:L:514:ASN:O	2.10	0.51
25:Z:67:ARG:NH1	27:b:50:TYR:O	2.39	0.51
37:l:132:TYR:HB3	37:l:137:LEU:HD13	1.92	0.51
10:J:134:MET:HE2	10:J:134:MET:HA	1.93	0.51
12:L:64:THR:HG23	12:L:64:THR:O	2.11	0.51
12:L:548:THR:HG22	12:L:548:THR:O	2.09	0.51
13:M:45:THR:HG22	13:M:45:THR:O	2.10	0.51
13:M:225:ILE:HD13	13:M:331:ASN:HB2	1.91	0.51
16:P:59:LEU:HA	16:P:62:MET:HE3	1.93	0.51
12:L:338:MET:HE2	12:L:461:SER:CB	2.41	0.51
11:K:73:VAL:O	11:K:77:LEU:HD23	2.10	0.51
2:B:135:TYR:HB2	9:I:119:ILE:HG21	1.91	0.51
14:N:62:THR:HG21	14:N:114:TRP:CG	2.46	0.51
40:o:91:HIS:HD2	40:o:92:LEU:HD22	1.75	0.51
1:A:58:VAL:HA	1:A:61:THR:HG22	1.93	0.51
3:C:28:TYR:OH	3:C:67:HIS:NE2	2.25	0.51
5:E:150:ASN:ND2	5:E:162:GLU:OE1	2.36	0.51
6:F:78:LYS:NZ	48:F:502:FMN:O5'	2.44	0.51
12:L:337:ALA:CB	12:L:457:LEU:HD13	2.41	0.51
16:P:115:ARG:NH1	16:P:119:GLN:OE1	2.43	0.51
25:Z:119:LEU:HD12	25:Z:121:GLY:H	1.75	0.51
3:C:57:VAL:CG1	3:C:120:ILE:HD11	2.40	0.51
23:X:19:VAL:HG22	23:X:23:VAL:CG1	2.40	0.51
23:X:150:ASN:ND2	33:h:118:GLY:O	2.44	0.51
7:G:333:ASP:OD2	7:G:622:ARG:NE	2.43	0.50
10:J:168:GLU:OE2	14:N:5:THR:HG21	2.10	0.50
12:L:10:LEU:HD13	34:i:78:MET:SD	2.51	0.50
21:V:102:LEU:HD12	21:V:103:VAL:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:81:ASP:OD2	38:m:71:ARG:NH2	2.44	0.50
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.41	0.50
7:G:452:VAL:HG23	7:G:452:VAL:O	2.11	0.50
14:N:242:THR:HG22	14:N:243:MET:HE2	1.91	0.50
15:O:104:ARG:NE	15:O:131:ASP:OD1	2.44	0.50
20:U:22:TYR:O	20:U:23:ASP:OD1	2.29	0.50
42:q:118:SER:O	42:q:123:GLN:NE2	2.45	0.50
10:J:112:VAL:HG21	30:e:73:ARG:HA	1.94	0.50
15:O:110:ASP:OD1	15:O:266:LYS:NZ	2.34	0.50
40:o:82:GLU:N	40:o:82:GLU:OE1	2.44	0.50
4:D:71:GLU:OE1	8:H:134:ARG:NH2	2.44	0.50
5:E:12:THR:HG22	5:E:13:PRO:CD	2.42	0.50
1:A:65:PHE:CE2	1:A:98:LEU:HD11	2.47	0.50
2:B:173:LEU:O	2:B:177:ILE:HD12	2.11	0.50
7:G:483:VAL:HG23	7:G:484:ALA:H	1.76	0.50
10:J:123:TRP:HZ3	25:Z:119:LEU:HD11	1.77	0.50
12:L:461:SER:O	12:L:461:SER:OG	2.28	0.50
13:M:364:LEU:HD23	13:M:369:LEU:HD22	1.93	0.50
14:N:319:LYS:HG2	15:O:267:THR:HG21	1.93	0.50
15:O:123:VAL:HG13	15:O:123:VAL:O	2.12	0.50
2:B:47:ILE:HD11	2:B:183:LEU:HD23	1.92	0.50
7:G:258:ILE:HG22	7:G:368:ILE:CD1	2.37	0.50
7:G:668:ILE:HG23	7:G:691:VAL:HG11	1.93	0.50
8:H:20:LEU:O	8:H:20:LEU:HD23	2.11	0.50
3:C:120:ILE:HG22	3:C:120:ILE:O	2.09	0.50
10:J:168:GLU:CG	14:N:5:THR:HG21	2.41	0.50
14:N:159:ILE:HD11	14:N:278:MET:CE	2.42	0.50
14:N:207:ILE:O	14:N:211:LEU:HD23	2.12	0.50
37:l:90:THR:HG22	38:m:10:LEU:HD13	1.94	0.50
8:H:89:LEU:HD11	8:H:240:ILE:HD12	1.93	0.50
4:D:112:MET:HE2	4:D:181:TYR:CE1	2.46	0.50
14:N:233:LEU:HD11	14:N:240:MET:CE	2.42	0.50
16:P:171:ILE:HG22	16:P:207:VAL:HG22	1.93	0.50
12:L:124:PHE:CE1	12:L:247:LEU:HG	2.47	0.49
13:M:344:MET:CE	13:M:423:MET:HE1	2.41	0.49
13:M:458:THR:O	41:p:149:TYR:OH	2.30	0.49
14:N:108:LEU:HD13	14:N:191:LEU:HD22	1.92	0.49
19:S:57:CYS:SG	19:S:58:SER:N	2.81	0.49
4:D:259:MET:HE1	4:D:405:MET:CE	2.42	0.49
6:F:203:PRO:O	6:F:361:GLN:NE2	2.45	0.49
8:H:70:LEU:HA	8:H:73:ILE:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:35:TYR:OH	34:i:73:HIS:NE2	2.33	0.49
12:L:285:THR:HG22	12:L:415:ALA:HB1	1.94	0.49
12:L:294:THR:HG22	12:L:294:THR:O	2.11	0.49
19:S:50:LEU:O	19:S:52:ILE:HD12	2.13	0.49
2:B:64:CYS:SG	4:D:190:HIS:NE2	2.78	0.49
1:A:94:LEU:HD22	10:J:152:MET:HE1	1.94	0.49
12:L:337:ALA:HB3	12:L:457:LEU:HD13	1.95	0.49
13:M:71:TRP:HZ3	32:g:67:VAL:HG11	1.78	0.49
6:F:113:HIS:HE2	44:s:32:TYR:HH	0.59	0.49
12:L:486:LEU:O	12:L:489:THR:HG22	2.12	0.49
13:M:109:THR:HG21	13:M:238:LEU:HD11	1.94	0.49
16:P:134:HIS:ND1	53:P:501:NDP:H5N	2.28	0.49
27:b:20:VAL:O	27:b:24:VAL:HG12	2.13	0.49
7:G:338:VAL:HG12	7:G:338:VAL:O	2.13	0.49
12:L:226:GLN:O	12:L:230:HIS:N	2.46	0.49
25:Z:116:VAL:HG23	25:Z:116:VAL:O	2.12	0.49
51:d:201:CDL:O1	51:d:201:CDL:OB9	2.31	0.49
51:i:201:CDL:OB4	41:p:48:ARG:NH1	2.46	0.49
39:n:18:LEU:HD13	39:n:67:GLU:CD	2.38	0.49
4:D:410:MET:HE1	8:H:283:ASP:CG	2.37	0.49
6:F:30:ASP:O	6:F:39:ARG:NH2	2.46	0.49
12:L:214:MET:HE2	12:L:214:MET:HA	1.95	0.49
35:j:59:TRP:HB3	35:j:64:LEU:HD11	1.95	0.49
40:o:88:TYR:O	40:o:92:LEU:HD23	2.13	0.49
3:C:117:ILE:HD12	3:C:117:ILE:N	2.28	0.49
8:H:55:LEU:HA	8:H:217:ALA:HB1	1.95	0.49
14:N:24:THR:HG22	30:e:18:MET:HE2	1.95	0.49
14:N:193:ILE:HD11	14:N:269:GLU:HB3	1.95	0.49
16:P:108:ASP:OD1	16:P:112:ASN:ND2	2.46	0.49
2:B:101:THR:HG21	4:D:85:2MR:HG2	1.93	0.49
2:B:164:GLU:OE2	9:I:57:GLY:N	2.44	0.49
3:C:133:GLU:OE2	4:D:430:ARG:NH2	2.46	0.49
9:I:50:ILE:HG22	42:q:58:ARG:HG3	1.95	0.48
16:P:22:THR:HG23	16:P:88:SER:HB3	1.94	0.48
20:U:66:ASP:O	20:U:70:LEU:HD23	2.13	0.48
35:j:50:HIS:O	35:j:50:HIS:ND1	2.46	0.48
14:N:313:MET:HE3	15:O:99:TRP:CH2	2.48	0.48
17:Q:9:GLN:C	17:Q:10:LEU:HD22	2.38	0.48
19:S:77:SER:O	19:S:79:ASN:N	2.46	0.48
5:E:145:LEU:HD12	5:E:153:MET:HE2	1.94	0.48
12:L:340:PHE:O	12:L:344:GLY:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:534:HIS:ND1	49:L:701:3PE:O12	2.42	0.48
12:L:575:THR:O	12:L:579:ASN:ND2	2.45	0.48
13:M:62:SER:OG	13:M:245:ARG:NH2	2.47	0.48
13:M:174:LEU:HA	13:M:179:LEU:HD11	1.96	0.48
23:X:48:GLU:OE2	23:X:134:ARG:NH1	2.36	0.48
3:C:169:THR:HG21	3:C:190:LEU:HD11	1.94	0.48
6:F:215:VAL:HG12	6:F:216:PHE:CD2	2.48	0.48
8:H:102:ILE:HD11	8:H:160:TYR:CD1	2.48	0.48
12:L:484:TRP:O	12:L:488:THR:OG1	2.29	0.48
13:M:395:LEU:HD21	38:m:100:TRP:CE2	2.48	0.48
21:V:77:GLU:O	21:V:81:LEU:HD23	2.13	0.48
34:i:82:HIS:ND1	41:p:36:TYR:OH	2.46	0.48
7:G:60:GLU:OE1	7:G:80:LEU:HD11	2.14	0.48
7:G:476:LYS:O	7:G:480:THR:HG23	2.14	0.48
8:H:123:SER:O	8:H:125:SER:N	2.46	0.48
10:J:154:VAL:HG11	14:N:31:VAL:HG11	1.95	0.48
16:P:26:ALA:HB3	16:P:47:ILE:HG23	1.94	0.48
19:S:35:PHE:HE1	19:S:87:THR:HG22	1.79	0.48
33:h:127:THR:HG22	33:h:128:PRO:HD2	1.95	0.48
6:F:92:TYR:HB2	6:F:220:THR:HG22	1.95	0.48
7:G:494:HIS:HB2	7:G:576:THR:HG22	1.95	0.48
12:L:451:MET:HE1	35:j:21:GLN:HB2	1.94	0.48
11:K:40:LEU:HD13	14:N:71:LEU:HD23	1.96	0.48
12:L:119:LYS:O	12:L:122:THR:OG1	2.30	0.48
13:M:189:SER:OG	13:M:190:TRP:N	2.47	0.48
35:j:52:SER:OG	35:j:53:TYR:N	2.47	0.48
4:D:423:ILE:HG23	4:D:428:ILE:HD11	1.95	0.48
7:G:331:LEU:HD22	7:G:525:LEU:CD2	2.36	0.48
5:E:104:THR:OG1	6:F:349:ARG:NH2	2.43	0.48
7:G:266:LYS:NZ	7:G:674:THR:OG1	2.34	0.48
11:K:4:THR:HG23	11:K:5:PHE:HD2	1.79	0.48
12:L:542:LEU:HD23	37:l:82:MET:CB	2.43	0.48
1:A:13:LEU:HD13	8:H:10:LEU:HD21	1.96	0.48
12:L:140:LEU:HD21	12:L:259:LEU:CD1	2.44	0.48
12:L:542:LEU:HD21	37:l:87:ARG:HH11	1.79	0.48
21:V:22:ARG:O	21:V:26:LEU:HD23	2.14	0.48
39:n:18:LEU:HD13	39:n:67:GLU:OE1	2.14	0.48
3:C:99:LEU:HD22	4:D:251:LEU:CD2	2.44	0.47
5:E:143:GLU:OE1	6:F:349:ARG:NH1	2.41	0.47
14:N:27:MET:HE2	14:N:74:ILE:HG21	1.96	0.47
4:D:149:ASN:HD22	4:D:149:ASN:C	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:259:MET:HE1	4:D:405:MET:HE2	1.96	0.47
6:F:96:ASN:ND2	6:F:187:GLY:O	2.37	0.47
6:F:253:THR:OG1	6:F:269:GLU:OE2	2.24	0.47
37:l:98:ASP:OD1	37:l:99:VAL:HG23	2.14	0.47
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.97	0.47
3:C:57:VAL:HG11	3:C:120:ILE:HD11	1.96	0.47
4:D:141:PHE:CZ	4:D:184:VAL:HG11	2.50	0.47
5:E:149:VAL:HG13	6:F:105:CYS:SG	2.54	0.47
1:A:13:LEU:CD1	8:H:10:LEU:HD21	2.44	0.47
6:F:215:VAL:HB	6:F:220:THR:HG21	1.96	0.47
13:M:341:THR:HG22	13:M:343:ILE:H	1.79	0.47
15:O:169:VAL:HG11	15:O:214:MET:HE3	1.96	0.47
4:D:247:ALA:HB1	21:V:10:LEU:HD23	1.97	0.47
7:G:231:MET:HE1	7:G:677:ILE:CG2	2.43	0.47
10:J:101:PHE:O	10:J:105:VAL:HG23	2.14	0.47
14:N:325:MET:HA	14:N:328:THR:HG22	1.97	0.47
16:P:334:THR:O	16:P:334:THR:HG22	2.14	0.47
7:G:483:VAL:HG23	7:G:484:ALA:N	2.29	0.47
11:K:82:SER:O	11:K:86:GLY:N	2.42	0.47
13:M:25:THR:O	13:M:29:SER:OG	2.25	0.47
23:X:24:LEU:HD21	25:Z:73:LEU:HD23	1.95	0.47
27:b:73:LEU:HD23	27:b:73:LEU:H	1.80	0.47
35:j:55:ASP:OD2	35:j:57:SER:OG	2.31	0.47
38:m:13:LEU:HD23	38:m:14:PRO:O	2.14	0.47
7:G:307:LEU:HD21	7:G:334:LEU:HD21	1.97	0.47
12:L:156:GLY:O	13:M:416:ARG:NH1	2.48	0.47
13:M:207:MET:HE1	13:M:240:SER:CB	2.45	0.47
32:g:116:ILE:HG23	41:p:159:LYS:HE2	1.97	0.47
37:l:127:VAL:HG12	37:l:128:GLY:O	2.15	0.47
1:A:115:GLU:O	4:D:74:ARG:NH2	2.47	0.47
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.22	0.47
7:G:367:THR:HG22	7:G:636:ILE:HD13	1.96	0.47
16:P:72:GLU:OE2	16:P:72:GLU:N	2.48	0.47
5:E:100:ILE:HG12	5:E:156:ILE:HD12	1.97	0.46
13:M:150:LEU:HD11	13:M:154:LEU:HD11	1.97	0.46
16:P:237:LEU:HD13	16:P:340:VAL:HG21	1.98	0.46
37:l:76:ILE:HD13	38:m:64:LEU:HD12	1.97	0.46
10:J:2:ASN:OD1	10:J:3:ASN:N	2.48	0.46
14:N:108:LEU:HD21	14:N:187:MET:HB3	1.98	0.46
14:N:300:THR:HG23	14:N:301:SER:N	2.29	0.46
23:X:43:MET:HE2	25:Z:72:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:118:LEU:HD21	41:p:162:MET:HB2	1.97	0.46
3:C:111:ALA:HB2	3:C:117:ILE:HD11	1.94	0.46
8:H:154:LEU:C	8:H:154:LEU:HD12	2.41	0.46
10:J:133:VAL:HG22	10:J:134:MET:H	1.80	0.46
12:L:304:PHE:HZ	12:L:526:LEU:HD11	1.81	0.46
12:L:319:MET:SD	12:L:319:MET:N	2.89	0.46
16:P:203:GLN:NE2	16:P:232:GLY:O	2.41	0.46
24:Y:104:THR:HG23	24:Y:104:THR:O	2.14	0.46
7:G:613:TYR:CD2	7:G:619:VAL:HG22	2.50	0.46
12:L:188:TRP:CD2	12:L:212:PRO:HG3	2.50	0.46
6:F:82:MET:CE	6:F:221:THR:HG23	2.45	0.46
7:G:395:ILE:O	7:G:399:TRP:N	2.48	0.46
7:G:604:SER:CB	7:G:611:LEU:HD13	2.45	0.46
9:I:45:ARG:NH2	43:r:19:LEU:HD22	2.30	0.46
23:X:20:SER:OG	23:X:21:SER:N	2.46	0.46
32:g:69:VAL:O	32:g:73:THR:HG23	2.16	0.46
7:G:243:ARG:O	7:G:244:THR:OG1	2.27	0.46
7:G:635:ASP:OD1	7:G:636:ILE:N	2.48	0.46
8:H:85:LEU:HG	8:H:233:LEU:HD21	1.98	0.46
11:K:59:ILE:HG21	14:N:84:TRP:CH2	2.51	0.46
16:P:129:PHE:HB3	16:P:160:PHE:CE2	2.50	0.46
1:A:68:GLU:HG2	1:A:98:LEU:HD22	1.98	0.46
6:F:357:GLU:O	6:F:407:LEU:HD11	2.16	0.46
8:H:2:PHE:CZ	8:H:95:LEU:HD21	2.51	0.46
12:L:345:SER:O	12:L:349:SER:OG	2.20	0.46
13:M:1:FME:HE1	13:M:58:SER:OG	2.15	0.46
13:M:65:LEU:HD13	13:M:110:PHE:CE1	2.51	0.46
16:P:249:THR:O	16:P:251:ARG:N	2.49	0.46
40:o:88:TYR:CZ	40:o:92:LEU:HD21	2.50	0.46
2:B:141:SER:OG	4:D:84:HIS:O	2.33	0.46
4:D:61:VAL:HG23	4:D:61:VAL:O	2.16	0.46
7:G:285:ARG:NH2	7:G:555:PRO:O	2.49	0.46
7:G:629:ASN:OD1	7:G:630:LEU:N	2.49	0.46
8:H:136:VAL:HG12	8:H:140:ILE:HD12	1.97	0.46
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.97	0.46
15:O:105:LEU:HD11	15:O:159:THR:HB	1.97	0.46
4:D:341:SER:OG	4:D:344:SER:OG	2.09	0.46
7:G:543:ILE:HD13	7:G:556:MET:CE	2.46	0.46
14:N:324:LEU:HD11	29:d:64:PHE:CZ	2.44	0.46
15:O:145:ARG:HD3	32:g:22:MET:HE3	1.97	0.46
7:G:423:GLY:HA3	7:G:428:ILE:HD11	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:88:PRO:HB3	8:H:98:LEU:HD12	1.98	0.45
9:I:114:ASP:OD1	9:I:116:THR:OG1	2.29	0.45
14:N:135:LYS:CG	14:N:187:MET:HE1	2.45	0.45
20:T:49:GLU:OE2	22:W:38:TYR:OH	2.31	0.45
1:A:82:ILE:HD12	1:A:82:ILE:H	1.81	0.45
2:B:135:TYR:CD2	9:I:119:ILE:HD13	2.51	0.45
4:D:381:ASP:O	4:D:383:SER:N	2.46	0.45
6:F:45:THR:HG22	6:F:49:LEU:HD13	1.98	0.45
13:M:24:TRP:CH2	13:M:96:ILE:HD11	2.50	0.45
13:M:442:ILE:HG21	32:g:68:LEU:HD13	1.98	0.45
4:D:345:LEU:HD22	7:G:103:LEU:HD12	1.99	0.45
8:H:102:ILE:HD11	8:H:154:LEU:CD2	2.47	0.45
13:M:231:LEU:HD23	13:M:235:LEU:HD12	1.98	0.45
15:O:24:VAL:HG22	15:O:122:VAL:HG22	1.97	0.45
35:j:61:ASP:OD1	40:o:106:ARG:NH2	2.49	0.45
37:l:76:ILE:CD1	38:m:64:LEU:HD12	2.46	0.45
4:D:109:VAL:HG11	4:D:152:MET:SD	2.56	0.45
4:D:202:ASP:OD1	4:D:203:LEU:N	2.46	0.45
7:G:443:LEU:HD12	7:G:443:LEU:O	2.15	0.45
29:d:26:LEU:O	29:d:26:LEU:HD23	2.17	0.45
1:A:65:PHE:CZ	1:A:98:LEU:HD11	2.52	0.45
7:G:447:LYS:O	7:G:483:VAL:HG12	2.15	0.45
9:I:147:GLU:OE1	17:Q:69:LEU:HD11	2.16	0.45
13:M:7:PRO:HB2	13:M:34:ILE:HD12	1.98	0.45
13:M:106:LEU:HD13	13:M:234:ILE:CG2	2.41	0.45
13:M:336:ARG:NH2	13:M:433:GLU:OE1	2.49	0.45
17:Q:128:THR:O	17:Q:128:THR:HG22	2.15	0.45
2:B:91:ARG:HD2	8:H:61:MET:HE2	1.99	0.45
8:H:172:MET:HE1	25:Z:49:MET:HG2	1.99	0.45
12:L:188:TRP:CD1	12:L:211:ILE:HD11	2.52	0.45
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.98	0.45
12:L:584:ILE:HD11	12:L:588:PHE:CE1	2.51	0.45
13:M:303:ILE:HG22	13:M:305:THR:HG23	1.97	0.45
6:F:376:MET:HE1	6:F:418:LEU:HD23	1.98	0.45
12:L:83:ASP:OD2	12:L:262:ARG:NH2	2.49	0.45
33:h:114:MET:HE3	33:h:120:GLY:HA3	1.98	0.45
7:G:199:VAL:HG12	7:G:208:LEU:HD11	1.99	0.45
7:G:145:LEU:HD22	7:G:269:PHE:CD2	2.52	0.45
7:G:379:LEU:HD23	7:G:452:VAL:HG22	1.96	0.45
12:L:546:LEU:O	12:L:551:THR:HG22	2.17	0.45
17:Q:93:ILE:HD12	17:Q:103:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:44:LEU:HD22	23:X:130:VAL:CG1	2.45	0.45
39:n:153:LEU:HD11	39:n:165:LEU:HD22	1.98	0.45
42:q:138:VAL:HG23	42:q:138:VAL:O	2.17	0.45
3:C:52:ILE:HG22	3:C:53:HIS:O	2.17	0.45
4:D:62:LEU:HD21	4:D:64:LEU:HD11	1.99	0.45
6:F:262:VAL:HG11	6:F:284:ALA:HB1	1.99	0.45
7:G:47:SER:O	7:G:161:ARG:NH1	2.41	0.45
14:N:156:MET:HA	14:N:159:ILE:HD12	1.99	0.45
4:D:222:ILE:CD1	4:D:304:MET:HE2	2.48	0.44
4:D:371:LYS:NZ	4:D:422:ASP:O	2.45	0.44
9:I:71:ARG:NH2	18:R:38:ASN:O	2.50	0.44
16:P:135:LEU:HD22	16:P:231:THR:HG22	1.99	0.44
25:Z:79:ASP:O	25:Z:83:LEU:HD23	2.17	0.44
4:D:182:GLU:OE2	9:I:60:SER:N	2.50	0.44
7:G:37:ILE:HD13	7:G:57:VAL:HG11	2.00	0.44
9:I:148:GLU:OE2	42:q:123:GLN:NE2	2.50	0.44
17:Q:89:LYS:NZ	17:Q:107:GLU:OE1	2.51	0.44
31:f:30:ASP:OD1	33:h:89:LYS:NZ	2.41	0.44
37:l:71:ASN:OD1	37:l:72:TRP:N	2.47	0.44
38:m:124:PHE:O	38:m:126:ILE:N	2.50	0.44
1:A:3:LEU:HD13	8:H:96:ILE:CD1	2.47	0.44
12:L:194:ASN:CG	12:L:194:ASN:O	2.60	0.44
4:D:66:LEU:H	4:D:66:LEU:HD23	1.83	0.44
8:H:236:ALA:HB1	8:H:259:PHE:HZ	1.82	0.44
12:L:230:HIS:N	12:L:231:PRO:CD	2.81	0.44
13:M:344:MET:HE2	13:M:423:MET:HE1	1.98	0.44
13:M:395:LEU:HD21	38:m:100:TRP:CZ2	2.52	0.44
17:Q:33:ARG:NH1	17:Q:60:ASP:O	2.51	0.44
33:h:30:MET:HG2	33:h:34:ILE:HD12	1.99	0.44
7:G:156:CYS:O	7:G:157:THR:OG1	2.36	0.44
12:L:86:SER:OG	12:L:132:THR:O	2.20	0.44
15:O:144:ILE:HG22	15:O:145:ARG:O	2.16	0.44
33:h:9:PHE:CE2	39:n:103:LEU:HD21	2.52	0.44
2:B:162:THR:HG23	4:D:188:ARG:HD2	2.00	0.44
7:G:43:HIS:O	7:G:44:GLU:HG2	2.18	0.44
7:G:364:LEU:HD12	7:G:576:THR:OG1	2.18	0.44
46:J:201:PC1:H153	16:P:251:ARG:HH12	1.83	0.44
12:L:355:ASP:OD2	12:L:357:ARG:NH2	2.50	0.44
12:L:519:TYR:O	12:L:520:SER:OG	2.30	0.44
23:X:126:LYS:O	23:X:128:THR:HG23	2.16	0.44
15:O:52:PRO:O	15:O:107:GLN:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:106:LEU:HD13	4:D:391:ILE:HG21	2.00	0.44
12:L:295:GLN:NE2	12:L:524:THR:O	2.51	0.44
12:L:252:MET:O	12:L:255:ALA:N	2.40	0.44
13:M:168:GLN:HG3	13:M:174:LEU:HD11	2.00	0.44
30:e:19:PHE:HB2	30:e:36:GLU:OE2	2.17	0.44
2:B:55:LEU:HD21	2:B:173:LEU:HD23	1.99	0.43
2:B:69:MET:HE3	2:B:86:PHE:CE2	2.53	0.43
5:E:87:TYR:CG	6:F:181:ALA:HB3	2.53	0.43
7:G:226:GLU:OE1	17:Q:36:ARG:NE	2.51	0.43
9:I:137:PRO:HB3	42:q:93:MET:HE1	2.00	0.43
14:N:329:LEU:HD11	51:N:401:CDL:H552	2.00	0.43
25:Z:113:THR:O	25:Z:113:THR:HG22	2.17	0.43
35:j:45:ASP:OD1	35:j:46:ALA:N	2.51	0.43
3:C:37:VAL:HA	3:C:52:ILE:HD13	1.99	0.43
8:H:179:TRP:N	8:H:180:PRO:CD	2.81	0.43
11:K:66:PHE:CZ	14:N:31:VAL:HG13	2.53	0.43
12:L:54:PHE:HB2	12:L:87:ILE:HD13	1.99	0.43
15:O:223:TYR:OH	15:O:237:ASP:OD2	2.31	0.43
18:R:12:THR:HA	18:R:35:VAL:HG21	2.01	0.43
1:A:68:GLU:HG2	1:A:98:LEU:HD13	1.99	0.43
8:H:296:LEU:HD21	49:H:401:3PE:H361	1.99	0.43
13:M:328:CYS:HB3	13:M:437:MET:HE1	2.00	0.43
16:P:48:PRO:HB3	16:P:73:TRP:CD1	2.54	0.43
39:n:151:GLU:OE1	39:n:151:GLU:N	2.51	0.43
6:F:297:VAL:HG22	6:F:336:VAL:HG12	2.00	0.43
24:Y:80:ARG:O	24:Y:82:LYS:N	2.51	0.43
14:N:187:MET:CG	14:N:190:MET:HE3	2.48	0.43
37:l:66:SER:O	37:l:67:GLU:HG2	2.18	0.43
40:o:21:ILE:O	40:o:23:SER:N	2.51	0.43
1:A:59:ALA:HB1	10:J:65:VAL:HG13	2.00	0.43
1:A:63:LEU:HD21	10:J:62:GLY:HA2	2.00	0.43
3:C:97:LEU:HG	3:C:99:LEU:HD12	2.01	0.43
12:L:567:SER:O	12:L:571:THR:HG22	2.19	0.43
12:L:597:LEU:HD21	24:Y:34:ILE:HD12	2.00	0.43
14:N:125:HIS:O	14:N:126:MET:HB2	2.18	0.43
14:N:135:LYS:CB	14:N:187:MET:HE1	2.49	0.43
16:P:22:THR:OG1	16:P:91:VAL:HG13	2.19	0.43
19:S:64:LEU:HB3	19:S:76:VAL:HG22	1.99	0.43
2:B:101:THR:HG21	4:D:85:2MR:CG	2.49	0.43
9:I:40:LEU:HD21	43:r:10:LEU:HD21	2.00	0.43
37:l:132:TYR:CB	37:l:137:LEU:HD13	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:LEU:HD13	4:D:93:TYR:CE1	2.54	0.43
4:D:234:ILE:HD12	4:D:234:ILE:H	1.83	0.43
16:P:244:TYR:CE1	16:P:334:THR:HG21	2.54	0.43
19:S:23:CYS:SG	19:S:60:VAL:N	2.88	0.43
21:V:22:ARG:HE	21:V:26:LEU:HD21	1.83	0.43
1:A:98:LEU:HD23	8:H:298:LEU:HD21	1.99	0.43
7:G:678:SER:O	7:G:681:SER:OG	2.36	0.43
9:I:134:VAL:HG21	9:I:167:ILE:HG21	2.00	0.43
10:J:147:CYS:O	30:e:16:HIS:NE2	2.51	0.43
12:L:260:LEU:HD23	12:L:277:MET:SD	2.59	0.43
13:M:83:HIS:O	13:M:84:LEU:HG	2.19	0.43
13:M:84:LEU:HD12	13:M:84:LEU:O	2.19	0.43
19:S:43:LEU:HD13	19:S:90:MET:HE3	2.00	0.43
2:B:91:ARG:NH1	8:H:61:MET:HE1	2.33	0.43
6:F:307:ILE:CD1	6:F:327:THR:HG21	2.49	0.43
17:Q:93:ILE:HD11	17:Q:105:VAL:CG2	2.49	0.43
20:U:30:LEU:O	20:U:31:SER:OG	2.34	0.43
21:V:93:MET:HE2	21:V:96:TRP:HE3	1.84	0.43
1:A:57:LEU:HD23	1:A:57:LEU:O	2.19	0.42
4:D:183:ARG:NH1	4:D:210:ASP:OD2	2.51	0.42
7:G:317:ALA:CB	7:G:331:LEU:HD21	2.48	0.42
14:N:83:THR:HG22	30:e:19:PHE:HB3	2.02	0.42
16:P:160:PHE:HD2	16:P:163:ALA:HB2	1.83	0.42
3:C:45:LEU:HD12	3:C:45:LEU:O	2.19	0.42
4:D:128:ILE:HD13	4:D:330:VAL:HG21	2.01	0.42
9:I:99:GLU:OE1	9:I:109:THR:OG1	2.31	0.42
13:M:367:LEU:HD12	13:M:367:LEU:O	2.19	0.42
16:P:215:VAL:O	16:P:218:THR:HG22	2.19	0.42
22:W:86:ILE:HG22	22:W:90:MET:HE3	2.01	0.42
28:c:33:GLN:O	28:c:37:GLU:N	2.48	0.42
1:A:38:GLU:O	1:A:38:GLU:HG3	2.19	0.42
4:D:300:ARG:NH2	4:D:420:THR:O	2.47	0.42
48:F:502:FMN:HO3'	48:F:502:FMN:C10	2.27	0.42
7:G:27:LEU:HD13	7:G:69:CYS:CA	2.49	0.42
12:L:233:LEU:HB3	12:L:234:PRO:HD3	2.01	0.42
14:N:136:ILE:HG12	14:N:205:LEU:HD21	2.00	0.42
16:P:63:GLY:HA3	16:P:68:LEU:HD11	2.01	0.42
31:f:39:LYS:O	31:f:41:MET:HE2	2.19	0.42
7:G:43:HIS:O	7:G:43:HIS:CG	2.73	0.42
12:L:532:ILE:O	12:L:536:ILE:HG22	2.19	0.42
13:M:207:MET:HE1	13:M:240:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:215:MET:HE1	14:N:247:MET:CB	2.49	0.42
1:A:38:GLU:OE2	4:D:50:ASN:N	2.50	0.42
13:M:433:GLU:O	13:M:437:MET:HE2	2.20	0.42
33:h:11:VAL:HG13	39:n:103:LEU:CD1	2.49	0.42
3:C:183:VAL:HB	22:W:103:THR:HG21	2.02	0.42
7:G:273:GLY:O	7:G:549:HIS:NE2	2.46	0.42
11:K:77:LEU:HD21	14:N:41:ILE:CG2	2.44	0.42
12:L:3:ILE:HD13	41:p:36:TYR:CD2	2.54	0.42
12:L:193:MET:SD	12:L:204:SER:OG	2.78	0.42
12:L:386:LEU:O	12:L:387:THR:HG22	2.19	0.42
2:B:180:GLU:O	16:P:52:ASP:OD1	2.38	0.42
4:D:149:ASN:O	4:D:149:ASN:ND2	2.49	0.42
7:G:511:VAL:O	7:G:511:VAL:HG22	2.19	0.42
14:N:126:MET:HE1	14:N:129:ILE:CD1	2.50	0.42
2:B:143:VAL:O	2:B:145:GLY:N	2.53	0.42
5:E:34:ILE:HD11	44:s:46:LEU:HD22	2.01	0.42
6:F:194:GLU:OE2	6:F:204:ARG:NH2	2.52	0.42
7:G:223:ARG:NH2	17:Q:81:ASN:OD1	2.51	0.42
7:G:662:VAL:CG2	7:G:666:LEU:HD11	2.49	0.42
8:H:185:TRP:O	8:H:189:THR:HG22	2.20	0.42
9:I:140:GLU:HG3	9:I:140:GLU:O	2.20	0.42
15:O:25:ILE:CD1	15:O:48:MET:HE1	2.48	0.42
16:P:324:TYR:O	16:P:325:ARG:HB3	2.19	0.42
4:D:330:VAL:HG23	4:D:331:SER:N	2.34	0.42
7:G:40:PHE:HB2	7:G:52:CYS:SG	2.59	0.42
7:G:334:LEU:HD11	7:G:603:LEU:HD22	2.02	0.42
13:M:361:MET:HB3	13:M:441:MET:HE2	2.02	0.42
19:S:84:ASP:OD1	19:S:85:GLU:N	2.53	0.42
1:A:80:GLN:OE1	25:Z:57:ARG:NH1	2.53	0.42
2:B:88:ALA:O	4:D:54:GLN:NE2	2.47	0.42
5:E:150:ASN:OD1	5:E:190:ARG:NH1	2.53	0.42
14:N:126:MET:HE2	14:N:129:ILE:HD12	2.02	0.42
4:D:83:LEU:O	4:D:83:LEU:HG	2.20	0.41
7:G:322:LEU:CD2	7:G:677:ILE:HD12	2.49	0.41
10:J:63:MET:HE2	10:J:63:MET:N	2.35	0.41
12:L:128:MET:HE1	12:L:252:MET:HA	2.02	0.41
13:M:207:MET:HG2	13:M:298:ILE:HD11	2.02	0.41
38:m:13:LEU:HD21	38:m:18:ASP:HA	2.02	0.41
4:D:149:ASN:C	4:D:149:ASN:ND2	2.78	0.41
8:H:235:ASN:OD1	8:H:267:SER:HA	2.20	0.41
10:J:154:VAL:CG1	14:N:31:VAL:HG11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:570:HIS:HD2	14:N:288:LEU:HD22	1.84	0.41
13:M:127:ILE:HD12	14:N:256:PRO:CG	2.50	0.41
13:M:168:GLN:HE21	13:M:174:LEU:HD11	1.85	0.41
13:M:195:LEU:HD23	13:M:195:LEU:O	2.19	0.41
14:N:271:MET:HE1	14:N:276:LEU:HD23	2.02	0.41
21:V:33:ILE:HD11	21:V:91:ARG:CZ	2.50	0.41
39:n:44:ARG:O	39:n:48:GLU:N	2.48	0.41
40:o:27:ASP:OD1	40:o:27:ASP:C	2.63	0.41
40:o:45:MET:SD	40:o:55:ARG:HB2	2.60	0.41
42:q:33:ILE:HG22	42:q:33:ILE:O	2.20	0.41
4:D:342:MET:HE3	4:D:346:ILE:HD11	2.02	0.41
12:L:232:TRP:O	12:L:236:ALA:N	2.52	0.41
14:N:193:ILE:HD12	14:N:266:ILE:HG23	2.02	0.41
20:T:44:SER:O	20:T:48:VAL:HG23	2.20	0.41
25:Z:53:ASN:OD1	25:Z:56:ARG:NH1	2.54	0.41
35:j:21:GLN:O	35:j:25:GLY:N	2.53	0.41
38:m:126:ILE:HD13	41:p:102:MET:HE2	2.02	0.41
42:q:6:VAL:HG11	43:r:4:THR:HG22	2.03	0.41
8:H:213:VAL:HG23	8:H:214:GLU:HG2	2.01	0.41
9:I:108:THR:OG1	9:I:153:LYS:NZ	2.49	0.41
12:L:72:ASN:O	12:L:73:SER:OG	2.20	0.41
12:L:568:THR:HA	12:L:571:THR:HG22	2.02	0.41
13:M:123:GLU:HB2	14:N:255:PRO:HG2	2.03	0.41
21:V:33:ILE:HD11	21:V:91:ARG:NH1	2.35	0.41
34:i:87:TYR:O	34:i:88:HIS:ND1	2.53	0.41
38:m:7:PRO:CG	38:m:13:LEU:HD12	2.51	0.41
8:H:24:GLU:OE1	8:H:271:LEU:HD22	2.20	0.41
8:H:31:MET:HE3	9:I:43:LEU:HD12	2.01	0.41
10:J:4:TYR:CD2	10:J:5:ILE:HD13	2.55	0.41
12:L:49:LEU:HB3	12:L:50:PRO:HD3	2.02	0.41
13:M:354:LEU:HD11	33:h:22:LEU:HD11	2.02	0.41
13:M:399:ASN:OD1	13:M:403:THR:OG1	2.38	0.41
14:N:146:TYR:N	14:N:147:PRO:CD	2.83	0.41
39:n:127:LEU:HD21	39:n:162:LEU:CD2	2.51	0.41
42:q:48:TYR:CE1	42:q:62:VAL:HG22	2.56	0.41
5:E:105:THR:HG22	5:E:106:THR:N	2.33	0.41
6:F:15:LEU:HD23	6:F:15:LEU:H	1.85	0.41
12:L:97:THR:HG21	12:L:125:LEU:CD1	2.49	0.41
13:M:61:LEU:CD1	13:M:244:ILE:HG21	2.51	0.41
13:M:168:GLN:NE2	13:M:174:LEU:HD11	2.35	0.41
3:C:131:GLU:OE2	3:C:142:PHE:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:111:MET:SD	6:F:138:ILE:HD12	2.61	0.41
7:G:382:THR:OG1	7:G:454:GLY:N	2.53	0.41
8:H:6:ILE:HD13	8:H:95:LEU:HD11	2.03	0.41
13:M:150:LEU:HD12	13:M:150:LEU:O	2.21	0.41
13:M:158:ILE:CG1	14:N:287:LEU:HD11	2.50	0.41
19:S:32:VAL:HG22	19:S:78:LEU:CD1	2.50	0.41
20:U:19:LEU:HD22	20:U:50:ILE:HD12	2.02	0.41
42:q:125:VAL:HG13	42:q:125:VAL:O	2.21	0.41
2:B:101:THR:HA	2:B:129:CYS:HB3	2.03	0.41
5:E:142:VAL:HG12	5:E:143:GLU:N	2.36	0.41
8:H:40:VAL:HG21	8:H:47:GLN:OE1	2.21	0.41
10:J:122:ASP:HA	25:Z:132:MET:HE2	2.02	0.41
12:L:140:LEU:HD21	12:L:259:LEU:HD13	2.03	0.41
14:N:62:THR:HG21	14:N:114:TRP:CD1	2.56	0.41
33:h:10:VAL:O	33:h:10:VAL:HG13	2.21	0.41
3:C:98:SER:O	3:C:99:LEU:HB2	2.21	0.41
7:G:145:LEU:O	7:G:211:LYS:N	2.46	0.41
10:J:94:LEU:O	10:J:98:MET:N	2.51	0.41
12:L:211:ILE:N	12:L:212:PRO:CD	2.84	0.41
13:M:36:LEU:HD13	32:g:67:VAL:HA	2.02	0.41
13:M:127:ILE:HB	13:M:128:PRO:HD3	2.01	0.41
13:M:299:ALA:O	13:M:303:ILE:HG12	2.21	0.41
14:N:45:ILE:O	14:N:45:ILE:CG2	2.67	0.41
15:O:90:ASP:O	15:O:92:ASN:N	2.51	0.41
16:P:263:TYR:CE2	16:P:284:VAL:HG13	2.56	0.41
17:Q:11:ILE:HG22	17:Q:12:THR:N	2.36	0.41
17:Q:77:ASP:OD1	17:Q:77:ASP:C	2.63	0.41
18:R:34:GLU:OE2	42:q:124:TYR:CD1	2.74	0.41
20:U:13:ASP:OD2	36:k:21:LEU:HD12	2.21	0.41
22:W:44:GLU:OE2	22:W:96:ILE:HA	2.20	0.41
35:j:62:GLU:OE1	35:j:62:GLU:N	2.53	0.41
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.03	0.41
13:M:61:LEU:HD11	13:M:244:ILE:HD13	2.02	0.41
14:N:208:TYR:CZ	14:N:212:THR:HG21	2.56	0.41
20:T:26:ASP:O	20:T:28:GLU:N	2.54	0.41
2:B:81:ARG:HD2	9:I:49:THR:HG21	2.02	0.40
2:B:112:LYS:O	2:B:116:GLN:HG2	2.21	0.40
9:I:106:ARG:O	9:I:107:ARG:HD2	2.20	0.40
12:L:383:MET:HE3	12:L:384:PRO:HD2	2.02	0.40
13:M:1:FME:HE2	13:M:111:SER:HB2	1.99	0.40
13:M:361:MET:CB	13:M:441:MET:HE2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:145:ARG:CD	32:g:22:MET:HE3	2.51	0.40
21:V:93:MET:HE2	21:V:96:TRP:CE3	2.56	0.40
32:g:105:ILE:O	32:g:105:ILE:HG23	2.20	0.40
33:h:64:TRP:CD2	33:h:77:ARG:HD3	2.56	0.40
36:k:32:THR:HG23	36:k:58:TYR:HB3	2.03	0.40
36:k:32:THR:O	36:k:35:GLU:HG2	2.21	0.40
2:B:124:VAL:HG22	2:B:154:ILE:HG22	2.02	0.40
4:D:245:VAL:O	4:D:245:VAL:HG13	2.19	0.40
15:O:206:TYR:O	15:O:211:LEU:HD23	2.22	0.40
19:S:35:PHE:CE1	19:S:87:THR:HG22	2.56	0.40
40:o:15:GLU:OE2	40:o:15:GLU:HA	2.22	0.40
43:r:26:ARG:HD2	43:r:30:ILE:HD11	2.03	0.40
4:D:44:VAL:O	4:D:44:VAL:HG23	2.20	0.40
5:E:116:ILE:HD12	5:E:164:LEU:CD1	2.51	0.40
12:L:166:THR:HG22	37:l:86:ASN:O	2.21	0.40
14:N:250:SER:O	14:N:259:GLY:HA3	2.20	0.40
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.22	0.40
23:X:109:CYS:SG	23:X:113:LYS:NZ	2.81	0.40
23:X:156:ASP:N	23:X:156:ASP:OD1	2.54	0.40
4:D:268:ASP:OD1	4:D:270:ARG:N	2.50	0.40
8:H:179:TRP:CE3	8:H:183:MET:HE2	2.56	0.40
10:J:134:MET:HE2	10:J:134:MET:CA	2.52	0.40
15:O:312:VAL:HG13	28:c:1:LYS:HA	2.04	0.40
18:R:28:PHE:HD1	42:q:125:VAL:HG11	1.87	0.40
31:f:43:PHE:O	31:f:44:GLN:C	2.65	0.40
41:p:102:MET:HE1	41:p:131:PHE:HE1	1.86	0.40
2:B:167:LEU:HD12	2:B:167:LEU:O	2.21	0.40
5:E:53:LEU:HD13	44:s:46:LEU:CD1	2.52	0.40
7:G:98:LEU:HD23	7:G:116:LEU:HD21	2.04	0.40
49:H:403:3PE:O12	10:J:49:SER:OG	2.36	0.40
9:I:76:GLU:OE1	9:I:76:GLU:HA	2.21	0.40
25:Z:105:VAL:HG13	25:Z:106:GLY:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
2	B	154/224 (69%)	142 (92%)	12 (8%)	0	100	100
3	C	205/263 (78%)	191 (93%)	14 (7%)	0	100	100
4	D	427/463 (92%)	398 (93%)	29 (7%)	0	100	100
5	E	210/248 (85%)	191 (91%)	19 (9%)	0	100	100
6	F	426/464 (92%)	392 (92%)	34 (8%)	0	100	100
7	G	686/727 (94%)	629 (92%)	57 (8%)	0	100	100
8	H	316/318 (99%)	296 (94%)	20 (6%)	0	100	100
9	I	176/212 (83%)	164 (93%)	12 (7%)	0	100	100
10	J	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
11	K	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
12	L	604/607 (100%)	559 (92%)	45 (8%)	0	100	100
13	M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	N	342/345 (99%)	324 (95%)	18 (5%)	0	100	100
15	O	318/355 (90%)	306 (96%)	12 (4%)	0	100	100
16	P	340/377 (90%)	302 (89%)	38 (11%)	0	100	100
17	Q	123/175 (70%)	116 (94%)	7 (6%)	0	100	100
18	R	92/116 (79%)	90 (98%)	2 (2%)	0	100	100
19	S	81/99 (82%)	68 (84%)	13 (16%)	0	100	100
20	T	74/156 (47%)	69 (93%)	5 (7%)	0	100	100
20	U	84/156 (54%)	78 (93%)	6 (7%)	0	100	100
21	V	112/116 (97%)	103 (92%)	9 (8%)	0	100	100
22	W	112/131 (86%)	107 (96%)	5 (4%)	0	100	100
23	X	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
24	Y	138/143 (96%)	132 (96%)	6 (4%)	0	100	100
25	Z	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
26	a	66/70 (94%)	65 (98%)	1 (2%)	0	100	100
27	b	78/84 (93%)	73 (94%)	5 (6%)	0	100	100
28	c	46/76 (60%)	43 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	d	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
30	e	103/106 (97%)	95 (92%)	8 (8%)	0	100	100
31	f	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
32	g	99/151 (66%)	91 (92%)	8 (8%)	0	100	100
33	h	136/189 (72%)	129 (95%)	7 (5%)	0	100	100
34	i	90/128 (70%)	84 (93%)	6 (7%)	0	100	100
35	j	60/105 (57%)	58 (97%)	2 (3%)	0	100	100
36	k	73/104 (70%)	72 (99%)	1 (1%)	0	100	100
37	l	152/186 (82%)	133 (88%)	19 (12%)	0	100	100
38	m	124/129 (96%)	115 (93%)	9 (7%)	0	100	100
39	n	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
40	o	109/137 (80%)	97 (89%)	12 (11%)	0	100	100
41	p	167/176 (95%)	157 (94%)	10 (6%)	0	100	100
42	q	142/145 (98%)	136 (96%)	6 (4%)	0	100	100
43	r	96/113 (85%)	86 (90%)	10 (10%)	0	100	100
44	s	39/104 (38%)	36 (92%)	3 (8%)	0	100	100
All	All	8087/9214 (88%)	7538 (93%)	549 (7%)	0	100	100

There are no Ramachandran outliers to report.

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	103/103 (100%)	103 (100%)	0	100	100
2	B	132/185 (71%)	132 (100%)	0	100	100
3	C	189/227 (83%)	189 (100%)	0	100	100
4	D	370/394 (94%)	370 (100%)	0	100	100
5	E	183/206 (89%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	343/370 (93%)	343 (100%)	0	100	100
7	G	580/610 (95%)	580 (100%)	0	100	100
8	H	279/279 (100%)	279 (100%)	0	100	100
9	I	152/178 (85%)	152 (100%)	0	100	100
10	J	136/137 (99%)	136 (100%)	0	100	100
11	K	87/87 (100%)	87 (100%)	0	100	100
12	L	548/549 (100%)	547 (100%)	1 (0%)	87	85
13	M	414/414 (100%)	414 (100%)	0	100	100
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	284/309 (92%)	284 (100%)	0	100	100
16	P	299/325 (92%)	299 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	79/96 (82%)	79 (100%)	0	100	100
19	S	74/80 (92%)	74 (100%)	0	100	100
20	T	70/135 (52%)	70 (100%)	0	100	100
20	U	79/135 (58%)	79 (100%)	0	100	100
21	V	101/102 (99%)	101 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	153/154 (99%)	153 (100%)	0	100	100
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	122/123 (99%)	122 (100%)	0	100	100
26	a	58/60 (97%)	58 (100%)	0	100	100
27	b	71/73 (97%)	71 (100%)	0	100	100
28	c	42/67 (63%)	42 (100%)	0	100	100
29	d	107/107 (100%)	107 (100%)	0	100	100
30	e	93/94 (99%)	93 (100%)	0	100	100
31	f	49/53 (92%)	49 (100%)	0	100	100
32	g	92/129 (71%)	92 (100%)	0	100	100
33	h	123/162 (76%)	123 (100%)	0	100	100
34	i	89/120 (74%)	89 (100%)	0	100	100
35	j	58/87 (67%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	k	58/78 (74%)	58 (100%)	0	100	100
37	l	139/161 (86%)	139 (100%)	0	100	100
38	m	112/114 (98%)	112 (100%)	0	100	100
39	n	162/164 (99%)	162 (100%)	0	100	100
40	o	104/121 (86%)	104 (100%)	0	100	100
41	p	154/158 (98%)	154 (100%)	0	100	100
42	q	129/130 (99%)	129 (100%)	0	100	100
43	r	89/96 (93%)	89 (100%)	0	100	100
44	s	40/95 (42%)	40 (100%)	0	100	100
All	All	7177/7948 (90%)	7176 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	207	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	19	HIS
3	C	71	GLN
3	C	145	HIS
5	E	27	ASN
5	E	57	GLN
6	F	200	GLN
6	F	421	HIS
7	G	475	GLN
7	G	582	GLN
11	K	25	HIS
12	L	226	GLN
12	L	323	HIS
13	M	48	ASN
13	M	138	ASN
13	M	170	HIS
13	M	192	ASN
13	M	331	ASN
13	M	338	HIS
13	M	390	ASN

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Mol	Chain	Res	Type
14	N	289	ASN
14	N	310	ASN
15	O	36	ASN
15	O	147	GLN
16	P	87	HIS
16	P	131	HIS
16	P	184	ASN
16	P	234	ASN
16	P	250	HIS
19	S	47	HIS
21	V	36	HIS
21	V	52	ASN
22	W	72	ASN
23	X	29	HIS
23	X	39	ASN
25	Z	54	GLN
25	Z	111	HIS
29	d	8	HIS
29	d	117	HIS
30	e	96	HIS
32	g	101	ASN
33	h	44	ASN
33	h	86	ASN
33	h	124	GLN
36	k	26	GLN
36	k	38	GLN
37	l	54	GLN
39	n	11	HIS
39	n	77	GLN
40	o	49	GLN
41	p	55	HIS
42	q	59	HIS
42	q	123	GLN
44	s	34	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

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
42	AME	q	1	42	9,10,11	1.55	1 (11%)	9,11,13	1.37	2 (22%)
10	FME	J	1	10	8,9,10	0.92	0	8,9,11	0.94	0
4	2MR	D	85	4	10,12,13	2.43	2 (20%)	5,13,15	1.25	1 (20%)
11	FME	K	1	11	8,9,10	1.00	0	8,9,11	1.29	1 (12%)
12	FME	L	1	12	8,9,10	0.97	0	8,9,11	0.89	0
43	AYA	r	1	43	6,7,8	1.86	2 (33%)	6,8,10	1.29	1 (16%)
14	FME	N	1	14	8,9,10	0.99	0	8,9,11	0.78	0
13	FME	M	1	13	8,9,10	1.01	0	8,9,11	0.86	0
8	FME	H	1	8	8,9,10	0.87	0	8,9,11	1.44	1 (12%)
1	FME	A	1	1	8,9,10	1.00	0	8,9,11	0.98	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	AME	q	1	42	-	3/9/10/12	-
10	FME	J	1	10	-	2/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
11	FME	K	1	11	-	4/7/9/11	-
12	FME	L	1	12	-	5/7/9/11	-
43	AYA	r	1	43	-	0/5/6/8	-
14	FME	N	1	14	-	1/7/9/11	-
13	FME	M	1	13	-	2/7/9/11	-
8	FME	H	1	8	-	4/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.03	1.43	1.33
42	q	1	AME	CT1-N	3.56	1.45	1.34
43	r	1	AYA	CT-N	3.38	1.45	1.34
43	r	1	AYA	OT-CT	-2.05	1.18	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	1	FME	C-CA-N	3.09	115.45	109.50
11	K	1	FME	C-CA-N	2.79	114.89	109.50
4	D	85	2MR	CD-NE-CZ	2.63	128.31	123.36
42	q	1	AME	O-C-CA	-2.36	118.70	124.77
42	q	1	AME	CT2-CT1-N	2.22	119.80	116.12
43	r	1	AYA	CM-CT-N	2.12	119.64	116.12

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	CB-CA-N-CN
8	H	1	FME	N-CA-CB-CG
8	H	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CA-N-CN
12	L	1	FME	N-CA-CB-CG
12	L	1	FME	O-C-CA-CB
42	q	1	AME	O-C-CA-CB
10	J	1	FME	CA-CB-CG-SD
14	N	1	FME	CA-CB-CG-SD
10	J	1	FME	N-CA-CB-CG
13	M	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
8	H	1	FME	CB-CG-SD-CE
42	q	1	AME	CB-CG-SD-CE
12	L	1	FME	CB-CG-SD-CE
11	K	1	FME	CA-CB-CG-SD
42	q	1	AME	CA-CB-CG-SD
12	L	1	FME	C-CA-CB-CG
13	M	1	FME	CB-CA-N-CN
11	K	1	FME	N-CA-CB-CG
11	K	1	FME	CB-CG-SD-CE

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Mol	Chain	Res	Type	Atoms
11	K	1	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	85	2MR	2	0
11	K	1	FME	1	0
13	M	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 1 is monoatomic - leaving 34 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
45	SF4	G	803	7	0,12,12	-	-	-		
49	3PE	H	403	-	43,43,50	0.93	4 (9%)	46,48,55	1.15	2 (4%)
49	3PE	M	502	-	41,41,50	0.95	3 (7%)	44,46,55	1.11	2 (4%)
51	CDL	d	201	-	58,58,99	1.03	6 (10%)	63,69,111	1.06	3 (4%)
46	PC1	Z	201	-	44,44,53	1.05	4 (9%)	50,52,61	1.04	2 (4%)
49	3PE	L	701	-	48,48,50	0.89	4 (8%)	51,53,55	1.12	2 (3%)
51	CDL	d	202	-	62,62,99	1.10	8 (12%)	68,74,111	1.17	4 (5%)
55	EHZ	U	201	20	31,36,37	1.56	5 (16%)	36,44,47	1.68	9 (25%)
53	NDP	P	501	-	51,52,52	2.17	5 (9%)	71,80,80	1.53	17 (23%)
51	CDL	L	703	-	73,73,99	1.02	8 (10%)	79,85,111	1.14	4 (5%)
49	3PE	H	401	-	50,50,50	0.87	4 (8%)	53,55,55	1.08	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	G	801	7	0,12,12	-	-	-		
49	3PE	Y	401	-	40,40,50	0.97	4 (10%)	43,45,55	1.06	2 (4%)
48	FMN	F	502	-	33,33,33	1.13	3 (9%)	48,50,50	1.34	7 (14%)
46	PC1	B	202	-	34,34,53	1.17	4 (11%)	40,42,61	1.08	2 (5%)
49	3PE	K	201	-	32,32,50	1.07	4 (12%)	35,37,55	1.21	2 (5%)
45	SF4	F	501	6	0,12,12	-	-	-		
46	PC1	B	203	-	42,42,53	1.05	4 (9%)	48,50,61	1.06	2 (4%)
45	SF4	B	201	2	0,12,12	-	-	-		
45	SF4	I	202	9	0,12,12	-	-	-		
51	CDL	r	201	-	56,56,99	1.16	8 (14%)	62,68,111	1.18	4 (6%)
49	3PE	L	704	-	48,48,50	0.89	4 (8%)	51,53,55	1.07	2 (3%)
49	3PE	M	501	-	36,36,50	1.03	4 (11%)	39,41,55	1.13	2 (5%)
51	CDL	N	401	-	64,64,99	1.09	8 (12%)	70,76,111	1.16	4 (5%)
49	3PE	L	702	-	41,41,50	0.97	4 (9%)	44,46,55	1.16	2 (4%)
47	FES	G	802	7	0,4,4	-	-	-		
45	SF4	I	201	9	0,12,12	-	-	-		
51	CDL	i	201	-	69,69,99	1.04	7 (10%)	75,81,111	1.18	5 (6%)
46	PC1	J	201	-	41,41,53	1.06	4 (9%)	47,49,61	1.07	2 (4%)
50	88I	H	402	-	45,45,45	1.91	9 (20%)	55,56,56	1.73	13 (23%)
51	CDL	X	201	-	66,66,99	1.06	8 (12%)	72,78,111	1.16	4 (5%)
55	EHZ	T	201	20	31,36,37	1.54	5 (16%)	36,44,47	1.45	4 (11%)
52	ATP	O	401	-	32,33,33	0.32	0	48,52,52	0.70	0
47	FES	E	301	5	0,4,4	-	-	-		

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	3PE	H	403	-	-	20/47/47/54	-
45	SF4	G	803	7	-	-	0/6/5/5
49	3PE	M	502	-	-	13/45/45/54	-
51	CDL	d	201	-	-	28/67/67/110	-
46	PC1	Z	201	-	-	18/48/48/57	-
49	3PE	L	701	-	-	16/52/52/54	-
55	EHZ	U	201	20	1/1/9/9	15/42/44/45	-
51	CDL	d	202	-	-	29/73/73/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	NDP	P	501	-	-	8/34/77/77	0/5/5/5
51	CDL	L	703	-	-	32/84/84/110	-
49	3PE	H	401	-	-	21/54/54/54	-
45	SF4	G	801	7	-	-	0/6/5/5
49	3PE	Y	401	-	-	14/44/44/54	-
48	FMN	F	502	-	-	11/18/18/18	0/3/3/3
46	PC1	B	202	-	-	14/38/38/57	-
49	3PE	K	201	-	-	14/36/36/54	-
45	SF4	F	501	6	-	-	0/6/5/5
46	PC1	B	203	-	-	12/46/46/57	-
45	SF4	B	201	2	-	-	0/6/5/5
45	SF4	I	202	9	-	-	0/6/5/5
51	CDL	r	201	-	-	25/67/67/110	-
49	3PE	L	704	-	-	23/52/52/54	-
49	3PE	M	501	-	-	15/40/40/54	-
51	CDL	N	401	-	-	34/75/75/110	-
49	3PE	L	702	-	-	16/45/45/54	-
51	CDL	i	201	-	-	29/80/80/110	-
45	SF4	I	201	9	-	-	0/6/5/5
47	FES	G	802	7	-	-	0/1/1/1
46	PC1	J	201	-	-	16/45/45/57	-
50	88I	H	402	-	-	17/37/67/67	0/3/3/3
55	EHZ	T	201	20	1/1/9/9	17/42/44/45	-
51	CDL	X	201	-	-	35/77/77/110	-
52	ATP	O	401	-	-	6/22/38/38	0/3/3/3
47	FES	E	301	5	-	-	0/1/1/1

All (131) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	P	501	NDP	P2B-O2B	12.01	1.80	1.59
50	H	402	88I	C4-C5	-9.38	1.32	1.54
55	U	201	EHZ	C15-N2	5.10	1.45	1.33
55	U	201	EHZ	C12-N1	4.97	1.45	1.33
55	T	201	EHZ	C15-N2	4.96	1.45	1.33
55	T	201	EHZ	C12-N1	4.91	1.45	1.33
53	P	501	NDP	PN-O5D	3.95	1.74	1.59
53	P	501	NDP	PA-O3	3.70	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	P	501	NDP	O2B-C2B	-3.29	1.32	1.44
50	H	402	88I	O4'-C4'	-3.13	1.38	1.45
50	H	402	88I	O3-C16	3.13	1.39	1.35
49	M	501	3PE	O21-C2	-2.80	1.40	1.46
51	d	202	CDL	OB6-CB4	-2.80	1.40	1.46
51	i	201	CDL	OA6-CA4	-2.79	1.40	1.46
49	M	502	3PE	O21-C2	-2.79	1.40	1.46
51	i	201	CDL	OB6-CB4	-2.78	1.40	1.46
51	L	703	CDL	OB6-CB4	-2.77	1.40	1.46
49	L	701	3PE	O21-C2	-2.75	1.40	1.46
49	H	401	3PE	O21-C2	-2.71	1.40	1.46
46	B	203	PC1	O21-C2	-2.71	1.40	1.46
51	N	401	CDL	OB6-CB4	-2.71	1.40	1.46
48	F	502	FMN	C4A-N5	2.70	1.36	1.30
51	r	201	CDL	OB6-CB4	-2.70	1.40	1.46
51	N	401	CDL	OA6-CA4	-2.69	1.40	1.46
46	J	201	PC1	O21-C2	-2.65	1.40	1.46
49	L	702	3PE	O21-C2	-2.64	1.40	1.46
51	X	201	CDL	OA6-CA4	-2.63	1.40	1.46
49	Y	401	3PE	O21-C2	-2.60	1.40	1.46
49	L	704	3PE	O31-C31	2.54	1.40	1.33
51	N	401	CDL	OA8-CA7	2.54	1.40	1.33
46	Z	201	PC1	O21-C2	-2.54	1.40	1.46
51	r	201	CDL	OA6-CA4	-2.53	1.40	1.46
46	B	202	PC1	O21-C2	-2.53	1.40	1.46
51	X	201	CDL	OB6-CB4	-2.53	1.40	1.46
49	L	704	3PE	O21-C2	-2.51	1.40	1.46
51	d	202	CDL	OA6-CA4	-2.51	1.40	1.46
50	H	402	88I	CAD-C1	2.50	1.57	1.52
49	K	201	3PE	O21-C2	-2.50	1.40	1.46
50	H	402	88I	O4'-C1'	-2.50	1.39	1.45
55	U	201	EHZ	O4-C15	-2.47	1.18	1.23
51	X	201	CDL	OB8-CB7	2.46	1.40	1.33
46	Z	201	PC1	O31-C31	2.45	1.40	1.33
51	r	201	CDL	OA8-CA7	2.44	1.40	1.33
51	L	703	CDL	OB8-CB7	2.43	1.40	1.33
49	H	403	3PE	O31-C31	2.43	1.40	1.33
49	H	401	3PE	O31-C3	-2.43	1.39	1.45
51	L	703	CDL	OA8-CA7	2.42	1.40	1.33
51	i	201	CDL	OB8-CB6	-2.41	1.39	1.45
46	B	202	PC1	O31-C31	2.41	1.40	1.33
51	d	202	CDL	OB8-CB7	2.41	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	d	201	CDL	OB8-CB7	2.40	1.40	1.33
51	r	201	CDL	OB8-CB7	2.40	1.40	1.33
51	N	401	CDL	OB8-CB7	2.40	1.40	1.33
51	d	202	CDL	OA8-CA7	2.39	1.40	1.33
51	L	703	CDL	OA6-CA4	-2.37	1.41	1.46
46	B	203	PC1	O31-C31	2.37	1.40	1.33
50	H	402	88I	C5-C16	2.36	1.54	1.51
49	H	403	3PE	O21-C2	-2.36	1.41	1.46
51	X	201	CDL	OA8-CA6	-2.36	1.39	1.45
55	T	201	EHZ	O4-C15	-2.35	1.18	1.23
49	Y	401	3PE	O31-C3	-2.35	1.39	1.45
49	M	501	3PE	O31-C3	-2.35	1.39	1.45
51	i	201	CDL	OA8-CA7	2.35	1.40	1.33
49	M	501	3PE	O31-C31	2.34	1.40	1.33
49	L	701	3PE	O31-C31	2.34	1.40	1.33
49	Y	401	3PE	O31-C31	2.34	1.40	1.33
51	d	201	CDL	OA8-CA7	2.32	1.40	1.33
55	T	201	EHZ	O3-C12	-2.32	1.18	1.23
49	L	702	3PE	O31-C31	2.32	1.40	1.33
49	L	702	3PE	O31-C3	-2.32	1.40	1.45
51	d	201	CDL	OA8-CA6	-2.32	1.40	1.45
46	B	202	PC1	O21-C21	2.31	1.40	1.34
50	H	402	88I	OP3-CAD	-2.30	1.38	1.43
46	Z	201	PC1	O21-C21	2.30	1.40	1.34
49	H	403	3PE	O31-C3	-2.29	1.40	1.45
49	K	201	3PE	O31-C31	2.29	1.40	1.33
51	i	201	CDL	OB8-CB7	2.29	1.40	1.33
55	U	201	EHZ	C9-S1	2.29	1.81	1.76
51	d	201	CDL	OB8-CB6	-2.29	1.40	1.45
49	M	502	3PE	O31-C31	2.28	1.40	1.33
51	d	201	CDL	OB6-CB4	-2.28	1.41	1.46
46	J	201	PC1	O31-C31	2.28	1.40	1.33
51	i	201	CDL	OA8-CA6	-2.28	1.40	1.45
51	d	202	CDL	OB8-CB6	-2.27	1.40	1.45
51	r	201	CDL	OB6-CB5	2.27	1.40	1.34
55	U	201	EHZ	O3-C12	-2.26	1.18	1.23
49	L	702	3PE	O21-C21	2.25	1.40	1.34
51	r	201	CDL	OB8-CB6	-2.23	1.40	1.45
51	X	201	CDL	OA8-CA7	2.23	1.39	1.33
51	N	401	CDL	OB8-CB6	-2.23	1.40	1.45
51	X	201	CDL	OA6-CA5	2.22	1.40	1.34
51	d	201	CDL	OB6-CB5	2.22	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	K	201	3PE	O31-C3	-2.21	1.40	1.45
46	J	201	PC1	O31-C3	-2.21	1.40	1.45
49	M	502	3PE	O31-C3	-2.21	1.40	1.45
48	F	502	FMN	C10-N1	2.19	1.37	1.33
51	r	201	CDL	OA6-CA5	2.19	1.40	1.34
51	L	703	CDL	OA8-CA6	-2.19	1.40	1.45
49	L	704	3PE	O21-C21	2.18	1.40	1.34
53	P	501	NDP	O5D-C5D	-2.18	1.36	1.44
46	B	203	PC1	O21-C21	2.17	1.40	1.34
49	K	201	3PE	O21-C21	2.17	1.40	1.34
51	d	202	CDL	OA8-CA6	-2.17	1.40	1.45
49	H	401	3PE	O31-C31	2.17	1.39	1.33
51	X	201	CDL	OB6-CB5	2.16	1.40	1.34
51	L	703	CDL	OB8-CB6	-2.16	1.40	1.45
49	L	701	3PE	O31-C3	-2.14	1.40	1.45
49	H	401	3PE	O21-C21	2.13	1.40	1.34
51	d	202	CDL	OA6-CA5	2.13	1.40	1.34
51	X	201	CDL	OB8-CB6	-2.13	1.40	1.45
55	T	201	EHZ	C9-S1	2.12	1.81	1.76
51	N	401	CDL	OA6-CA5	2.12	1.40	1.34
51	L	703	CDL	OA6-CA5	2.12	1.40	1.34
46	B	202	PC1	O31-C3	-2.11	1.40	1.45
46	B	203	PC1	O31-C3	-2.11	1.40	1.45
51	N	401	CDL	OB6-CB5	2.08	1.40	1.34
46	J	201	PC1	O21-C21	2.08	1.40	1.34
49	L	701	3PE	O21-C21	2.07	1.40	1.34
51	i	201	CDL	OA6-CA5	2.07	1.40	1.34
51	L	703	CDL	OB6-CB5	2.07	1.40	1.34
49	Y	401	3PE	O21-C21	2.07	1.40	1.34
46	Z	201	PC1	O31-C3	-2.07	1.40	1.45
51	r	201	CDL	OA8-CA6	-2.06	1.40	1.45
51	N	401	CDL	OA8-CA6	-2.04	1.40	1.45
49	H	403	3PE	O21-C21	2.04	1.40	1.34
51	d	202	CDL	OB6-CB5	2.03	1.40	1.34
50	H	402	88I	O2'-C2'	-2.01	1.40	1.45
48	F	502	FMN	C4A-C10	-2.01	1.38	1.44
50	H	402	88I	O2'-C1	-2.01	1.40	1.45
49	L	704	3PE	O31-C3	-2.01	1.40	1.45
49	M	501	3PE	O21-C21	2.01	1.39	1.34

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	T	201	EHZ	C8-C9-S1	6.01	121.14	113.56
55	U	201	EHZ	C8-C9-S1	5.40	120.38	113.56
50	H	402	88I	C29-C28-C5'	-5.40	105.27	114.11
49	L	701	3PE	O21-C21-C22	4.52	121.25	111.48
49	K	201	3PE	O21-C21-C22	4.48	121.17	111.48
49	L	702	3PE	O21-C21-C22	4.46	121.13	111.48
53	P	501	NDP	P2B-O2B-C2B	-4.29	111.96	123.43
51	i	201	CDL	OB6-CB5-C51	4.25	120.68	111.48
46	B	202	PC1	O21-C21-C22	4.21	120.59	111.48
51	N	401	CDL	OA6-CA5-C11	4.20	120.56	111.48
49	M	502	3PE	O21-C21-C22	4.17	120.51	111.48
51	X	201	CDL	OA6-CA5-C11	4.17	120.50	111.48
51	r	201	CDL	OA6-CA5-C11	4.14	120.44	111.48
49	H	403	3PE	O21-C21-C22	4.12	120.39	111.48
51	L	703	CDL	OA6-CA5-C11	4.10	120.34	111.48
51	L	703	CDL	OB6-CB5-C51	4.10	120.34	111.48
46	Z	201	PC1	O21-C21-C22	4.06	120.25	111.48
51	X	201	CDL	OB6-CB5-C51	4.03	120.20	111.48
46	B	203	PC1	O21-C21-C22	3.99	120.12	111.48
51	r	201	CDL	OB6-CB5-C51	3.95	120.03	111.48
51	d	201	CDL	OB6-CB5-C51	3.90	119.92	111.48
49	M	501	3PE	O21-C21-C22	3.85	119.81	111.48
51	d	202	CDL	OB6-CB5-C51	3.85	119.81	111.48
49	H	401	3PE	O21-C21-C22	3.84	119.80	111.48
51	N	401	CDL	OB6-CB5-C51	3.84	119.79	111.48
51	d	202	CDL	OA6-CA5-C11	3.84	119.79	111.48
51	i	201	CDL	OA6-CA5-C11	3.84	119.78	111.48
49	Y	401	3PE	O21-C21-C22	3.84	119.78	111.48
46	J	201	PC1	O21-C21-C22	3.83	119.77	111.48
49	L	704	3PE	O21-C21-C22	3.80	119.69	111.48
48	F	502	FMN	C4-N3-C2	-3.77	118.95	125.64
53	P	501	NDP	O2B-P2B-O1X	-3.74	96.00	109.33
50	H	402	88I	O3-C16-O3'	3.53	125.63	121.26
50	H	402	88I	O3-C17-C4	3.51	109.92	103.42
55	U	201	EHZ	C16-C15-N2	3.39	122.92	116.48
53	P	501	NDP	O3-PA-O1A	-3.35	100.64	110.70
49	H	403	3PE	O31-C31-C32	3.30	121.89	111.83
48	F	502	FMN	C4A-C10-N10	3.15	121.00	116.48
50	H	402	88I	O4'-C1'-C24	3.11	109.61	104.34
50	H	402	88I	C6-C5-C16	3.08	121.55	112.07
46	J	201	PC1	O31-C31-C32	3.07	121.19	111.83
55	U	201	EHZ	C13-C12-N1	3.01	121.83	116.34
55	T	201	EHZ	O2-C9-S1	-3.01	118.85	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	d	202	CDL	OA8-CA7-C31	2.97	120.90	111.83
51	N	401	CDL	OA8-CA7-C31	2.94	120.79	111.83
51	r	201	CDL	OA8-CA7-C31	2.93	120.78	111.83
51	X	201	CDL	OB8-CB7-C71	2.89	120.64	111.83
49	M	501	3PE	O31-C31-C32	2.85	120.53	111.83
50	H	402	88I	C25-C24-C1'	-2.84	97.64	103.14
49	L	702	3PE	O31-C31-C32	2.83	120.47	111.83
48	F	502	FMN	C4A-C4-N3	2.82	120.42	113.25
49	L	704	3PE	O31-C31-C32	2.82	120.42	111.83
49	H	401	3PE	O31-C31-C32	2.81	120.42	111.83
51	L	703	CDL	OB8-CB7-C71	2.79	120.35	111.83
46	B	203	PC1	O31-C31-C32	2.79	120.33	111.83
53	P	501	NDP	PA-O5B-C5B	-2.76	105.53	121.35
50	H	402	88I	C18-C17-C4	-2.76	110.01	115.89
46	Z	201	PC1	O31-C31-C32	2.74	120.20	111.83
50	H	402	88I	O5'-C5'-C4'	2.74	115.80	109.98
51	d	201	CDL	OA8-CA7-C31	2.72	120.13	111.83
49	K	201	3PE	O31-C31-C32	2.71	120.10	111.83
49	L	701	3PE	O31-C31-C32	2.71	120.09	111.83
51	d	202	CDL	OB8-CB7-C71	2.70	120.07	111.83
46	B	202	PC1	O31-C31-C32	2.69	120.05	111.83
53	P	501	NDP	C2A-N1A-C6A	-2.66	114.35	118.73
48	F	502	FMN	O4-C4-C4A	-2.66	119.50	126.53
51	i	201	CDL	OA8-CA7-C31	2.66	119.94	111.83
48	F	502	FMN	C4A-C10-N1	-2.64	118.12	124.59
51	d	201	CDL	OB8-CB7-C71	2.64	119.88	111.83
51	r	201	CDL	OB8-CB7-C71	2.64	119.87	111.83
51	i	201	CDL	OB8-CB7-C71	2.63	119.85	111.83
51	L	703	CDL	OA8-CA7-C31	2.62	119.82	111.83
53	P	501	NDP	PN-O5D-C5D	-2.62	106.35	121.35
53	P	501	NDP	O3X-P2B-O2X	2.57	117.45	107.80
49	Y	401	3PE	O31-C31-C32	2.54	119.57	111.83
55	U	201	EHZ	C19-C17-C16	2.53	113.08	108.77
51	X	201	CDL	OA8-CA7-C31	2.53	119.54	111.83
50	H	402	88I	O3-C16-C5	-2.47	107.16	109.93
51	N	401	CDL	OB8-CB7-C71	2.47	119.36	111.83
53	P	501	NDP	O2N-PN-O3	2.47	113.94	107.27
55	U	201	EHZ	O2-C9-C8	-2.46	119.87	123.74
53	P	501	NDP	O2N-PN-O1N	2.40	123.63	112.44
55	T	201	EHZ	C10-C11-N1	-2.40	107.41	112.41
55	T	201	EHZ	O2-C9-C8	-2.38	120.00	123.74
49	M	502	3PE	O31-C31-C32	2.34	118.98	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	H	402	88I	C4-C5-C16	2.34	105.81	102.18
50	H	402	88I	C8-CAD-C1	2.33	117.61	112.12
48	F	502	FMN	C4-C4A-C10	2.33	120.92	116.93
55	U	201	EHZ	O4-C15-N2	-2.31	118.09	122.98
55	U	201	EHZ	O2-C9-S1	-2.31	119.75	122.68
55	U	201	EHZ	C11-N1-C12	-2.24	118.65	122.82
50	H	402	88I	O2'-C2'-C21	2.23	108.13	104.34
53	P	501	NDP	O4B-C4B-C3B	2.22	109.56	105.15
53	P	501	NDP	C5B-C4B-C3B	-2.21	107.24	115.21
50	H	402	88I	O2'-C1-C20	2.21	108.09	104.34
51	i	201	CDL	CB4-OB6-CB5	-2.21	112.51	117.80
48	F	502	FMN	C10-C4A-N5	-2.20	120.32	124.81
55	U	201	EHZ	C10-S1-C9	2.16	108.21	101.84
53	P	501	NDP	C3N-C2N-N1N	-2.13	120.07	123.20
53	P	501	NDP	N3A-C2A-N1A	2.13	131.81	128.58
53	P	501	NDP	C5A-C4A-N3A	-2.12	123.79	126.72
53	P	501	NDP	O5D-PN-O1N	-2.12	100.55	108.94
53	P	501	NDP	N3A-C4A-N9A	2.08	130.71	127.17
53	P	501	NDP	O3X-P2B-O2B	-2.03	97.92	105.85

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
55	T	201	EHZ	C16
55	U	201	EHZ	C16

All (498) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	O13-C11-C12-N
46	B	203	PC1	C11-O13-P-O14
46	B	203	PC1	O13-C11-C12-N
46	B	203	PC1	O22-C21-O21-C2
46	B	203	PC1	C22-C21-O21-C2
46	J	201	PC1	C11-O13-P-O12
46	J	201	PC1	C1-O11-P-O12
46	J	201	PC1	C1-O11-P-O13
46	J	201	PC1	O21-C2-C3-O31
46	Z	201	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
46	Z	201	PC1	C11-O13-P-O14
46	Z	201	PC1	C11-O13-P-O11
46	Z	201	PC1	C1-O11-P-O14
46	Z	201	PC1	O13-C11-C12-N
48	F	502	FMN	N10-C1'-C2'-O2'
48	F	502	FMN	N10-C1'-C2'-C3'
48	F	502	FMN	C1'-C2'-C3'-O3'
48	F	502	FMN	C1'-C2'-C3'-C4'
48	F	502	FMN	C3'-C4'-C5'-O5'
48	F	502	FMN	O4'-C4'-C5'-O5'
48	F	502	FMN	C5'-O5'-P-O2P
48	F	502	FMN	C5'-O5'-P-O3P
49	H	401	3PE	C11-O13-P-O11
49	H	401	3PE	C11-O13-P-O14
49	H	401	3PE	C12-C11-O13-P
49	H	403	3PE	C1-O11-P-O12
49	H	403	3PE	C1-O11-P-O14
49	H	403	3PE	C11-O13-P-O11
49	H	403	3PE	C11-O13-P-O12
49	H	403	3PE	O13-C11-C12-N
49	K	201	3PE	C11-O13-P-O11
49	K	201	3PE	O32-C31-O31-C3
49	L	701	3PE	C1-O11-P-O12
49	L	701	3PE	C1-O11-P-O13
49	L	701	3PE	C1-O11-P-O14
49	L	701	3PE	O22-C21-O21-C2
49	L	702	3PE	C11-O13-P-O11
49	L	702	3PE	C11-O13-P-O12
49	L	702	3PE	C11-O13-P-O14
49	L	702	3PE	C22-C21-O21-C2
49	L	704	3PE	C1-O11-P-O12
49	L	704	3PE	C11-O13-P-O11
49	L	704	3PE	C11-O13-P-O12
49	L	704	3PE	C12-C11-O13-P
49	M	501	3PE	C11-O13-P-O11
49	M	501	3PE	C11-O13-P-O14
49	M	501	3PE	C22-C21-O21-C2
49	M	502	3PE	C11-O13-P-O11
49	M	502	3PE	C11-O13-P-O12
49	M	502	3PE	O22-C21-O21-C2
49	M	502	3PE	C22-C21-O21-C2
49	Y	401	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
49	Y	401	3PE	C11-O13-P-O12
50	H	402	88I	C25-C4'-C5'-C28
50	H	402	88I	C25-C4'-C5'-O5'
50	H	402	88I	O4'-C4'-C5'-C28
50	H	402	88I	O4'-C4'-C5'-O5'
50	H	402	88I	C16-C5-C6-C13
50	H	402	88I	C4-C5-C6-C13
51	L	703	CDL	CB3-OB5-PB2-OB2
51	L	703	CDL	CB3-OB5-PB2-OB3
51	L	703	CDL	CB3-OB5-PB2-OB4
51	L	703	CDL	OB7-CB5-OB6-CB4
51	N	401	CDL	CA3-OA5-PA1-OA2
51	N	401	CDL	CA3-OA5-PA1-OA3
51	N	401	CDL	CA3-OA5-PA1-OA4
51	N	401	CDL	CB2-OB2-PB2-OB3
51	N	401	CDL	CB2-OB2-PB2-OB4
51	N	401	CDL	CB2-OB2-PB2-OB5
51	X	201	CDL	O1-C1-CA2-OA2
51	X	201	CDL	CB2-C1-CA2-OA2
51	X	201	CDL	C1-CA2-OA2-PA1
51	X	201	CDL	CA2-OA2-PA1-OA3
51	X	201	CDL	CA2-OA2-PA1-OA4
51	X	201	CDL	CA2-OA2-PA1-OA5
51	X	201	CDL	CA3-OA5-PA1-OA2
51	X	201	CDL	CA3-OA5-PA1-OA3
51	X	201	CDL	CA3-OA5-PA1-OA4
51	X	201	CDL	CB2-OB2-PB2-OB3
51	X	201	CDL	CB3-OB5-PB2-OB2
51	X	201	CDL	CB3-OB5-PB2-OB3
51	X	201	CDL	CB3-OB5-PB2-OB4
51	X	201	CDL	C51-CB5-OB6-CB4
51	d	201	CDL	O1-C1-CB2-OB2
51	d	201	CDL	CA2-OA2-PA1-OA5
51	d	201	CDL	CB3-OB5-PB2-OB2
51	d	201	CDL	CB3-OB5-PB2-OB3
51	d	201	CDL	CB3-OB5-PB2-OB4
51	d	201	CDL	C51-CB5-OB6-CB4
51	d	202	CDL	CB2-C1-CA2-OA2
51	d	202	CDL	CB2-OB2-PB2-OB3
51	d	202	CDL	CB2-OB2-PB2-OB5
51	i	201	CDL	C1-CA2-OA2-PA1
51	i	201	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
51	i	201	CDL	CB2-OB2-PB2-OB5
51	i	201	CDL	CB3-OB5-PB2-OB2
51	i	201	CDL	CB3-OB5-PB2-OB3
51	i	201	CDL	OB6-CB4-CB6-OB8
51	r	201	CDL	CA3-OA5-PA1-OA2
51	r	201	CDL	CA3-OA5-PA1-OA3
51	r	201	CDL	CA3-OA5-PA1-OA4
51	r	201	CDL	CB2-OB2-PB2-OB4
51	r	201	CDL	CB2-OB2-PB2-OB5
51	r	201	CDL	OB6-CB4-CB6-OB8
52	O	401	ATP	PB-O3B-PG-O2G
52	O	401	ATP	C5'-O5'-PA-O2A
52	O	401	ATP	C5'-O5'-PA-O3A
53	P	501	NDP	C5B-O5B-PA-O1A
53	P	501	NDP	C5B-O5B-PA-O2A
53	P	501	NDP	C5B-O5B-PA-O3
53	P	501	NDP	O4D-C4D-C5D-O5D
55	T	201	EHZ	C7-C8-C9-S1
55	T	201	EHZ	C12-C13-C14-N2
55	T	201	EHZ	N2-C15-C16-O5
55	T	201	EHZ	C16-C17-C20-O6
55	T	201	EHZ	C18-C17-C20-O6
55	T	201	EHZ	C19-C17-C20-O6
55	U	201	EHZ	C16-C15-N2-C14
55	U	201	EHZ	C15-C16-C17-C18
55	U	201	EHZ	C15-C16-C17-C19
55	U	201	EHZ	C15-C16-C17-C20
55	U	201	EHZ	O5-C16-C17-C18
55	U	201	EHZ	O5-C16-C17-C19
55	U	201	EHZ	O5-C16-C17-C20
46	J	201	PC1	O32-C31-O31-C3
49	H	403	3PE	O32-C31-O31-C3
49	L	704	3PE	O32-C31-O31-C3
51	X	201	CDL	OA9-CA7-OA8-CA6
49	H	403	3PE	C32-C31-O31-C3
49	L	704	3PE	C32-C31-O31-C3
49	M	501	3PE	O32-C31-O31-C3
51	d	202	CDL	OA9-CA7-OA8-CA6
51	d	202	CDL	OB9-CB7-OB8-CB6
51	i	201	CDL	OB9-CB7-OB8-CB6
51	r	201	CDL	OA9-CA7-OA8-CA6
51	X	201	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
51	i	201	CDL	OA7-CA5-OA6-CA4
51	i	201	CDL	OB7-CB5-OB6-CB4
46	J	201	PC1	C32-C31-O31-C3
49	H	401	3PE	C32-C31-O31-C3
49	K	201	3PE	C32-C31-O31-C3
49	M	501	3PE	C32-C31-O31-C3
51	X	201	CDL	C31-CA7-OA8-CA6
51	d	202	CDL	C71-CB7-OB8-CB6
51	r	201	CDL	C31-CA7-OA8-CA6
49	L	701	3PE	C22-C21-O21-C2
51	L	703	CDL	C51-CB5-OB6-CB4
51	i	201	CDL	C51-CB5-OB6-CB4
51	d	202	CDL	C31-CA7-OA8-CA6
51	i	201	CDL	C71-CB7-OB8-CB6
49	H	401	3PE	O32-C31-O31-C3
49	Y	401	3PE	O32-C31-O31-C3
51	N	401	CDL	OB9-CB7-OB8-CB6
49	L	702	3PE	O22-C21-O21-C2
49	M	501	3PE	O22-C21-O21-C2
51	d	201	CDL	OB7-CB5-OB6-CB4
51	L	703	CDL	O1-C1-CB2-OB2
51	d	202	CDL	O1-C1-CA2-OA2
51	L	703	CDL	C71-CB7-OB8-CB6
51	L	703	CDL	OB9-CB7-OB8-CB6
55	U	201	EHZ	O4-C15-N2-C14
49	H	403	3PE	C22-C21-O21-C2
51	i	201	CDL	C11-CA5-OA6-CA4
53	P	501	NDP	O4B-C4B-C5B-O5B
49	Y	401	3PE	C32-C31-O31-C3
51	N	401	CDL	C71-CB7-OB8-CB6
51	d	201	CDL	CB4-CB3-OB5-PB2
49	H	403	3PE	O22-C21-O21-C2
46	B	203	PC1	C32-C31-O31-C3
51	N	401	CDL	C31-CA7-OA8-CA6
51	X	201	CDL	C71-CB7-OB8-CB6
51	d	201	CDL	C31-CA7-OA8-CA6
51	d	201	CDL	C71-CB7-OB8-CB6
53	P	501	NDP	O4D-C1D-N1N-C6N
51	d	201	CDL	OA5-CA3-CA4-OA6
46	B	203	PC1	O32-C31-O31-C3
51	N	401	CDL	OA9-CA7-OA8-CA6
46	Z	201	PC1	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
49	L	704	3PE	O21-C2-C3-O31
49	L	701	3PE	C21-C22-C23-C24
51	X	201	CDL	OB9-CB7-OB8-CB6
51	d	201	CDL	OB9-CB7-OB8-CB6
53	P	501	NDP	C3B-C4B-C5B-O5B
51	r	201	CDL	C71-CB7-OB8-CB6
46	J	201	PC1	C21-C22-C23-C24
51	X	201	CDL	CA5-C11-C12-C13
51	d	201	CDL	OA9-CA7-OA8-CA6
51	i	201	CDL	CA5-C11-C12-C13
51	N	401	CDL	C51-CB5-OB6-CB4
51	N	401	CDL	OB7-CB5-OB6-CB4
51	d	201	CDL	CA2-C1-CB2-OB2
51	d	201	CDL	OA5-CA3-CA4-CA6
53	P	501	NDP	C3D-C4D-C5D-O5D
49	L	701	3PE	C32-C31-O31-C3
50	H	402	88I	CAC-C8-CAD-C1
49	L	704	3PE	C22-C21-O21-C2
51	r	201	CDL	OB9-CB7-OB8-CB6
46	B	202	PC1	C2-C1-O11-P
51	L	703	CDL	OA5-CA3-CA4-OA6
51	r	201	CDL	C51-CB5-OB6-CB4
51	L	703	CDL	OB6-CB4-CB6-OB8
49	K	201	3PE	C25-C26-C27-C28
49	L	702	3PE	C23-C24-C25-C26
49	L	704	3PE	C38-C39-C3A-C3B
50	H	402	88I	C10-C11-C12-C13
50	H	402	88I	C29-C30-C31-C32
51	L	703	CDL	C74-C75-C76-C77
46	J	201	PC1	C33-C34-C35-C36
49	L	704	3PE	O22-C21-O21-C2
49	L	701	3PE	C22-C23-C24-C25
49	L	704	3PE	C31-C32-C33-C34
49	M	502	3PE	C3A-C3B-C3C-C3D
51	L	703	CDL	C11-CA5-OA6-CA4
55	U	201	EHZ	C5-C6-C7-C8
49	L	702	3PE	C26-C27-C28-C29
49	L	701	3PE	O32-C31-O31-C3
49	H	401	3PE	C25-C26-C27-C28
51	N	401	CDL	C31-C32-C33-C34
51	L	703	CDL	CA2-C1-CB2-OB2
49	L	701	3PE	C27-C28-C29-C2A

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Mol	Chain	Res	Type	Atoms
51	i	201	CDL	CB7-C71-C72-C73
51	X	201	CDL	C33-C34-C35-C36
49	L	701	3PE	C35-C36-C37-C38
49	L	702	3PE	C2A-C2B-C2C-C2D
49	M	502	3PE	C3D-C3E-C3F-C3G
49	M	502	3PE	C36-C37-C38-C39
48	F	502	FMN	O2'-C2'-C3'-C4'
49	H	403	3PE	C34-C35-C36-C37
51	i	201	CDL	C18-C19-C20-C21
51	L	703	CDL	OA7-CA5-OA6-CA4
51	r	201	CDL	OB7-CB5-OB6-CB4
51	L	703	CDL	C11-C12-C13-C14
46	Z	201	PC1	C29-C2A-C2B-C2C
51	r	201	CDL	C31-C32-C33-C34
51	d	201	CDL	C58-C59-C60-C61
46	B	202	PC1	C22-C21-O21-C2
49	H	401	3PE	C22-C21-O21-C2
51	N	401	CDL	C11-CA5-OA6-CA4
51	d	202	CDL	C51-CB5-OB6-CB4
55	U	201	EHZ	C12-C13-C14-N2
49	H	401	3PE	O22-C21-O21-C2
51	N	401	CDL	OA7-CA5-OA6-CA4
50	H	402	88I	CAA-C7-CAB-C2
51	L	703	CDL	C35-C36-C37-C38
55	U	201	EHZ	C5-C6-C7-O1
51	L	703	CDL	CB5-C51-C52-C53
46	B	203	PC1	C37-C38-C39-C3A
51	L	703	CDL	C76-C77-C78-C79
49	Y	401	3PE	C35-C36-C37-C38
49	M	502	3PE	O21-C2-C3-O31
49	Y	401	3PE	O21-C2-C3-O31
49	Y	401	3PE	C32-C33-C34-C35
51	N	401	CDL	C51-C52-C53-C54
51	N	401	CDL	C1-CA2-OA2-PA1
46	B	202	PC1	O22-C21-O21-C2
50	H	402	88I	CAB-C2-CAC-C8
55	T	201	EHZ	O4-C15-C16-O5
49	L	704	3PE	C23-C24-C25-C26
51	N	401	CDL	C78-C79-C80-C81
51	i	201	CDL	C31-C32-C33-C34
51	d	202	CDL	OB7-CB5-OB6-CB4
49	H	403	3PE	C39-C3A-C3B-C3C

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Mol	Chain	Res	Type	Atoms
51	N	401	CDL	CA5-C11-C12-C13
46	B	203	PC1	C1-C2-C3-O31
46	J	201	PC1	C1-C2-C3-O31
46	Z	201	PC1	C1-C2-C3-O31
49	L	704	3PE	C1-C2-C3-O31
51	N	401	CDL	CB3-CB4-CB6-OB8
51	i	201	CDL	CA3-CA4-CA6-OA8
51	r	201	CDL	CB3-CB4-CB6-OB8
49	L	702	3PE	C32-C33-C34-C35
49	M	502	3PE	C32-C33-C34-C35
51	N	401	CDL	C77-C78-C79-C80
49	H	401	3PE	C32-C33-C34-C35
51	L	703	CDL	C16-C17-C18-C19
51	i	201	CDL	C23-C24-C25-C26
48	F	502	FMN	C5'-O5'-P-O1P
51	N	401	CDL	C74-C75-C76-C77
49	H	403	3PE	C3-C2-O21-C21
51	L	703	CDL	CA6-CA4-OA6-CA5
49	Y	401	3PE	C34-C35-C36-C37
49	L	704	3PE	C28-C29-C2A-C2B
50	H	402	88I	C31-C32-C33-C34
51	L	703	CDL	C52-C53-C54-C55
51	i	201	CDL	C22-C23-C24-C25
51	N	401	CDL	C55-C56-C57-C58
49	L	702	3PE	C33-C34-C35-C36
55	T	201	EHZ	C7-C8-C9-O2
51	d	202	CDL	C11-CA5-OA6-CA4
51	d	202	CDL	CA5-C11-C12-C13
55	T	201	EHZ	O4-C15-C16-C17
48	F	502	FMN	O2'-C2'-C3'-O3'
49	M	502	3PE	C24-C25-C26-C27
51	d	202	CDL	C79-C80-C81-C82
46	B	203	PC1	C35-C36-C37-C38
51	N	401	CDL	OA5-CA3-CA4-CA6
50	H	402	88I	C12-C13-C6-C5
55	T	201	EHZ	N2-C15-C16-C17
51	L	703	CDL	C51-C52-C53-C54
51	i	201	CDL	C31-CA7-OA8-CA6
50	H	402	88I	C11-C10-C9-CAA
49	H	401	3PE	C29-C2A-C2B-C2C
51	L	703	CDL	CB2-C1-CA2-OA2
49	M	501	3PE	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
49	Y	401	3PE	C1-C2-C3-O31
51	L	703	CDL	CB3-CB4-CB6-OB8
51	X	201	CDL	C71-C72-C73-C74
46	Z	201	PC1	C32-C33-C34-C35
49	K	201	3PE	O11-C1-C2-O21
51	N	401	CDL	OA5-CA3-CA4-OA6
51	L	703	CDL	O1-C1-CA2-OA2
51	L	703	CDL	C1-CA2-OA2-PA1
51	d	202	CDL	C1-CA2-OA2-PA1
55	T	201	EHZ	O1-C7-C8-C9
49	K	201	3PE	C33-C34-C35-C36
49	L	702	3PE	C2D-C2E-C2F-C2G
49	H	403	3PE	C32-C33-C34-C35
49	H	401	3PE	C21-C22-C23-C24
55	U	201	EHZ	C1-C2-C3-C4
49	Y	401	3PE	C26-C27-C28-C29
49	L	701	3PE	C29-C2A-C2B-C2C
55	T	201	EHZ	C6-C7-C8-C9
51	L	703	CDL	C31-C32-C33-C34
50	H	402	88I	CAC-C8-CAD-OP3
51	d	202	CDL	OA7-CA5-OA6-CA4
49	H	403	3PE	C36-C37-C38-C39
49	K	201	3PE	O11-C1-C2-C3
51	L	703	CDL	OA5-CA3-CA4-CA6
51	d	202	CDL	OA5-CA3-CA4-CA6
51	i	201	CDL	OA9-CA7-OA8-CA6
51	d	202	CDL	C76-C77-C78-C79
51	N	401	CDL	C76-C77-C78-C79
51	r	201	CDL	CA3-CA4-OA6-CA5
51	d	201	CDL	C72-C73-C74-C75
46	B	202	PC1	C12-C11-O13-P
49	L	701	3PE	C12-C11-O13-P
49	L	702	3PE	C12-C11-O13-P
49	H	401	3PE	O21-C2-C3-O31
51	X	201	CDL	C56-C57-C58-C59
46	J	201	PC1	O13-C11-C12-N
51	X	201	CDL	C32-C33-C34-C35
46	Z	201	PC1	C34-C35-C36-C37
51	d	201	CDL	C75-C76-C77-C78
46	B	202	PC1	C21-C22-C23-C24
51	r	201	CDL	C11-C12-C13-C14
55	U	201	EHZ	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
51	r	201	CDL	C1-CA2-OA2-PA1
55	T	201	EHZ	C11-C10-S1-C9
51	N	401	CDL	OB5-CB3-CB4-OB6
51	r	201	CDL	OA5-CA3-CA4-OA6
55	T	201	EHZ	C1-C2-C3-C4
49	L	701	3PE	C39-C3A-C3B-C3C
49	M	501	3PE	O21-C2-C3-O31
51	N	401	CDL	OB6-CB4-CB6-OB8
51	X	201	CDL	OA6-CA4-CA6-OA8
51	i	201	CDL	OA6-CA4-CA6-OA8
49	Y	401	3PE	C33-C34-C35-C36
51	i	201	CDL	CB3-CB4-CB6-OB8
51	d	202	CDL	C33-C34-C35-C36
46	B	202	PC1	C1-O11-P-O13
46	J	201	PC1	C11-O13-P-O14
46	J	201	PC1	C11-O13-P-O11
49	H	403	3PE	C1-O11-P-O13
49	K	201	3PE	C11-O13-P-O14
49	L	704	3PE	C1-O11-P-O13
49	L	704	3PE	C1-O11-P-O14
49	M	501	3PE	C11-O13-P-O12
51	L	703	CDL	CA3-OA5-PA1-OA3
51	d	201	CDL	CA2-OA2-PA1-OA3
51	i	201	CDL	CA2-OA2-PA1-OA4
51	i	201	CDL	CA2-OA2-PA1-OA5
51	r	201	CDL	CB2-OB2-PB2-OB3
52	O	401	ATP	C5'-O5'-PA-O1A
51	d	201	CDL	C72-C71-CB7-OB8
51	r	201	CDL	CA4-CA3-OA5-PA1
49	Y	401	3PE	C21-C22-C23-C24
51	L	703	CDL	C54-C55-C56-C57
49	L	702	3PE	C3-C2-O21-C21
51	X	201	CDL	CB3-CB4-OB6-CB5
51	d	201	CDL	CB6-CB4-OB6-CB5
51	d	202	CDL	CA6-CA4-OA6-CA5
51	d	202	CDL	C32-C33-C34-C35
51	i	201	CDL	C16-C17-C18-C19
49	H	403	3PE	C31-C32-C33-C34
51	r	201	CDL	CA5-C11-C12-C13
51	d	201	CDL	C31-C32-C33-C34
51	d	201	CDL	C52-C53-C54-C55
49	L	704	3PE	C2A-C2B-C2C-C2D

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Mol	Chain	Res	Type	Atoms
51	r	201	CDL	OA7-CA5-OA6-CA4
46	B	203	PC1	C32-C33-C34-C35
46	B	203	PC1	O21-C2-C3-O31
49	M	502	3PE	C1-C2-C3-O31
49	M	501	3PE	C31-C32-C33-C34
49	L	702	3PE	O21-C21-C22-C23
49	K	201	3PE	C27-C28-C29-C2A
51	d	202	CDL	C72-C73-C74-C75
51	N	401	CDL	C83-C84-C85-C86
46	B	202	PC1	C34-C35-C36-C37
51	X	201	CDL	C61-C62-C63-C64
51	X	201	CDL	C52-C53-C54-C55
49	M	501	3PE	C25-C26-C27-C28
49	L	702	3PE	C34-C35-C36-C37
51	N	401	CDL	CA4-CA3-OA5-PA1
46	J	201	PC1	C38-C39-C3A-C3B
51	i	201	CDL	C14-C15-C16-C17
49	L	704	3PE	C2-C1-O11-P
51	d	202	CDL	CA4-CA3-OA5-PA1
51	X	201	CDL	C13-C14-C15-C16
51	r	201	CDL	OA5-CA3-CA4-CA6
51	N	401	CDL	C80-C81-C82-C83
51	d	202	CDL	C75-C76-C77-C78
51	r	201	CDL	C71-C72-C73-C74
46	Z	201	PC1	C2C-C2D-C2E-C2F
46	Z	201	PC1	C36-C37-C38-C39
55	T	201	EHZ	C21-C22-C23-C24
51	N	401	CDL	C84-C85-C86-C87
49	H	401	3PE	C2D-C2E-C2F-C2G
46	J	201	PC1	C26-C27-C28-C29
49	M	502	3PE	C23-C24-C25-C26
55	T	201	EHZ	C13-C14-N2-C15
51	d	202	CDL	OA5-CA3-CA4-OA6
51	r	201	CDL	C11-CA5-OA6-CA4
51	X	201	CDL	C59-C60-C61-C62
49	H	401	3PE	C22-C23-C24-C25
49	M	502	3PE	C35-C36-C37-C38
51	N	401	CDL	OB5-CB3-CB4-CB6
51	d	201	CDL	OB5-CB3-CB4-CB6
51	d	202	CDL	OA6-CA4-CA6-OA8
49	M	501	3PE	C34-C35-C36-C37
49	H	401	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
51	X	201	CDL	C63-C64-C65-C66
52	O	401	ATP	PB-O3B-PG-O1G
49	L	701	3PE	C26-C27-C28-C29
51	d	202	CDL	C31-C32-C33-C34
51	i	201	CDL	C11-C12-C13-C14
49	M	501	3PE	C39-C3A-C3B-C3C
51	d	202	CDL	C73-C74-C75-C76
49	H	403	3PE	C3C-C3D-C3E-C3F
49	M	501	3PE	C2-C1-O11-P
50	H	402	88I	C28-C29-C30-C31
51	X	201	CDL	CA3-CA4-CA6-OA8
55	T	201	EHZ	C10-C11-N1-C12
49	H	401	3PE	C35-C36-C37-C38
49	K	201	3PE	O21-C21-C22-C23
49	M	501	3PE	C12-C11-O13-P
50	H	402	88I	C10-C9-CAA-C7
46	Z	201	PC1	C11-C12-N-C14
46	J	201	PC1	C35-C36-C37-C38
46	B	202	PC1	O21-C21-C22-C23
46	Z	201	PC1	O21-C21-C22-C23
51	L	703	CDL	C12-C11-CA5-OA6
46	B	203	PC1	C3C-C3D-C3E-C3F
51	X	201	CDL	C62-C63-C64-C65
49	H	401	3PE	C28-C29-C2A-C2B
49	K	201	3PE	O31-C31-C32-C33
46	Z	201	PC1	C28-C29-C2A-C2B
49	H	403	3PE	O21-C21-C22-C23
49	L	704	3PE	O21-C21-C22-C23
46	J	201	PC1	C3A-C3B-C3C-C3D
49	L	704	3PE	C2B-C2C-C2D-C2E
51	d	201	CDL	C56-C57-C58-C59
49	H	401	3PE	C2-C1-O11-P
49	K	201	3PE	C2-C1-O11-P
49	Y	401	3PE	O31-C31-C32-C33
49	L	704	3PE	O31-C31-C32-C33
51	d	202	CDL	C12-C11-CA5-OA6
51	X	201	CDL	C55-C56-C57-C58
46	B	202	PC1	C24-C25-C26-C27
46	Z	201	PC1	C11-C12-N-C13
51	X	201	CDL	C31-C32-C33-C34
46	B	202	PC1	O22-C21-C22-C23
55	U	201	EHZ	C2-C3-C4-C5

Continued on next page...

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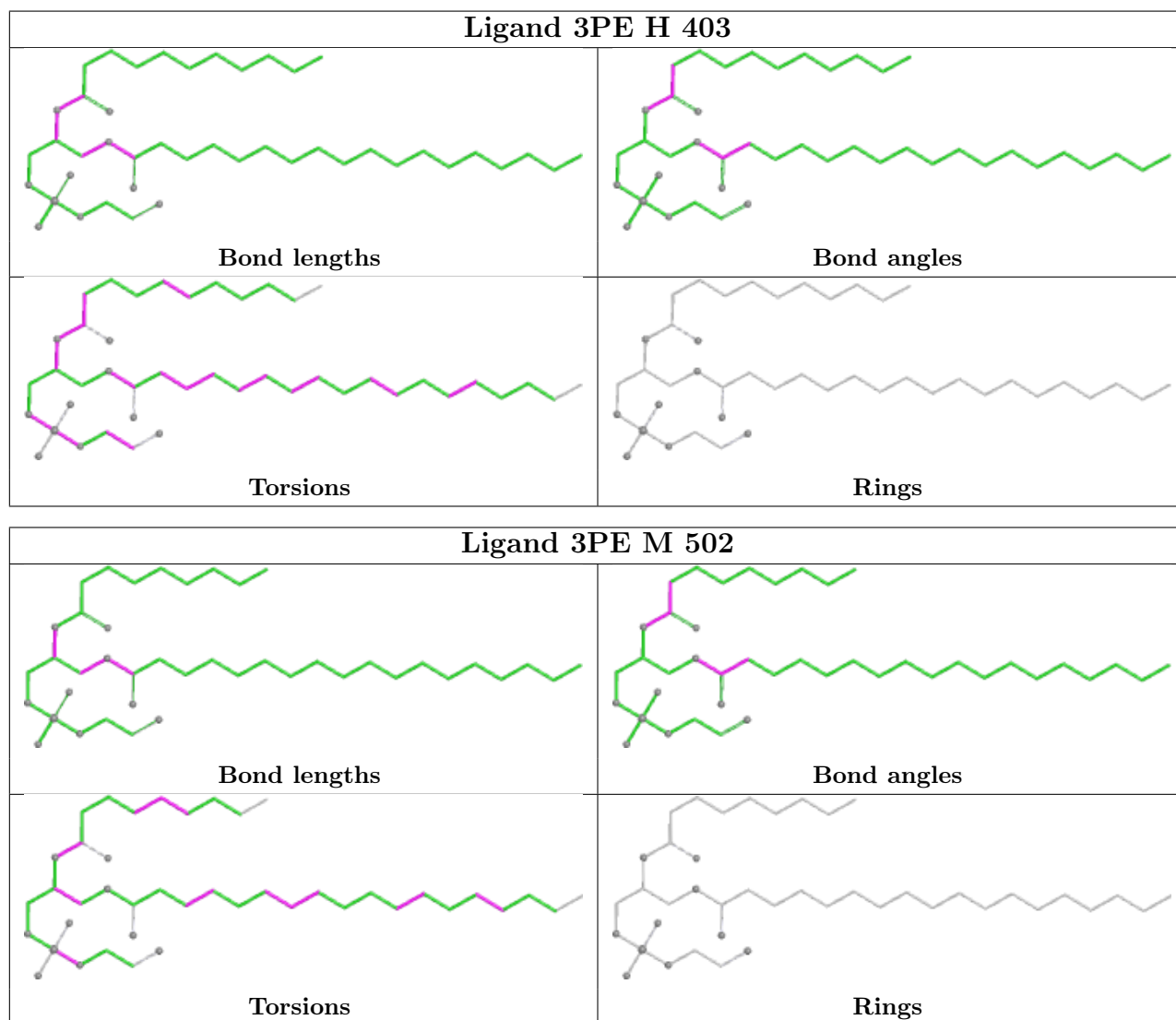
Mol	Chain	Res	Type	Atoms
49	H	401	3PE	C3E-C3F-C3G-C3H
46	Z	201	PC1	C2A-C2B-C2C-C2D
49	L	704	3PE	O32-C31-C32-C33
46	Z	201	PC1	C11-C12-N-C15
51	i	201	CDL	C72-C71-CB7-OB8
51	d	202	CDL	C12-C11-CA5-OA7
49	H	403	3PE	C24-C25-C26-C27
49	L	704	3PE	O22-C21-C22-C23
49	K	201	3PE	O22-C21-C22-C23
49	H	401	3PE	C3C-C3D-C3E-C3F
52	O	401	ATP	O4'-C4'-C5'-O5'
49	H	403	3PE	O22-C21-C22-C23
49	K	201	3PE	O32-C31-C32-C33
51	L	703	CDL	C12-C11-CA5-OA7
49	H	401	3PE	C1-C2-C3-O31
55	U	201	EHZ	N2-C15-C16-O5
49	Y	401	3PE	O32-C31-C32-C33
51	N	401	CDL	C52-C51-CB5-OB6
51	d	201	CDL	C52-C51-CB5-OB6
49	L	702	3PE	C24-C25-C26-C27
51	d	201	CDL	C32-C31-CA7-OA8
51	d	201	CDL	C71-C72-C73-C74
49	L	701	3PE	C28-C29-C2A-C2B

There are no ring outliers.

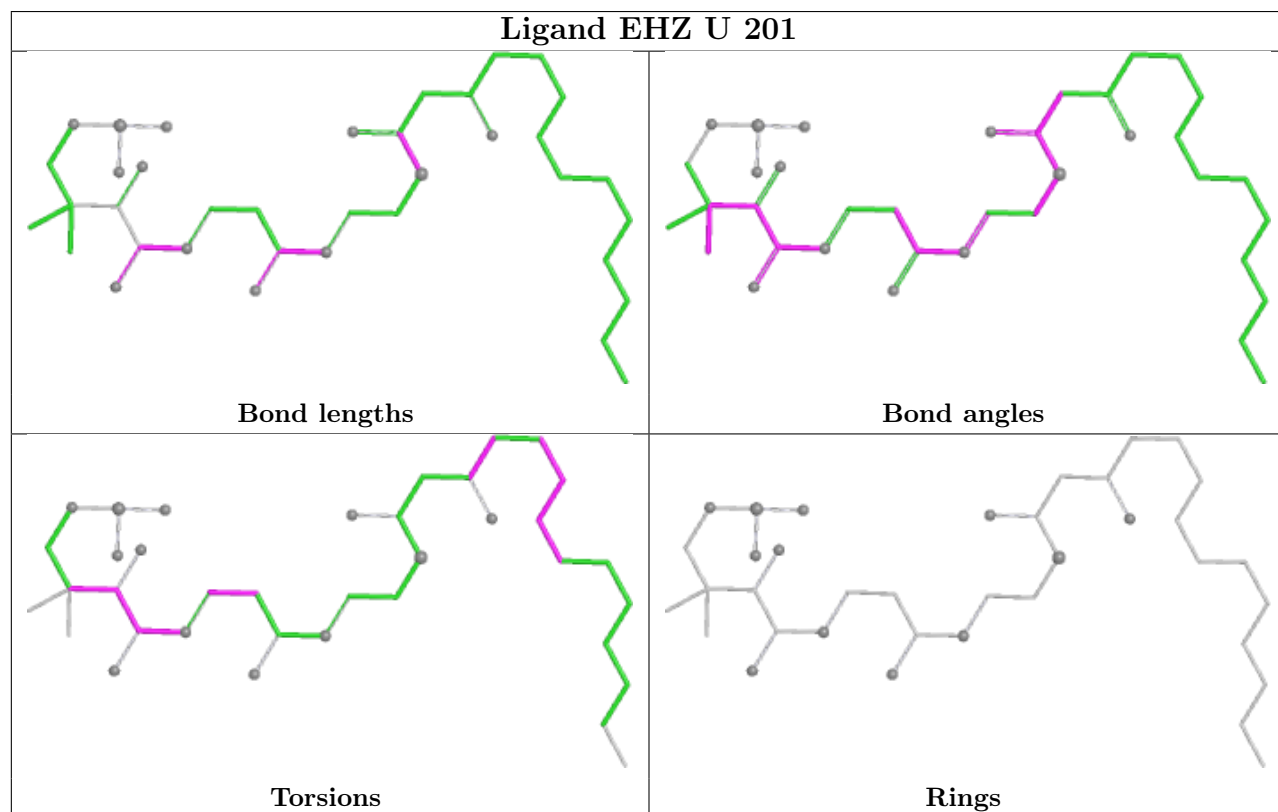
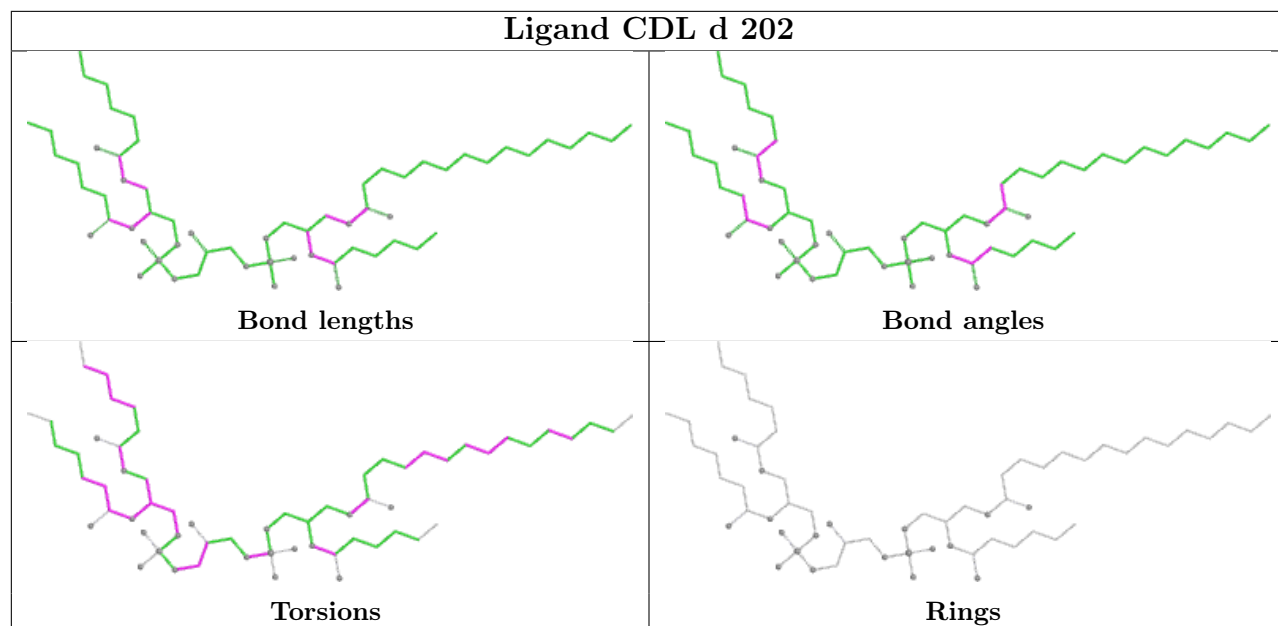
13 monomers are involved in 20 short contacts:

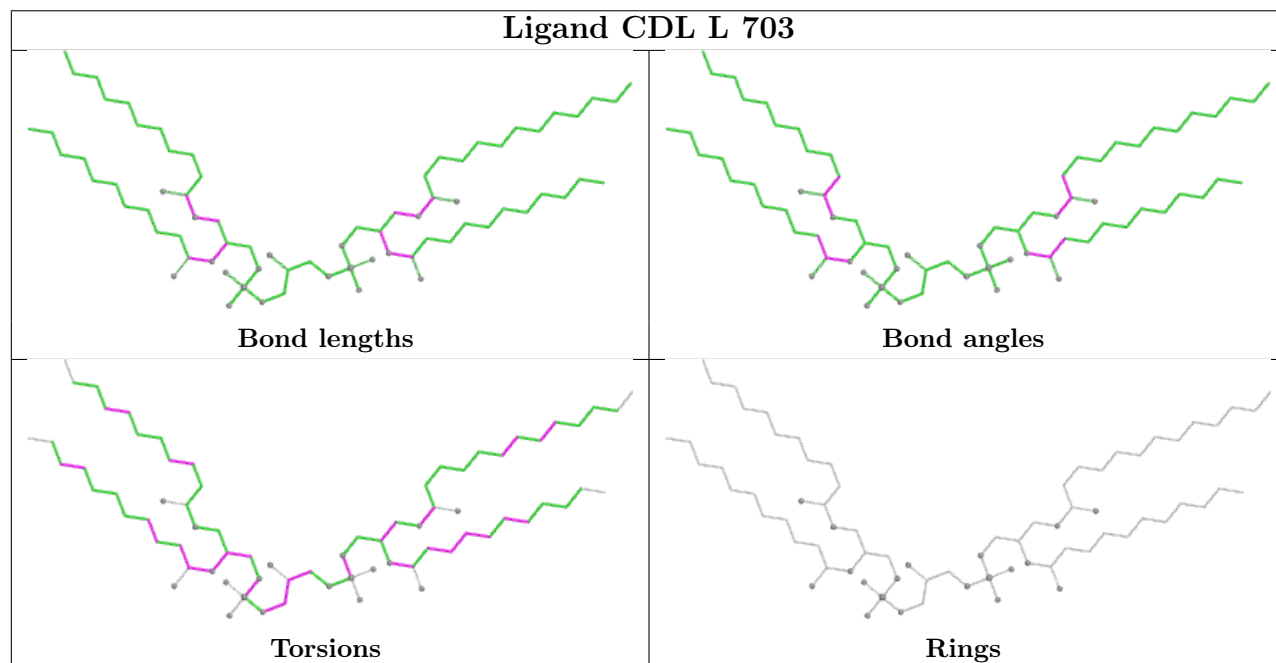
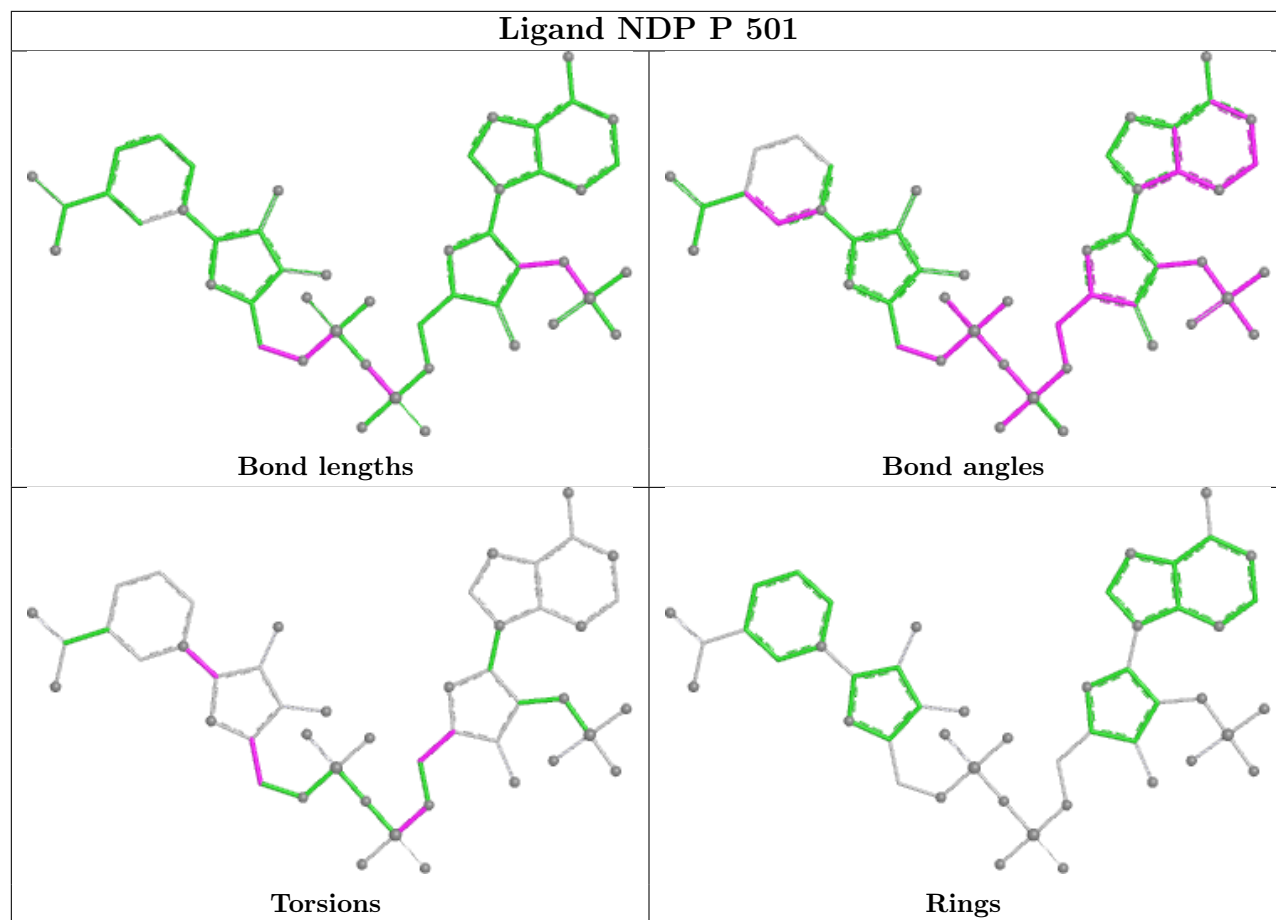
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	H	403	3PE	2	0
51	d	201	CDL	1	0
49	L	701	3PE	1	0
55	U	201	EHZ	1	0
53	P	501	NDP	2	0
49	H	401	3PE	1	0
48	F	502	FMN	4	0
51	N	401	CDL	1	0
49	L	702	3PE	1	0
51	i	201	CDL	1	0
46	J	201	PC1	2	0
55	T	201	EHZ	2	0
52	O	401	ATP	1	0

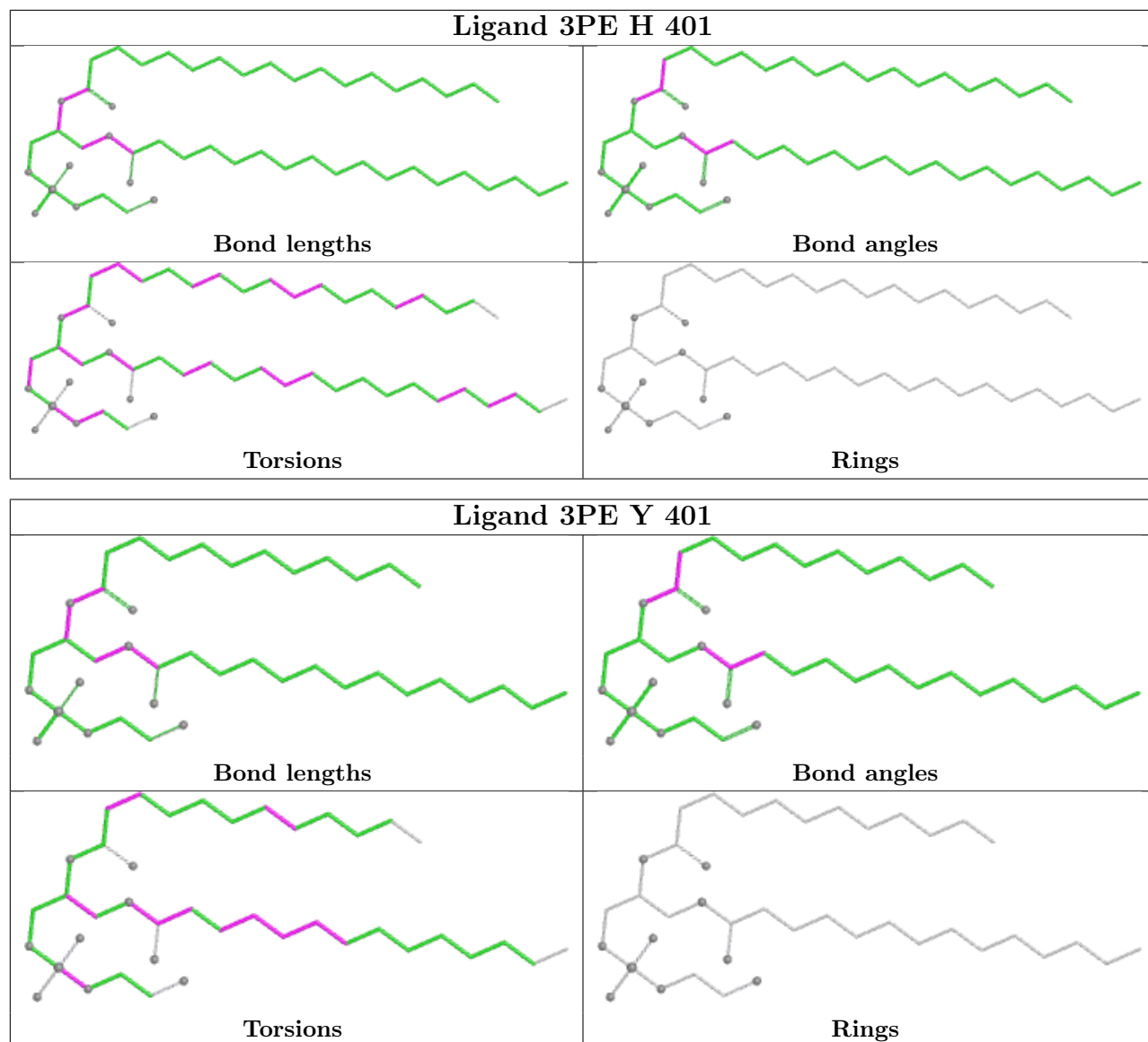
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

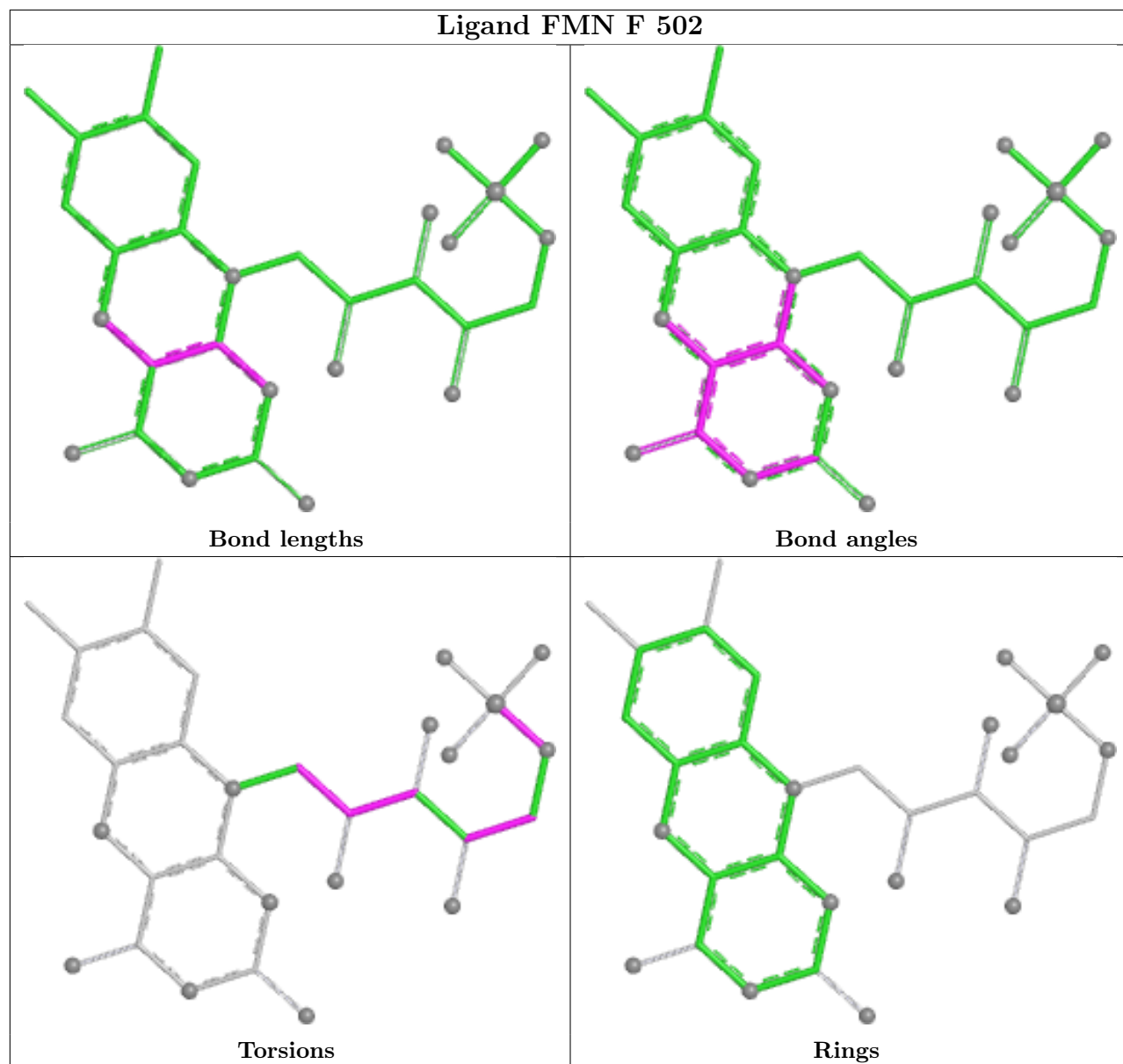


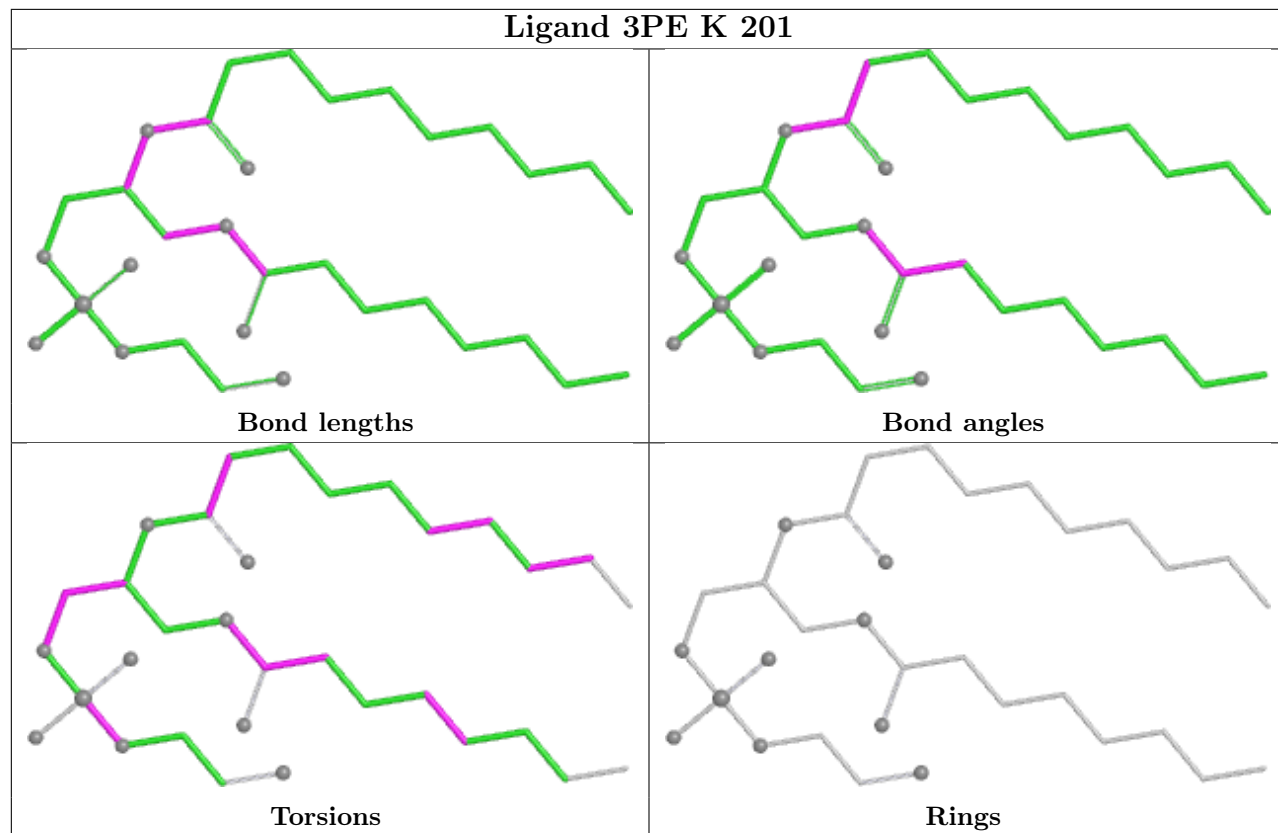
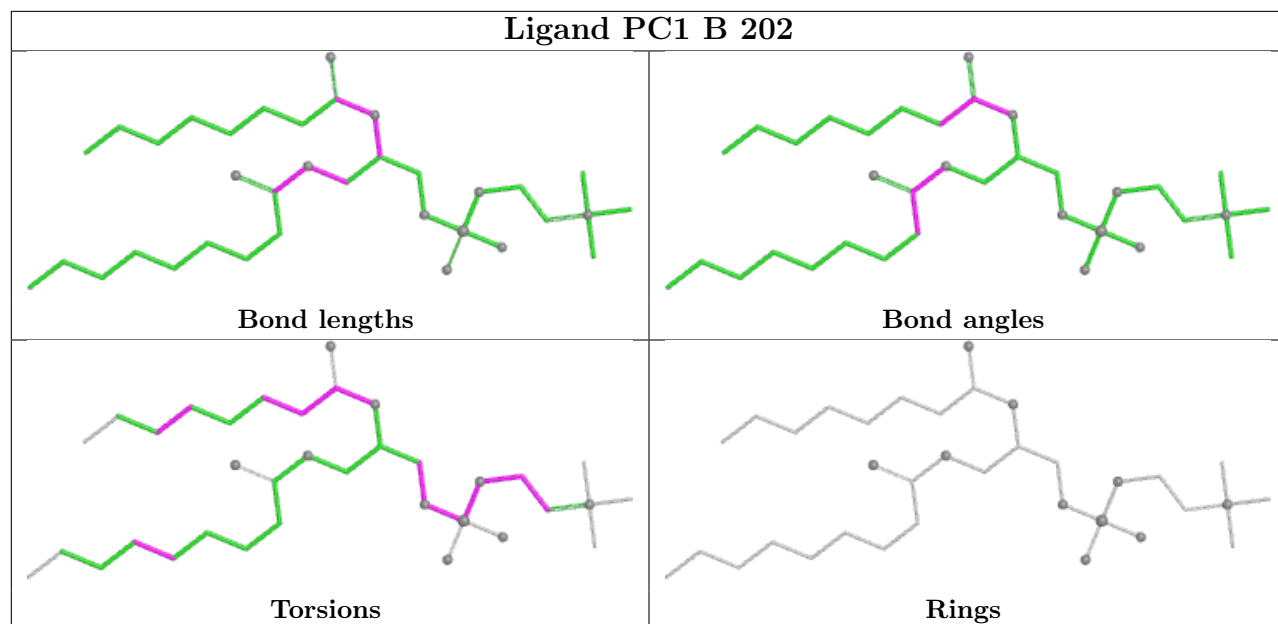


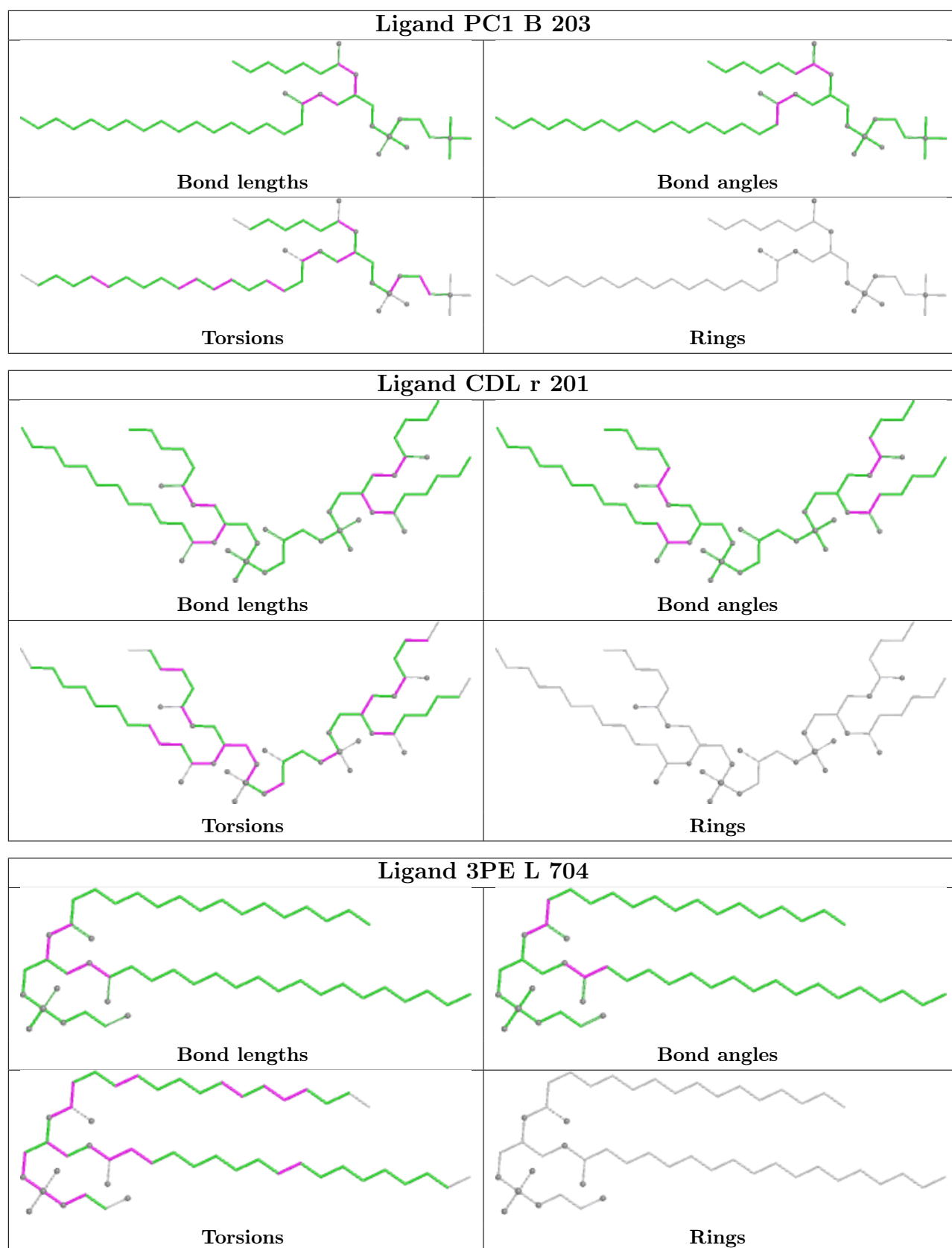


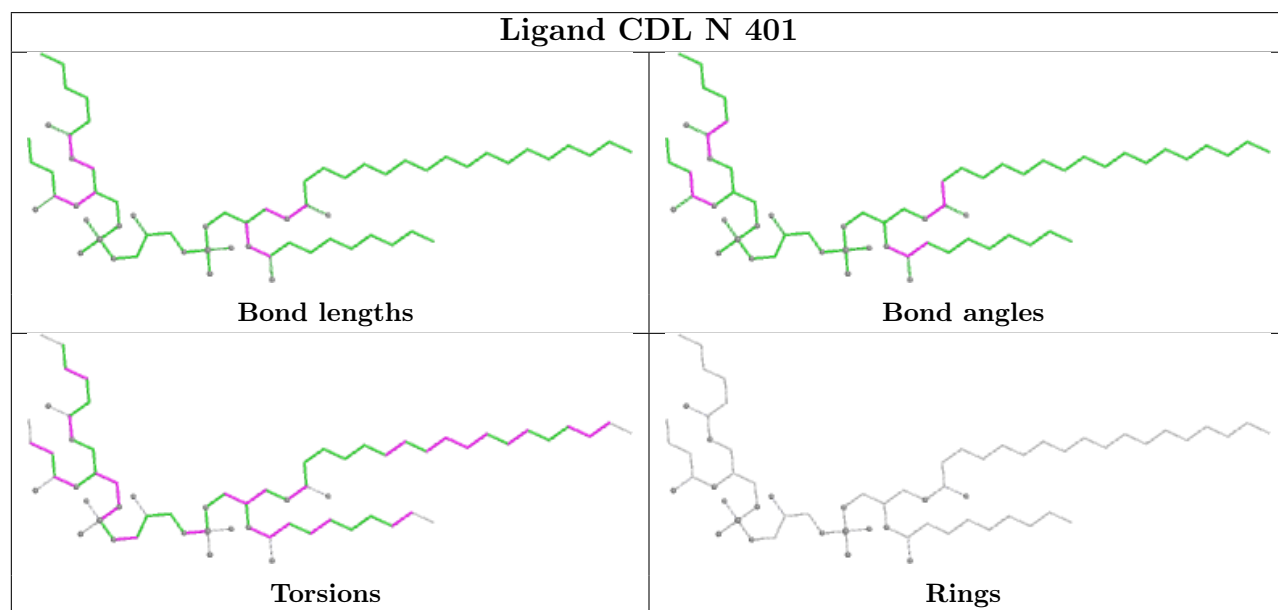
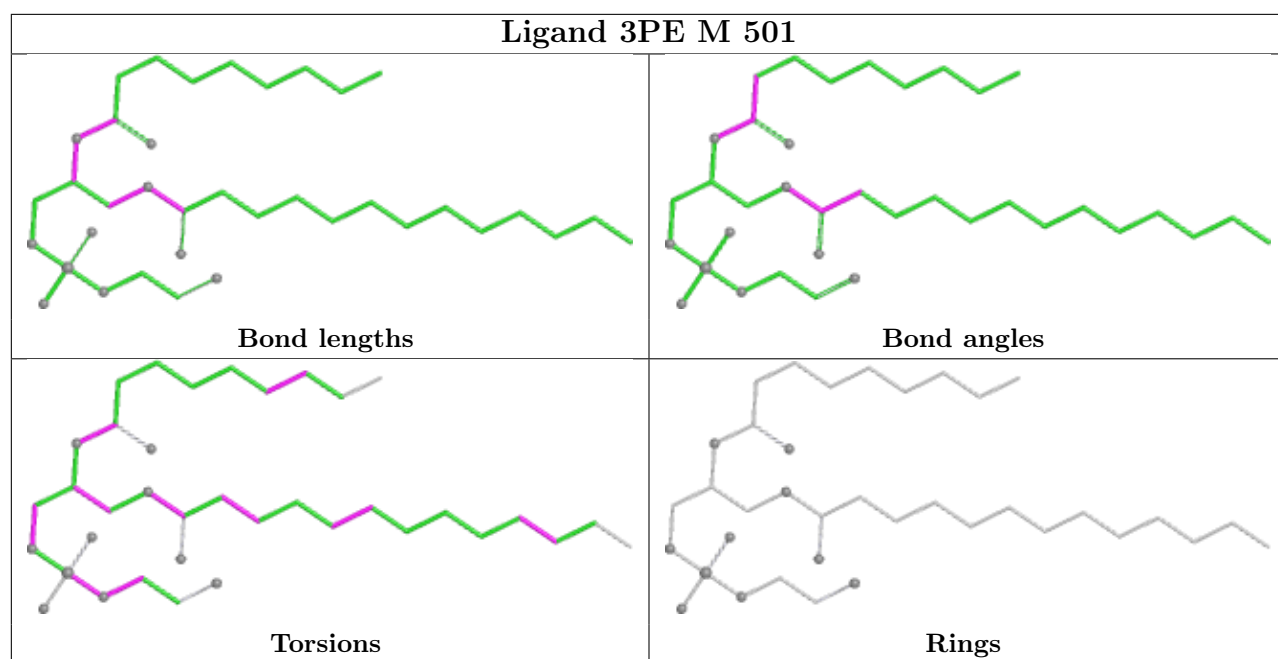


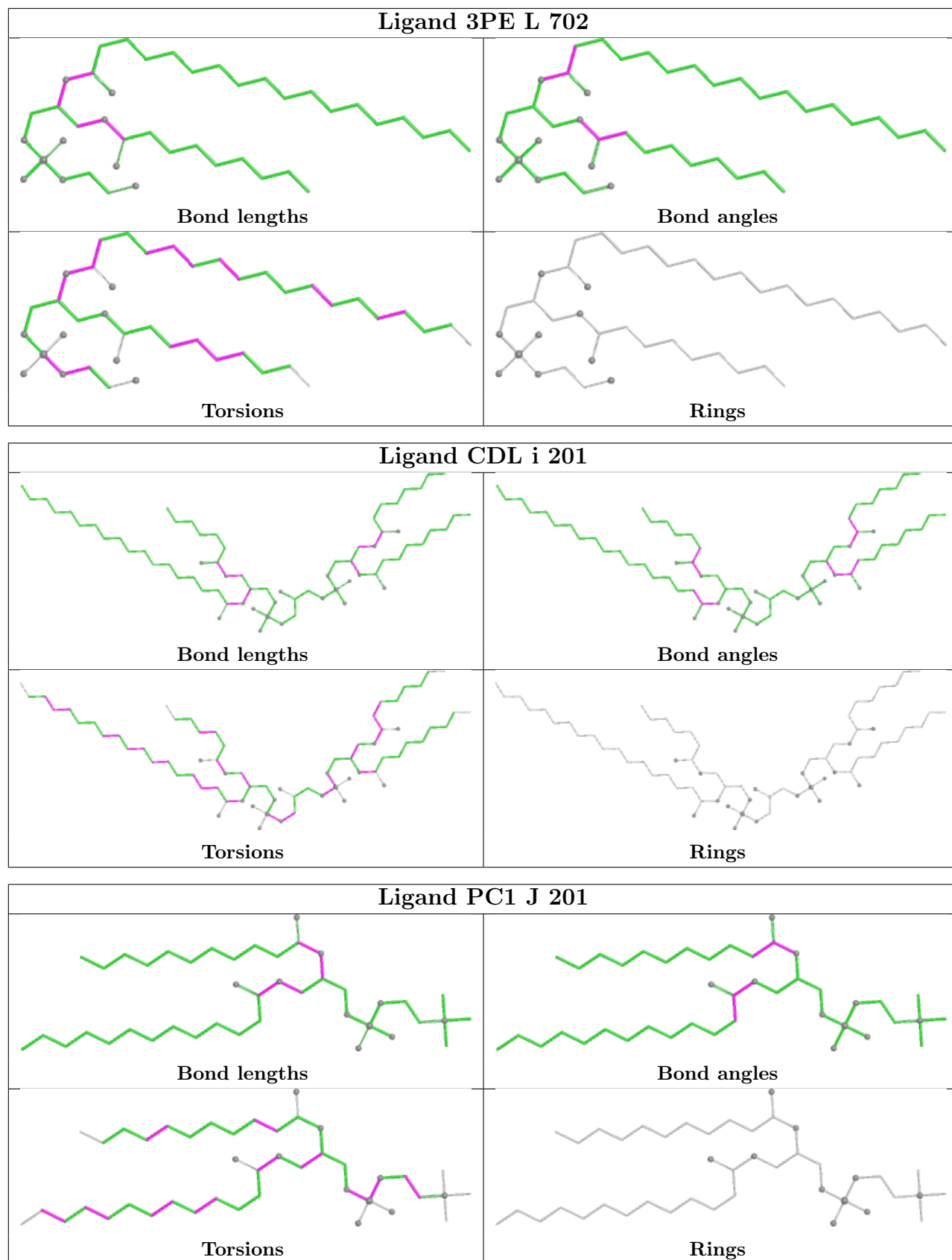


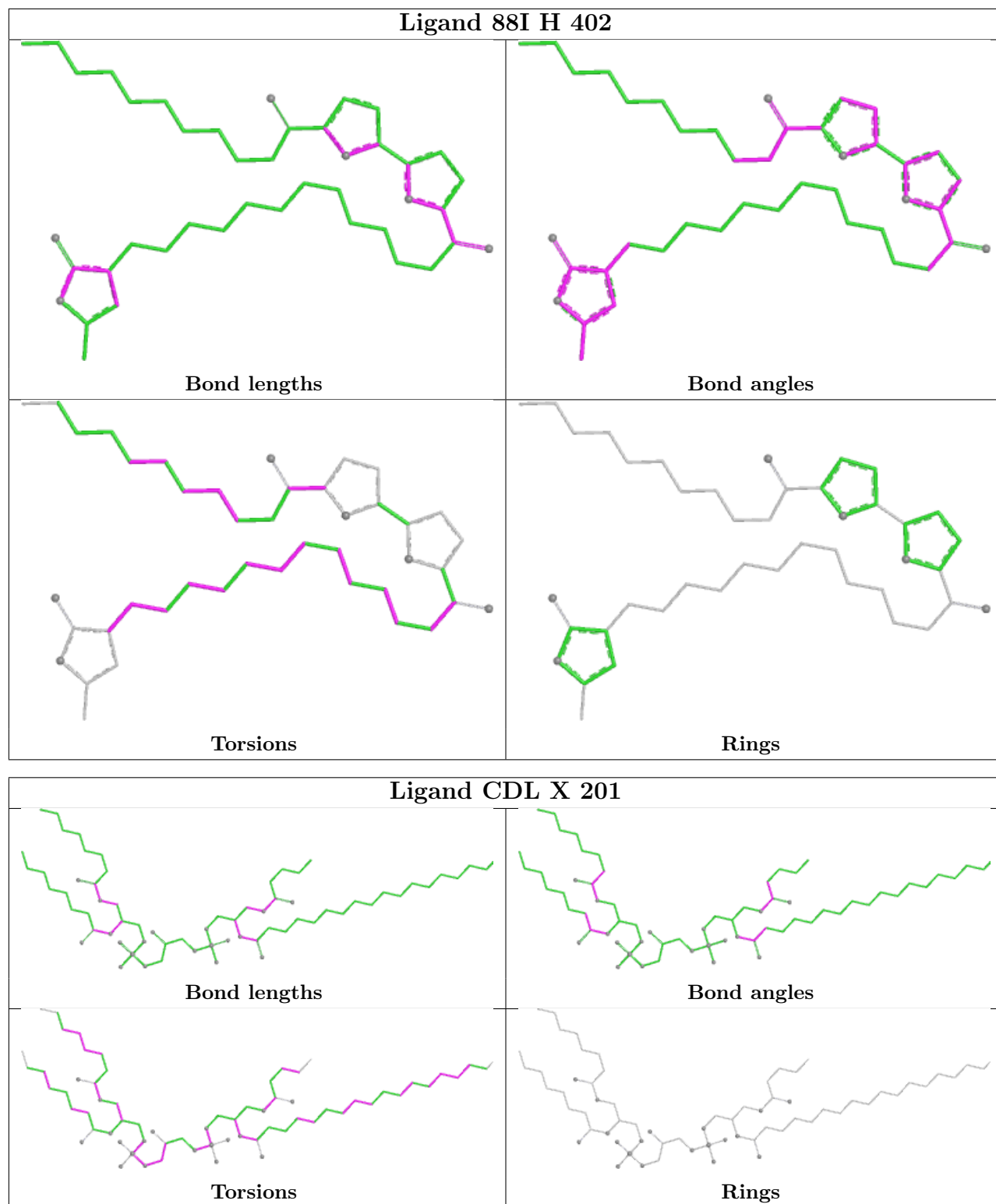


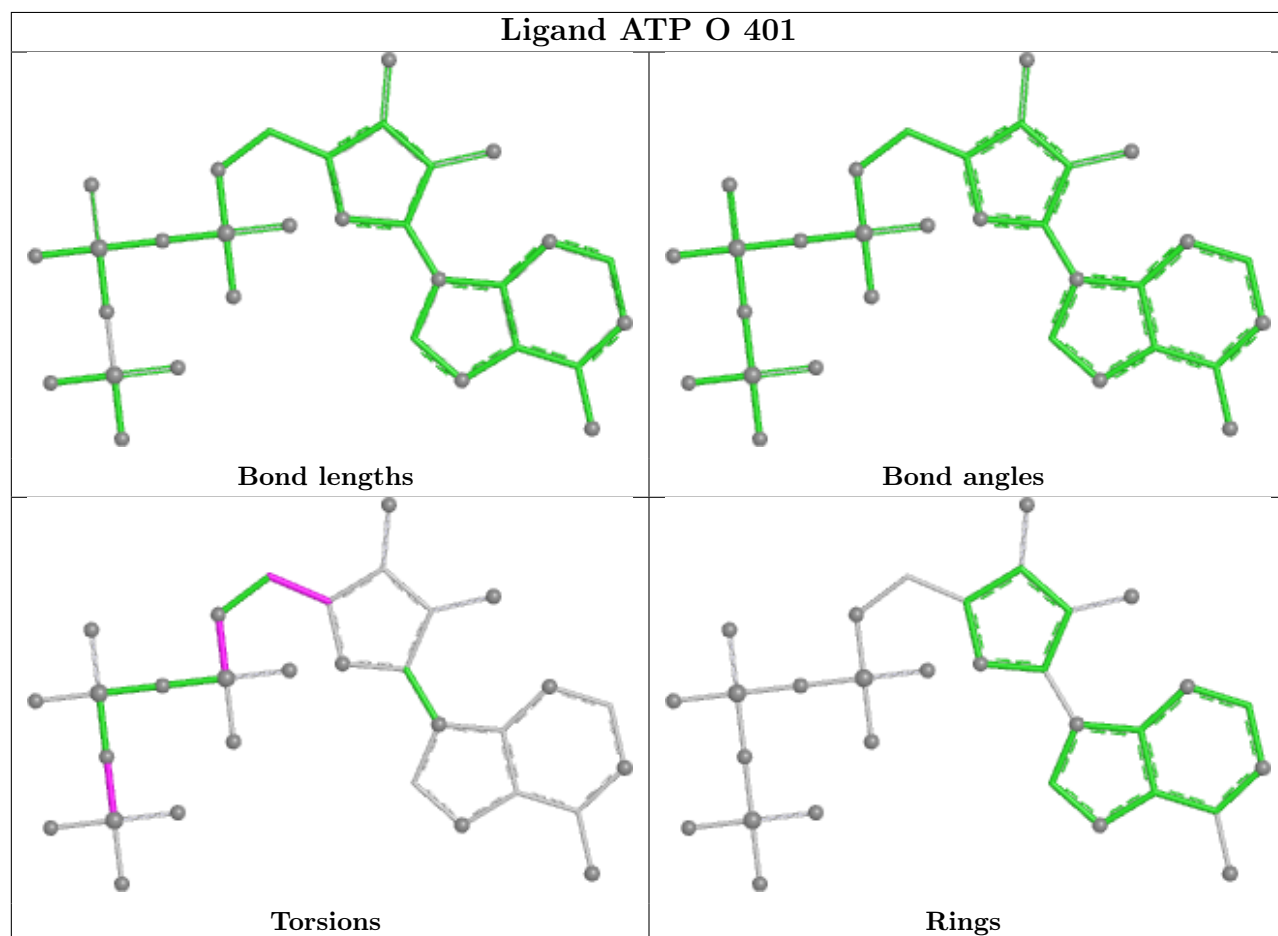
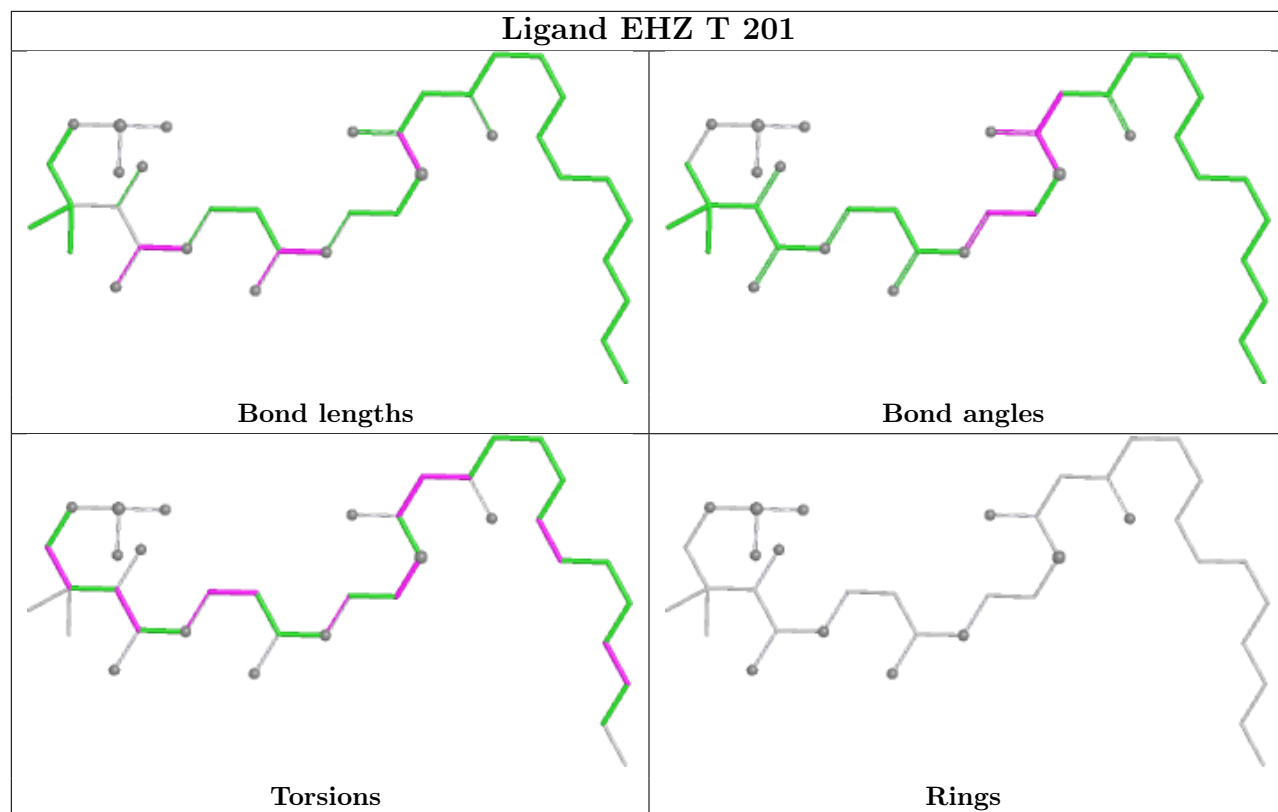












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

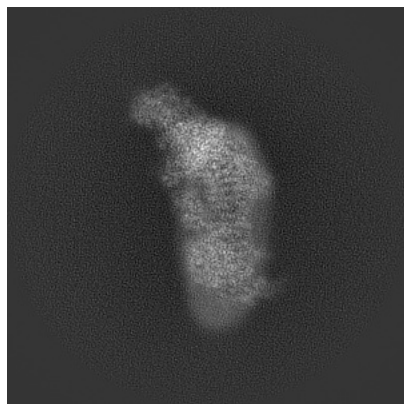
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13611. These allow visual inspection of the internal detail of the map and identification of artifacts.

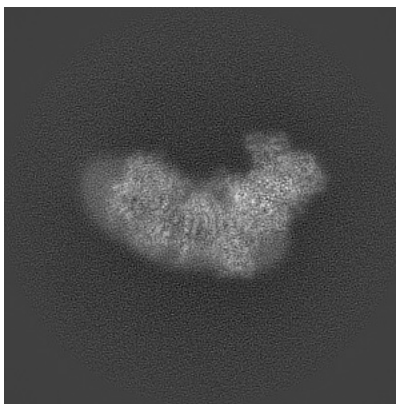
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

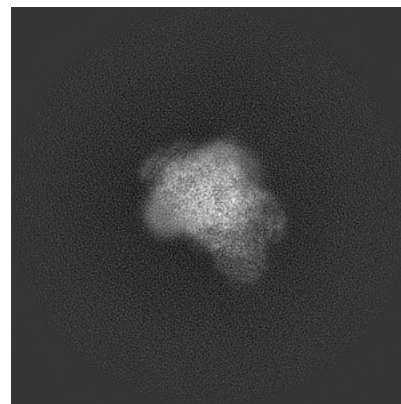
6.1.1 Primary map



X

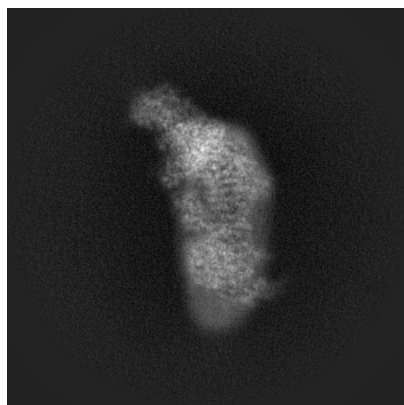


Y

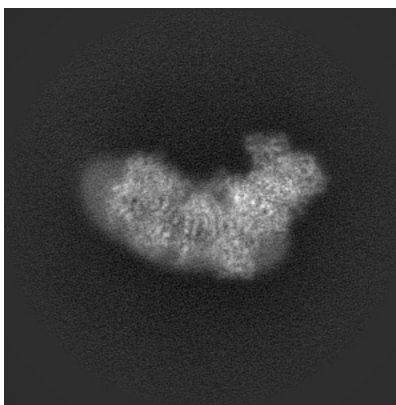


Z

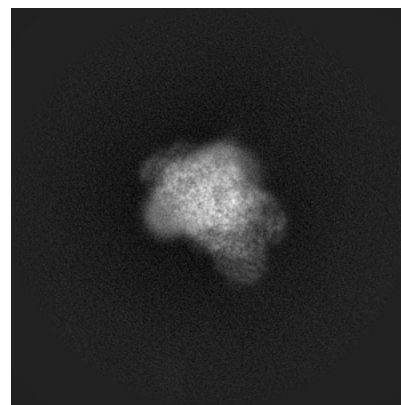
6.1.2 Raw map



X



Y

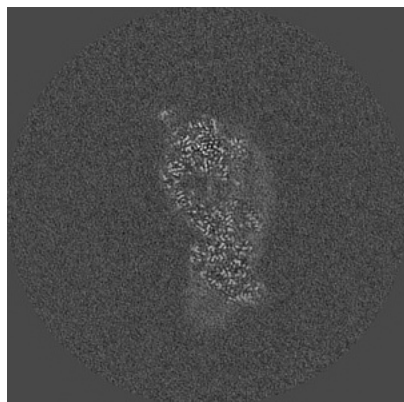


Z

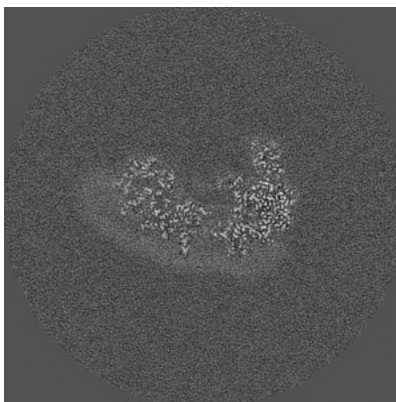
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

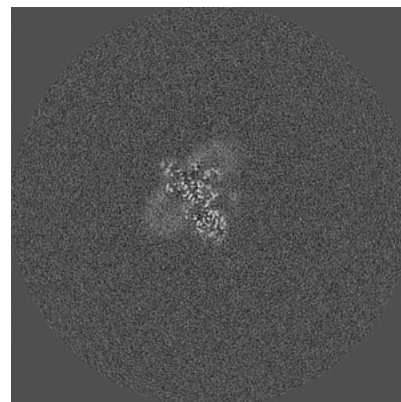
6.2.1 Primary map



X Index: 225

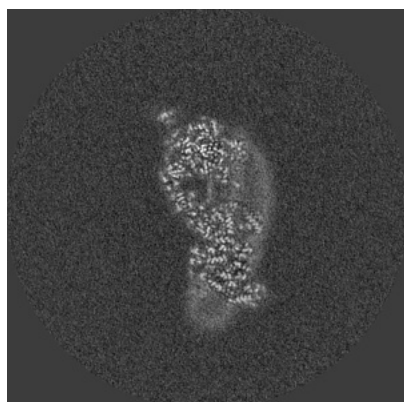


Y Index: 225

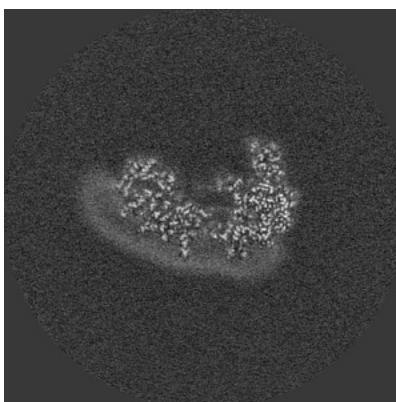


Z Index: 225

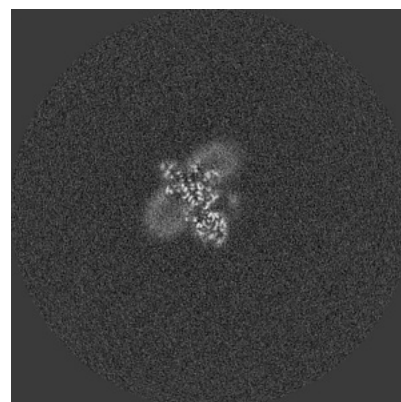
6.2.2 Raw map



X Index: 225



Y Index: 225

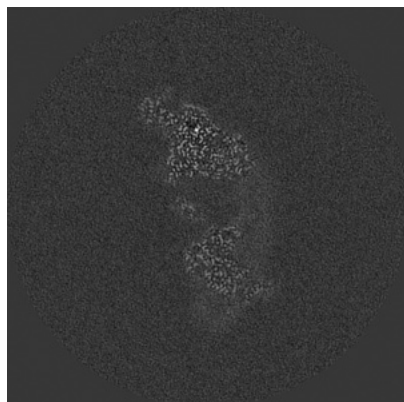


Z Index: 225

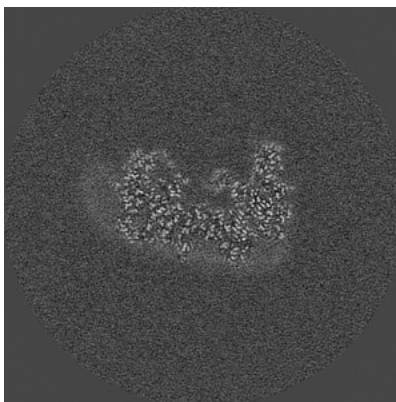
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

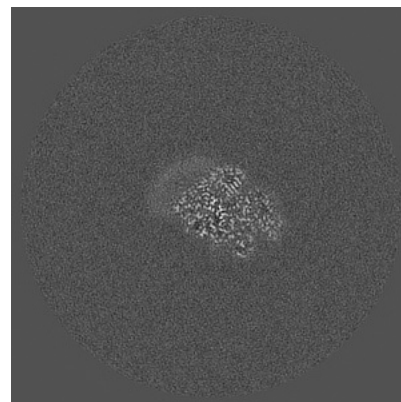
6.3.1 Primary map



X Index: 240

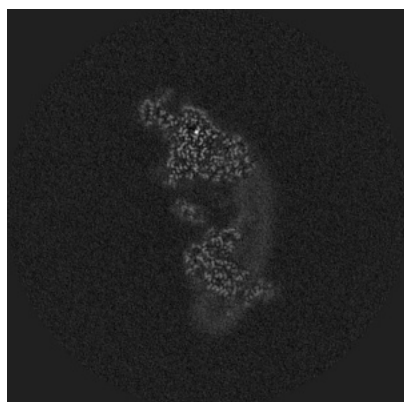


Y Index: 235

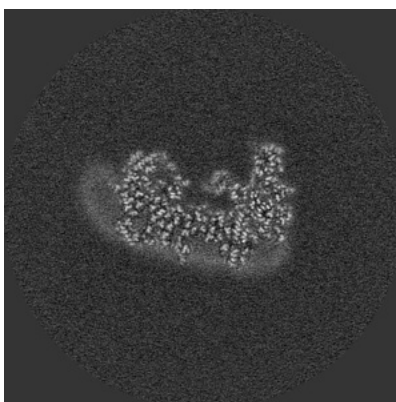


Z Index: 297

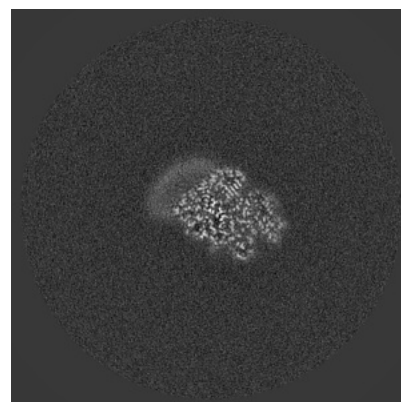
6.3.2 Raw map



X Index: 240



Y Index: 235

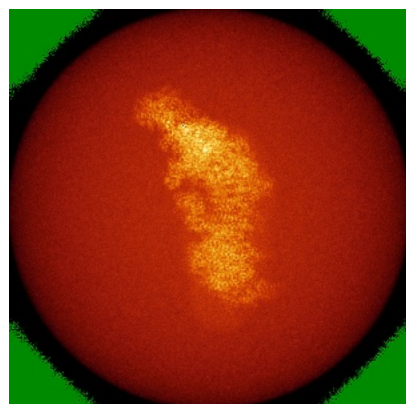


Z Index: 297

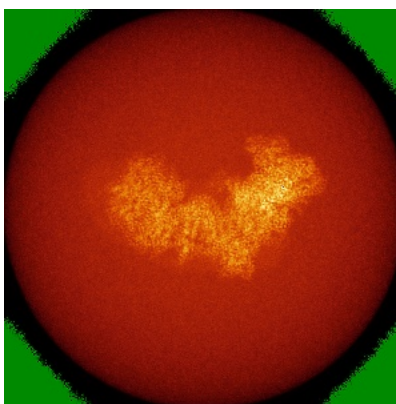
The images above show the largest variance slices of the map in three orthogonal directions.

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

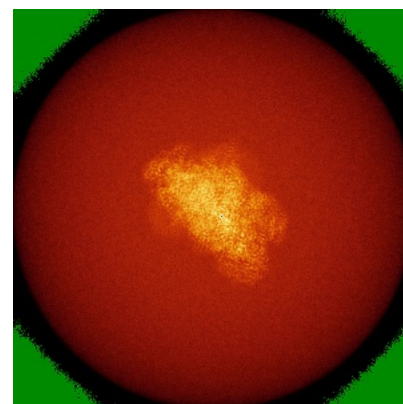
6.4.1 Primary map



X

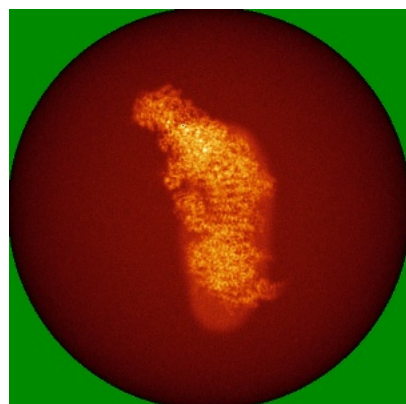


Y

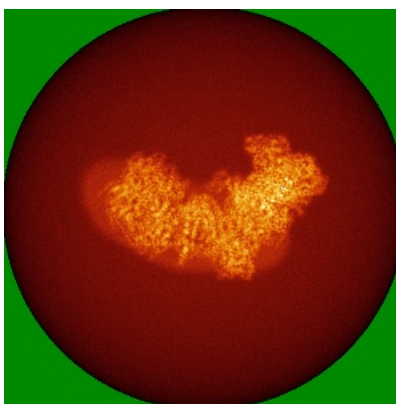


Z

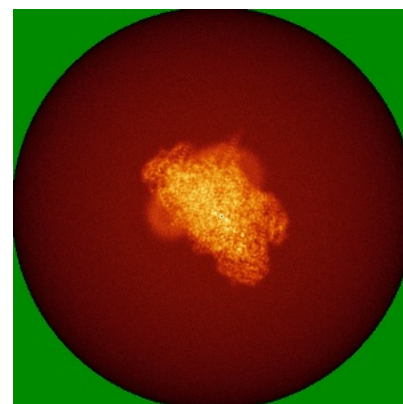
6.4.2 Raw map



X



Y

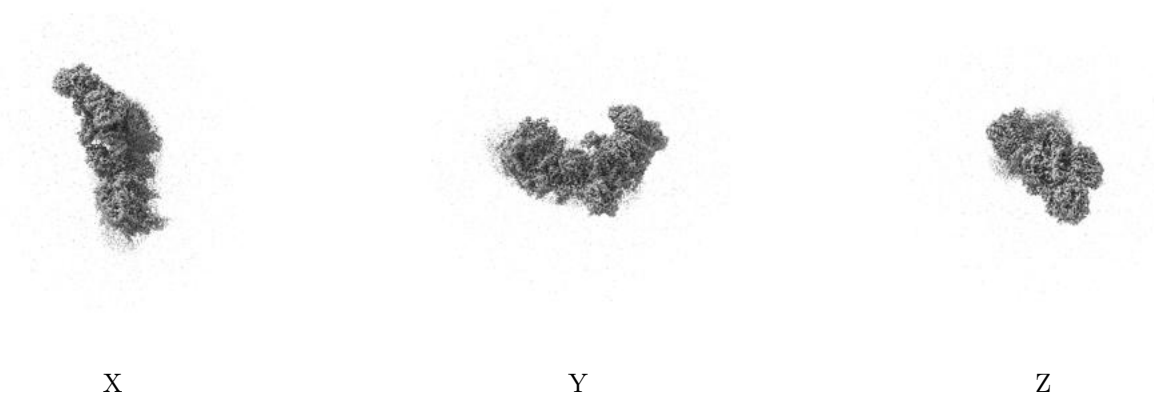


Z

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

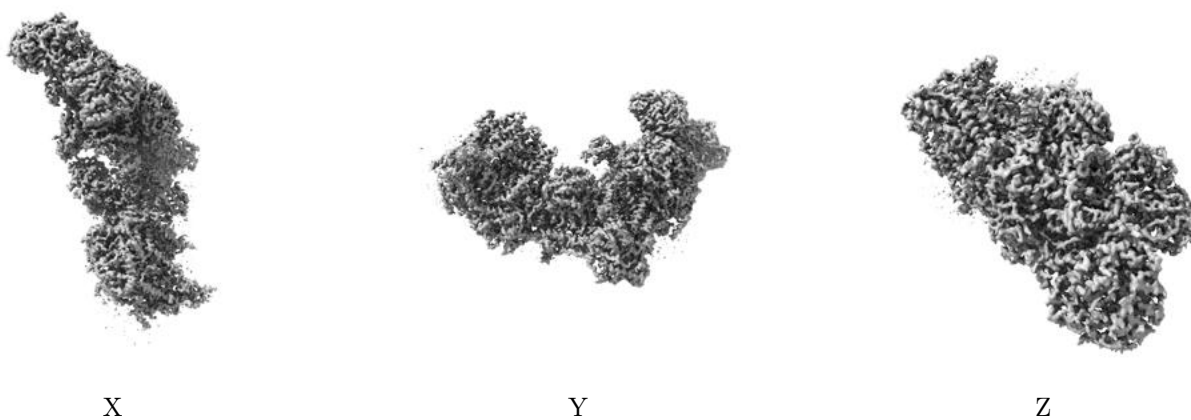
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

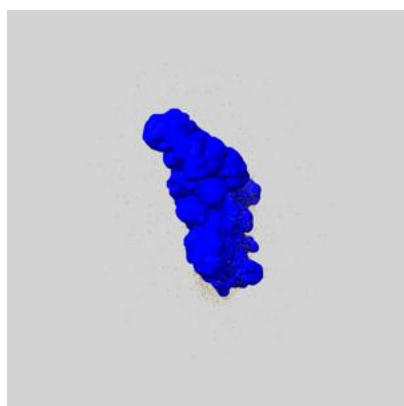
6.6 Mask visualisation [i](#)

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

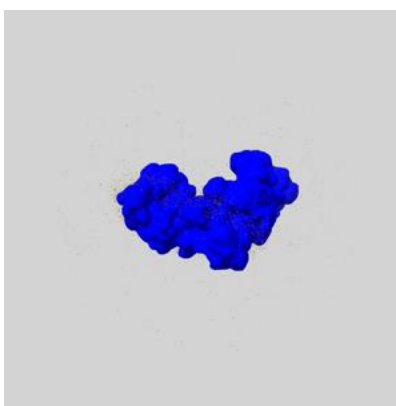
A mask typically either:

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

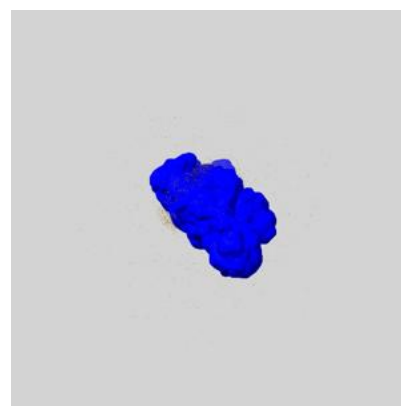
6.6.1 emd_13611_msk_1.map [i](#)



X



Y

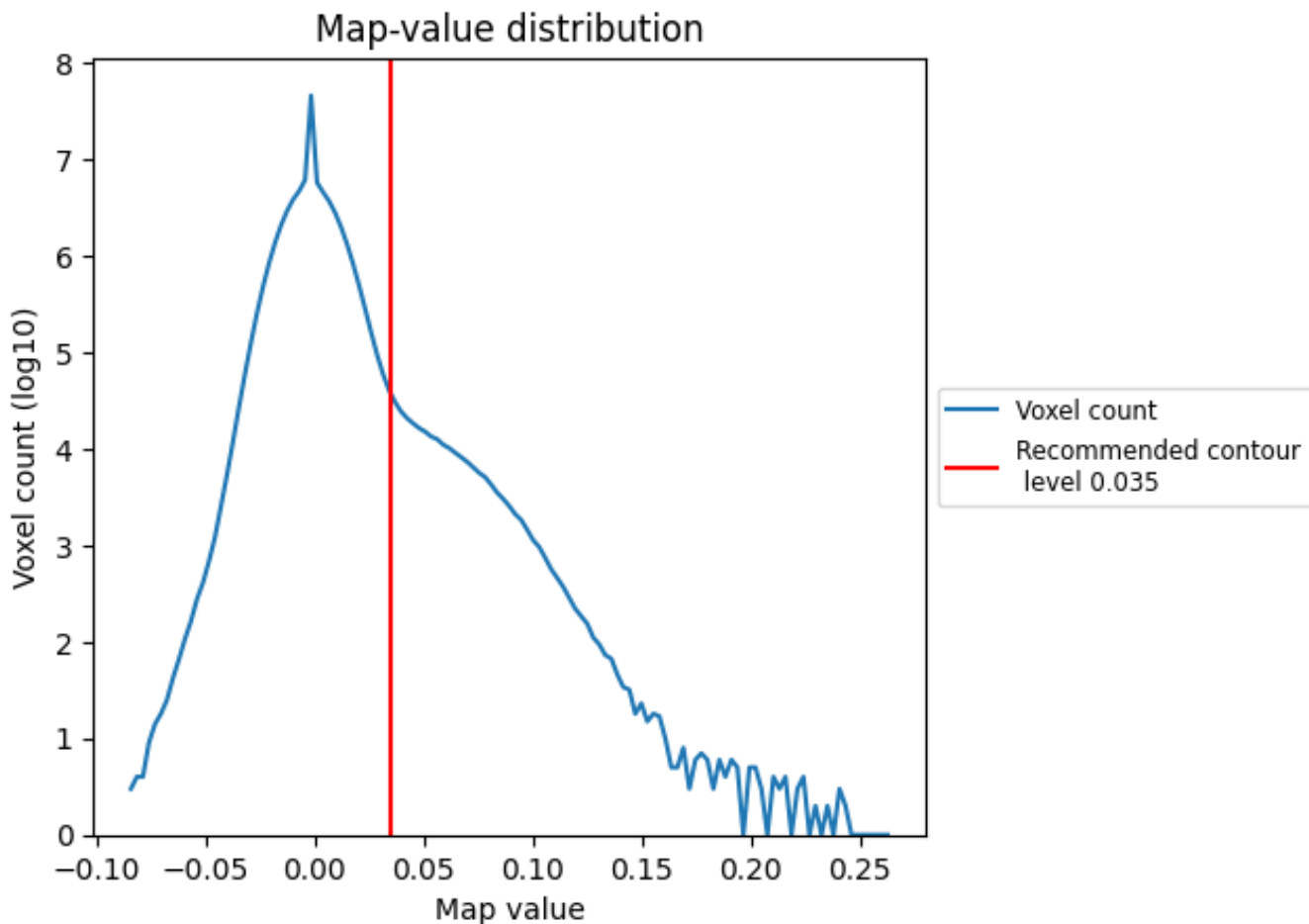


Z

7 Map analysis [i](#)

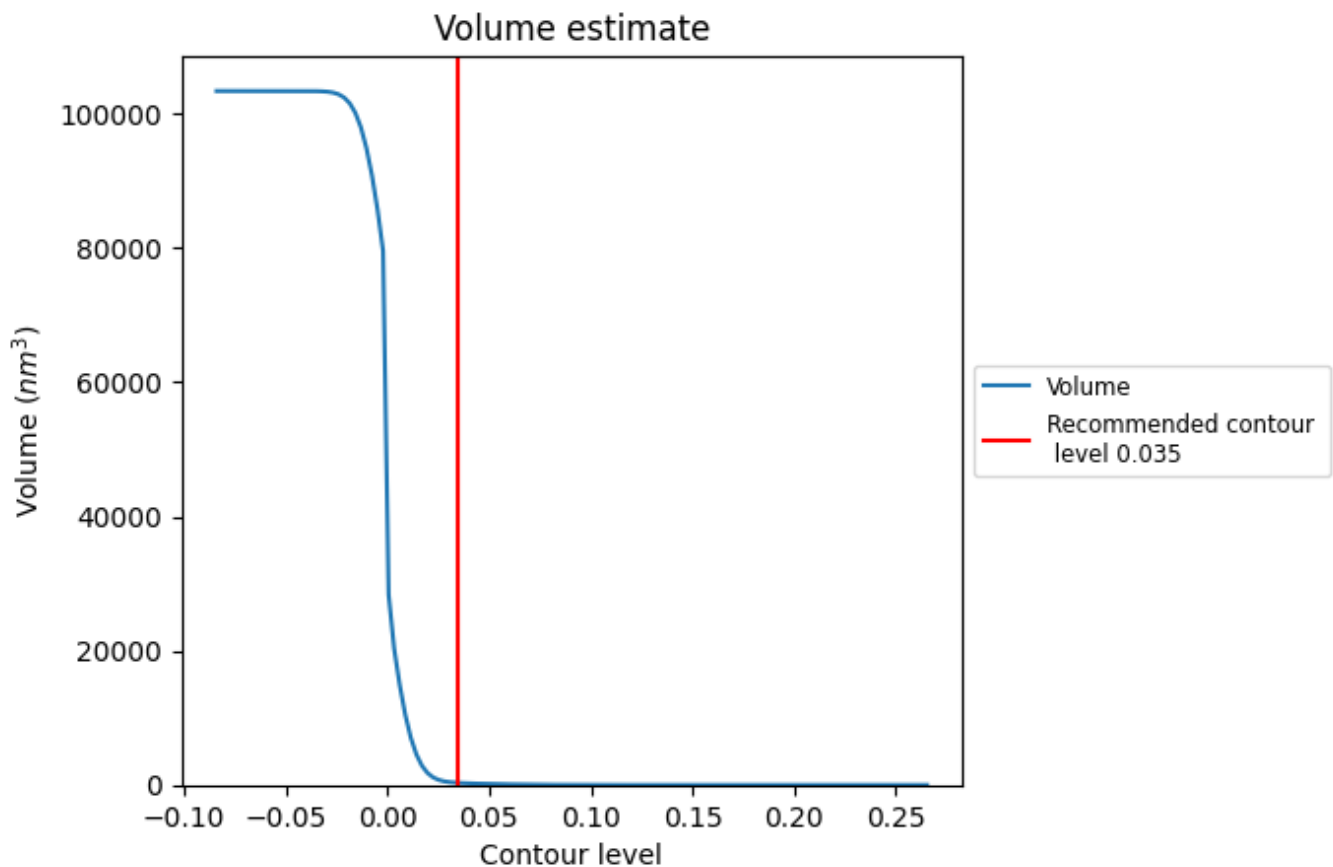
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

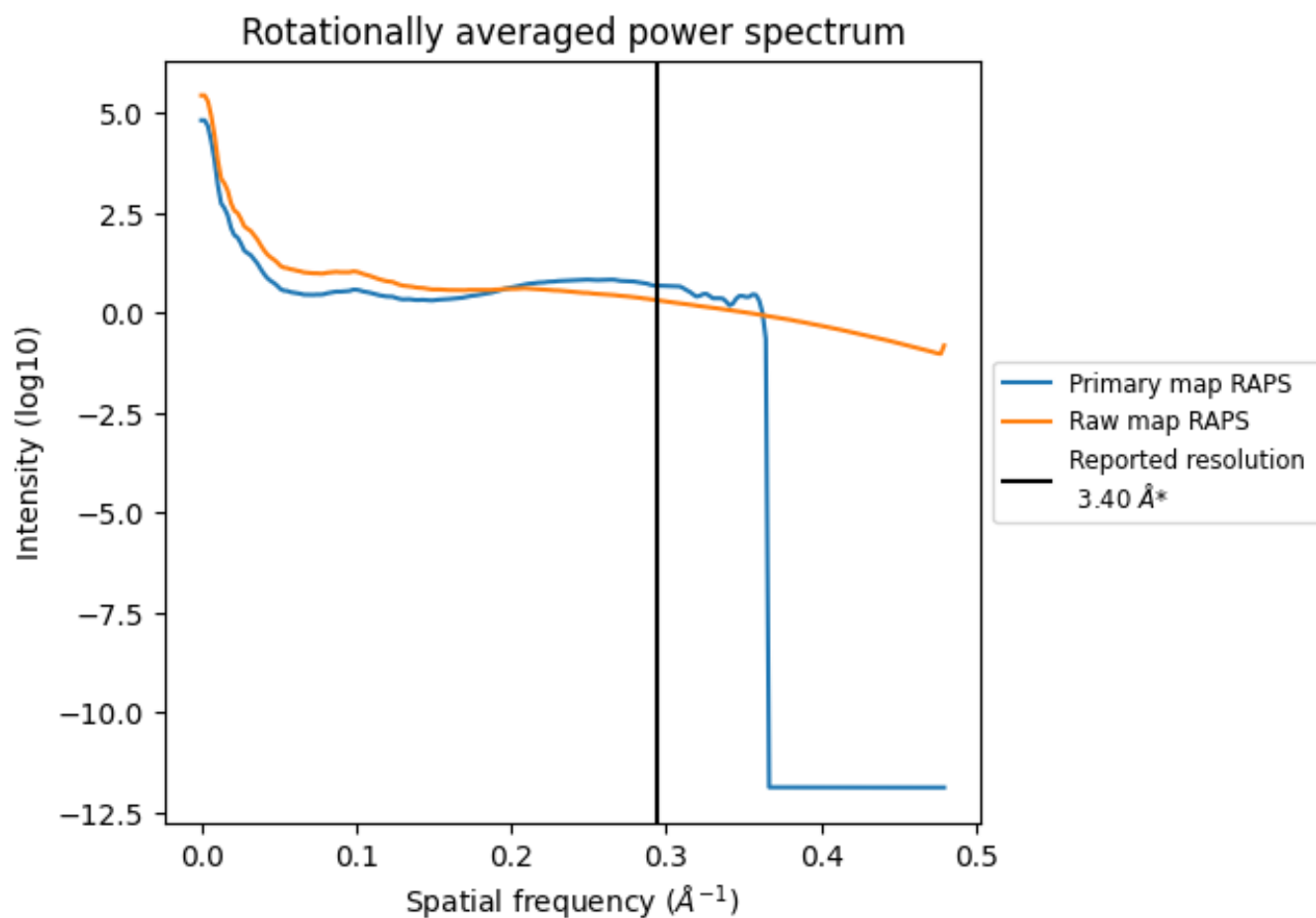
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm^3 ; this corresponds to an approximate mass of 276 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](#)

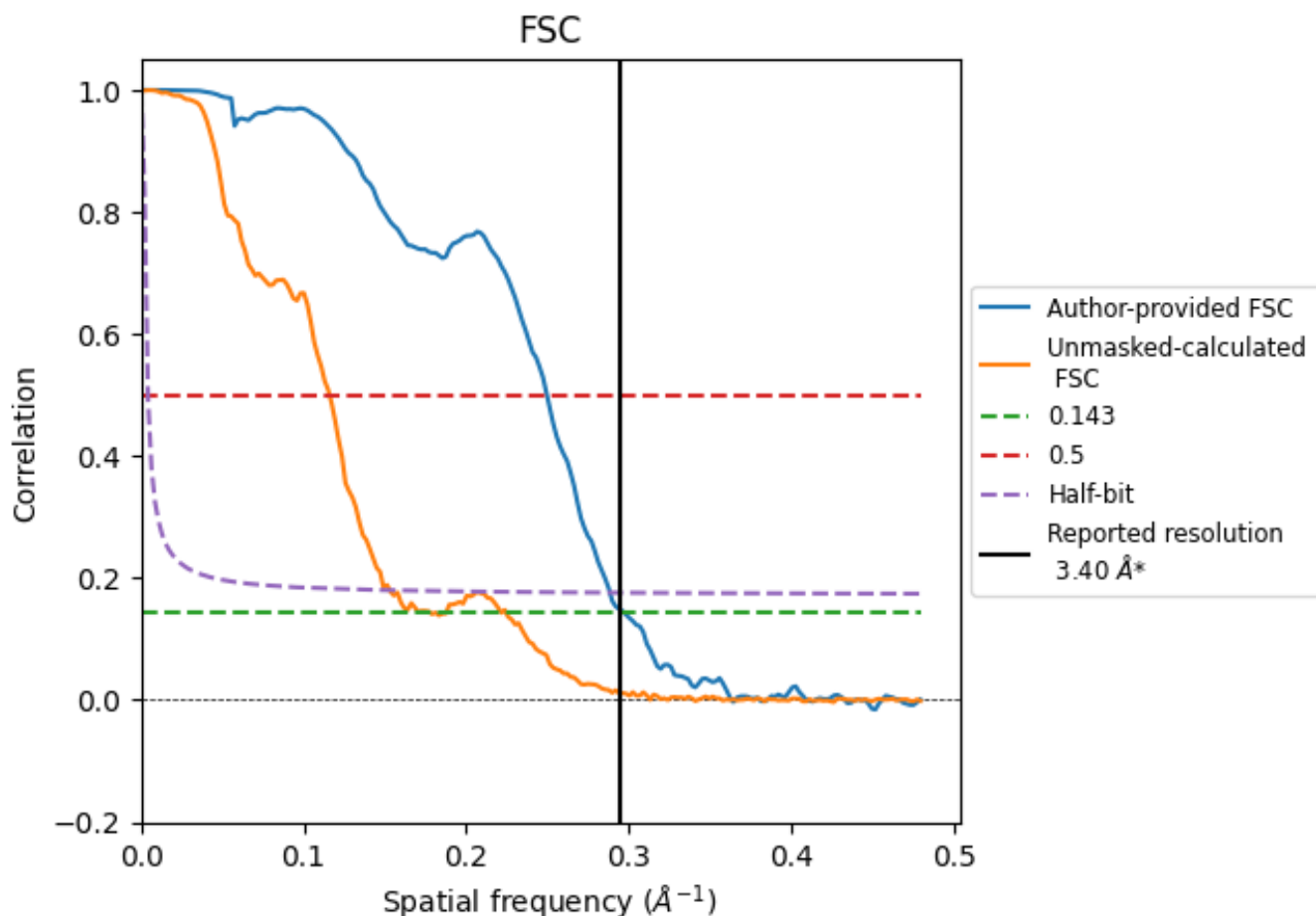


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

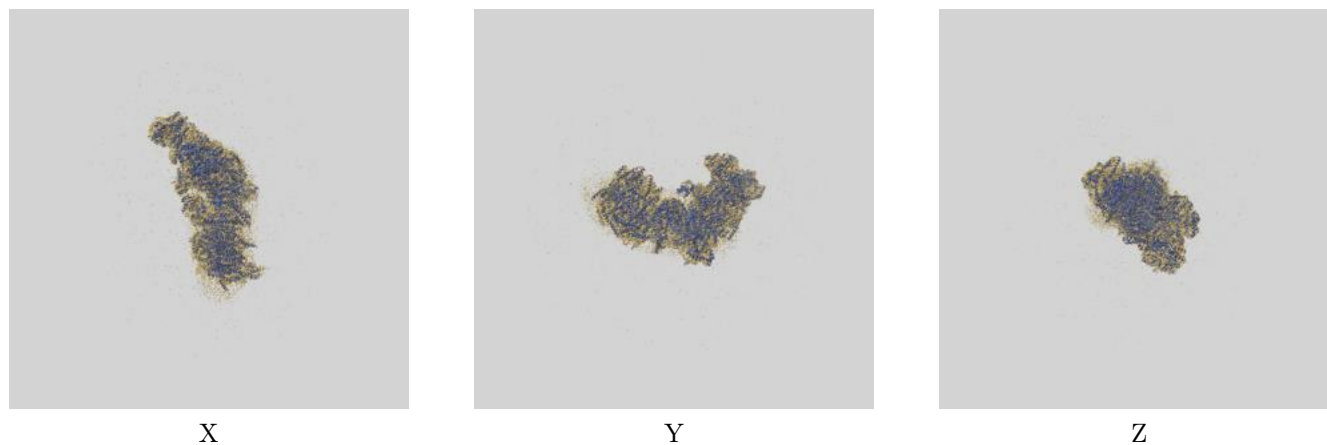
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	4.01	3.47
Unmasked-calculated*	5.62	8.64	6.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.62 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

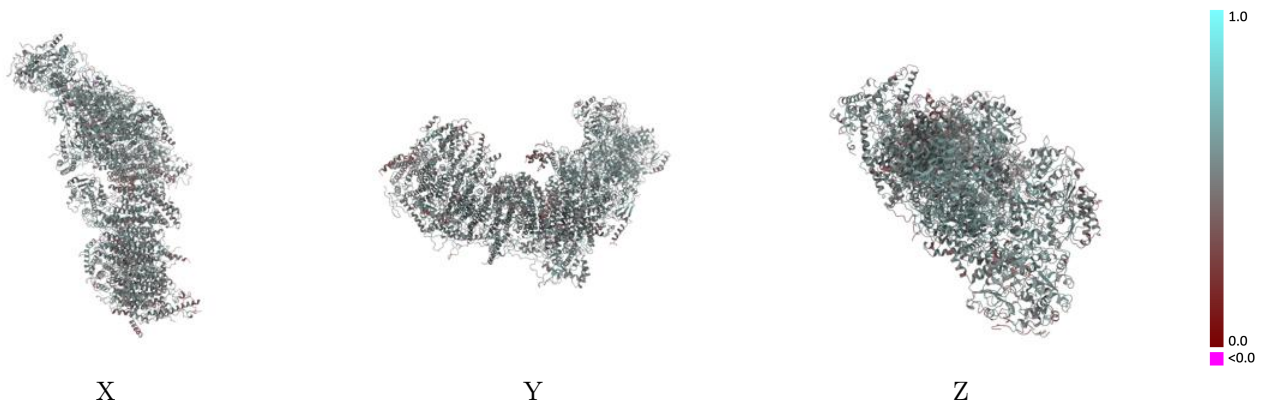
This section contains information regarding the fit between EMDB map EMD-13611 and PDB model 7PSA. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



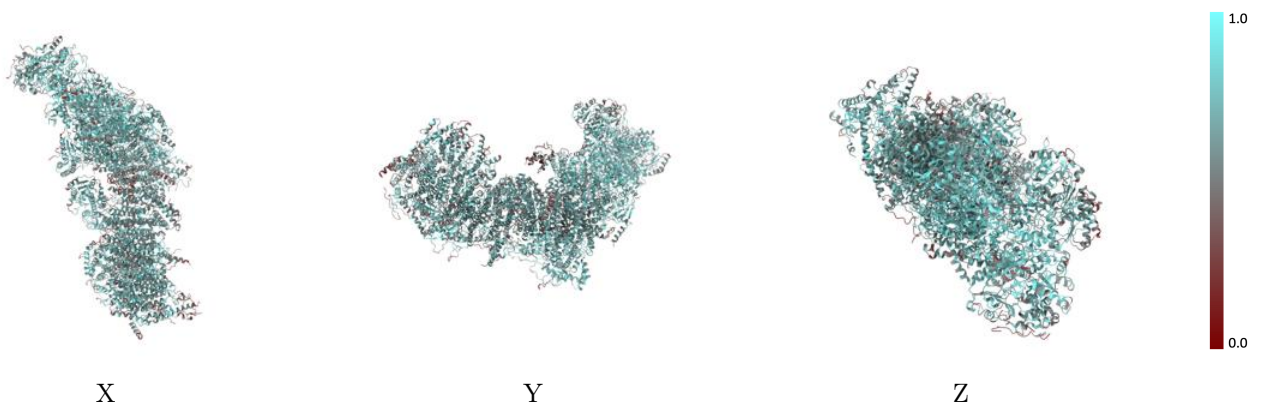
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



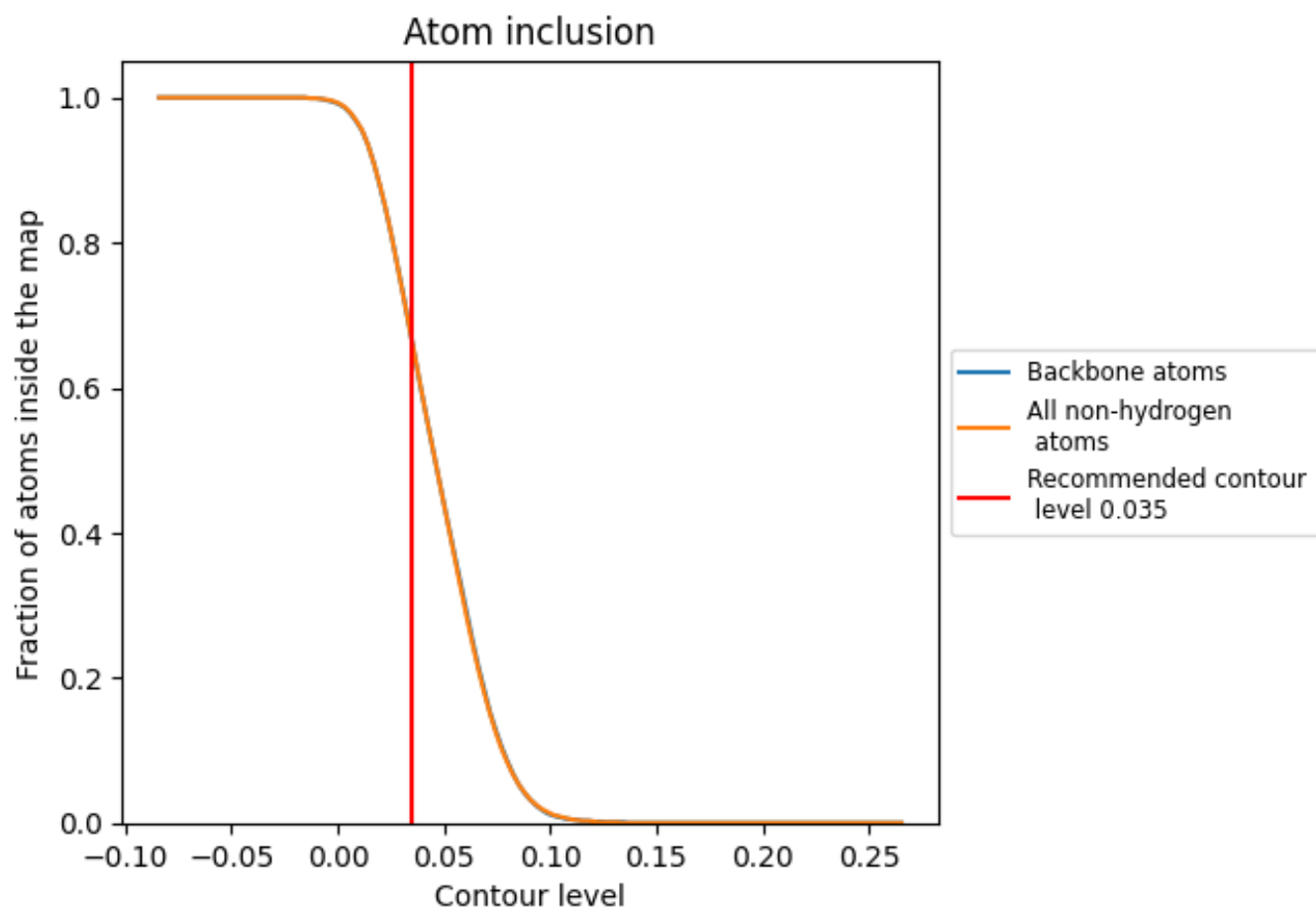
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6630	 0.5160
A	 0.6680	 0.5230
B	 0.7740	 0.5590
C	 0.7680	 0.5570
D	 0.7380	 0.5470
E	 0.6500	 0.4990
F	 0.6760	 0.5100
G	 0.6890	 0.5230
H	 0.6920	 0.5320
I	 0.7640	 0.5460
J	 0.6080	 0.4800
K	 0.6770	 0.5360
L	 0.6550	 0.5180
M	 0.6990	 0.5390
N	 0.6860	 0.5340
O	 0.6980	 0.5290
P	 0.6870	 0.5250
Q	 0.6920	 0.5360
R	 0.7160	 0.5480
S	 0.6020	 0.4820
T	 0.3890	 0.4050
U	 0.5980	 0.4740
V	 0.6320	 0.5060
W	 0.6760	 0.5230
X	 0.6400	 0.4970
Y	 0.5700	 0.4840
Z	 0.6690	 0.5070
a	 0.7260	 0.5320
b	 0.6320	 0.5050
c	 0.5690	 0.4670
d	 0.6520	 0.5160
e	 0.6600	 0.5130
f	 0.5530	 0.4620
g	 0.6260	 0.5080
h	 0.7040	 0.5300



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	 0.5900	 0.4940
j	 0.5650	 0.4560
k	 0.5590	 0.4620
l	 0.6590	 0.5050
m	 0.6140	 0.4750
n	 0.6300	 0.4940
o	 0.5650	 0.4490
p	 0.6450	 0.4930
q	 0.7040	 0.5310
r	 0.6230	 0.5010
s	 0.6330	 0.5040