



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:26 PM UTC

PDB ID : 8Q0Q / pdb_00008q0q
EMDB ID : EMD-18059
Title : Outward-facing, slack proteoliposome complex I at 3.6 Å. Initially purified in DDM
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-07-28
Resolution : 3.60 Å (reported)
Based on initial model : 7QSO

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

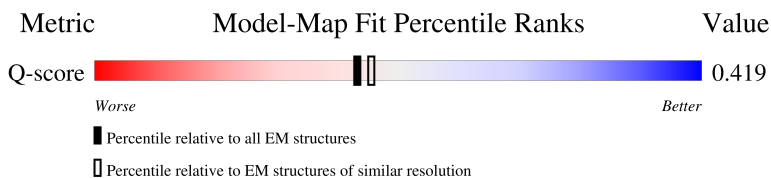
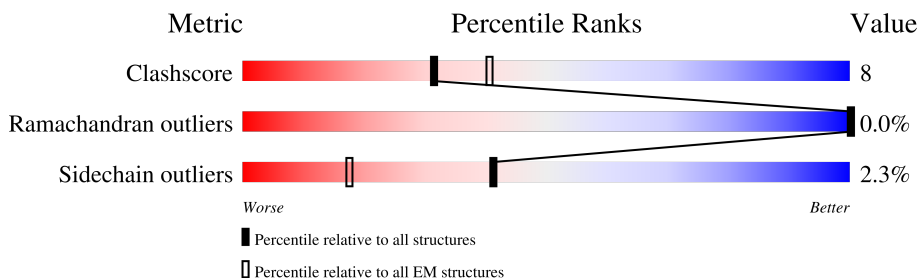
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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.



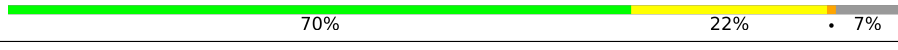
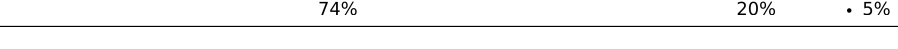
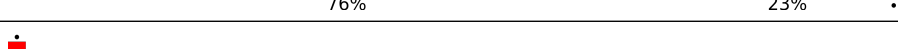
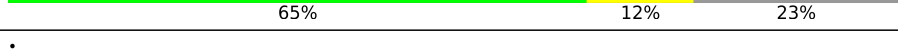
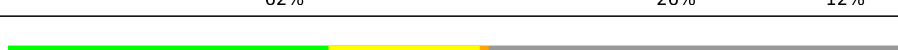
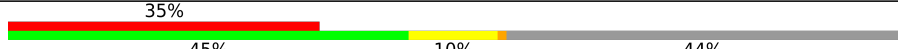
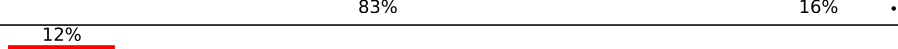
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	217187	24013	-
Ramachandran outliers	211220	23611	-
Sidechain outliers	210688	23127	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	 67% 22% 10%
2	B	216	 62% 12% 27%
3	C	266	 60% 18% 21%
4	D	463	 67% 16% 16%

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Mol	Chain	Length	Quality of chain
5	E	249	
6	F	464	
7	G	727	
8	H	318	
9	I	212	
10	J	175	
11	K	98	
12	L	606	
13	M	459	
14	N	347	
15	O	343	
16	P	380	
17	Q	175	
18	R	124	
19	S	99	
20	T	156	
20	U	156	
21	V	116	
22	W	128	
23	X	172	
24	Y	141	
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	154	
33	h	189	
34	i	128	
35	j	108	
36	k	98	
37	l	186	
38	m	129	
39	n	179	
40	o	137	
41	p	176	
42	q	145	
43	r	113	
44	s	109	

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
47	SF4	B	202	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 65579 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	104	Total	C	N	O	S	0	0
			842	575	119	143	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	158	Total	C	N	O	S	0	0
			1260	803	227	216	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	210	Total	C	N	O	S	0	0
			1743	1123	299	318	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	388	Total	C	N	O	S	0	0
			3110	1984	538	564	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	variant	UNP P17694

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1659	1059	278	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	432	Total	C	N	O	S	0	0
			3324	2094	594	616	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	689	Total	C	N	O	S	0	0
			5284	3310	921	1014	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	318	Total	C	N	O	S	0	0
			2509	1681	385	420	23		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	160	Total	C	N	O	S	0	0
			1219	823	172	212	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	86	Total	C	N	O	S	0	0
			647	425	96	111	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	547	Total	C	N	O	S	0	0
			4334	2880	667	746	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3654	2436	570	609	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	347	Total	C	N	O	S	0	0
			2733	1817	416	457	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2589	1662	429	488	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	255	LYS	ASN	variant	UNP P34942

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	320	Total	C	N	O	S	0	0
			2560	1652	452	451	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1016	641	181	191	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	96	Total	C	N	O	S	0	0
			740	454	140	143	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	87	Total	C	N	O	S	0	0
			701	439	133	127	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	84	Total	C	N	O	S	0	0
			681	439	100	137	5		
20	U	88	Total	C	N	O	S	0	0
			707	454	104	144	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	113	Total	C	N	O	S	0	0
			919	595	155	166	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	115	Total	C	N	O	S	0	0
			977	625	181	167	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1402	887	253	252	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	33	Total	C	N	O	S	0	0
			248	162	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	142	Total	C	N	O	S	0	0
			1157	743	202	203	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	70	Total	C	N	O	S	0	0
			569	365	104	95	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			654	427	109	116	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	c	48	Total	C	N	O	0	0
			405	268	69	68		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	120	Total	C	N	O	S	0	0
			999	650	172	172	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	99	Total	C	N	O	S	0	0
			829	523	158	142	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	57	Total	C	N	O	S	0	0
			492	322	86	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	90	Total	C	N	O	S	0	0
			750	483	124	139	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	143	Total	C	N	O	S	0	0
			1186	776	203	205	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	127	Total	C	N	O	S	0	0
			1097	722	191	183	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	70	Total	C	N	O	S	0	0
			592	387	98	106	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	81	Total	C	N	O	S	0	0
			653	427	110	114	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1314	850	216	240	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	128	Total	C	N	O	S	0	0
			1070	686	188	196			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	171	Total	C	N	O	S	0	0
			1487	952	272	256	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	120	Total	C	N	O	S	0	0
			1035	645	199	183	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	173	Total	C	N	O	S	0	0
			1455	912	268	267	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	145	Total	C	N	O	S	0	0
			1212	780	216	211	5		

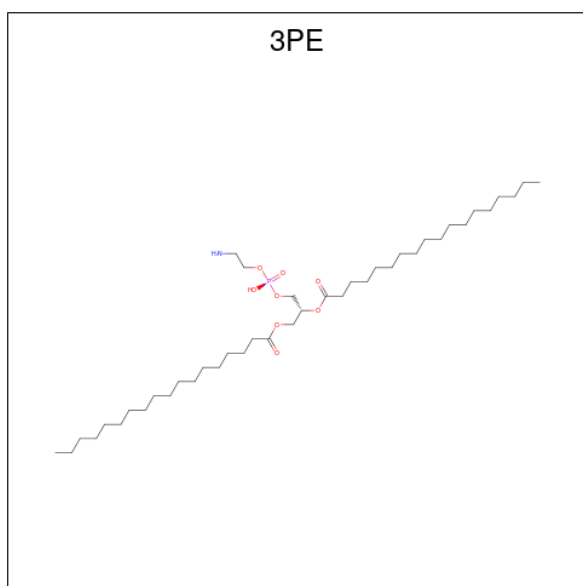
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	96	Total	C	N	O	S	0	0
			785	496	146	140	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	45	Total	C	N	O	S	0	0
			380	238	67	74	1		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



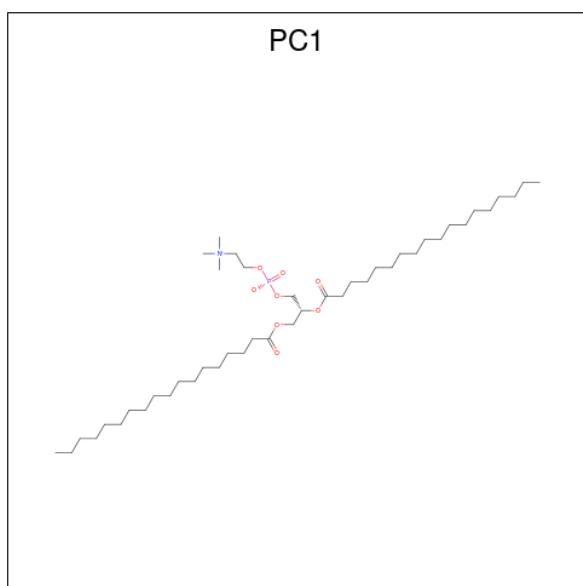
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	I	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	J	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	M	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	M	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	O	1	Total	C	N	O	P	0
			35	25	1	8	1	

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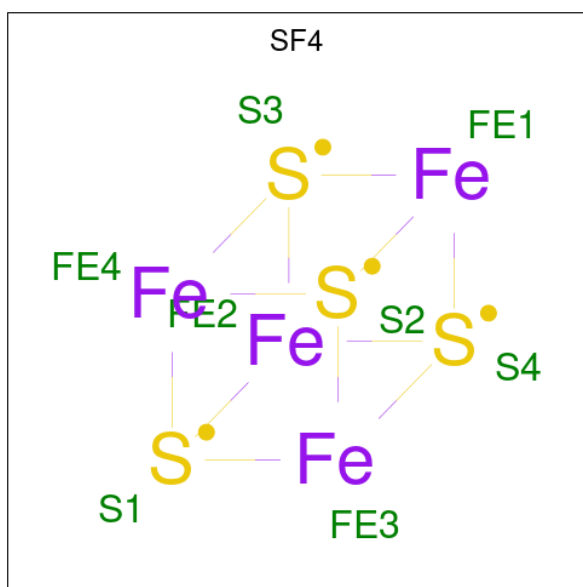
Mol	Chain	Residues	Atoms					AltConf
45	Z	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	h	1	Total	C	N	O	P	0
			32	22	1	8	1	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



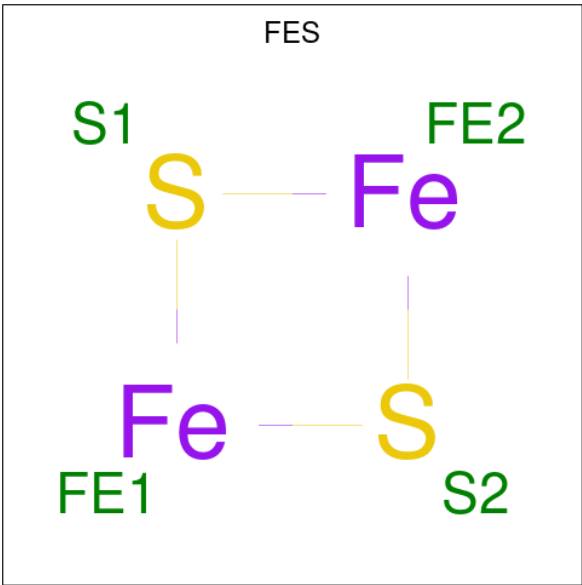
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
46	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	H	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	d	1	Total	C	N	O	P	0
			33	23	1	8	1	
46	q	1	Total	C	N	O	P	0
			37	27	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



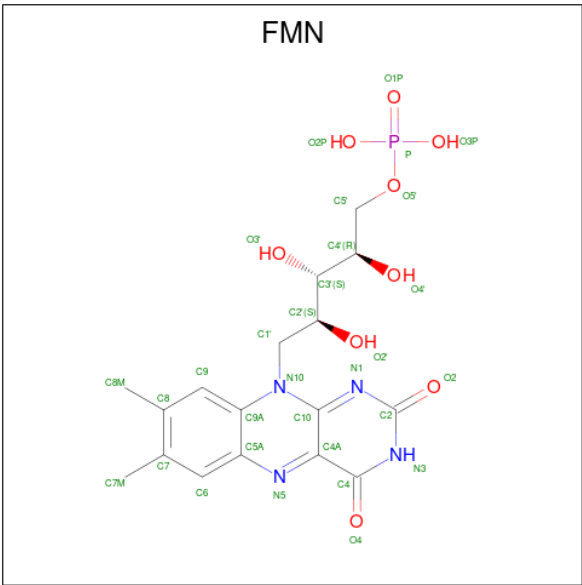
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
48	E	1	Total	Fe	S	0
			4	2	2	
48	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).

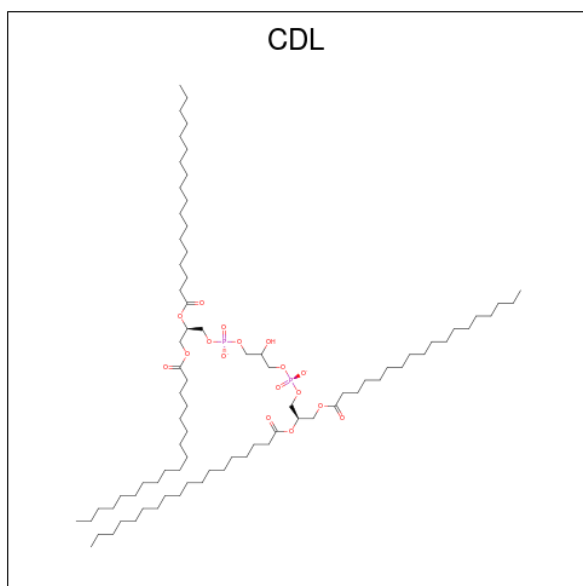


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

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



Mol	Chain	Residues	Atoms				AltConf
51	N	1	Total	C	O	P	0
			73	54	17	2	
51	X	1	Total	C	O	P	0
			79	60	17	2	
51	d	1	Total	C	O	P	0
			65	46	17	2	
51	q	1	Total	C	O	P	0
			60	41	17	2	

- Molecule 52 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
52	O	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
53	O	1	Total Mg 1 1	0

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).

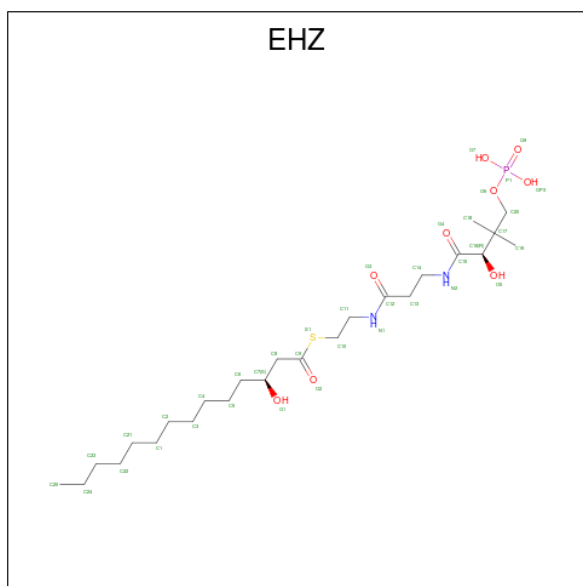


Mol	Chain	Residues	Atoms					AltConf
54	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

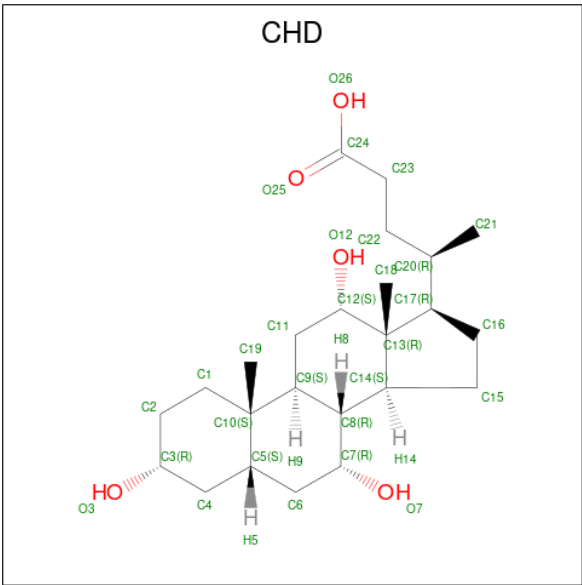
Mol	Chain	Residues	Atoms		AltConf
55	R	1	Total	Zn	0
			1	1	

- Molecule 56 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



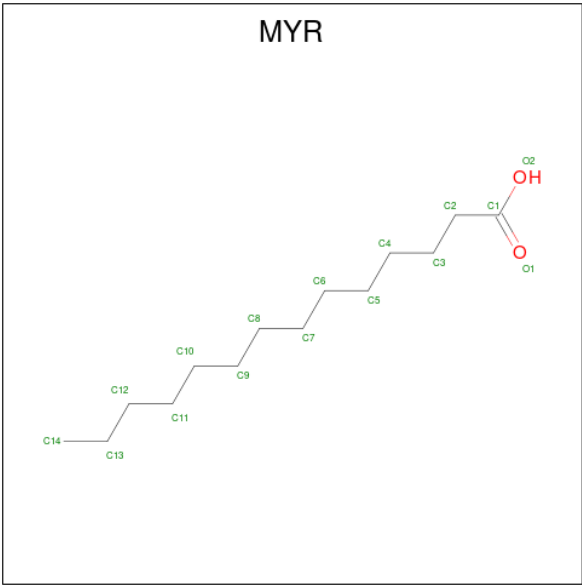
Mol	Chain	Residues	Atoms						AltConf
56	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
56	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 57 is CHOLIC ACID (CCD ID: CHD) (formula: C₂₄H₄₀O₅).



Mol	Chain	Residues	Atoms			AltConf
57	i	1	Total	C	O	0
			29	24	5	

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).

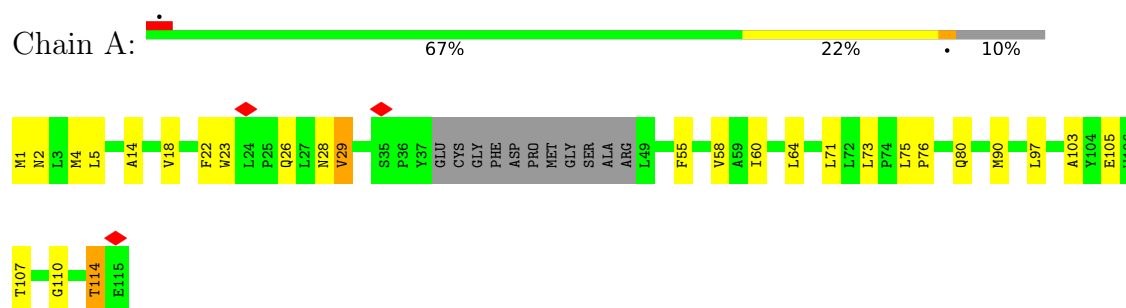


Mol	Chain	Residues	Atoms			AltConf
58	o	1	Total	C	O	0
			15	14	1	

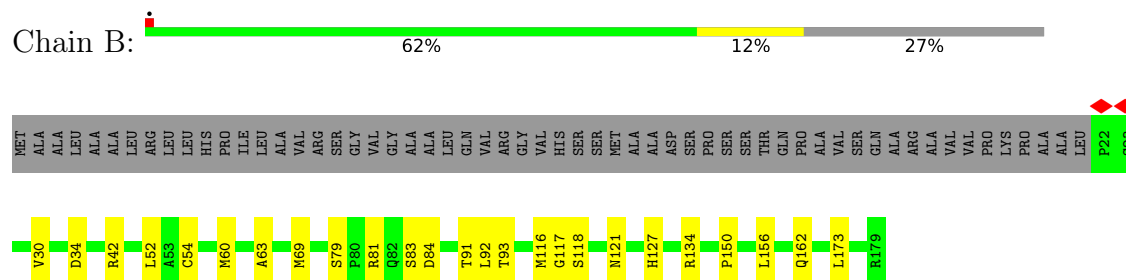
3 Residue-property plots [i](#)

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

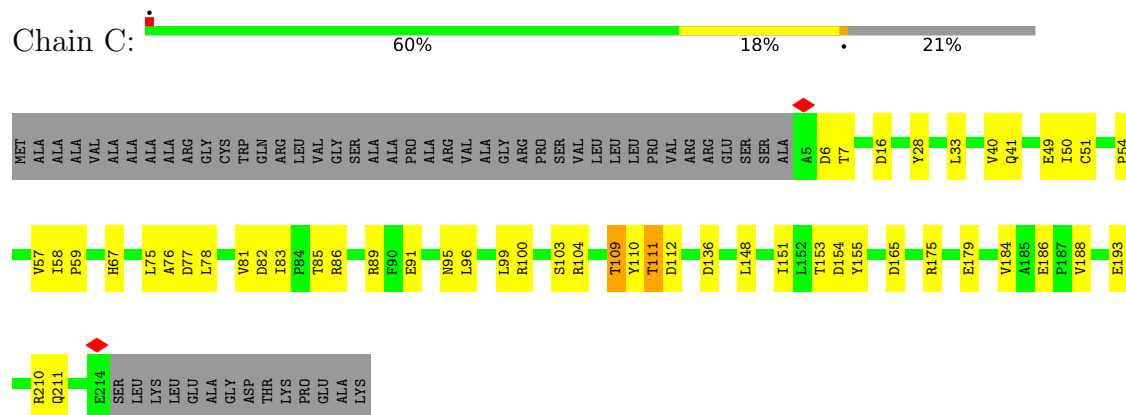
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



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

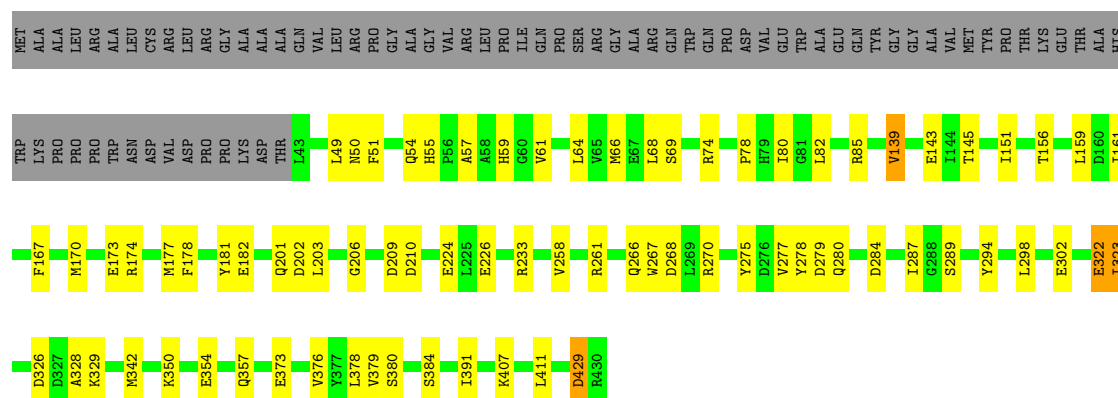


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



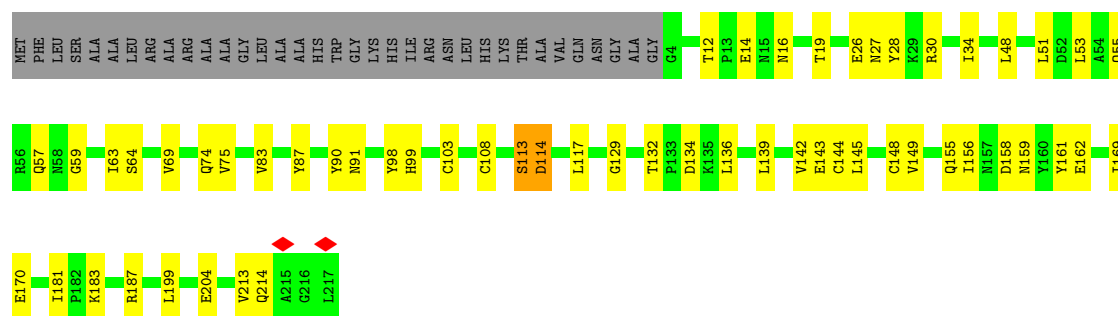
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:  67% 16% 16%



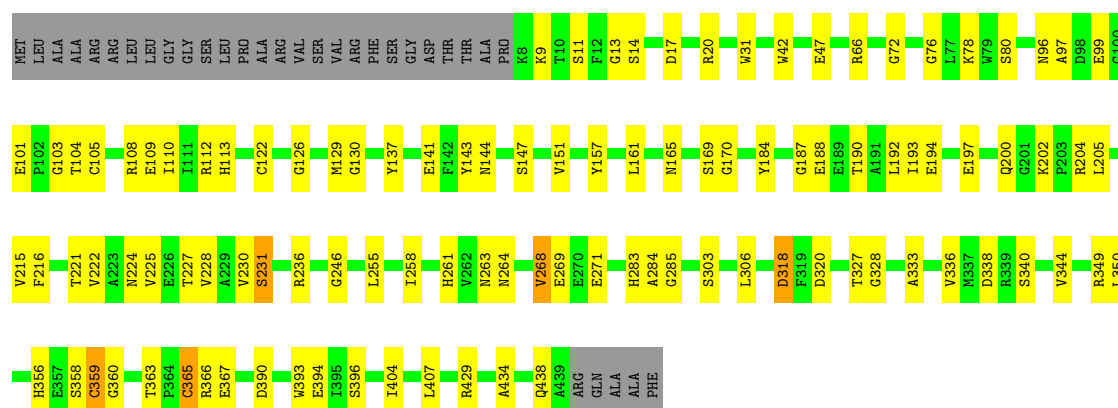
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:  63% 22% 14%



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

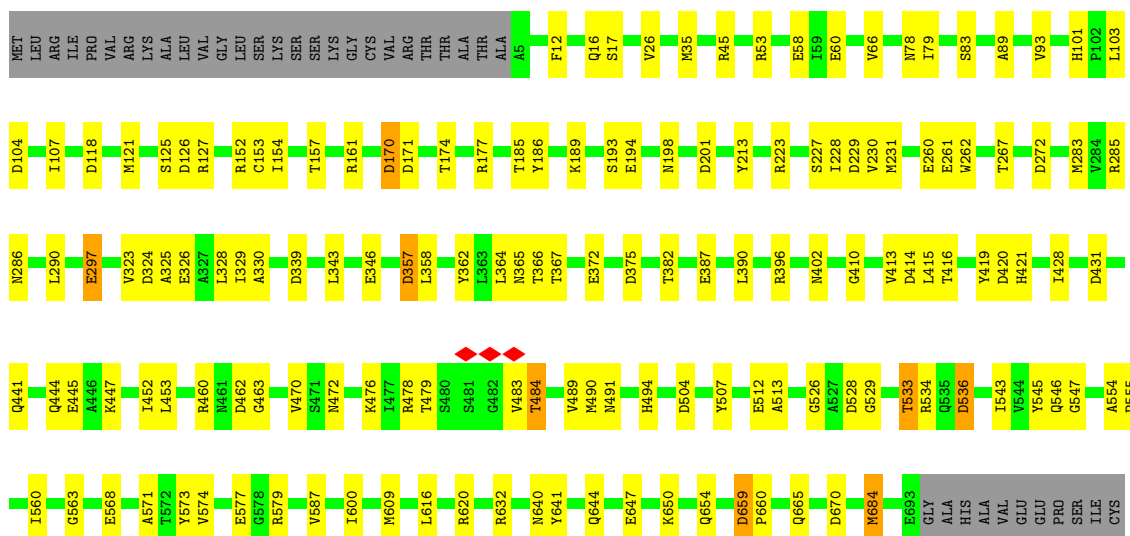
Chain F:  70% 22% 7%



- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

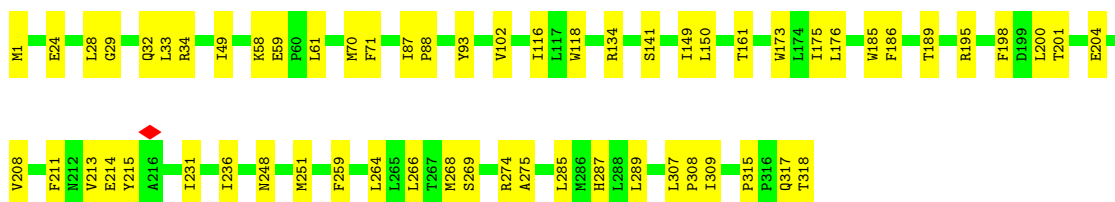
Chain G:  74% 20% 5%





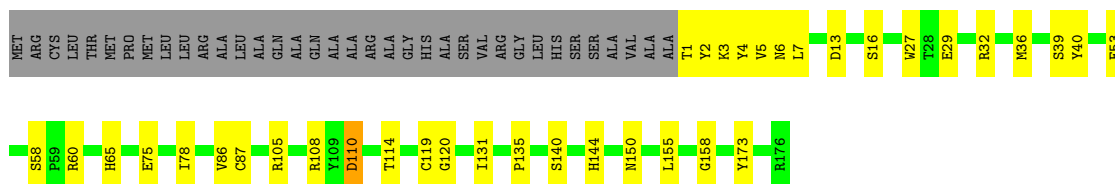
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 81% 19%



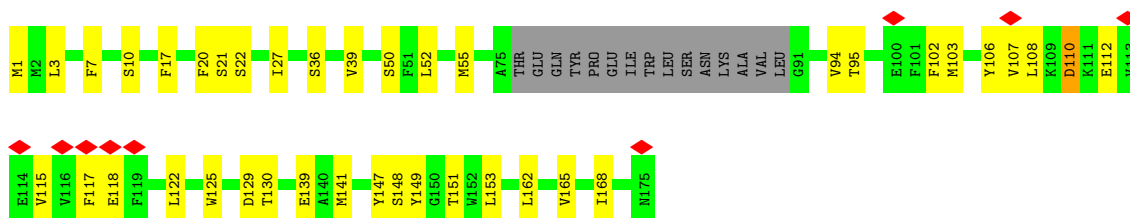
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I: 66% 17% 17%



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

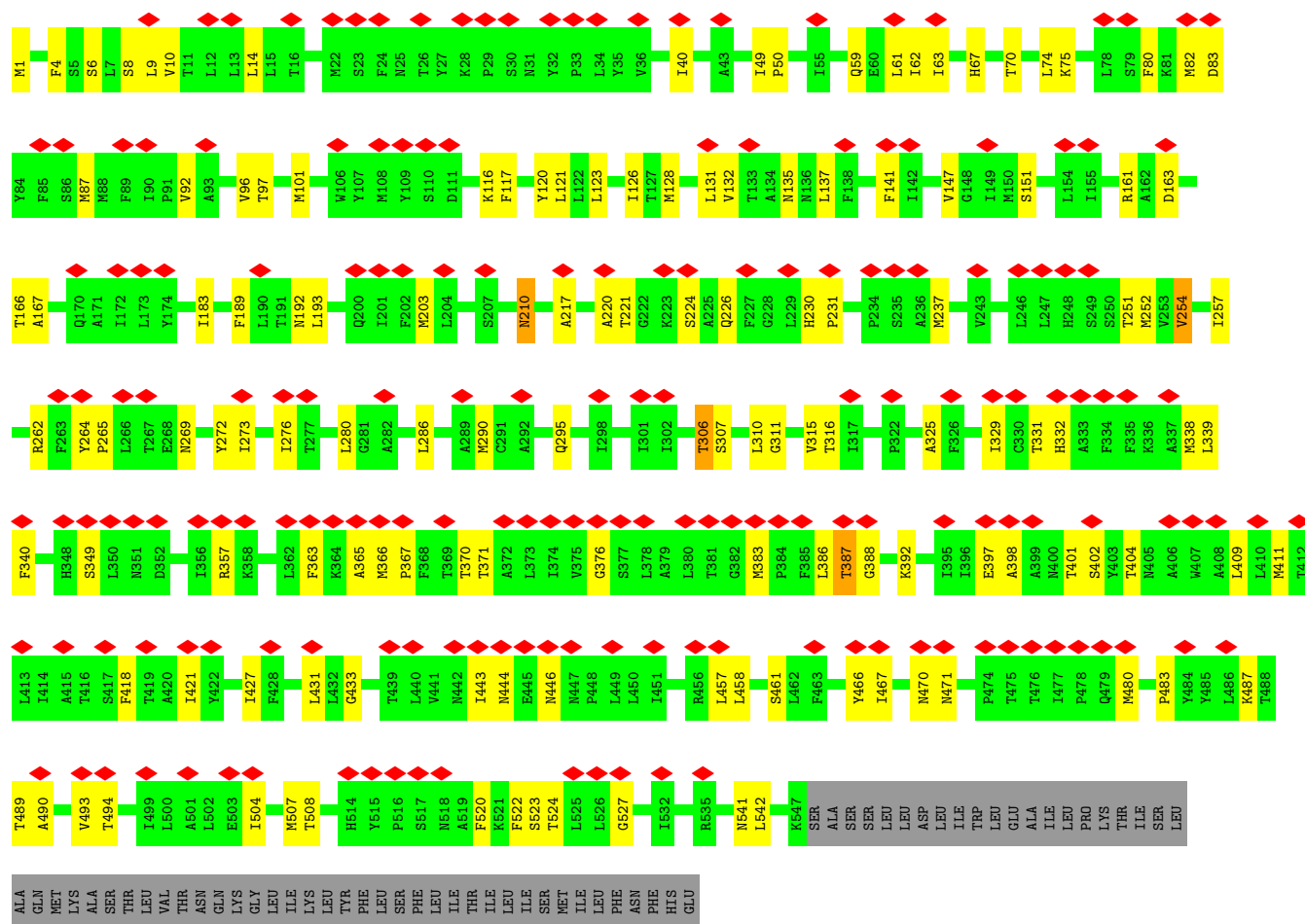
Chain J: 5% 69% 22% 9%



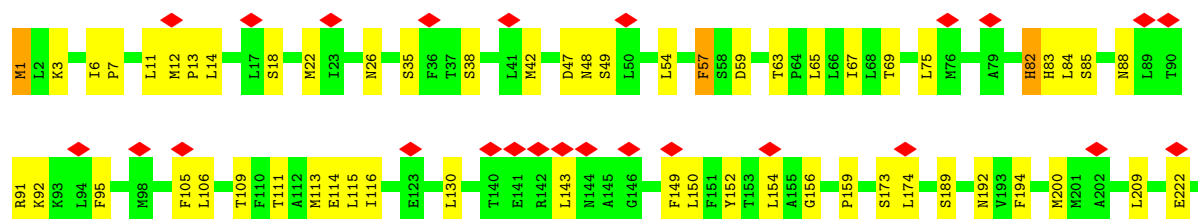
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

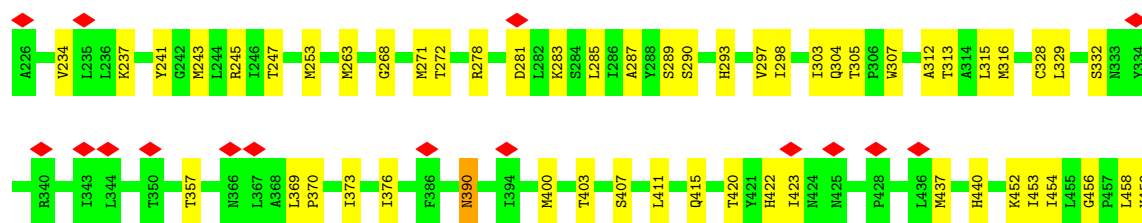


Chain L: 30% 67% 22% 10%



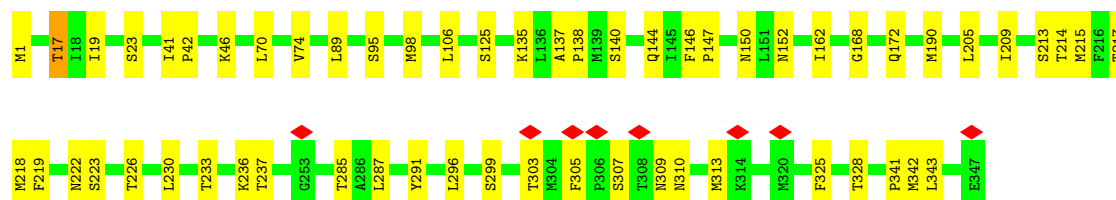
Chain M:





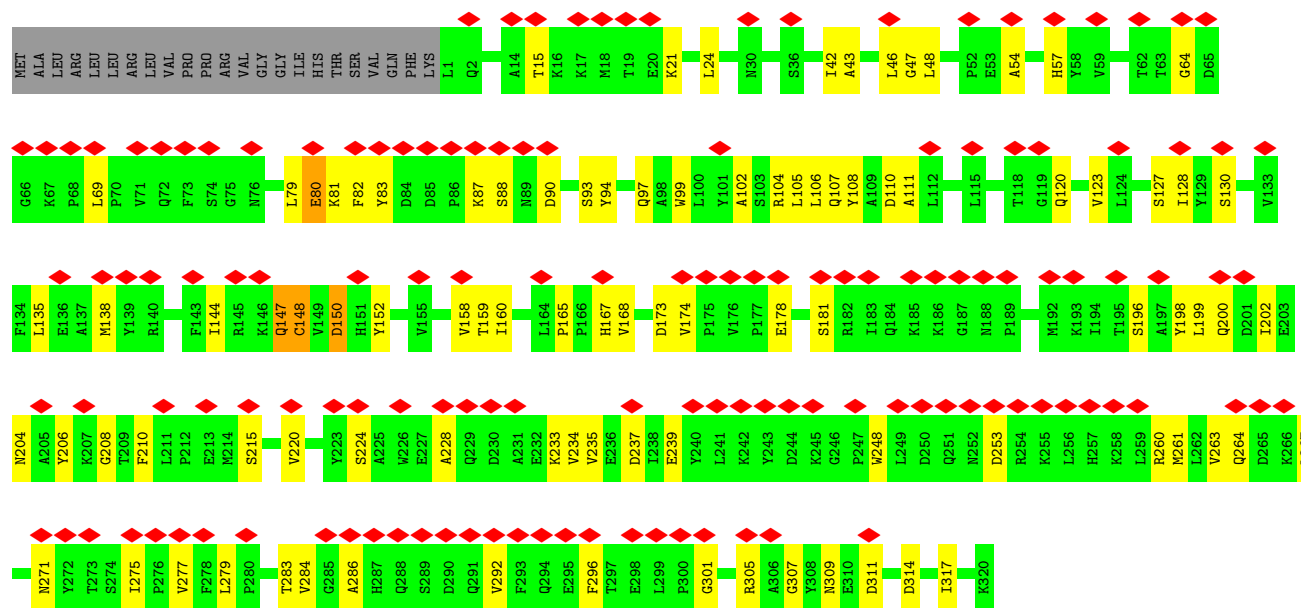
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 83% 16%



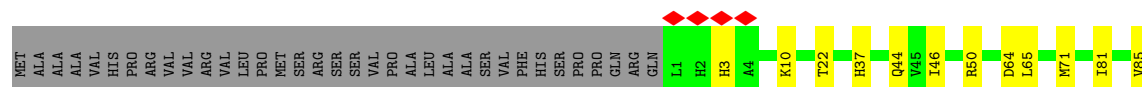
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

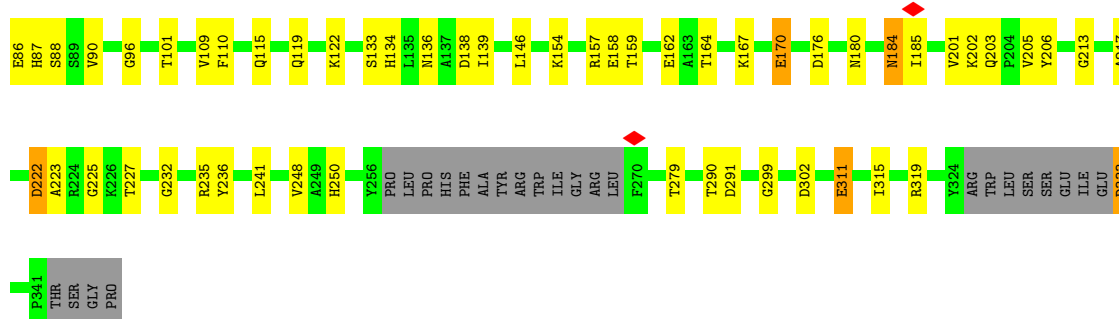
Chain O: 40% 66% 27% 7%



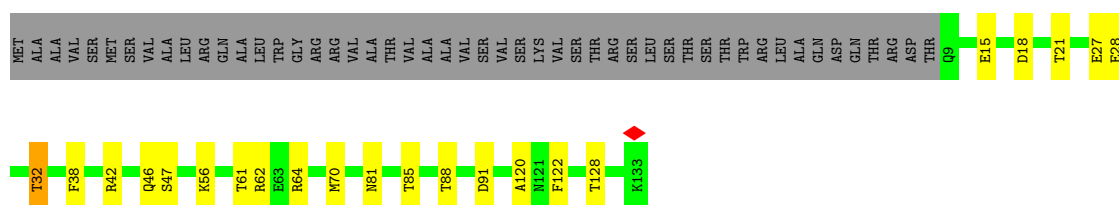
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 67% 16% 16%

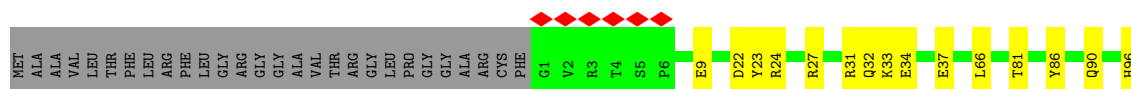




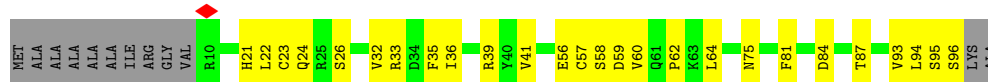
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



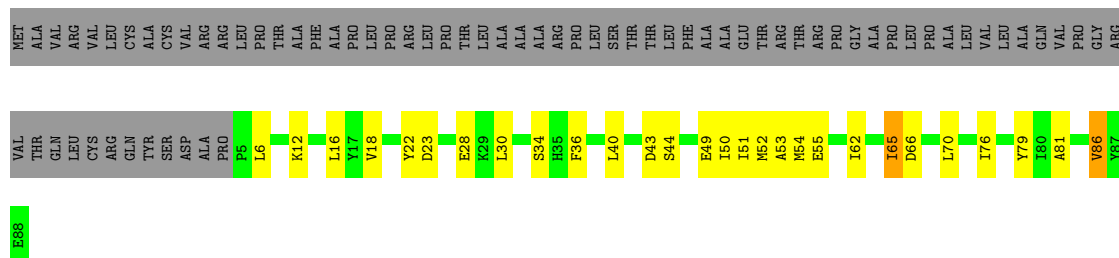
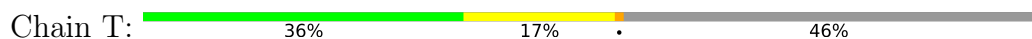
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



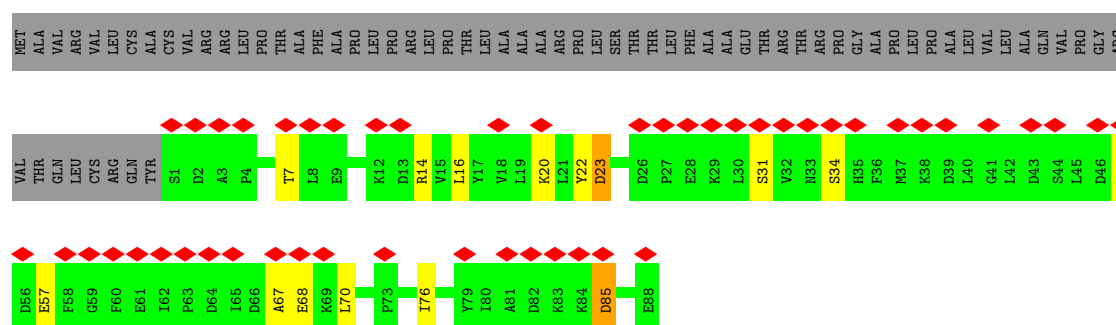
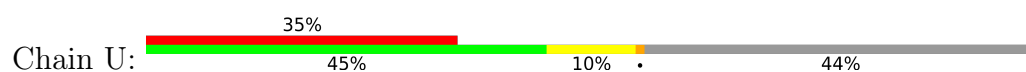
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



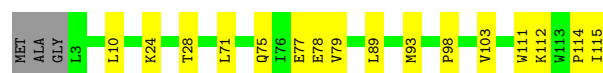
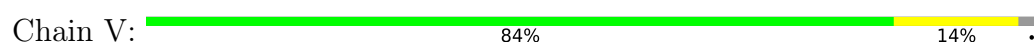
- Molecule 20: Acyl carrier protein, mitochondrial



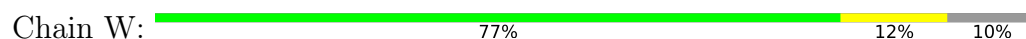
- Molecule 20: Acyl carrier protein, mitochondrial



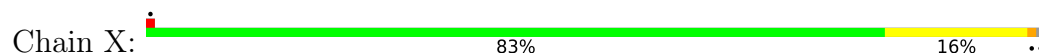
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



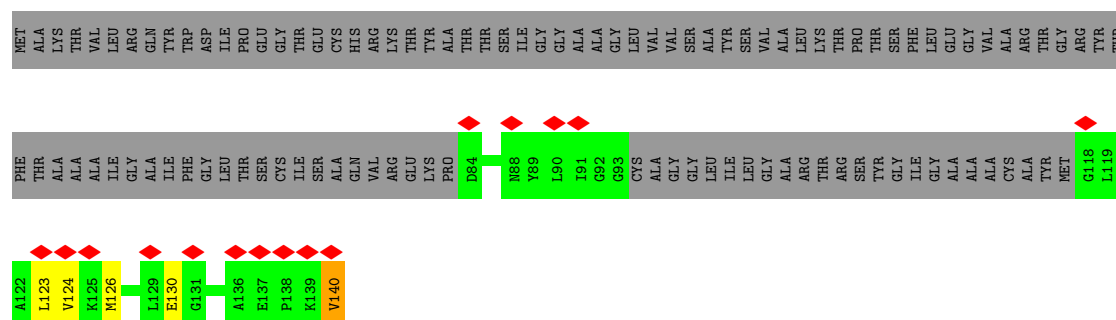
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



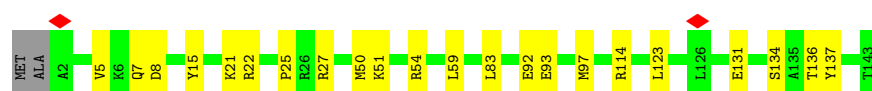
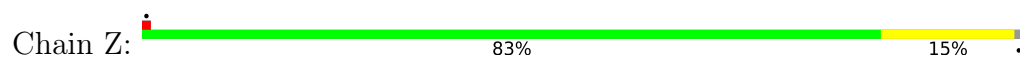
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



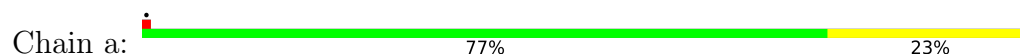
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



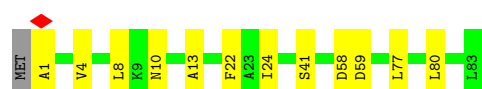
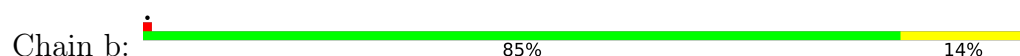
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



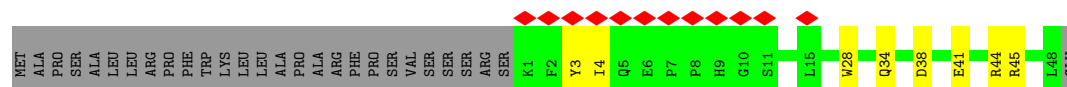
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



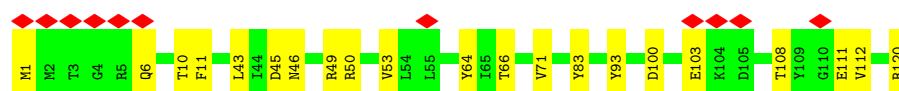
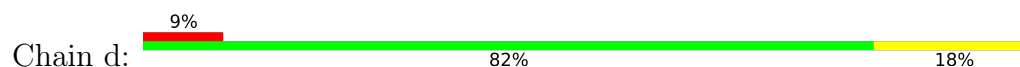
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



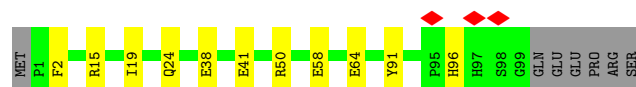
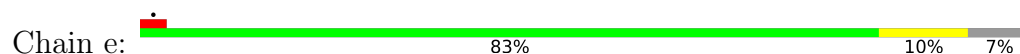
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



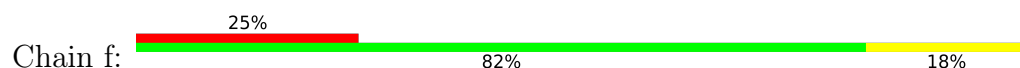
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

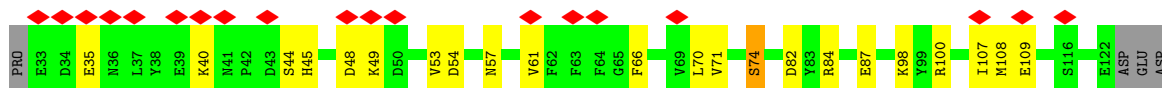
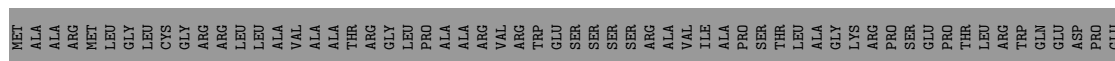


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

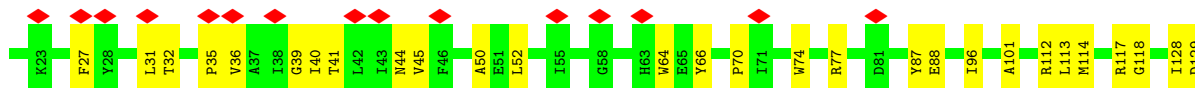
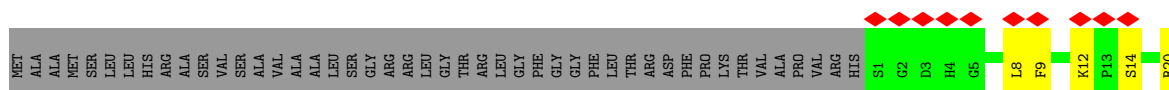




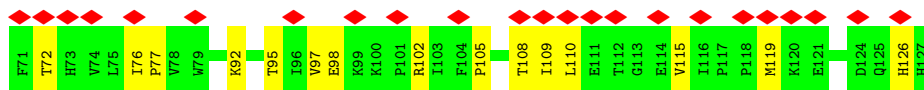
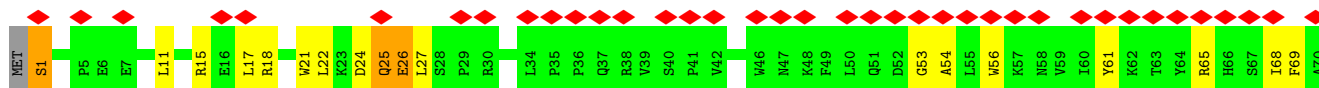
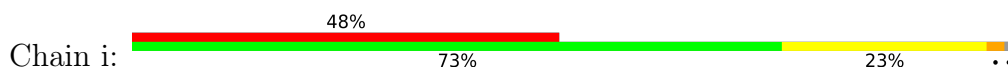
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



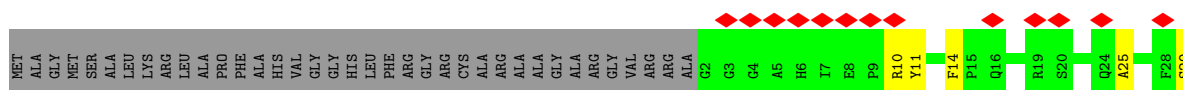
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

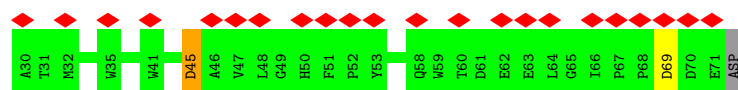


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

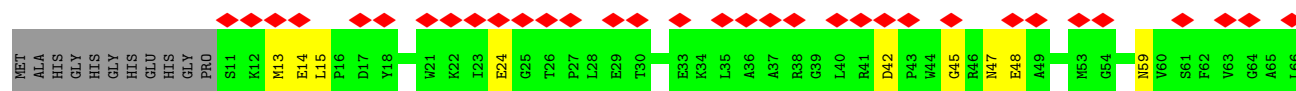


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

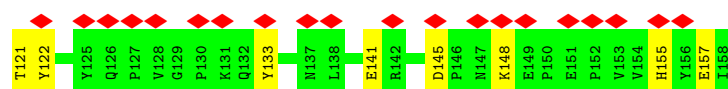
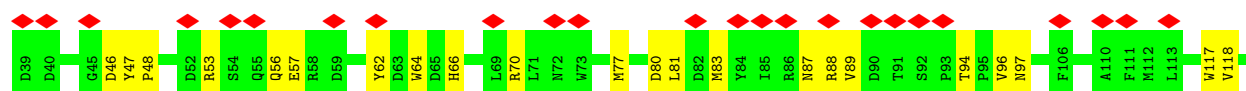
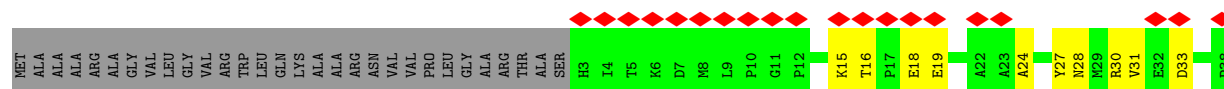




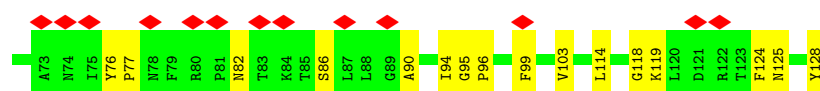
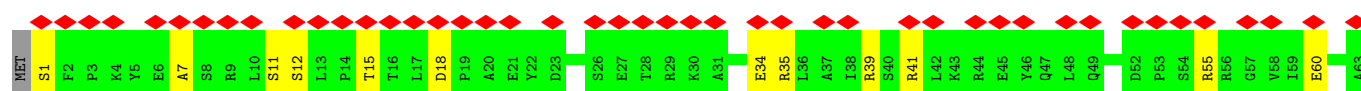
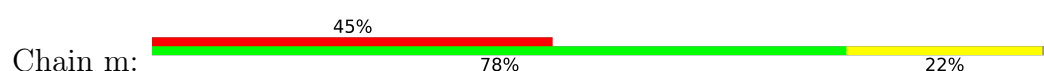
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



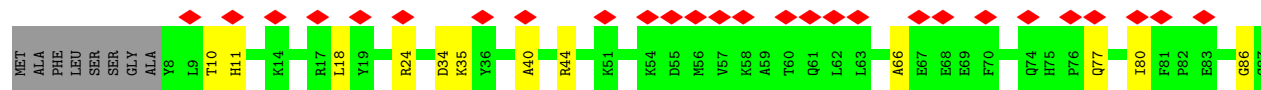
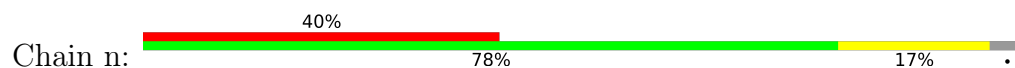
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

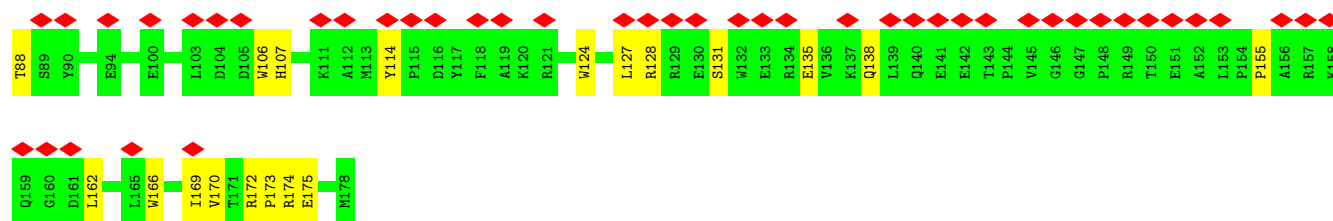


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

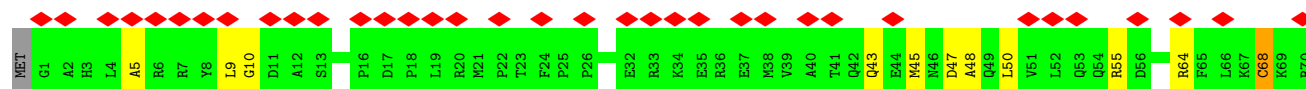
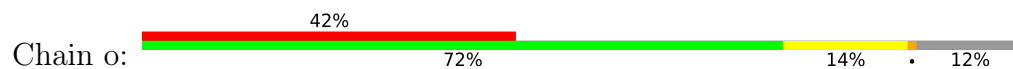


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

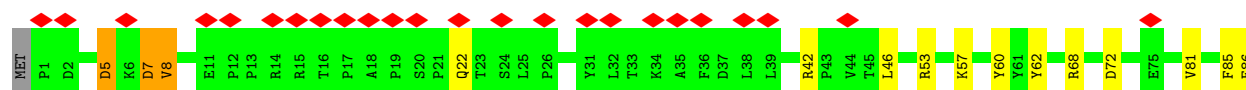
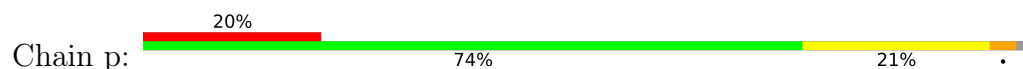




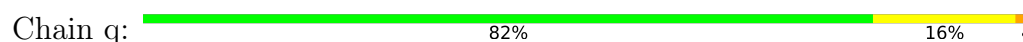
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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



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

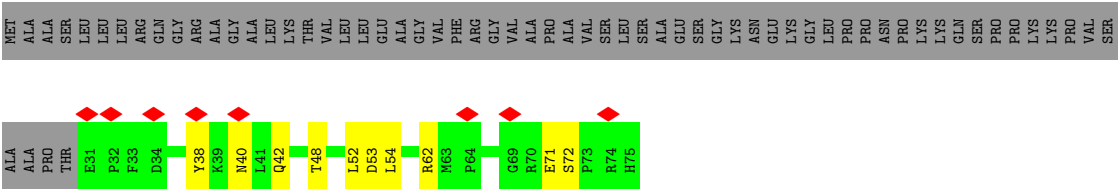


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45544	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 ($e^-/\text{\AA}^2$)	39.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	486.0, 486.0, 486.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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: FES, NDP, FME, FMN, PC1, MG, EHZ, SAC, 2MR, ZN, CDL, CHD, 3PE, AYA, DGT, MYR, SF4, AME, K

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	0.24	0/854	0.28	0/1170
2	B	0.37	0/1292	0.32	0/1747
3	C	0.32	0/1794	0.32	0/2443
4	D	0.34	0/3170	0.33	0/4285
5	E	0.18	0/1699	0.30	0/2312
6	F	0.20	0/3398	0.28	0/4591
7	G	0.26	0/5372	0.29	0/7281
8	H	0.29	0/2571	0.31	0/3513
9	I	0.38	0/1445	0.34	0/1956
10	J	0.23	0/1239	0.29	0/1677
11	K	0.23	0/646	0.28	0/872
12	L	0.12	0/4443	0.25	0/6047
13	M	0.15	0/3738	0.25	0/5097
14	N	0.21	0/2792	0.27	0/3800
15	O	0.12	0/2651	0.25	0/3587
16	P	0.23	0/2626	0.27	0/3557
17	Q	0.30	0/1039	0.28	0/1404
18	R	0.24	0/753	0.29	0/1014
19	S	0.16	0/712	0.26	0/957
20	T	0.15	0/692	0.27	0/932
20	U	0.12	0/719	0.24	0/971
21	V	0.22	0/939	0.24	0/1272
22	W	0.24	0/1001	0.27	0/1345
23	X	0.18	0/1439	0.26	0/1942
24	Y	0.11	0/252	0.26	0/340
25	Z	0.20	0/1186	0.26	0/1599
26	a	0.24	0/584	0.27	0/786
27	b	0.19	0/667	0.27	0/916
28	c	0.16	0/418	0.24	0/567
29	d	0.17	0/1018	0.24	0/1375
30	e	0.19	0/850	0.26	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.15	0/505	0.26	0/681
32	g	0.12	0/772	0.25	0/1046
33	h	0.15	0/1221	0.26	0/1651
34	i	0.12	0/1127	0.27	0/1534
35	j	0.10	0/619	0.23	0/848
36	k	0.09	0/672	0.21	0/906
37	l	0.11	0/1369	0.26	0/1873
38	m	0.12	0/1088	0.27	0/1472
39	n	0.10	0/1540	0.23	0/2085
40	o	0.10	0/1060	0.22	0/1420
41	p	0.12	0/1489	0.25	0/2008
42	q	0.26	0/1242	0.29	0/1688
43	r	0.25	0/798	0.29	0/1079
44	s	0.12	0/392	0.23	0/531
All	All	0.22	0/65893	0.27	0/89313

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	842	0	882	23	0
2	B	1260	0	1269	22	0
3	C	1743	0	1690	34	0
4	D	3110	0	3088	61	0
5	E	1659	0	1664	41	0
6	F	3324	0	3279	76	0
7	G	5284	0	5306	112	0
8	H	2509	0	2621	39	0
9	I	1414	0	1370	34	0
10	J	1219	0	1227	38	0
11	K	647	0	690	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4334	0	4451	102	0
13	M	3654	0	3852	73	0
14	N	2733	0	2912	39	0
15	O	2589	0	2566	61	0
16	P	2560	0	2581	39	0
17	Q	1016	0	1014	12	0
18	R	740	0	714	10	0
19	S	701	0	717	20	0
20	T	681	0	677	20	0
20	U	707	0	700	14	0
21	V	919	0	961	11	0
22	W	977	0	994	10	0
23	X	1402	0	1379	23	0
24	Y	248	0	247	5	0
25	Z	1157	0	1156	17	0
26	a	569	0	568	10	0
27	b	654	0	663	9	0
28	c	405	0	409	6	0
29	d	999	0	988	15	0
30	e	829	0	829	11	0
31	f	492	0	501	9	0
32	g	750	0	711	20	0
33	h	1186	0	1193	37	0
34	i	1097	0	1108	31	0
35	j	592	0	528	4	0
36	k	653	0	639	11	0
37	l	1314	0	1210	27	0
38	m	1070	0	1068	17	0
39	n	1487	0	1433	32	0
40	o	1035	0	1002	13	0
41	p	1455	0	1430	37	0
42	q	1212	0	1183	16	0
43	r	785	0	795	12	0
44	s	380	0	349	10	0
45	A	43	0	63	4	0
45	I	84	0	122	6	0
45	J	39	0	52	0	0
45	M	77	0	105	5	0
45	O	35	0	44	2	0
45	Z	49	0	75	1	0
45	d	49	0	75	1	0
45	h	32	0	38	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	A	50	0	77	2	0
46	B	51	0	79	2	0
46	H	43	0	63	0	0
46	d	33	0	40	5	0
46	q	37	0	48	0	0
47	B	8	0	0	2	0
47	F	8	0	0	1	0
47	G	16	0	0	0	0
47	I	16	0	0	1	0
48	E	4	0	0	0	0
48	G	4	0	0	1	0
49	F	31	0	19	2	0
50	G	1	0	0	0	0
51	N	73	0	90	2	0
51	X	79	0	105	1	0
51	d	65	0	77	1	0
51	q	60	0	64	0	0
52	O	31	0	12	2	0
53	O	1	0	0	0	0
54	P	48	0	24	2	0
55	R	1	0	0	0	0
56	T	37	0	0	1	0
56	U	37	0	0	0	0
57	i	29	0	38	2	0
58	o	15	0	27	0	0
All	All	65579	0	65951	1085	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 8.

All (1085) 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)
7:G:58:GLU:OE1	7:G:83:SER:OG	1.83	0.95
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.03	0.92
12:L:265:PRO:O	12:L:269:ASN:ND2	2.04	0.90
12:L:67:HIS:HE2	12:L:70:THR:HG1	1.08	0.90
14:N:140:SER:O	14:N:144:GLN:NE2	2.05	0.89
16:P:22:THR:OG1	16:P:88:SER:OG	1.85	0.89
31:f:46:ARG:NH1	31:f:47:GLU:O	2.05	0.88
4:D:326:ASP:OD1	7:G:127:ARG:NH2	2.06	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:140:ASP:O	41:p:157:LYS:NZ	2.07	0.88
13:M:35:SER:O	13:M:38:SER:OG	1.91	0.88
16:P:203:GLN:N	16:P:291:ASP:OD2	2.07	0.87
13:M:289:SER:O	13:M:293:HIS:ND1	2.08	0.87
13:M:47:ASP:OD2	41:p:93:ARG:NH1	2.08	0.85
6:F:157:TYR:OH	44:s:62:ARG:NH1	2.10	0.85
29:d:112:VAL:O	41:p:159:LYS:NZ	2.11	0.83
12:L:542:LEU:O	13:M:278:ARG:NH1	2.11	0.83
4:D:74:ARG:O	4:D:407:LYS:NZ	2.12	0.83
5:E:108:CYS:O	5:E:113:SER:OG	1.95	0.83
12:L:427:ILE:HG23	12:L:431:LEU:HD12	1.61	0.83
14:N:19:ILE:O	14:N:23:SER:OG	1.96	0.82
7:G:297:GLU:N	7:G:297:GLU:OE1	2.13	0.81
19:S:39:ARG:NH1	19:S:87:THR:OG1	2.12	0.81
39:n:131:SER:OG	39:n:135:GLU:OE2	1.98	0.81
7:G:382:THR:OG1	7:G:387:GLU:OE1	1.99	0.81
12:L:490:ALA:O	12:L:494:THR:OG1	1.99	0.81
15:O:178:GLU:OE1	15:O:181:SER:OG	1.98	0.81
6:F:78:LYS:NZ	49:F:501:FMN:O3P	2.13	0.81
33:h:129:ASP:OD1	33:h:130:LYS:N	2.14	0.81
15:O:47:GLY:O	15:O:120:GLN:NE2	2.13	0.80
12:L:295:GLN:NE2	39:n:77:GLN:OE1	2.14	0.80
16:P:154:LYS:NZ	16:P:158:GLU:OE2	2.13	0.80
5:E:183:LYS:O	5:E:187:ARG:NH1	2.14	0.80
15:O:94:TYR:OH	15:O:148:CYS:O	2.00	0.80
33:h:87:TYR:OH	41:p:86:GLU:OE1	1.98	0.80
6:F:358:SER:OG	6:F:365:CYS:SG	2.38	0.80
16:P:162:GLU:OE1	16:P:162:GLU:N	2.13	0.80
7:G:641:TYR:OH	19:S:56:GLU:OE2	1.99	0.79
6:F:17:ASP:OD1	6:F:20:ARG:NH1	2.14	0.79
2:B:93:THR:OG1	4:D:82:LEU:O	2.00	0.79
7:G:194:GLU:N	7:G:194:GLU:OE1	2.15	0.79
6:F:9:LYS:NZ	6:F:11:SER:O	2.12	0.79
45:M:501:3PE:H2B2	45:M:501:3PE:H262	1.65	0.79
8:H:32:GLN:OE1	8:H:34:ARG:NH2	2.15	0.79
10:J:7:PHE:O	10:J:10:SER:OG	2.01	0.79
56:T:101:EHZ:N1	56:T:101:EHZ:O5	2.16	0.78
3:C:211:GLN:NE2	21:V:114:PRO:O	2.15	0.78
12:L:444:ASN:OD1	12:L:446:ASN:ND2	2.17	0.78
4:D:201:GLN:OE1	9:I:60:ARG:NH1	2.17	0.78
13:M:65:LEU:O	13:M:69:THR:OG1	2.00	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:415:LEU:O	7:G:416:THR:OG1	2.01	0.78
41:p:72:ASP:OD1	41:p:90:GLN:NE2	2.16	0.78
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.64	0.78
36:k:24:GLU:OE1	36:k:24:GLU:N	2.17	0.77
31:f:8:ARG:NE	31:f:8:ARG:O	2.17	0.77
7:G:609:MET:SD	7:G:609:MET:N	2.57	0.77
32:g:35:GLU:OE2	32:g:40:LYS:NZ	2.16	0.77
32:g:45:HIS:N	32:g:54:ASP:OD2	2.17	0.77
14:N:125:SER:OG	51:N:401:CDL:OA3	2.01	0.77
37:l:33:ASP:OD2	38:m:35:ARG:NH2	2.17	0.77
12:L:166:THR:OG1	37:l:87:ASN:ND2	2.18	0.77
19:S:24:GLN:OE1	19:S:24:GLN:N	2.18	0.77
7:G:632:ARG:NH1	19:S:58:SER:OG	2.18	0.77
37:l:28:ASN:OD1	38:m:41:ARG:NH2	2.18	0.76
9:I:27:TRP:NE1	45:I:201:3PE:O22	2.18	0.76
14:N:299:SER:O	14:N:303:THR:OG1	2.02	0.76
16:P:176:ASP:OD1	16:P:180:ASN:ND2	2.19	0.76
12:L:6:SER:O	12:L:10:VAL:HG13	1.85	0.76
20:T:55:GLU:OE2	20:T:62:ILE:N	2.19	0.76
10:J:94:VAL:O	10:J:95:THR:OG1	2.03	0.76
20:T:43:ASP:OD1	20:T:44:SER:N	2.18	0.76
4:D:202:ASP:OD1	4:D:203:LEU:N	2.18	0.76
13:M:105:PHE:O	13:M:109:THR:OG1	2.04	0.76
8:H:186:PHE:O	8:H:189:THR:OG1	2.04	0.76
16:P:157:ARG:NH1	16:P:225:GLY:O	2.19	0.76
16:P:164:THR:OG1	16:P:223:ALA:O	2.03	0.75
4:D:69:SER:OG	4:D:74:ARG:NE	2.19	0.75
34:i:26:GLU:OE1	34:i:26:GLU:N	2.19	0.75
7:G:45:ARG:NH1	7:G:260:GLU:OE1	2.19	0.75
7:G:445:GLU:O	7:G:447:LYS:NZ	2.18	0.75
40:o:82:GLU:N	40:o:82:GLU:OE1	2.20	0.74
14:N:213:SER:O	14:N:217:THR:OG1	2.05	0.74
30:e:58:GLU:N	30:e:58:GLU:OE1	2.20	0.74
6:F:318:ASP:N	6:F:318:ASP:OD1	2.17	0.74
23:X:58:GLU:N	23:X:58:GLU:OE1	2.20	0.74
37:l:15:LYS:N	37:l:19:GLU:OE1	2.20	0.74
12:L:161:ARG:NH1	39:n:88:THR:O	2.20	0.74
23:X:68:GLU:OE2	23:X:72:GLN:NE2	2.21	0.74
28:c:41:GLU:OE2	28:c:45:ARG:NE	2.21	0.74
38:m:99:PHE:O	38:m:103:VAL:HG23	1.88	0.74
3:C:77:ASP:OD1	3:C:78:LEU:N	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:467:ILE:O	12:L:471:ASN:ND2	2.21	0.73
13:M:14:LEU:O	13:M:18:SER:OG	2.05	0.73
6:F:165:ASN:OD1	6:F:170:GLY:N	2.22	0.73
4:D:206:GLY:N	25:Z:8:ASP:OD2	2.21	0.73
29:d:11:PHE:N	46:d:202:PC1:O12	2.21	0.73
13:M:329:LEU:O	13:M:332:SER:OG	2.06	0.73
10:J:17:PHE:O	10:J:21:SER:OG	2.06	0.73
26:a:55:SER:O	26:a:64:LYS:NZ	2.22	0.73
16:P:333:ASP:OD1	16:P:333:ASP:N	2.22	0.72
7:G:414:ASP:OD1	7:G:415:LEU:N	2.22	0.72
40:o:45:MET:O	40:o:55:ARG:NH2	2.22	0.72
20:U:16:LEU:O	20:U:20:LYS:N	2.22	0.72
7:G:16:GLN:NE2	7:G:17:SER:O	2.21	0.72
9:I:29:GLU:N	9:I:29:GLU:OE1	2.23	0.72
17:Q:15:GLU:OE1	22:W:73:THR:OG1	2.01	0.72
20:U:49:GLU:OE2	39:n:44:ARG:NH1	2.22	0.72
4:D:357:GLN:OE1	4:D:357:GLN:N	2.23	0.72
15:O:147:GLN:N	15:O:147:GLN:OE1	2.23	0.72
29:d:45:ASP:OD2	29:d:64:TYR:OH	2.07	0.71
8:H:266:LEU:O	8:H:269:SER:OG	2.07	0.71
5:E:156:ILE:HD13	5:E:161:TYR:CE2	2.26	0.71
37:l:30:ARG:NE	38:m:34:GLU:OE1	2.23	0.71
12:L:397:GLU:O	12:L:401:THR:OG1	2.04	0.71
3:C:148:LEU:O	22:W:87:MET:HE2	1.91	0.71
23:X:110:VAL:O	23:X:115:GLY:N	2.24	0.71
12:L:433:GLY:O	36:k:59:ASN:ND2	2.23	0.70
4:D:350:LYS:NZ	7:G:118:ASP:OD1	2.18	0.70
7:G:547:GLY:O	7:G:563:GLY:N	2.24	0.70
18:R:22:ASP:OD1	18:R:23:TYR:N	2.24	0.70
37:l:145:ASP:OD2	37:l:148:LYS:NZ	2.18	0.70
4:D:322:GLU:N	4:D:322:GLU:OE1	2.23	0.70
16:P:311:GLU:OE1	16:P:311:GLU:N	2.23	0.70
20:U:85:ASP:OD2	39:n:175:GLU:N	2.23	0.70
5:E:26:GLU:N	5:E:26:GLU:OE1	2.24	0.70
7:G:632:ARG:NH2	19:S:58:SER:O	2.24	0.70
16:P:157:ARG:NH2	16:P:227:THR:OG1	2.24	0.70
6:F:363:THR:OG1	6:F:366:ARG:NH2	2.24	0.70
5:E:98:TYR:N	5:E:136:LEU:O	2.24	0.70
44:s:40:ASN:ND2	44:s:40:ASN:O	2.24	0.70
7:G:644:GLN:N	7:G:644:GLN:OE1	2.24	0.70
4:D:429:ASP:N	4:D:429:ASP:OD1	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:157:GLU:OE1	40:o:96:LYS:NZ	2.21	0.69
17:Q:42:ARG:NH1	17:Q:46:GLN:O	2.25	0.69
1:A:80:GLN:NE2	8:H:315:PRO:O	2.26	0.69
2:B:162:GLN:OE1	9:I:140:SER:OG	2.10	0.69
9:I:13:ASP:OD1	9:I:16:SER:OG	2.03	0.69
18:R:37:GLU:OE1	18:R:37:GLU:N	2.25	0.69
37:l:66:HIS:O	37:l:70:ARG:N	2.26	0.69
6:F:394:GLU:OE2	43:r:50:ASN:N	2.25	0.69
12:L:147:VAL:O	12:L:151:SER:OG	2.07	0.68
2:B:116:MET:SD	2:B:156:LEU:HD22	2.34	0.68
7:G:577:GLU:OE2	7:G:579:ARG:NH2	2.27	0.68
41:p:117:GLY:O	41:p:120:HIS:ND1	2.26	0.68
31:f:42:LEU:O	41:p:68:ARG:NH2	2.26	0.68
14:N:341:PRO:O	29:d:83:TYR:OH	2.12	0.68
10:J:52:LEU:N	10:J:139:GLU:OE2	2.25	0.67
15:O:158:VAL:HG13	15:O:159:THR:HG23	1.77	0.67
3:C:33:LEU:HD23	21:V:98:PRO:HB3	1.77	0.67
5:E:30:ARG:NH1	44:s:53:ASP:OD1	2.28	0.67
9:I:32:ARG:NH2	25:Z:25:PRO:O	2.27	0.67
6:F:129:MET:HE1	6:F:221:THR:HG21	1.77	0.67
20:T:28:GLU:N	20:T:28:GLU:OE1	2.28	0.67
13:M:143:LEU:HD22	13:M:222:GLU:OE2	1.93	0.67
16:P:122:LYS:NZ	16:P:159:THR:O	2.22	0.67
29:d:93:TYR:OH	33:h:117:ARG:NH2	2.28	0.67
4:D:210:ASP:OD1	43:r:31:SER:OG	2.13	0.67
7:G:512:GLU:OE1	7:G:513:ALA:N	2.29	0.66
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.14	0.66
33:h:9:PHE:HA	34:i:27:LEU:HD21	1.78	0.66
31:f:41:SER:O	31:f:45:LYS:N	2.28	0.66
7:G:285:ARG:NH2	7:G:555:PRO:O	2.29	0.66
14:N:70:LEU:O	14:N:74:VAL:HG23	1.95	0.66
18:R:9:GLU:OE2	18:R:33:LYS:NZ	2.20	0.66
6:F:356:HIS:O	7:G:177:ARG:NH2	2.28	0.66
32:g:48:ASP:OD1	32:g:49:LYS:N	2.26	0.66
6:F:263:ASN:ND2	6:F:285:GLY:O	2.27	0.66
15:O:198:TYR:CE2	15:O:202:ILE:HD11	2.30	0.66
7:G:358:LEU:HD23	7:G:641:TYR:HB2	1.77	0.65
10:J:103:MET:O	10:J:107:VAL:N	2.25	0.65
15:O:307:GLY:N	28:c:3:TYR:OH	2.30	0.65
3:C:54:PRO:O	3:C:57:VAL:HG23	1.96	0.65
13:M:403:THR:O	13:M:407:SER:OG	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:55:GLN:O	5:E:59:GLY:N	2.28	0.65
12:L:83:ASP:OD2	12:L:262:ARG:NH1	2.29	0.65
13:M:453:ILE:HG13	13:M:454:ILE:HG23	1.79	0.65
23:X:143:SER:OG	30:e:38:GLU:OE1	2.11	0.65
34:i:61:TYR:OH	34:i:65:ARG:NH1	2.30	0.65
36:k:47:ASN:ND2	36:k:48:GLU:OE2	2.29	0.65
13:M:91:ARG:NH1	45:O:401:3PE:O22	2.29	0.65
37:l:133:TYR:O	37:l:155:HIS:NE2	2.30	0.65
14:N:106:LEU:O	14:N:135:LYS:NZ	2.29	0.65
41:p:8:VAL:O	41:p:108:ARG:NH2	2.30	0.65
7:G:441:GLN:NE2	7:G:444:GLN:OE1	2.30	0.64
23:X:25:LYS:NZ	23:X:94:GLN:O	2.22	0.64
17:Q:56:LYS:NZ	17:Q:85:THR:OG1	2.26	0.64
23:X:10:GLU:N	23:X:10:GLU:OE1	2.30	0.64
3:C:109:THR:OG1	3:C:110:TYR:N	2.27	0.64
20:T:49:GLU:OE2	22:W:63:ARG:NH2	2.30	0.64
13:M:88:ASN:O	13:M:92:LYS:N	2.29	0.64
15:O:80:GLU:N	15:O:80:GLU:OE1	2.31	0.64
21:V:71:LEU:HD13	21:V:79:VAL:HG11	1.80	0.64
6:F:47:GLU:N	6:F:47:GLU:OE1	2.30	0.64
3:C:136:ASP:OD2	3:C:151:ILE:N	2.31	0.64
4:D:173:GLU:OE2	43:r:24:GLN:NE2	2.31	0.64
4:D:182:GLU:OE1	9:I:58:SER:OG	2.14	0.64
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.30	0.64
16:P:115:GLN:NE2	16:P:119:GLN:OE1	2.30	0.64
39:n:138:GLN:NE2	39:n:155:PRO:O	2.31	0.64
12:L:220:ALA:O	12:L:224:SER:OG	2.08	0.64
16:P:10:LYS:NZ	22:W:126:ASP:OD2	2.30	0.64
34:i:21:TRP:NE1	39:n:172:ARG:O	2.31	0.64
42:q:2:GLU:N	42:q:2:GLU:OE1	2.30	0.64
15:O:305:ARG:O	15:O:309:ASN:ND2	2.30	0.63
23:X:154:GLU:N	23:X:154:GLU:OE1	2.31	0.63
5:E:204:GLU:N	5:E:204:GLU:OE1	2.32	0.63
15:O:83:TYR:OH	52:O:402:DGT:H2'	1.98	0.63
41:p:103:ASN:O	41:p:107:GLU:N	2.31	0.63
1:A:71:LEU:O	10:J:147:TYR:OH	2.11	0.63
13:M:150:LEU:HD22	14:N:291:TYR:CD1	2.32	0.63
13:M:297:VAL:HG13	13:M:312:ALA:HB1	1.79	0.63
46:d:202:PC1:H322	46:d:202:PC1:C13	2.28	0.63
37:l:53:ARG:NH2	38:m:12:SER:OG	2.31	0.63
13:M:192:ASN:HB2	13:M:253:MET:HE1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:THR:OG1	3:C:112:ASP:N	2.29	0.63
22:W:22:ARG:N	22:W:26:GLU:OE1	2.32	0.63
10:J:55:MET:HE2	10:J:55:MET:HA	1.80	0.63
5:E:214:GLN:NE2	6:F:236:ARG:O	2.32	0.62
17:Q:88:THR:OG1	17:Q:91:ASP:OD2	2.16	0.62
29:d:120:ARG:NH1	41:p:144:ASP:OD2	2.32	0.62
37:l:56:GLN:OE1	37:l:70:ARG:NH1	2.32	0.62
28:c:41:GLU:OE2	28:c:44:ARG:NH2	2.32	0.62
7:G:53:ARG:N	48:G:803:FES:S2	2.72	0.62
40:o:79:CYS:O	40:o:83:ARG:N	2.31	0.62
45:I:201:3PE:H2F1	45:I:204:3PE:H2A2	1.81	0.62
11:K:1:FME:O	11:K:3:MET:N	2.33	0.62
29:d:46:ASN:O	29:d:50:ARG:N	2.32	0.62
39:n:131:SER:CB	39:n:162:LEU:HD12	2.30	0.62
12:L:311:GLY:O	12:L:315:VAL:HG23	2.00	0.62
19:S:58:SER:O	19:S:60:VAL:HG13	1.98	0.62
25:Z:21:LYS:NZ	43:r:108:ASP:OD1	2.30	0.62
29:d:103:GLU:OE1	29:d:103:GLU:N	2.32	0.62
40:o:72:SER:O	40:o:75:ASN:N	2.33	0.62
15:O:165:PRO:O	15:O:248:TRP:NE1	2.33	0.62
20:T:16:LEU:HD13	20:T:30:LEU:HD11	1.81	0.62
23:X:170:THR:OG1	51:X:201:CDL:OA7	2.17	0.62
24:Y:120:THR:O	24:Y:124:VAL:HG23	2.00	0.62
33:h:12:LYS:O	39:n:106:TRP:NE1	2.33	0.62
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.82	0.61
7:G:396:ARG:NH1	7:G:416:THR:O	2.32	0.61
13:M:65:LEU:O	13:M:69:THR:N	2.30	0.61
3:C:179:GLU:OE1	16:P:37:HIS:NE2	2.33	0.61
3:C:86:ARG:NH1	3:C:91:GLU:OE1	2.32	0.61
9:I:75:GLU:O	9:I:105:ARG:NH1	2.33	0.61
21:V:77:GLU:N	21:V:77:GLU:OE1	2.33	0.61
32:g:82:ASP:OD1	32:g:87:GLU:N	2.33	0.61
22:W:95:VAL:HG12	22:W:95:VAL:O	2.01	0.61
2:B:81:ARG:NH2	8:H:214:GLU:O	2.33	0.61
6:F:165:ASN:OD1	6:F:169:SER:N	2.32	0.61
13:M:114:GLU:OE1	13:M:116:ILE:N	2.33	0.61
12:L:4:PHE:O	12:L:8:SER:OG	2.17	0.61
13:M:59:ASP:O	13:M:63:THR:OG1	2.18	0.61
36:k:14:GLU:N	36:k:14:GLU:OE1	2.34	0.61
11:K:9:MET:HE2	11:K:43:MET:HE3	1.82	0.61
3:C:6:ASP:OD1	3:C:7:THR:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:150:ASN:OD1	30:e:50:ARG:NH1	2.33	0.60
8:H:102:VAL:HG13	8:H:150:LEU:HD21	1.83	0.60
13:M:281:ASP:OD1	13:M:283:LYS:N	2.34	0.60
38:m:90:ALA:O	38:m:94:ILE:HG22	2.02	0.60
13:M:1:FME:CE	13:M:111:THR:HG21	2.31	0.60
12:L:132:VAL:O	12:L:262:ARG:NH2	2.34	0.60
15:O:292:VAL:O	15:O:296:PHE:N	2.34	0.60
10:J:141:MET:HA	10:J:141:MET:HE2	1.83	0.60
12:L:63:ILE:O	12:L:80:PHE:N	2.32	0.60
42:q:42:ASP:OD1	42:q:46:ASN:N	2.35	0.60
4:D:145:THR:HG1	4:D:181:TYR:HH	1.49	0.60
6:F:96:ASN:ND2	6:F:187:GLY:O	2.34	0.60
14:N:226:THR:O	14:N:230:LEU:N	2.35	0.59
43:r:32:LYS:O	43:r:35:GLN:NE2	2.35	0.59
5:E:53:LEU:HD13	44:s:52:LEU:CD1	2.31	0.59
14:N:287:LEU:O	14:N:291:TYR:N	2.30	0.59
1:A:60:ILE:HG21	10:J:168:ILE:HG21	1.85	0.59
15:O:88:SER:OG	15:O:90:ASP:OD1	2.19	0.59
18:R:27:ARG:O	18:R:31:ARG:NH2	2.34	0.59
23:X:102:GLN:N	23:X:102:GLN:OE1	2.32	0.59
39:n:162:LEU:HD13	39:n:166:TRP:NE1	2.18	0.59
45:A:201:3PE:H2B2	27:b:22:PHE:CE1	2.38	0.59
4:D:224:GLU:OE1	9:I:40:TYR:OH	2.20	0.59
11:K:12:PHE:O	11:K:15:SER:OG	2.20	0.59
4:D:287:ILE:O	9:I:5:VAL:HG22	2.03	0.59
7:G:372:GLU:O	7:G:402:ASN:ND2	2.35	0.59
10:J:118:GLU:N	10:J:118:GLU:OE1	2.35	0.59
11:K:9:MET:HE2	11:K:43:MET:CE	2.33	0.59
12:L:520:PHE:O	12:L:524:THR:N	2.33	0.59
6:F:188:GLU:OE1	6:F:190:THR:N	2.36	0.59
14:N:89:LEU:HD11	14:N:98:MET:SD	2.42	0.59
37:l:62:TYR:OH	38:m:39:ARG:NH2	2.35	0.59
1:A:73:LEU:CD1	10:J:55:MET:HE1	2.32	0.58
6:F:344:VAL:HG21	6:F:429:ARG:HE	1.68	0.58
8:H:248:ASN:OD1	8:H:251:MET:N	2.33	0.58
20:T:34:SER:HB3	20:T:40:LEU:HD21	1.86	0.58
37:l:24:ALA:HB3	37:l:31:VAL:HG22	1.84	0.58
37:l:118:VAL:O	37:l:122:TYR:N	2.35	0.58
7:G:231:MET:HE2	7:G:231:MET:HA	1.85	0.58
13:M:459:TYR:O	32:g:84:ARG:NH1	2.37	0.58
4:D:55:HIS:O	4:D:57:ALA:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:119:MET:HE1	40:o:64:ARG:HB2	1.84	0.58
37:l:77:MET:CE	37:l:81:LEU:HD22	2.33	0.58
5:E:155:GLN:C	5:E:156:ILE:HD12	2.28	0.58
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.34	0.58
13:M:11:FME:HE3	13:M:111:THR:HG21	1.85	0.58
7:G:325:ALA:O	7:G:329:ILE:HG22	2.03	0.58
57:i:201:CHD:H212	57:i:201:CHD:H12	1.84	0.58
17:Q:28:GLU:O	17:Q:32:THR:OG1	2.18	0.58
46:d:202:PC1:H322	46:d:202:PC1:H133	1.86	0.58
42:q:76:ASP:N	42:q:76:ASP:OD1	2.37	0.58
33:h:74:TRP:CE3	45:h:201:3PE:H251	2.39	0.57
5:E:51:LEU:HD23	5:E:69:VAL:HG21	1.85	0.57
6:F:99:GLU:OE2	6:F:104:THR:HG22	2.04	0.57
15:O:57:HIS:NE2	15:O:69:LEU:O	2.37	0.57
15:O:150:ASP:OD1	15:O:150:ASP:N	2.34	0.57
2:B:42:ARG:NH2	46:B:201:PC1:O14	2.34	0.57
5:E:16:ASN:OD1	5:E:19:THR:N	2.38	0.57
6:F:261:HIS:N	6:F:336:VAL:O	2.37	0.57
42:q:142:THR:HG22	42:q:144:TYR:H	1.69	0.57
6:F:393:TRP:O	6:F:396:SER:OG	2.19	0.57
18:R:22:ASP:OD1	18:R:24:ARG:N	2.35	0.57
6:F:268:VAL:HG21	6:F:283:HIS:ND1	2.19	0.57
12:L:357:ARG:NH1	39:n:77:GLN:O	2.36	0.57
32:g:66:PHE:HA	32:g:70:LEU:HD12	1.85	0.57
3:C:154:ASP:OD1	3:C:155:TYR:N	2.38	0.57
12:L:489:THR:O	12:L:493:VAL:HG22	2.04	0.57
23:X:120:ASP:N	23:X:123:ASP:OD2	2.36	0.57
7:G:489:VAL:O	7:G:491:ASN:ND2	2.38	0.57
35:j:10:ARG:NH1	35:j:14:PHE:O	2.34	0.57
3:C:33:LEU:HD21	21:V:93:MET:HE1	1.86	0.57
23:X:133:ASP:OD1	23:X:133:ASP:N	2.35	0.57
33:h:70:PRO:O	33:h:74:TRP:N	2.32	0.57
7:G:375:ASP:OD1	7:G:375:ASP:N	2.34	0.56
13:M:22:MET:O	13:M:26:ASN:ND2	2.38	0.56
5:E:53:LEU:HD13	44:s:52:LEU:HD13	1.87	0.56
6:F:113:HIS:NE2	44:s:38:TYR:OH	2.34	0.56
6:F:200:GLN:OE1	6:F:202:LYS:NZ	2.33	0.56
9:I:114:THR:HG21	9:I:144:HIS:NE2	2.20	0.56
23:X:97:ARG:HD3	25:Z:59:LEU:HD13	1.86	0.56
41:p:134:VAL:O	41:p:138:TYR:N	2.32	0.56
10:J:108:LEU:HD13	10:J:112:GLU:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:237:LYS:NZ	13:M:316:MET:O	2.38	0.56
15:O:15:THR:OG1	15:O:253:ASP:OD1	2.17	0.56
16:P:86:GLU:OE1	16:P:87:HIS:NE2	2.39	0.56
19:S:23:CYS:SG	19:S:24:GLN:N	2.78	0.56
38:m:82:ASN:O	38:m:86:SER:OG	2.24	0.56
1:A:28:ASN:ND2	46:A:202:PC1:O32	2.35	0.56
14:N:190:MET:HE2	14:N:205:LEU:HA	1.87	0.56
36:k:70:PHE:O	36:k:74:PHE:N	2.31	0.56
19:S:26:SER:O	19:S:33:ARG:NH2	2.37	0.56
26:a:40:HIS:N	26:a:44:GLN:OE1	2.36	0.56
3:C:82:ASP:OD1	3:C:83:ILE:N	2.39	0.56
7:G:103:LEU:O	18:R:86:TYR:OH	2.22	0.56
12:L:367:PRO:O	12:L:371:THR:N	2.39	0.56
15:O:138:MET:HE2	15:O:144:ILE:CG2	2.36	0.56
37:l:18:GLU:N	37:l:18:GLU:OE1	2.38	0.56
37:l:141:GLU:N	37:l:141:GLU:OE1	2.39	0.56
1:A:23:TRP:O	1:A:26:GLN:N	2.38	0.56
2:B:127:HIS:O	2:B:134:ARG:NH1	2.39	0.56
8:H:70:MET:HE3	8:H:118:TRP:CD1	2.41	0.56
12:L:137:LEU:O	12:L:141:PHE:N	2.32	0.56
14:N:144:GLN:OE1	30:e:2:PHE:N	2.39	0.56
3:C:210:ARG:NH2	7:G:35:MET:SD	2.79	0.56
7:G:362:TYR:O	7:G:494:HIS:NE2	2.38	0.56
9:I:7:LEU:HD23	43:r:111:TYR:HE2	1.71	0.56
13:M:1:FME:O1	13:M:3:LYS:NZ	2.39	0.56
42:q:65:THR:O	42:q:73:THR:OG1	2.24	0.56
2:B:79:SER:O	2:B:83:SER:OG	2.24	0.55
12:L:504:ILE:HA	12:L:507:MET:HE3	1.88	0.55
16:P:64:ASP:OD1	16:P:65:LEU:N	2.34	0.55
4:D:342:MET:HE2	7:G:101:HIS:HD2	1.71	0.55
10:J:115:VAL:O	10:J:117:PHE:N	2.40	0.55
13:M:189:SER:OG	24:Y:130:GLU:OE2	2.24	0.55
32:g:109:GLU:O	41:p:141:ARG:NE	2.40	0.55
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.38	0.55
6:F:101:GLU:OE2	6:F:303:SER:OG	2.22	0.55
7:G:262:TRP:HB2	7:G:390:LEU:HD11	1.89	0.55
7:G:413:VAL:O	7:G:419:TYR:OH	2.10	0.55
34:i:22:LEU:HD22	39:n:174:ARG:CG	2.37	0.55
5:E:132:THR:OG1	5:E:134:ASP:OD1	2.18	0.55
8:H:195:ARG:HD3	8:H:231:ILE:HD11	1.88	0.55
13:M:271:MET:HE2	13:M:271:MET:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:s:71:GLU:OE1	44:s:71:GLU:N	2.40	0.55
20:T:12:LYS:O	20:T:16:LEU:HD23	2.07	0.55
9:I:150:ASN:CG	42:q:124:TYR:HH	2.10	0.55
12:L:387:THR:OG1	12:L:461:SER:O	2.24	0.55
23:X:48:GLU:OE1	23:X:134:ARG:NH2	2.37	0.55
7:G:193:SER:OG	7:G:194:GLU:OE1	2.24	0.55
45:I:201:3PE:H2G2	45:Z:201:3PE:H2I3	1.89	0.55
6:F:197:GLU:HG3	6:F:215:VAL:HG23	1.89	0.54
23:X:141:TYR:O	25:Z:114:ARG:NH1	2.41	0.54
12:L:402:SER:O	12:L:404:THR:HG23	2.07	0.54
39:n:127:LEU:HG	39:n:162:LEU:HD11	1.88	0.54
41:p:53:ARG:O	41:p:57:LYS:N	2.35	0.54
7:G:272:ASP:OD1	7:G:272:ASP:N	2.40	0.54
9:I:110:ASP:N	9:I:110:ASP:OD1	2.37	0.54
12:L:117:PHE:CE2	12:L:121:LEU:HD11	2.42	0.54
13:M:130:LEU:HD21	13:M:149:PHE:CZ	2.43	0.54
18:R:32:GLN:NE2	18:R:34:GLU:OE1	2.39	0.54
4:D:151:ILE:CD1	4:D:177:MET:HE1	2.38	0.54
34:i:53:GLY:O	34:i:54:ALA:HB3	2.08	0.54
41:p:81:VAL:O	41:p:85:PHE:N	2.40	0.54
4:D:328:ALA:N	7:G:126:ASP:OD2	2.38	0.54
6:F:434:ALA:O	6:F:438:GLN:N	2.39	0.54
15:O:311:ASP:OD1	15:O:311:ASP:N	2.40	0.54
5:E:143:GLU:OE1	6:F:349:ARG:NH2	2.40	0.54
7:G:229:ASP:OD1	7:G:230:VAL:N	2.41	0.54
10:J:27:ILE:H	10:J:27:ILE:HD12	1.73	0.54
11:K:55:LEU:HD12	30:e:24:GLN:OE1	2.07	0.54
12:L:59:GLN:OE1	12:L:61:LEU:HD11	2.08	0.54
4:D:302:GLU:OE2	9:I:3:LYS:NZ	2.28	0.54
7:G:366:THR:O	7:G:367:THR:OG1	2.17	0.54
10:J:22:SER:O	11:K:22:TYR:OH	2.26	0.54
20:U:22:TYR:HD2	20:U:50:ILE:HD11	1.73	0.54
15:O:275:ILE:O	15:O:277:VAL:HG23	2.07	0.54
40:o:86:TRP:NE1	40:o:90:GLU:OE2	2.41	0.54
3:C:75:LEU:HD12	3:C:96:LEU:HD23	1.90	0.54
12:L:123:LEU:HD23	12:L:126:ILE:HD12	1.90	0.54
2:B:52:LEU:HD13	2:B:91:THR:O	2.08	0.53
5:E:149:VAL:HG22	6:F:105:CYS:SG	2.48	0.53
6:F:224:ASN:OD1	6:F:225:VAL:N	2.41	0.53
13:M:411:LEU:HD12	13:M:415:GLN:HG3	1.90	0.53
13:M:152:TYR:O	13:M:156:GLY:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:168:GLY:O	14:N:172:GLN:NE2	2.42	0.53
20:T:6:LEU:HD13	20:T:86:VAL:HA	1.90	0.53
32:g:98:LYS:NZ	41:p:5:ASP:OD2	2.42	0.53
7:G:125:SER:OG	7:G:126:ASP:N	2.41	0.53
12:L:306:THR:HG23	12:L:332:HIS:NE2	2.23	0.53
24:Y:140:VAL:HG12	33:h:112:ARG:HB2	1.90	0.53
29:d:43:LEU:HD22	29:d:53:VAL:HG12	1.88	0.53
9:I:108:ARG:NH1	17:Q:70:MET:O	2.40	0.53
36:k:71:LYS:O	36:k:75:ALA:N	2.38	0.53
15:O:107:GLN:O	15:O:111:ALA:N	2.40	0.53
6:F:338:ASP:OD1	6:F:340:SER:OG	2.22	0.53
7:G:472:ASN:OD1	7:G:650:LYS:NZ	2.37	0.53
20:T:81:ALA:HB1	20:T:86:VAL:HG22	1.90	0.53
25:Z:50:MET:SD	25:Z:54:ARG:NH2	2.82	0.53
39:n:18:LEU:HD21	39:n:66:ALA:HB1	1.91	0.53
2:B:81:ARG:NH1	8:H:213:VAL:O	2.41	0.53
46:B:201:PC1:H3E2	46:B:201:PC1:H3I3	1.89	0.53
8:H:93:TYR:OH	26:a:35:GLU:OE2	2.25	0.53
13:M:243:MET:O	13:M:247:THR:HG23	2.09	0.53
14:N:46:LYS:NZ	51:N:401:CDL:OA3	2.42	0.53
16:P:201:VAL:HG11	16:P:235:ARG:HE	1.73	0.53
4:D:139:VAL:HG21	4:D:277:VAL:HG22	1.91	0.53
34:i:97:VAL:HG11	41:p:114:GLN:HB3	1.90	0.53
1:A:14:ALA:O	1:A:18:VAL:HG23	2.09	0.53
26:a:42:PRO:O	26:a:46:TYR:N	2.40	0.53
9:I:36:MET:O	9:I:39:SER:OG	2.23	0.53
14:N:89:LEU:HD12	14:N:95:SER:HA	1.90	0.53
9:I:135:PRO:HB2	42:q:93:MET:HE1	1.91	0.52
24:Y:123:LEU:HD23	24:Y:126:MET:CE	2.39	0.52
6:F:109:GLU:OE1	6:F:112:ARG:NH2	2.41	0.52
7:G:528:ASP:OD2	7:G:545:TYR:OH	2.25	0.52
15:O:43:ALA:O	15:O:47:GLY:N	2.42	0.52
16:P:46:ILE:N	16:P:46:ILE:HD12	2.23	0.52
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.38	0.52
15:O:235:VAL:O	15:O:239:GLU:N	2.42	0.52
15:O:93:SER:O	15:O:97:GLN:N	2.39	0.52
16:P:222:ASP:OD1	16:P:222:ASP:N	2.43	0.52
40:o:5:ALA:O	40:o:10:GLY:N	2.43	0.52
6:F:246:GLY:N	6:F:271:GLU:OE2	2.40	0.52
12:L:508:THR:O	39:n:35:LYS:NZ	2.34	0.52
20:T:51:ILE:HG21	22:W:36:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:GLU:OE2	4:D:278:TYR:OH	2.16	0.52
7:G:365:ASN:ND2	7:G:490:MET:O	2.41	0.52
9:I:65:HIS:CE1	47:I:202:SF4:S2	3.02	0.52
20:T:65:ILE:HG23	20:T:66:ASP:OD1	2.10	0.52
1:A:64:LEU:HD11	10:J:168:ILE:HD12	1.92	0.52
4:D:209:ASP:OD1	25:Z:15:TYR:OH	2.23	0.52
5:E:156:ILE:HD13	5:E:161:TYR:CD2	2.45	0.52
16:P:202:LYS:O	16:P:236:TYR:N	2.42	0.52
22:W:51:LEU:HD22	22:W:103:MET:SD	2.50	0.52
23:X:146:ARG:NH2	30:e:41:GLU:OE1	2.43	0.52
29:d:108:THR:N	29:d:111:GLU:OE1	2.38	0.52
5:E:83:VAL:HG13	5:E:87:TYR:HE2	1.74	0.52
12:L:383:MET:HB3	12:L:386:LEU:HD12	1.91	0.52
15:O:173:ASP:OD1	15:O:174:VAL:N	2.43	0.52
8:H:29:GLY:O	8:H:33:LEU:N	2.42	0.52
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.42	0.52
12:L:418:PHE:CD1	12:L:421:ILE:HD12	2.45	0.52
13:M:241:TYR:OH	13:M:245:ARG:NH2	2.43	0.52
15:O:82:PHE:CE1	15:O:138:MET:HE3	2.45	0.52
3:C:193:GLU:OE1	17:Q:64:ARG:NE	2.37	0.52
5:E:55:GLN:OE1	5:E:91:ASN:ND2	2.38	0.52
7:G:357:ASP:N	7:G:357:ASP:OD1	2.42	0.52
12:L:147:VAL:O	12:L:151:SER:N	2.36	0.52
4:D:50:ASN:OD1	4:D:51:PHE:N	2.44	0.51
27:b:58:ASP:OD1	27:b:59:ASP:N	2.42	0.51
29:d:45:ASP:OD1	29:d:49:ARG:NH1	2.39	0.51
33:h:112:ARG:HH22	33:h:113:LEU:HD21	1.76	0.51
1:A:105:GLU:O	1:A:110:GLY:N	2.43	0.51
2:B:34:ASP:N	2:B:173:LEU:HD12	2.25	0.51
7:G:170:ASP:N	7:G:170:ASP:OD1	2.42	0.51
4:D:139:VAL:HG21	4:D:277:VAL:CG2	2.40	0.51
12:L:404:THR:OG1	12:L:409:LEU:HD22	2.11	0.51
20:U:85:ASP:N	20:U:85:ASP:OD1	2.40	0.51
32:g:57:ASN:O	32:g:61:VAL:HG23	2.11	0.51
4:D:342:MET:HE2	7:G:101:HIS:CD2	2.46	0.51
5:E:48:LEU:O	5:E:90:TYR:OH	2.28	0.51
33:h:50:ALA:HB2	41:p:60:TYR:CE2	2.46	0.51
3:C:136:ASP:OD1	3:C:153:THR:OG1	2.21	0.51
9:I:155:LEU:O	9:I:158:GLY:N	2.44	0.51
25:Z:92:GLU:OE1	30:e:91:TYR:OH	2.28	0.51
4:D:279:ASP:OD1	4:D:279:ASP:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:284:ASP:OD1	9:I:1:THR:HG21	2.11	0.51
6:F:359:CYS:SG	6:F:360:GLY:N	2.84	0.51
8:H:200:LEU:HD12	8:H:204:GLU:OE2	2.11	0.51
30:e:19:ILE:HD11	33:h:132:LEU:HB2	1.93	0.51
6:F:228:VAL:O	6:F:231:SER:OG	2.28	0.51
26:a:34:LYS:NZ	26:a:61:TYR:O	2.30	0.51
12:L:9:LEU:HD11	12:L:63:ILE:HG21	1.92	0.51
14:N:342:MET:HB3	45:d:201:3PE:H2I2	1.93	0.51
37:l:16:THR:N	37:l:19:GLU:OE1	2.41	0.50
13:M:150:LEU:HD22	14:N:291:TYR:CE1	2.47	0.50
19:S:57:CYS:SG	19:S:58:SER:N	2.84	0.50
2:B:91:THR:HG22	2:B:92:LEU:N	2.25	0.50
14:N:307:SER:O	15:O:284:VAL:N	2.39	0.50
16:P:138:ASP:OD1	16:P:139:ILE:N	2.44	0.50
39:n:131:SER:HB3	39:n:162:LEU:HD12	1.94	0.50
41:p:108:ARG:NH1	41:p:130:GLN:OE1	2.43	0.50
42:q:62:VAL:HG22	42:q:63:ILE:N	2.26	0.50
4:D:80:ILE:O	4:D:82:LEU:N	2.45	0.50
7:G:223:ARG:NH2	17:Q:81:ASN:OD1	2.39	0.50
16:P:213:GLY:O	16:P:217:ALA:N	2.43	0.50
34:i:72:THR:HA	34:i:76:ILE:HD12	1.94	0.50
32:g:107:ILE:HG13	41:p:105:ILE:HD11	1.93	0.50
33:h:27:PHE:O	33:h:31:LEU:N	2.41	0.50
4:D:379:VAL:HG12	4:D:380:SER:N	2.27	0.50
6:F:306:LEU:C	6:F:306:LEU:HD12	2.36	0.50
12:L:97:THR:HG22	12:L:101:MET:HG2	1.94	0.50
15:O:204:ASN:O	15:O:208:GLY:N	2.44	0.50
20:U:22:TYR:CD2	20:U:50:ILE:HD11	2.47	0.50
46:d:202:PC1:H322	46:d:202:PC1:H132	1.93	0.50
33:h:41:THR:O	33:h:45:VAL:HG23	2.11	0.50
21:V:112:LYS:NZ	21:V:115:ILE:O	2.45	0.50
40:o:43:GLN:NE2	40:o:47:ASP:OD1	2.45	0.50
1:A:64:LEU:HD13	10:J:165:VAL:HG22	1.94	0.49
7:G:328:LEU:O	7:G:507:TYR:OH	2.28	0.49
8:H:134:ARG:NH2	8:H:204:GLU:OE1	2.45	0.49
8:H:141:SER:HB3	8:H:289:LEU:HD23	1.93	0.49
9:I:131:ILE:HG23	9:I:131:ILE:O	2.12	0.49
12:L:62:ILE:N	34:i:97:VAL:O	2.42	0.49
15:O:106:LEU:O	15:O:110:ASP:N	2.37	0.49
25:Z:93:GLU:O	25:Z:97:MET:N	2.42	0.49
27:b:77:LEU:O	27:b:80:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:28:TRP:NE1	29:d:66:THR:OG1	2.45	0.49
6:F:366:ARG:NE	6:F:367:GLU:OE2	2.43	0.49
10:J:102:PHE:O	10:J:103:MET:HB2	2.12	0.49
16:P:81:ILE:O	16:P:85:VAL:HG22	2.12	0.49
35:j:11:TYR:CD2	36:k:15:LEU:HD22	2.47	0.49
6:F:215:VAL:HG22	6:F:216:PHE:CD2	2.46	0.49
21:V:75:GLN:N	21:V:78:GLU:OE1	2.46	0.49
31:f:41:SER:OG	33:h:88:GLU:OE2	2.16	0.49
41:p:88:GLU:OE2	41:p:151:ALA:N	2.40	0.49
6:F:110:ILE:HD11	6:F:255:LEU:CD1	2.42	0.49
6:F:204:ARG:C	6:F:205:LEU:HD12	2.38	0.49
12:L:40:ILE:HD12	12:L:40:ILE:H	1.78	0.49
42:q:69:ASN:OD1	42:q:112:ASN:ND2	2.42	0.49
14:N:313:MET:HE1	15:O:102:ALA:HB1	1.95	0.49
7:G:536:ASP:OD1	7:G:536:ASP:N	2.46	0.49
12:L:135:ASN:O	12:L:135:ASN:ND2	2.46	0.49
12:L:221:THR:HG23	12:L:226:GLN:HB2	1.95	0.49
16:P:248:VAL:O	16:P:250:HIS:ND1	2.41	0.49
8:H:236:ILE:HG23	8:H:259:PHE:CZ	2.48	0.49
10:J:148:SER:OG	10:J:149:TYR:N	2.45	0.49
12:L:466:TYR:O	12:L:470:ASN:ND2	2.41	0.49
24:Y:140:VAL:HG12	33:h:112:ARG:CB	2.42	0.49
33:h:74:TRP:CG	45:h:201:3PE:H232	2.47	0.49
37:l:117:TRP:O	37:l:121:THR:N	2.39	0.49
38:m:76:TYR:N	38:m:77:PRO:CD	2.76	0.49
6:F:192:LEU:C	6:F:192:LEU:HD23	2.37	0.49
13:M:115:LEU:HD12	13:M:174:LEU:HD22	1.95	0.49
15:O:196:SER:O	15:O:199:LEU:N	2.46	0.49
32:g:66:PHE:O	32:g:71:VAL:HG23	2.11	0.49
33:h:32:THR:O	33:h:36:VAL:HG23	2.13	0.49
1:A:4:MET:N	1:A:4:MET:HE2	2.27	0.49
14:N:214:THR:HG22	14:N:218:MET:HE2	1.94	0.49
32:g:98:LYS:HB2	41:p:8:VAL:HG22	1.95	0.49
4:D:151:ILE:HG23	4:D:170:MET:HB3	1.95	0.48
4:D:277:VAL:O	4:D:280:GLN:N	2.46	0.48
13:M:150:LEU:HD11	13:M:154:LEU:HD11	1.93	0.48
7:G:362:TYR:OH	7:G:504:ASP:OD1	2.19	0.48
7:G:665:GLN:NE2	7:G:670:ASP:O	2.45	0.48
9:I:1:THR:HG22	9:I:2:TYR:N	2.28	0.48
12:L:203:MET:HE1	41:p:124:CYS:HB2	1.95	0.48
12:L:357:ARG:NH2	39:n:77:GLN:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:313:MET:HE3	15:O:99:TRP:CH2	2.48	0.48
15:O:279:LEU:O	15:O:283:THR:OG1	2.29	0.48
15:O:314:ASP:HB2	15:O:317:ILE:HD11	1.94	0.48
34:i:25:GLN:N	34:i:25:GLN:OE1	2.46	0.48
10:J:153:LEU:HD23	10:J:153:LEU:O	2.13	0.48
19:S:57:CYS:HB3	19:S:60:VAL:HG11	1.96	0.48
32:g:53:VAL:O	32:g:57:ASN:N	2.37	0.48
4:D:233:ARG:NH1	45:I:201:3PE:O14	2.46	0.48
4:D:329:LYS:NZ	7:G:121:MET:O	2.46	0.48
5:E:14:GLU:O	5:E:19:THR:OG1	2.30	0.48
5:E:142:VAL:HG21	5:E:145:LEU:HD21	1.95	0.48
12:L:273:ILE:HD13	12:L:276:ILE:HD12	1.96	0.48
20:T:6:LEU:HD13	20:T:86:VAL:HG12	1.95	0.48
28:c:34:GLN:NE2	28:c:38:ASP:OD2	2.46	0.48
12:L:62:ILE:HD11	41:p:114:GLN:NE2	2.28	0.48
12:L:237:MET:HE2	12:L:237:MET:HA	1.94	0.48
12:L:290:MET:SD	12:L:523:SER:OG	2.69	0.48
15:O:261:MET:SD	15:O:264:GLN:NE2	2.87	0.48
3:C:175:ARG:NH2	3:C:186:GLU:OE2	2.45	0.48
6:F:76:GLY:O	6:F:80:SER:OG	2.28	0.48
12:L:365:ALA:HB1	12:L:443:ILE:HG21	1.94	0.48
7:G:153:CYS:SG	7:G:154:ILE:N	2.87	0.48
12:L:338:MET:HB2	12:L:457:LEU:HD13	1.96	0.48
15:O:64:GLY:O	28:c:4:ILE:HG22	2.14	0.48
16:P:136:ASN:O	16:P:146:LEU:HD22	2.13	0.48
33:h:40:ILE:HG22	33:h:44:ASN:OD1	2.13	0.48
33:h:74:TRP:CH2	45:h:201:3PE:H262	2.49	0.48
6:F:122:CYS:O	6:F:126:GLY:N	2.42	0.48
6:F:143:TYR:OH	44:s:48:THR:O	2.29	0.48
7:G:366:THR:OG1	7:G:491:ASN:ND2	2.42	0.48
12:L:522:PHE:O	12:L:527:GLY:N	2.41	0.48
2:B:117:GLY:O	2:B:121:ASN:ND2	2.47	0.48
13:M:84:LEU:HD11	13:M:95:PHE:CD2	2.49	0.48
14:N:233:THR:HG23	14:N:237:THR:HG23	1.96	0.48
32:g:107:ILE:HG21	41:p:105:ILE:HD11	1.96	0.48
4:D:178:PHE:O	4:D:182:GLU:N	2.43	0.48
7:G:453:LEU:HD22	7:G:470:VAL:HG21	1.96	0.48
23:X:120:ASP:N	23:X:120:ASP:OD1	2.47	0.48
32:g:44:SER:O	33:h:20:ARG:NH2	2.43	0.48
33:h:35:PRO:O	33:h:39:GLY:N	2.38	0.48
13:M:369:LEU:HD12	13:M:370:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:134:HIS:NE2	16:P:170:GLU:OE2	2.46	0.47
3:C:28:TYR:OH	3:C:67:HIS:NE2	2.30	0.47
7:G:198:ASN:O	7:G:201:ASP:N	2.47	0.47
12:L:458:LEU:HD23	12:L:458:LEU:O	2.14	0.47
16:P:184:ASN:N	16:P:184:ASN:OD1	2.47	0.47
31:f:39:ASN:N	33:h:88:GLU:OE1	2.44	0.47
45:A:201:3PE:H2E1	27:b:22:PHE:CD1	2.48	0.47
7:G:104:ASP:OD2	7:G:152:ARG:NE	2.45	0.47
10:J:108:LEU:HD13	10:J:112:GLU:HB2	1.96	0.47
12:L:307:SER:HA	12:L:310:LEU:HD12	1.97	0.47
13:M:200:MET:HE1	13:M:243:MET:HG2	1.96	0.47
36:k:42:ASP:OD2	36:k:45:GLY:N	2.47	0.47
12:L:74:LEU:HD12	12:L:75:LYS:N	2.28	0.47
15:O:196:SER:O	15:O:200:GLN:N	2.42	0.47
20:U:70:LEU:HD13	20:U:76:ILE:HG12	1.95	0.47
38:m:95:GLY:N	38:m:96:PRO:HD2	2.29	0.47
41:p:127:GLU:N	41:p:127:GLU:OE1	2.48	0.47
5:E:143:GLU:O	5:E:144:CYS:C	2.57	0.47
35:j:25:ALA:O	35:j:29:SER:N	2.37	0.47
7:G:26:VAL:HG13	7:G:79:ILE:HD13	1.96	0.47
7:G:227:SER:OG	7:G:228:ILE:N	2.47	0.47
17:Q:120:ALA:O	17:Q:128:THR:OG1	2.27	0.47
20:T:36:PHE:CD1	20:T:40:LEU:HD12	2.49	0.47
33:h:112:ARG:NH2	33:h:113:LEU:HD21	2.30	0.47
34:i:18:ARG:NH1	39:n:173:PRO:O	2.47	0.47
1:A:103:ALA:O	1:A:107:THR:HG23	2.15	0.47
4:D:156:THR:O	4:D:159:LEU:N	2.47	0.47
6:F:31:TRP:NE1	44:s:42:GLN:OE1	2.43	0.47
7:G:410:GLY:O	7:G:421:HIS:NE2	2.43	0.47
7:G:616:LEU:HD11	7:G:620:ARG:NE	2.30	0.47
8:H:264:LEU:HD21	26:a:16:LEU:HD12	1.95	0.47
12:L:183:ILE:HD13	13:M:400:MET:HE1	1.96	0.47
12:L:480:MET:O	12:L:487:LYS:NZ	2.42	0.47
13:M:285:LEU:HD23	13:M:285:LEU:C	2.40	0.47
20:T:23:ASP:OD1	20:T:23:ASP:N	2.47	0.47
25:Z:27:ARG:NH1	43:r:14:ALA:O	2.47	0.47
29:d:100:ASP:OD2	33:h:117:ARG:NH1	2.47	0.47
34:i:18:ARG:NH2	39:n:173:PRO:O	2.48	0.47
41:p:100:GLU:O	41:p:103:ASN:N	2.47	0.47
2:B:84:ASP:OD1	8:H:58:LYS:NZ	2.45	0.47
4:D:233:ARG:NE	9:I:29:GLU:OE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:452:ILE:HD12	7:G:452:ILE:N	2.29	0.47
8:H:87:ILE:N	8:H:88:PRO:CD	2.78	0.47
14:N:106:LEU:HD21	14:N:138:PRO:HB2	1.96	0.47
15:O:48:LEU:HD12	15:O:123:VAL:HG23	1.96	0.47
34:i:102:ARG:NH2	40:o:48:ALA:O	2.39	0.47
43:r:3:ALA:O	43:r:8:GLN:NE2	2.43	0.47
5:E:162:GLU:OE2	6:F:108:ARG:NH1	2.43	0.47
7:G:571:ALA:HB3	7:G:573:TYR:CE2	2.50	0.47
9:I:4:TYR:CE1	43:r:105:LEU:HD21	2.50	0.47
9:I:173:TYR:CD2	18:R:66:LEU:HD21	2.49	0.47
13:M:390:ASN:OD1	13:M:390:ASN:N	2.45	0.47
33:h:128:ILE:HG22	33:h:129:ASP:O	2.15	0.47
40:o:5:ALA:O	40:o:9:LEU:N	2.41	0.47
13:M:313:THR:HG21	13:M:456:GLY:N	2.30	0.47
1:A:2:ASN:O	1:A:5:LEU:N	2.47	0.46
2:B:81:ARG:CZ	8:H:61:LEU:HD22	2.44	0.46
6:F:184:TYR:CE1	49:F:501:FMN:H6	2.50	0.46
13:M:82:HIS:O	13:M:85:SER:OG	2.25	0.46
31:f:26:LEU:O	31:f:30:ASN:N	2.45	0.46
1:A:97:LEU:HD22	10:J:162:LEU:HD22	1.96	0.46
3:C:104:ARG:NH2	4:D:373:GLU:OE2	2.40	0.46
6:F:194:GLU:OE2	6:F:204:ARG:NE	2.31	0.46
7:G:60:GLU:OE1	7:G:78:ASN:ND2	2.43	0.46
8:H:317:GLN:NE2	10:J:141:MET:HE1	2.30	0.46
12:L:189:PHE:O	12:L:193:LEU:N	2.49	0.46
33:h:8:LEU:O	34:i:27:LEU:HD11	2.15	0.46
20:T:54:MET:HE3	20:T:76:ILE:HD13	1.96	0.46
41:p:5:ASP:OD1	41:p:7:ASP:N	2.49	0.46
4:D:161:ILE:HG22	4:D:161:ILE:O	2.16	0.46
5:E:158:ASP:O	6:F:144:ASN:ND2	2.48	0.46
7:G:684:MET:HA	7:G:684:MET:HE2	1.98	0.46
20:U:55:GLU:OE1	39:n:24:ARG:NH2	2.49	0.46
23:X:72:GLN:O	23:X:76:HIS:ND1	2.48	0.46
36:k:13:MET:O	36:k:15:LEU:HD23	2.15	0.46
5:E:129:GLY:N	5:E:139:LEU:O	2.41	0.46
6:F:66:ARG:NE	6:F:72:GLY:O	2.42	0.46
7:G:229:ASP:OD2	7:G:267:THR:OG1	2.21	0.46
12:L:226:GLN:O	12:L:230:HIS:N	2.49	0.46
15:O:127:SER:N	15:O:130:SER:OG	2.35	0.46
6:F:258:ILE:N	6:F:258:ILE:HD12	2.31	0.46
8:H:309:ILE:O	27:b:41:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:52:MET:HE1	22:W:39:TYR:CG	2.51	0.46
1:A:90:MET:SD	10:J:151:THR:HG23	2.56	0.46
4:D:233:ARG:NH1	45:I:201:3PE:O21	2.49	0.46
6:F:268:VAL:HG11	6:F:283:HIS:HB3	1.98	0.46
7:G:533:THR:OG1	7:G:534:ARG:N	2.48	0.46
8:H:141:SER:O	8:H:289:LEU:HD21	2.15	0.46
12:L:273:ILE:HA	12:L:276:ILE:HD12	1.98	0.46
15:O:224:SER:O	15:O:228:ALA:N	2.45	0.46
34:i:17:LEU:O	34:i:21:TRP:N	2.39	0.46
9:I:173:TYR:CG	18:R:66:LEU:HD21	2.51	0.46
20:U:23:ASP:OD1	20:U:23:ASP:N	2.49	0.46
37:l:94:THR:OG1	37:l:96:VAL:O	2.34	0.46
45:A:201:3PE:H2B2	45:A:201:3PE:H2E2	1.73	0.46
3:C:99:LEU:HD12	3:C:99:LEU:H	1.81	0.46
5:E:155:GLN:HA	5:E:159:ASN:O	2.16	0.46
7:G:420:ASP:OD1	7:G:421:HIS:N	2.49	0.46
12:L:331:THR:HB	12:L:387:THR:HG22	1.97	0.46
13:M:297:VAL:HG13	13:M:312:ALA:CB	2.45	0.46
14:N:309:ASN:HA	15:O:284:VAL:HG21	1.96	0.46
1:A:73:LEU:HD13	10:J:55:MET:HE1	1.96	0.46
4:D:266:GLN:HA	4:D:287:ILE:HD11	1.98	0.45
7:G:326:GLU:OE1	7:G:326:GLU:N	2.48	0.45
14:N:236:LYS:HG3	14:N:237:THR:HG22	1.97	0.45
15:O:196:SER:HA	15:O:199:LEU:HD12	1.97	0.45
22:W:98:GLN:O	22:W:101:HIS:N	2.49	0.45
32:g:70:LEU:O	32:g:74:SER:OG	2.33	0.45
6:F:97:ALA:HB3	6:F:137:TYR:O	2.16	0.45
6:F:327:THR:OG1	6:F:328:GLY:N	2.50	0.45
13:M:6:ILE:N	13:M:7:PRO:HD2	2.31	0.45
5:E:63:ILE:HG23	5:E:64:SER:N	2.32	0.45
7:G:89:ALA:O	7:G:93:VAL:HG23	2.16	0.45
7:G:228:ILE:HG22	7:G:229:ASP:N	2.31	0.45
15:O:105:LEU:HD12	15:O:128:ILE:HG21	1.97	0.45
34:i:105:PRO:HG2	34:i:119:MET:HE2	1.98	0.45
45:A:201:3PE:H2E1	27:b:22:PHE:HD1	1.81	0.45
6:F:13:GLY:O	6:F:14:SER:OG	2.32	0.45
6:F:407:LEU:C	6:F:407:LEU:HD23	2.42	0.45
12:L:131:LEU:HD23	12:L:131:LEU:C	2.42	0.45
33:h:52:LEU:HD12	41:p:62:TYR:O	2.17	0.45
34:i:65:ARG:HB3	57:i:201:CHD:H191	1.99	0.45
7:G:616:LEU:HD11	7:G:620:ARG:HE	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:226:GLN:HB3	12:L:280:LEU:HD11	1.98	0.45
12:L:365:ALA:HB1	12:L:443:ILE:HD13	1.99	0.45
14:N:343:LEU:C	14:N:343:LEU:HD12	2.42	0.45
30:e:15:ARG:HH21	33:h:132:LEU:HD21	1.81	0.45
39:n:127:LEU:CD1	39:n:162:LEU:HD11	2.47	0.45
7:G:330:ALA:O	7:G:600:ILE:HG21	2.16	0.45
12:L:338:MET:CA	12:L:457:LEU:HD13	2.47	0.45
34:i:24:ASP:OD2	39:n:124:TRP:NE1	2.50	0.45
40:o:68:CYS:O	40:o:72:SER:N	2.42	0.45
7:G:107:ILE:HG22	9:I:78:ILE:HD12	1.98	0.45
7:G:157:THR:O	7:G:161:ARG:NE	2.36	0.45
12:L:230:HIS:N	12:L:231:PRO:CD	2.80	0.45
14:N:219:PHE:O	14:N:223:SER:N	2.45	0.45
15:O:138:MET:HE2	15:O:144:ILE:HG21	1.99	0.45
38:m:114:LEU:O	38:m:118:GLY:N	2.50	0.45
8:H:201:THR:HG21	8:H:211:PHE:CE1	2.50	0.45
12:L:4:PHE:CE1	12:L:87:MET:HE3	2.52	0.45
45:O:401:3PE:H252	45:O:401:3PE:H282	1.80	0.45
32:g:98:LYS:CB	41:p:8:VAL:HG22	2.47	0.45
39:n:124:TRP:O	39:n:128:ARG:N	2.49	0.45
4:D:54:GLN:OE1	4:D:61:VAL:HG12	2.17	0.45
5:E:103:CYS:HB2	5:E:145:LEU:HD12	1.98	0.45
5:E:156:ILE:HD12	5:E:156:ILE:N	2.32	0.45
6:F:197:GLU:OE2	6:F:216:PHE:N	2.41	0.45
6:F:205:LEU:HD11	6:F:404:ILE:HD13	1.99	0.45
7:G:323:VAL:HG12	7:G:324:ASP:N	2.32	0.45
15:O:215:SER:HA	15:O:220:VAL:HG23	1.98	0.45
16:P:203:GLN:NE2	16:P:232:GLY:O	2.46	0.45
37:l:27:TYR:OH	37:l:46:ASP:OD1	2.30	0.45
42:q:39:VAL:HG23	42:q:50:GLU:HG2	1.99	0.45
6:F:338:ASP:OD1	6:F:338:ASP:C	2.60	0.44
7:G:476:LYS:O	7:G:479:THR:OG1	2.29	0.44
7:G:526:GLY:N	7:G:546:GLN:O	2.50	0.44
12:L:411:MET:N	12:L:411:MET:HE2	2.33	0.44
13:M:106:LEU:HD13	13:M:234:VAL:HG11	1.99	0.44
16:P:315:ILE:O	16:P:319:ARG:N	2.51	0.44
4:D:268:ASP:OD2	4:D:270:ARG:NH2	2.44	0.44
5:E:162:GLU:OE2	6:F:108:ARG:NH2	2.50	0.44
7:G:53:ARG:O	7:G:93:VAL:HG21	2.17	0.44
10:J:3:LEU:HD21	10:J:125:TRP:CD1	2.52	0.44
12:L:116:LYS:NZ	12:L:120:TYR:OH	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:17:THR:HG23	14:N:137:ALA:HB2	1.98	0.44
15:O:135:LEU:HD22	15:O:152:TYR:CD2	2.51	0.44
15:O:206:TYR:HA	15:O:210:PHE:HB3	1.99	0.44
27:b:4:VAL:O	27:b:8:LEU:N	2.45	0.44
39:n:169:ILE:O	39:n:172:ARG:NH1	2.42	0.44
4:D:66:MET:HE1	4:D:411:LEU:HD11	2.00	0.44
7:G:431:ASP:OD1	7:G:431:ASP:N	2.50	0.44
10:J:17:PHE:HA	10:J:20:PHE:CE2	2.52	0.44
10:J:106:TYR:N	10:J:106:TYR:CD1	2.85	0.44
13:M:328:CYS:C	13:M:437:MET:HE1	2.42	0.44
14:N:305:PHE:O	15:O:286:ALA:HB2	2.17	0.44
34:i:11:LEU:O	34:i:15:ARG:N	2.38	0.44
6:F:147:SER:O	6:F:151:VAL:N	2.40	0.44
32:g:108:MET:CB	41:p:134:VAL:HG13	2.48	0.44
34:i:18:ARG:NH1	39:n:172:ARG:O	2.51	0.44
4:D:289:SER:OG	9:I:6:ASN:O	2.25	0.44
5:E:48:LEU:CD1	5:E:83:VAL:HG11	2.47	0.44
5:E:114:ASP:O	5:E:117:LEU:N	2.50	0.44
16:P:299:GLY:N	16:P:302:ASP:OD2	2.50	0.44
40:o:68:CYS:O	40:o:72:SER:OG	2.36	0.44
5:E:114:ASP:OD1	5:E:114:ASP:N	2.49	0.44
7:G:659:ASP:OD1	7:G:659:ASP:N	2.47	0.44
9:I:119:CYS:SG	9:I:120:GLY:N	2.91	0.44
21:V:10:LEU:N	21:V:10:LEU:HD23	2.32	0.44
34:i:108:THR:OG1	34:i:115:VAL:HG22	2.18	0.44
12:L:92:VAL:O	12:L:96:VAL:HG23	2.17	0.44
12:L:272:TYR:CE2	12:L:276:ILE:HD11	2.53	0.44
37:l:53:ARG:NE	37:l:57:GLU:OE2	2.51	0.44
4:D:233:ARG:NH2	9:I:29:GLU:OE2	2.50	0.44
21:V:24:LYS:O	21:V:28:THR:OG1	2.30	0.44
46:d:202:PC1:H382	46:d:202:PC1:H352	1.57	0.44
34:i:92:LYS:HB2	34:i:95:THR:HG21	1.99	0.44
12:L:251:THR:O	12:L:254:VAL:HG22	2.18	0.44
12:L:338:MET:HA	12:L:457:LEU:HD13	2.00	0.44
12:L:483:PRO:O	12:L:487:LYS:N	2.48	0.44
14:N:162:ILE:HG22	14:N:285:THR:HG21	1.99	0.44
16:P:290:THR:HG22	16:P:291:ASP:N	2.33	0.44
20:T:50:ILE:O	20:T:53:ALA:N	2.50	0.44
34:i:27:LEU:HD22	39:n:114:TYR:CE2	2.53	0.44
4:D:201:GLN:C	4:D:323:ILE:HD12	2.43	0.43
12:L:418:PHE:HD1	12:L:421:ILE:HD12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:48:ASN:OD1	13:M:49:SER:N	2.51	0.43
13:M:420:THR:HB	13:M:423:ILE:HD12	2.01	0.43
15:O:54:ALA:HB2	15:O:104:ARG:HA	2.00	0.43
33:h:50:ALA:HB2	41:p:60:TYR:HE2	1.83	0.43
35:j:45:ASP:OD1	35:j:45:ASP:N	2.51	0.43
42:q:1:AME:O	42:q:4:LEU:N	2.51	0.43
6:F:264:ASN:N	6:F:284:ALA:O	2.50	0.43
8:H:28:LEU:HD22	8:H:275:ALA:HB2	2.00	0.43
12:L:163:ASP:O	12:L:167:ALA:N	2.38	0.43
13:M:26:ASN:OD1	31:f:13:HIS:NE2	2.50	0.43
45:M:502:3PE:H2D2	45:M:502:3PE:H2G1	1.66	0.43
16:P:201:VAL:HB	16:P:290:THR:HG23	2.01	0.43
2:B:91:THR:HG22	2:B:92:LEU:H	1.84	0.43
4:D:277:VAL:O	4:D:279:ASP:N	2.51	0.43
8:H:307:LEU:HB3	8:H:308:PRO:HD3	2.00	0.43
10:J:110:ASP:OD1	10:J:110:ASP:N	2.51	0.43
12:L:257:ILE:HG21	12:L:329:ILE:HD11	2.00	0.43
15:O:128:ILE:HD12	15:O:160:ILE:HG13	2.00	0.43
3:C:188:VAL:O	3:C:188:VAL:HG13	2.18	0.43
6:F:227:THR:O	6:F:230:VAL:HG22	2.19	0.43
7:G:460:ARG:NH1	7:G:660:PRO:O	2.51	0.43
10:J:108:LEU:HD13	10:J:112:GLU:HA	2.00	0.43
12:L:316:THR:HB	12:L:325:ALA:HB2	2.00	0.43
13:M:54:LEU:HD21	33:h:96:ILE:HG21	2.00	0.43
14:N:41:ILE:N	14:N:42:PRO:HD2	2.34	0.43
29:d:71:VAL:HG11	51:d:203:CDL:H431	2.01	0.43
30:e:15:ARG:NH2	33:h:132:LEU:HD21	2.34	0.43
3:C:81:VAL:O	3:C:83:ILE:HD12	2.19	0.43
7:G:185:THR:O	7:G:186:TYR:HB3	2.18	0.43
7:G:261:GLU:OE1	17:Q:42:ARG:NH2	2.52	0.43
7:G:283:MET:HE1	42:q:137:TRP:CZ3	2.53	0.43
4:D:261:ARG:NH1	4:D:267:TRP:O	2.50	0.43
10:J:125:TRP:CB	25:Z:136:THR:HG21	2.49	0.43
12:L:217:ALA:O	12:L:221:THR:OG1	2.31	0.43
12:L:286:LEU:HD23	12:L:286:LEU:C	2.44	0.43
12:L:339:LEU:HD21	12:L:376:GLY:HA3	2.01	0.43
20:T:70:LEU:N	20:T:70:LEU:HD23	2.34	0.43
33:h:14:SER:OG	39:n:107:HIS:N	2.50	0.43
2:B:150:PRO:HB3	47:B:202:SF4:S1	2.59	0.43
4:D:49:LEU:C	4:D:49:LEU:HD23	2.43	0.43
8:H:149:ILE:HG21	8:H:185:TRP:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:318:THR:HG23	26:a:41:TYR:HE2	1.84	0.43
14:N:325:PHE:O	14:N:328:THR:N	2.51	0.43
33:h:114:MET:O	33:h:118:GLY:N	2.49	0.43
36:k:76:ALA:O	36:k:80:ALA:N	2.45	0.43
37:l:30:ARG:NH1	37:l:33:ASP:OD1	2.51	0.43
39:n:162:LEU:HD13	39:n:166:TRP:CE2	2.53	0.43
4:D:64:LEU:HD12	4:D:78:PRO:HA	2.00	0.43
6:F:268:VAL:HG22	6:F:269:GLU:O	2.19	0.43
7:G:286:ASN:OD1	7:G:290:LEU:N	2.51	0.43
12:L:210:ASN:N	12:L:210:ASN:OD1	2.51	0.43
26:a:1:MET:HB2	26:a:3:PHE:CE2	2.54	0.43
5:E:148:CYS:SG	6:F:104:THR:N	2.92	0.43
6:F:193:ILE:HG23	6:F:215:VAL:HB	2.00	0.43
10:J:130:THR:HG21	25:Z:123:LEU:HD12	2.01	0.43
12:L:49:ILE:HB	12:L:50:PRO:HD3	2.01	0.43
13:M:75:LEU:HD23	13:M:440:HIS:CE1	2.54	0.43
13:M:159:PRO:HB3	45:M:502:3PE:H291	2.01	0.43
13:M:173:SER:HB2	33:h:101:ALA:HB2	2.01	0.43
13:M:373:ILE:HA	13:M:376:ILE:HD12	2.00	0.43
14:N:146:PHE:N	14:N:147:PRO:CD	2.82	0.43
17:Q:61:THR:HG22	17:Q:62:ARG:N	2.34	0.43
26:a:52:ARG:O	26:a:55:SER:OG	2.31	0.43
38:m:76:TYR:CG	38:m:77:PRO:HD3	2.54	0.43
2:B:81:ARG:NE	8:H:61:LEU:HD22	2.34	0.42
6:F:126:GLY:O	6:F:130:GLY:N	2.51	0.42
6:F:320:ASP:OD1	6:F:320:ASP:N	2.50	0.42
8:H:116:ILE:HG22	8:H:116:ILE:O	2.18	0.42
4:D:202:ASP:OD2	25:Z:7:GLN:NE2	2.53	0.42
7:G:574:VAL:HG13	7:G:579:ARG:O	2.18	0.42
13:M:54:LEU:HD12	13:M:54:LEU:H	1.85	0.42
41:p:112:CYS:O	41:p:116:GLU:HG2	2.19	0.42
2:B:63:ALA:HB2	2:B:69:MET:HE2	2.01	0.42
2:B:83:SER:O	8:H:58:LYS:NZ	2.43	0.42
4:D:68:LEU:HD21	4:D:411:LEU:HD13	2.01	0.42
4:D:174:ARG:HA	4:D:177:MET:HE3	2.02	0.42
7:G:171:ASP:OD2	7:G:189:LYS:NZ	2.45	0.42
7:G:478:ARG:HA	7:G:483:VAL:HG21	2.02	0.42
32:g:108:MET:HB2	41:p:134:VAL:HG13	2.02	0.42
33:h:64:TRP:CG	33:h:77:ARG:HB3	2.54	0.42
34:i:97:VAL:HG12	34:i:98:GLU:N	2.34	0.42
1:A:114:THR:HG23	8:H:287:HIS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:128:MET:O	12:L:132:VAL:HG13	2.19	0.42
12:L:349:SER:OG	12:L:366:MET:SD	2.78	0.42
13:M:143:LEU:HD13	13:M:222:GLU:OE2	2.18	0.42
15:O:21:LYS:NZ	15:O:46:LEU:O	2.43	0.42
45:h:201:3PE:H252	45:h:201:3PE:H282	1.63	0.42
13:M:209:LEU:HD13	13:M:298:ILE:HD13	2.01	0.42
19:S:22:LEU:HD11	19:S:36:ILE:HD12	2.02	0.42
19:S:35:PHE:CD1	19:S:35:PHE:C	2.98	0.42
34:i:54:ALA:HB1	34:i:56:TRP:CZ3	2.54	0.42
7:G:365:ASN:N	7:G:491:ASN:OD1	2.52	0.42
7:G:554:ALA:HB3	7:G:555:PRO:HD3	2.01	0.42
12:L:388:GLY:O	12:L:392:LYS:N	2.39	0.42
45:M:501:3PE:H2B2	45:M:501:3PE:C26	2.40	0.42
15:O:267:LEU:O	15:O:271:ASN:N	2.53	0.42
16:P:185:ILE:HD12	16:P:279:THR:OG1	2.19	0.42
16:P:205:VAL:HG22	16:P:206:TYR:N	2.35	0.42
23:X:153:VAL:N	29:d:6:GLN:OE1	2.52	0.42
1:A:64:LEU:HD13	10:J:165:VAL:CG2	2.49	0.42
3:C:89:ARG:NH2	3:C:165:ASP:OD1	2.48	0.42
6:F:13:GLY:N	6:F:271:GLU:OE1	2.43	0.42
6:F:188:GLU:OE1	6:F:190:THR:OG1	2.26	0.42
7:G:343:LEU:HD22	7:G:343:LEU:N	2.35	0.42
8:H:173:TRP:HB3	8:H:175:ILE:HG22	2.01	0.42
10:J:50:SER:N	10:J:139:GLU:OE1	2.52	0.42
20:U:31:SER:OG	20:U:34:SER:OG	2.12	0.42
37:l:47:TYR:CG	37:l:48:PRO:HD2	2.55	0.42
38:m:114:LEU:HD22	38:m:119:LYS:HB2	2.01	0.42
3:C:16:ASP:OD1	3:C:16:ASP:N	2.53	0.42
6:F:197:GLU:OE1	6:F:204:ARG:NH2	2.53	0.42
7:G:104:ASP:OD2	7:G:152:ARG:NH2	2.48	0.42
19:S:22:LEU:HD13	19:S:32:VAL:HG12	2.02	0.42
19:S:94:LEU:O	19:S:95:SER:OG	2.27	0.42
27:b:10:ASN:O	27:b:13:ALA:N	2.43	0.42
4:D:258:VAL:O	4:D:258:VAL:HG12	2.19	0.42
8:H:195:ARG:O	8:H:198:PHE:N	2.52	0.42
15:O:260:ARG:HA	15:O:263:VAL:HG22	2.02	0.42
16:P:133:SER:O	16:P:167:LYS:HA	2.19	0.42
37:l:80:ASP:HB3	37:l:83:MET:HE2	2.00	0.42
7:G:12:PHE:HA	7:G:16:GLN:O	2.20	0.42
13:M:303:ILE:C	13:M:304:GLN:HG2	2.43	0.42
2:B:60:MET:O	2:B:63:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:ASP:OD1	3:C:82:ASP:C	2.63	0.41
6:F:221:THR:HG22	6:F:222:VAL:N	2.34	0.41
10:J:52:LEU:HD23	11:K:61:ILE:HD11	2.02	0.41
10:J:108:LEU:HD22	10:J:112:GLU:HA	2.02	0.41
12:L:203:MET:HE2	41:p:109:LEU:HG	2.02	0.41
13:M:57:PHE:HB3	13:M:113:MET:HE2	2.02	0.41
13:M:263:MET:N	13:M:263:MET:SD	2.93	0.41
13:M:452:LYS:HB2	13:M:459:TYR:CE2	2.55	0.41
19:S:60:VAL:HG23	19:S:60:VAL:O	2.20	0.41
34:i:97:VAL:HG13	41:p:115:ARG:HB2	2.02	0.41
43:r:61:GLU:O	43:r:63:MET:HE2	2.19	0.41
2:B:118:SER:N	47:B:202:SF4:S3	2.93	0.41
7:G:358:LEU:HD23	7:G:641:TYR:CB	2.49	0.41
7:G:654:GLN:OE1	7:G:654:GLN:N	2.53	0.41
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.84	0.41
14:N:215:MET:HE3	14:N:219:PHE:CZ	2.55	0.41
15:O:79:LEU:HD21	52:O:402:DGT:O3'	2.19	0.41
19:S:22:LEU:HD21	19:S:56:GLU:HG2	2.03	0.41
5:E:213:VAL:HG12	5:E:214:GLN:O	2.20	0.41
7:G:415:LEU:C	7:G:416:THR:HG1	2.11	0.41
7:G:462:ASP:O	7:G:463:GLY:C	2.63	0.41
13:M:268:GLY:O	13:M:272:THR:HG23	2.20	0.41
19:S:21:HIS:O	19:S:62:PRO:HA	2.21	0.41
26:a:43:TYR:CZ	26:a:47:LEU:HD11	2.55	0.41
10:J:129:ASP:OD1	10:J:129:ASP:N	2.50	0.41
12:L:151:SER:OG	12:L:252:MET:SD	2.78	0.41
12:L:398:ALA:HA	12:L:401:THR:OG1	2.20	0.41
6:F:42:TRP:CZ2	6:F:161:LEU:HD13	2.56	0.41
6:F:103:GLY:O	6:F:333:ALA:HB1	2.21	0.41
6:F:390:ASP:O	6:F:393:TRP:HB3	2.21	0.41
7:G:213:TYR:O	7:G:213:TYR:CG	2.74	0.41
8:H:71:PHE:O	8:H:215:TYR:OH	2.31	0.41
8:H:208:VAL:O	8:H:208:VAL:HG13	2.20	0.41
10:J:36:SER:HA	10:J:39:VAL:HG22	2.02	0.41
12:L:82:MET:HB3	12:L:87:MET:HE2	2.02	0.41
12:L:316:THR:HG21	12:L:325:ALA:N	2.36	0.41
12:L:363:PHE:CD2	12:L:370:THR:HG21	2.55	0.41
13:M:12:MET:HB2	13:M:13:PRO:HD3	2.03	0.41
19:S:93:VAL:O	19:S:96:SER:OG	2.35	0.41
21:V:89:LEU:HD11	21:V:93:MET:HE2	2.02	0.41
42:q:62:VAL:CG2	42:q:63:ILE:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:76:ALA:N	3:C:95:ASN:O	2.53	0.41
3:C:99:LEU:HD12	3:C:99:LEU:N	2.36	0.41
8:H:49:ILE:N	8:H:49:ILE:HD12	2.35	0.41
20:U:47:GLN:NE2	20:U:70:LEU:O	2.46	0.41
1:A:28:ASN:C	1:A:29:VAL:HG22	2.45	0.41
1:A:55:PHE:O	1:A:58:VAL:HG12	2.20	0.41
3:C:100:ARG:O	43:r:100:ILE:HG22	2.20	0.41
7:G:568:GLU:HG2	7:G:587:VAL:HG23	2.03	0.41
9:I:86:VAL:O	9:I:87:CYS:C	2.64	0.41
11:K:82:SER:O	11:K:86:GLY:N	2.44	0.41
12:L:67:HIS:CE1	12:L:70:THR:HG1	2.33	0.41
15:O:158:VAL:CG1	15:O:159:THR:HG23	2.48	0.41
15:O:199:LEU:HA	15:O:202:ILE:HD12	2.01	0.41
16:P:96:GLY:O	54:P:501:NDP:H8A	2.20	0.41
18:R:81:THR:OG1	18:R:90:GLN:OE1	2.23	0.41
20:U:14:ARG:NH2	20:U:57:GLU:O	2.54	0.41
13:M:287:ALA:O	13:M:290:SER:OG	2.32	0.41
17:Q:18:ASP:OD1	17:Q:18:ASP:C	2.63	0.41
23:X:52:PRO:HB2	25:Z:83:LEU:HD11	2.02	0.41
3:C:41:GLN:NE2	3:C:49:GLU:OE1	2.50	0.41
3:C:58:ILE:HB	3:C:59:PRO:HD3	2.03	0.41
4:D:226:GLU:OE1	25:Z:22:ARG:NE	2.51	0.41
5:E:34:ILE:HD11	44:s:52:LEU:HD22	2.03	0.41
7:G:283:MET:HE1	42:q:137:TRP:HZ3	1.85	0.41
7:G:324:ASP:HB2	7:G:571:ALA:HB1	2.02	0.41
7:G:428:ILE:O	7:G:431:ASP:N	2.54	0.41
7:G:483:VAL:HG12	7:G:484:THR:N	2.36	0.41
7:G:640:ASN:C	7:G:641:TYR:CG	2.99	0.41
13:M:42:MET:HG3	13:M:67:ILE:HD11	2.02	0.41
13:M:458:LEU:HD22	13:M:458:LEU:H	1.86	0.41
14:N:150:ASN:OD1	14:N:152:ASN:N	2.54	0.41
15:O:233:LYS:O	15:O:237:ASP:N	2.41	0.41
16:P:50:ARG:NE	54:P:501:NDP:O1X	2.45	0.41
20:T:22:TYR:OH	20:T:49:GLU:OE1	2.28	0.41
20:U:68:GLU:HB3	34:i:1:SAC:H2A2	2.03	0.41
30:e:64:GLU:HA	30:e:64:GLU:OE1	2.21	0.41
34:i:76:ILE:HB	34:i:77:PRO:HD3	2.03	0.41
39:n:124:TRP:HZ3	39:n:170:VAL:HG11	1.86	0.41
41:p:42:ARG:O	41:p:46:LEU:N	2.44	0.41
7:G:647:GLU:OE1	19:S:41:VAL:HG11	2.20	0.41
45:I:201:3PE:H3C2	27:b:24:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:40:ILE:HD12	12:L:40:ILE:N	2.36	0.41
13:M:422:HIS:O	38:m:55:ARG:NH2	2.50	0.41
20:T:76:ILE:O	20:T:79:TYR:N	2.54	0.41
23:X:108:GLU:O	23:X:112:ASP:N	2.40	0.41
23:X:142:HIS:CD2	23:X:142:HIS:N	2.89	0.41
39:n:40:ALA:O	39:n:44:ARG:N	2.40	0.41
4:D:294:TYR:CE2	4:D:298:LEU:HD11	2.56	0.40
5:E:169:ILE:HG23	5:E:170:GLU:N	2.36	0.40
12:L:286:LEU:HD23	12:L:286:LEU:O	2.21	0.40
14:N:310:ASN:OD1	14:N:310:ASN:N	2.53	0.40
16:P:109:VAL:HG23	16:P:110:PHE:CD2	2.56	0.40
19:S:64:LEU:O	19:S:75:ASN:HA	2.21	0.40
20:U:47:GLN:NE2	20:U:67:ALA:O	2.54	0.40
23:X:110:VAL:O	23:X:114:LEU:N	2.54	0.40
37:l:88:ARG:O	37:l:89:VAL:C	2.64	0.40
39:n:10:THR:HG22	39:n:11:HIS:N	2.36	0.40
1:A:23:TRP:O	1:A:26:GLN:HB2	2.20	0.40
2:B:60:MET:HE2	4:D:167:PHE:CE1	2.57	0.40
3:C:40:VAL:HG22	3:C:50:ILE:HD13	2.02	0.40
12:L:14:LEU:HD11	34:i:69:PHE:CE2	2.56	0.40
15:O:42:ILE:HD11	15:O:234:VAL:HG11	2.03	0.40
15:O:108:TYR:HB2	15:O:128:ILE:HG23	2.03	0.40
32:g:100:ARG:NH1	32:g:107:ILE:O	2.53	0.40
42:q:95:ASP:N	43:r:34:THR:OG1	2.54	0.40
1:A:75:LEU:N	1:A:76:PRO:HD2	2.37	0.40
6:F:359:CYS:N	47:F:502:SF4:S4	2.89	0.40
12:L:192:ASN:O	38:m:124:PHE:HB2	2.21	0.40
12:L:264:TYR:N	12:L:265:PRO:CD	2.85	0.40
12:L:433:GLY:N	36:k:59:ASN:OD1	2.49	0.40
13:M:11:LEU:O	13:M:14:LEU:HB3	2.20	0.40
13:M:194:PHE:HD2	45:M:502:3PE:H2B2	1.87	0.40
14:N:209:ILE:O	14:N:213:SER:OG	2.35	0.40
15:O:167:HIS:CE1	15:O:248:TRP:CD2	3.09	0.40
25:Z:136:THR:HG22	25:Z:137:TYR:CE1	2.56	0.40
37:l:64:TRP:CD1	37:l:70:ARG:HA	2.56	0.40
13:M:173:SER:CB	33:h:101:ALA:HB2	2.52	0.40
13:M:411:LEU:HD12	13:M:415:GLN:CG	2.52	0.40
16:P:46:ILE:HG23	16:P:71:MET:HE3	2.03	0.40
31:f:42:LEU:N	31:f:42:LEU:HD12	2.37	0.40
33:h:129:ASP:OD1	33:h:131:GLU:N	2.37	0.40
39:n:80:ILE:HG21	39:n:86:GLY:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:5:ASP:OD1	41:p:5:ASP:C	2.65	0.40
1:A:29:VAL:O	46:A:202:PC1:H133	2.22	0.40
3:C:51:CYS:HB3	21:V:111:TRP:CZ2	2.56	0.40
5:E:199:LEU:HD12	5:E:199:LEU:N	2.36	0.40
7:G:346:GLU:OE2	7:G:529:GLY:N	2.49	0.40
15:O:105:LEU:HA	15:O:128:ILE:HG22	2.04	0.40
15:O:301:GLY:HA2	15:O:309:ASN:CB	2.50	0.40
25:Z:131:GLU:O	25:Z:134:SER:HB3	2.21	0.40
34:i:109:ILE:HG22	34:i:110:LEU:N	2.36	0.40
38:m:7:ALA:HB1	38:m:11:SER:O	2.22	0.40
38:m:99:PHE:CE2	38:m:103:VAL:HG21	2.56	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	100/115 (87%)	87 (87%)	12 (12%)	1 (1%)	12	45
2	B	156/216 (72%)	147 (94%)	9 (6%)	0	100	100
3	C	208/266 (78%)	185 (89%)	23 (11%)	0	100	100
4	D	385/463 (83%)	359 (93%)	26 (7%)	0	100	100
5	E	212/249 (85%)	195 (92%)	17 (8%)	0	100	100
6	F	430/464 (93%)	403 (94%)	27 (6%)	0	100	100
7	G	687/727 (94%)	632 (92%)	55 (8%)	0	100	100
8	H	316/318 (99%)	300 (95%)	16 (5%)	0	100	100
9	I	174/212 (82%)	160 (92%)	14 (8%)	0	100	100
10	J	156/175 (89%)	132 (85%)	24 (15%)	0	100	100
11	K	84/98 (86%)	79 (94%)	4 (5%)	1 (1%)	10	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	L	545/606 (90%)	518 (95%)	27 (5%)	0	100	100
13	M	457/459 (100%)	432 (94%)	25 (6%)	0	100	100
14	N	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
15	O	318/343 (93%)	305 (96%)	13 (4%)	0	100	100
16	P	314/380 (83%)	288 (92%)	26 (8%)	0	100	100
17	Q	123/175 (70%)	113 (92%)	10 (8%)	0	100	100
18	R	94/124 (76%)	82 (87%)	12 (13%)	0	100	100
19	S	85/99 (86%)	80 (94%)	5 (6%)	0	100	100
20	T	82/156 (53%)	80 (98%)	2 (2%)	0	100	100
20	U	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
21	V	111/116 (96%)	105 (95%)	6 (5%)	0	100	100
22	W	113/128 (88%)	104 (92%)	9 (8%)	0	100	100
23	X	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
24	Y	29/141 (21%)	27 (93%)	2 (7%)	0	100	100
25	Z	140/144 (97%)	133 (95%)	7 (5%)	0	100	100
26	a	68/70 (97%)	68 (100%)	0	0	100	100
27	b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	c	46/76 (60%)	46 (100%)	0	0	100	100
29	d	118/120 (98%)	110 (93%)	8 (7%)	0	100	100
30	e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
31	f	55/57 (96%)	52 (94%)	3 (6%)	0	100	100
32	g	88/154 (57%)	79 (90%)	9 (10%)	0	100	100
33	h	141/189 (75%)	131 (93%)	10 (7%)	0	100	100
34	i	125/128 (98%)	116 (93%)	9 (7%)	0	100	100
35	j	68/108 (63%)	62 (91%)	6 (9%)	0	100	100
36	k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	l	154/186 (83%)	138 (90%)	16 (10%)	0	100	100
38	m	126/129 (98%)	118 (94%)	8 (6%)	0	100	100
39	n	169/179 (94%)	160 (95%)	9 (5%)	0	100	100
40	o	118/137 (86%)	109 (92%)	9 (8%)	0	100	100
41	p	171/176 (97%)	162 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	q	143/145 (99%)	133 (93%)	10 (7%)	0	100	100
43	r	92/113 (81%)	79 (86%)	13 (14%)	0	100	100
44	s	43/109 (39%)	42 (98%)	1 (2%)	0	100	100
All	All	7901/9213 (86%)	7377 (93%)	522 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	2	SER
1	A	29	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	92/100 (92%)	90 (98%)	2 (2%)	45	65
2	B	134/175 (77%)	132 (98%)	2 (2%)	57	70
3	C	190/228 (83%)	185 (97%)	5 (3%)	40	62
4	D	334/392 (85%)	324 (97%)	10 (3%)	36	59
5	E	183/205 (89%)	175 (96%)	8 (4%)	25	52
6	F	345/368 (94%)	338 (98%)	7 (2%)	48	66
7	G	578/608 (95%)	565 (98%)	13 (2%)	45	65
8	H	274/274 (100%)	269 (98%)	5 (2%)	51	68
9	I	151/175 (86%)	150 (99%)	1 (1%)	76	78
10	J	127/141 (90%)	125 (98%)	2 (2%)	55	69
11	K	73/85 (86%)	69 (94%)	4 (6%)	19	47
12	L	479/533 (90%)	473 (99%)	6 (1%)	61	72
13	M	412/412 (100%)	404 (98%)	8 (2%)	50	67
14	N	315/315 (100%)	312 (99%)	3 (1%)	68	75
15	O	283/303 (93%)	275 (97%)	8 (3%)	38	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	276/327 (84%)	266 (96%)	10 (4%)	31	56
17	Q	112/153 (73%)	106 (95%)	6 (5%)	20	47
18	R	79/97 (81%)	78 (99%)	1 (1%)	61	72
19	S	77/82 (94%)	74 (96%)	3 (4%)	28	54
20	T	78/135 (58%)	75 (96%)	3 (4%)	29	55
20	U	81/135 (60%)	78 (96%)	3 (4%)	30	56
21	V	101/102 (99%)	100 (99%)	1 (1%)	68	75
22	W	108/114 (95%)	105 (97%)	3 (3%)	38	60
23	X	154/155 (99%)	151 (98%)	3 (2%)	50	67
24	Y	25/102 (24%)	24 (96%)	1 (4%)	28	54
25	Z	120/121 (99%)	118 (98%)	2 (2%)	53	69
26	a	59/59 (100%)	59 (100%)	0	100	100
27	b	71/72 (99%)	71 (100%)	0	100	100
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	105/105 (100%)	104 (99%)	1 (1%)	68	75
30	e	89/96 (93%)	88 (99%)	1 (1%)	65	74
31	f	54/54 (100%)	54 (100%)	0	100	100
32	g	81/131 (62%)	80 (99%)	1 (1%)	63	73
33	h	124/158 (78%)	122 (98%)	2 (2%)	55	69
34	i	120/121 (99%)	116 (97%)	4 (3%)	33	58
35	j	61/84 (73%)	59 (97%)	2 (3%)	33	58
36	k	63/76 (83%)	62 (98%)	1 (2%)	55	69
37	l	140/159 (88%)	139 (99%)	1 (1%)	76	78
38	m	113/114 (99%)	108 (96%)	5 (4%)	25	52
39	n	156/161 (97%)	155 (99%)	1 (1%)	78	79
40	o	109/120 (91%)	104 (95%)	5 (5%)	24	51
41	p	156/157 (99%)	149 (96%)	7 (4%)	24	51
42	q	130/130 (100%)	123 (95%)	7 (5%)	20	47
43	r	86/97 (89%)	86 (100%)	0	100	100
44	s	44/92 (48%)	42 (96%)	2 (4%)	24	51
All	All	6986/7891 (88%)	6826 (98%)	160 (2%)	41	64

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	PHE
1	A	114	THR
2	B	30	VAL
2	B	54	CYS
3	C	85	THR
3	C	103	SER
3	C	109	THR
3	C	111	THR
3	C	184	VAL
4	D	59	HIS
4	D	139	VAL
4	D	275	TYR
4	D	322	GLU
4	D	323	ILE
4	D	376	VAL
4	D	378	LEU
4	D	384	SER
4	D	391	ILE
4	D	429	ASP
5	E	12	THR
5	E	28	TYR
5	E	74	GLN
5	E	75	VAL
5	E	99	HIS
5	E	113	SER
5	E	114	ASP
5	E	181	ILE
6	F	141	GLU
6	F	231	SER
6	F	268	VAL
6	F	318	ASP
6	F	350	LEU
6	F	359	CYS
6	F	365	CYS
7	G	66	VAL
7	G	170	ASP
7	G	174	THR
7	G	297	GLU
7	G	339	ASP
7	G	357	ASP
7	G	484	THR
7	G	533	THR

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Mol	Chain	Res	Type
7	G	536	ASP
7	G	543	ILE
7	G	560	ILE
7	G	659	ASP
7	G	684	MET
8	H	59	GLU
8	H	161	THR
8	H	176	LEU
8	H	268	MET
8	H	285	LEU
9	I	110	ASP
10	J	110	ASP
10	J	122	LEU
11	K	31	LEU
11	K	78	LEU
11	K	84	THR
11	K	85	TYR
12	L	210	ASN
12	L	254	VAL
12	L	306	THR
12	L	340	PHE
12	L	387	THR
12	L	541	ASN
13	M	57	PHE
13	M	82	HIS
13	M	83	HIS
13	M	305	THR
13	M	307	TRP
13	M	315	LEU
13	M	357	THR
13	M	390	ASN
14	N	17	THR
14	N	222	ASN
14	N	296	LEU
15	O	24	LEU
15	O	80	GLU
15	O	81	LYS
15	O	87	LYS
15	O	147	GLN
15	O	148	CYS
15	O	150	ASP
15	O	168	VAL

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Mol	Chain	Res	Type
16	P	3	HIS
16	P	44	GLN
16	P	90	VAL
16	P	101	THR
16	P	170	GLU
16	P	184	ASN
16	P	222	ASP
16	P	241	LEU
16	P	311	GLU
16	P	333	ASP
17	Q	21	THR
17	Q	27	GLU
17	Q	32	THR
17	Q	38	PHE
17	Q	47	SER
17	Q	122	PHE
18	R	96	HIS
19	S	59	ASP
19	S	81	PHE
19	S	84	ASP
20	T	18	VAL
20	T	65	ILE
20	T	86	VAL
20	U	7	THR
20	U	23	ASP
20	U	85	ASP
21	V	103	VAL
22	W	48	LEU
22	W	100	THR
22	W	118	LEU
23	X	120	ASP
23	X	133	ASP
23	X	156	ASP
24	Y	140	VAL
25	Z	5	VAL
25	Z	51	LYS
29	d	10	THR
30	e	96	HIS
32	g	74	SER
33	h	66	TYR
33	h	134	ASP
34	i	25	GLN

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Mol	Chain	Res	Type
34	i	26	GLU
34	i	68	ILE
34	i	126	HIS
35	j	45	ASP
35	j	69	ASP
36	k	90	GLN
37	l	97	ASN
38	m	15	THR
38	m	18	ASP
38	m	60	GLU
38	m	125	ASN
38	m	128	TYR
39	n	34	ASP
40	o	50	LEU
40	o	68	CYS
40	o	76	PHE
40	o	79	CYS
40	o	91	HIS
41	p	5	ASP
41	p	7	ASP
41	p	8	VAL
41	p	22	GLN
41	p	88	GLU
41	p	127	GLU
41	p	135	VAL
42	q	4	LEU
42	q	32	ASP
42	q	59	HIS
42	q	76	ASP
42	q	101	LYS
42	q	130	THR
42	q	145	LYS
44	s	54	LEU
44	s	72	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	160	HIS
6	F	144	ASN
6	F	257	ASN
7	G	7	ASN

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Mol	Chain	Res	Type
7	G	336	ASN
7	G	517	ASN
8	H	250	HIS
11	K	25	HIS
12	L	56	HIS
12	L	541	ASN
13	M	279	GLN
15	O	204	ASN
16	P	180	ASN
17	Q	46	GLN
23	X	29	HIS
25	Z	7	GLN
26	a	27	HIS
27	b	70	GLN
31	f	5	GLN
34	i	82	HIS
34	i	127	HIS
35	j	16	GLN
36	k	58	ASN
37	l	87	ASN
41	p	139	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

14 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	$\# Z > 2$
27	AYA	b	1	27	6,7,8	1.92	1 (16%)	6,8,10	1.37	1 (16%)
8	FME	H	1	8	8,9,10	1.50	1 (12%)	8,9,11	1.46	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	FME	J	1	10	8,9,10	1.53	1 (12%)	8,9,11	1.41	1 (12%)
14	FME	N	1	14	8,9,10	1.51	1 (12%)	8,9,11	1.36	1 (12%)
42	AME	q	1	42	9,10,11	1.52	1 (11%)	9,11,13	1.44	1 (11%)
1	FME	A	1	1	8,9,10	1.52	1 (12%)	8,9,11	1.48	2 (25%)
38	SAC	m	1	38	7,8,9	1.79	2 (28%)	7,9,11	1.86	1 (14%)
34	SAC	i	1	34	7,8,9	1.72	1 (14%)	7,9,11	1.28	1 (14%)
13	FME	M	1	13	8,9,10	1.51	1 (12%)	8,9,11	1.46	1 (12%)
29	AME	d	1	29	9,10,11	1.50	1 (11%)	9,11,13	1.20	0
43	AYA	r	1	43	6,7,8	1.84	2 (33%)	6,8,10	1.36	1 (16%)
12	FME	L	1	12	8,9,10	1.52	1 (12%)	8,9,11	1.46	2 (25%)
4	2MR	D	85	4	10,12,13	2.38	2 (20%)	5,13,15	1.63	2 (40%)
11	FME	K	1	11	8,9,10	1.53	1 (12%)	8,9,11	1.34	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	AYA	b	1	27	-	0/5/6/8	-
8	FME	H	1	8	-	4/7/9/11	-
10	FME	J	1	10	-	4/7/9/11	-
14	FME	N	1	14	-	4/7/9/11	-
42	AME	q	1	42	-	2/9/10/12	-
1	FME	A	1	1	-	3/7/9/11	-
38	SAC	m	1	38	-	3/7/8/10	-
34	SAC	i	1	34	-	2/7/8/10	-
13	FME	M	1	13	-	2/7/9/11	-
29	AME	d	1	29	-	1/9/10/12	-
43	AYA	r	1	43	-	0/5/6/8	-
12	FME	L	1	12	-	3/7/9/11	-
4	2MR	D	85	4	-	0/10/13/15	-
11	FME	K	1	11	-	3/7/9/11	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.25	1.44	1.33
4	D	85	2MR	CZ-NE	4.87	1.44	1.34
11	K	1	FME	CN-N	3.91	1.46	1.33
10	J	1	FME	CN-N	3.77	1.45	1.33
14	N	1	FME	CN-N	3.77	1.45	1.33
12	L	1	FME	CN-N	3.76	1.45	1.33
8	H	1	FME	CN-N	3.73	1.45	1.33
1	A	1	FME	CN-N	3.72	1.45	1.33
38	m	1	SAC	C1A-N	3.72	1.46	1.34
13	M	1	FME	CN-N	3.69	1.45	1.33
27	b	1	AYA	CT-N	3.61	1.46	1.34
42	q	1	AME	CT1-N	3.52	1.45	1.34
34	i	1	SAC	C1A-N	3.49	1.45	1.34
29	d	1	AME	CT1-N	3.43	1.45	1.34
43	r	1	AYA	CT-N	3.35	1.45	1.34
38	m	1	SAC	OAC-C1A	-2.02	1.18	1.23
43	r	1	AYA	OT-CT	-2.02	1.18	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	m	1	SAC	C2A-C1A-N	3.67	122.21	116.12
42	q	1	AME	CT2-CT1-N	2.63	120.48	116.12
27	b	1	AYA	CM-CT-N	2.42	120.13	116.12
4	D	85	2MR	CD-NE-CZ	-2.42	118.82	123.36
1	A	1	FME	CA-N-CN	-2.32	119.26	122.82
43	r	1	AYA	CM-CT-N	2.30	119.94	116.12
34	i	1	SAC	C2A-C1A-N	2.28	119.90	116.12
4	D	85	2MR	CQ2-NH2-CZ	-2.28	118.75	123.65
14	N	1	FME	O1-CN-N	-2.22	119.58	125.32
12	L	1	FME	CA-N-CN	-2.21	119.42	122.82
11	K	1	FME	O1-CN-N	-2.19	119.67	125.32
8	H	1	FME	O1-CN-N	-2.15	119.75	125.32
10	J	1	FME	O1-CN-N	-2.10	119.90	125.32
13	M	1	FME	O1-CN-N	-2.07	119.97	125.32
1	A	1	FME	O1-CN-N	-2.07	119.97	125.32
8	H	1	FME	CA-N-CN	-2.03	119.69	122.82
12	L	1	FME	O1-CN-N	-2.01	120.12	125.32
8	H	1	FME	CE-SD-CG	2.00	110.68	100.32

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
8	H	1	FME	C-CA-CB-CG
8	H	1	FME	O-C-CA-CB
10	J	1	FME	O1-CN-N-CA
10	J	1	FME	N-CA-CB-CG
10	J	1	FME	C-CA-CB-CG
11	K	1	FME	O1-CN-N-CA
11	K	1	FME	CB-CA-N-CN
12	L	1	FME	O1-CN-N-CA
14	N	1	FME	O1-CN-N-CA
14	N	1	FME	C-CA-CB-CG
38	m	1	SAC	O-C-CA-CB
12	L	1	FME	CA-CB-CG-SD
38	m	1	SAC	C2A-C1A-N-CA
38	m	1	SAC	OAC-C1A-N-CA
14	N	1	FME	N-CA-CB-CG
14	N	1	FME	CB-CG-SD-CE
13	M	1	FME	CA-CB-CG-SD
42	q	1	AME	CA-CB-CG-SD
8	H	1	FME	CB-CG-SD-CE
8	H	1	FME	N-CA-CB-CG
13	M	1	FME	CB-CG-SD-CE
11	K	1	FME	CA-CB-CG-SD
12	L	1	FME	CB-CG-SD-CE
34	i	1	SAC	CB-CA-N-C1A
34	i	1	SAC	C-CA-N-C1A
42	q	1	AME	CB-CA-N-CT1
10	J	1	FME	CB-CA-N-CN
29	d	1	AME	CA-CB-CG-SD

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
42	q	1	AME	1	0
34	i	1	SAC	1	0
13	M	1	FME	3	0
11	K	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 3 are 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
54	NDP	P	501	-	51,52,52	3.99	27 (52%)	71,80,80	2.01	14 (19%)
46	PC1	A	202	-	49,49,53	1.01	4 (8%)	55,57,61	1.00	2 (3%)
56	EHZ	U	101	20	31,36,37	1.60	5 (16%)	36,44,47	1.68	8 (22%)
45	3PE	d	201	-	48,48,50	0.88	4 (8%)	51,53,55	1.10	2 (3%)
48	FES	G	803	7	0,4,4	-	-	-	-	-
52	DGT	O	402	53	32,33,33	3.32	14 (43%)	48,52,52	1.93	14 (29%)
47	SF4	F	502	6	0,12,12	-	-	-	-	-
45	3PE	Z	201	-	48,48,50	0.88	4 (8%)	51,53,55	1.07	2 (3%)
47	SF4	B	202	2	0,12,12	-	-	-	-	-
48	FES	E	301	5	0,4,4	-	-	-	-	-
46	PC1	d	202	-	32,32,53	1.21	4 (12%)	38,40,61	1.10	2 (5%)
45	3PE	I	204	-	32,32,50	1.07	4 (12%)	35,37,55	1.12	2 (5%)
47	SF4	G	802	7	0,12,12	-	-	-	-	-
51	CDL	q	702	-	59,59,99	1.12	6 (10%)	65,71,111	1.15	4 (6%)
45	3PE	J	201	-	38,38,50	1.00	4 (10%)	41,43,55	1.11	2 (4%)
57	CHD	i	201	-	32,32,32	3.27	10 (31%)	51,51,51	2.13	18 (35%)
45	3PE	O	401	-	34,34,50	1.03	4 (11%)	37,39,55	1.14	2 (5%)
46	PC1	q	701	-	36,36,53	1.13	4 (11%)	42,44,61	1.03	2 (4%)
49	FMN	F	501	-	33,33,33	2.71	10 (30%)	48,50,50	1.71	11 (22%)
46	PC1	B	201	-	50,50,53	1.01	4 (8%)	56,58,61	1.02	2 (3%)
47	SF4	G	801	7	0,12,12	-	-	-	-	-
56	EHZ	T	101	20	31,36,37	1.62	5 (16%)	36,44,47	1.84	10 (27%)
47	SF4	I	202	9	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	CDL	N	401	-	72,72,99	1.02	8 (11%)	78,84,111	1.09	4 (5%)
51	CDL	X	201	-	78,78,99	0.99	7 (8%)	84,90,111	1.14	6 (7%)
45	3PE	h	201	-	31,31,50	1.09	4 (12%)	34,36,55	1.21	2 (5%)
45	3PE	I	201	-	50,50,50	0.87	2 (4%)	53,55,55	1.15	3 (5%)
45	3PE	M	502	-	38,38,50	0.98	4 (10%)	41,43,55	1.14	2 (4%)
45	3PE	A	201	-	42,42,50	0.93	4 (9%)	45,47,55	1.15	2 (4%)
45	3PE	M	501	-	37,37,50	0.99	4 (10%)	40,42,55	1.23	3 (7%)
47	SF4	I	203	9	0,12,12	-	-	-	-	-
51	CDL	d	203	-	64,64,99	1.07	7 (10%)	70,76,111	1.11	5 (7%)
58	MYR	o	201	40	13,14,15	0.43	0	12,13,15	0.81	0
46	PC1	H	401	-	42,42,53	1.08	4 (9%)	48,50,61	1.10	2 (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
54	NDP	P	501	-	-	8/34/77/77	0/5/5/5
46	PC1	A	202	-	-	19/53/53/57	-
56	EHZ	U	101	20	-	23/42/44/45	-
45	3PE	d	201	-	-	18/52/52/54	-
52	DGT	O	402	53	-	6/22/34/34	0/3/3/3
48	FES	G	803	7	-	-	0/1/1/1
47	SF4	F	502	6	-	-	0/6/5/5
45	3PE	Z	201	-	-	22/52/52/54	-
47	SF4	B	202	2	-	-	0/6/5/5
48	FES	E	301	5	-	-	0/1/1/1
46	PC1	d	202	-	-	20/36/36/57	-
45	3PE	I	204	-	-	18/36/36/54	-
47	SF4	G	802	7	-	-	0/6/5/5
51	CDL	q	702	-	-	35/70/70/110	-
45	3PE	J	201	-	-	19/42/42/54	-
57	CHD	i	201	-	-	3/9/74/74	0/4/4/4
45	3PE	O	401	-	-	12/38/38/54	-
46	PC1	q	701	-	-	19/40/40/57	-
49	FMN	F	501	-	-	9/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	B	201	-	-	20/54/54/57	-
47	SF4	G	801	7	-	-	0/6/5/5
56	EHZ	T	101	20	-	14/42/44/45	-
47	SF4	I	202	9	-	-	0/6/5/5
51	CDL	X	201	-	-	36/89/89/110	-
51	CDL	N	401	-	-	38/83/83/110	-
45	3PE	h	201	-	-	18/35/35/54	-
45	3PE	I	201	-	-	19/54/54/54	-
45	3PE	M	502	-	-	21/42/42/54	-
45	3PE	A	201	-	-	18/46/46/54	-
45	3PE	M	501	-	-	19/41/41/54	-
51	CDL	d	203	-	-	26/75/75/110	-
47	SF4	I	203	9	-	-	0/6/5/5
58	MYR	o	201	40	-	6/12/12/13	-
46	PC1	H	401	-	-	13/46/46/57	-

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	501	NDP	PA-O3	10.02	1.70	1.59
57	i	201	CHD	C11-C12	9.38	1.68	1.53
54	P	501	NDP	C2B-C1B	-9.21	1.30	1.53
52	O	402	DGT	O6-C6	8.71	1.40	1.23
54	P	501	NDP	O4B-C1B	8.33	1.61	1.42
54	P	501	NDP	O4D-C1D	8.25	1.61	1.42
54	P	501	NDP	C7N-N7N	7.64	1.55	1.33
54	P	501	NDP	C2D-C1D	-7.27	1.30	1.53
54	P	501	NDP	C6N-C5N	7.08	1.54	1.33
57	i	201	CHD	C16-C15	6.89	1.72	1.54
52	O	402	DGT	C5-N7	6.72	1.52	1.39
54	P	501	NDP	O4D-C4D	-6.49	1.30	1.45
49	F	501	FMN	C4A-N5	6.41	1.44	1.30
49	F	501	FMN	C10-N1	6.36	1.46	1.33
57	i	201	CHD	C13-C17	5.90	1.65	1.55
57	i	201	CHD	C8-C9	5.72	1.64	1.53
56	T	101	EHZ	C15-N2	5.56	1.46	1.33
57	i	201	CHD	C20-C17	-5.52	1.44	1.54
49	F	501	FMN	C5A-N5	5.51	1.49	1.39
54	P	501	NDP	C6A-N6A	5.48	1.48	1.34
54	P	501	NDP	O4B-C4B	-5.47	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	501	NDP	P2B-O2B	5.37	1.68	1.59
52	O	402	DGT	PB-O3A	5.20	1.65	1.59
56	U	101	EHZ	C12-N1	5.18	1.45	1.33
56	U	101	EHZ	C15-N2	5.17	1.45	1.33
52	O	402	DGT	PB-O3B	5.15	1.65	1.59
57	i	201	CHD	O12-C12	-5.13	1.35	1.43
52	O	402	DGT	PA-O3A	5.12	1.65	1.59
56	T	101	EHZ	C12-N1	5.10	1.45	1.33
49	F	501	FMN	C2-N1	4.96	1.47	1.36
52	O	402	DGT	C2-N2	4.90	1.45	1.34
52	O	402	DGT	C2-N1	4.83	1.49	1.37
57	i	201	CHD	C6-C5	4.79	1.61	1.53
49	F	501	FMN	C9A-N10	4.67	1.49	1.41
54	P	501	NDP	PN-O3	4.62	1.64	1.59
54	P	501	NDP	C2N-C3N	4.55	1.47	1.35
49	F	501	FMN	C2-N3	4.51	1.48	1.39
54	P	501	NDP	C5A-C4A	-4.44	1.31	1.39
52	O	402	DGT	C2-N3	4.39	1.43	1.33
52	O	402	DGT	C8-N9	-4.34	1.27	1.37
54	P	501	NDP	O7N-C7N	-4.12	1.14	1.24
57	i	201	CHD	C15-C14	4.11	1.62	1.54
54	P	501	NDP	C8A-N9A	-4.03	1.30	1.37
52	O	402	DGT	C4-N9	-3.85	1.28	1.38
54	P	501	NDP	O2D-C2D	3.74	1.52	1.43
49	F	501	FMN	C4-N3	3.70	1.45	1.38
49	F	501	FMN	C10-N10	3.39	1.44	1.37
57	i	201	CHD	C6-C7	3.38	1.59	1.52
54	P	501	NDP	C4N-C3N	3.19	1.56	1.50
51	q	702	CDL	OB6-CB4	-3.00	1.39	1.46
49	F	501	FMN	O2-C2	-2.99	1.18	1.24
51	X	201	CDL	OA6-CA4	-2.92	1.39	1.46
45	I	201	3PE	O21-C2	-2.89	1.39	1.46
46	B	201	PC1	O21-C2	-2.85	1.39	1.46
49	F	501	FMN	O4-C4	-2.82	1.18	1.23
46	A	202	PC1	O21-C2	-2.82	1.40	1.46
54	P	501	NDP	C5A-N7A	-2.82	1.33	1.39
51	d	203	CDL	OA6-CA4	-2.79	1.40	1.46
46	H	401	PC1	O21-C2	-2.78	1.40	1.46
51	q	702	CDL	OA6-CA4	-2.75	1.40	1.46
51	X	201	CDL	OB6-CB4	-2.74	1.40	1.46
51	N	401	CDL	OB6-CB4	-2.74	1.40	1.46
46	d	202	PC1	O21-C2	-2.74	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	501	NDP	C4N-C5N	2.74	1.56	1.49
45	d	201	3PE	O21-C2	-2.70	1.40	1.46
45	A	201	3PE	O21-C2	-2.69	1.40	1.46
51	N	401	CDL	OA6-CA4	-2.69	1.40	1.46
45	I	204	3PE	O21-C2	-2.69	1.40	1.46
45	M	502	3PE	O21-C2	-2.68	1.40	1.46
45	J	201	3PE	O21-C2	-2.66	1.40	1.46
52	O	402	DGT	C1'-N9	-2.63	1.41	1.48
45	h	201	3PE	O21-C2	-2.60	1.40	1.46
45	O	401	3PE	O21-C2	-2.58	1.40	1.46
51	X	201	CDL	OB8-CB7	2.54	1.40	1.33
46	q	701	PC1	O21-C2	-2.54	1.40	1.46
54	P	501	NDP	O3D-C3D	-2.53	1.36	1.43
51	d	203	CDL	OB8-CB7	2.53	1.40	1.33
46	A	202	PC1	O31-C31	2.52	1.40	1.33
54	P	501	NDP	O3B-C3B	-2.52	1.36	1.43
51	q	702	CDL	OB8-CB7	2.51	1.40	1.33
45	I	201	3PE	O31-C3	-2.51	1.39	1.45
45	Z	201	3PE	O21-C2	-2.47	1.40	1.46
45	Z	201	3PE	O31-C31	2.47	1.40	1.33
51	N	401	CDL	OB8-CB7	2.47	1.40	1.33
51	q	702	CDL	OA8-CA6	-2.46	1.39	1.45
57	i	201	CHD	C13-C12	-2.45	1.50	1.54
54	P	501	NDP	C6N-N1N	2.41	1.43	1.37
46	d	202	PC1	O31-C31	2.41	1.40	1.33
46	B	201	PC1	O31-C31	2.41	1.40	1.33
45	M	501	3PE	O21-C2	-2.40	1.41	1.46
56	T	101	EHZ	O4-C15	-2.38	1.18	1.23
45	h	201	3PE	O31-C31	2.37	1.40	1.33
45	I	204	3PE	O31-C3	-2.37	1.39	1.45
54	P	501	NDP	C7N-C3N	2.36	1.53	1.48
54	P	501	NDP	PA-O5B	2.36	1.68	1.59
45	J	201	3PE	O31-C31	2.35	1.40	1.33
45	A	201	3PE	O31-C3	-2.35	1.39	1.45
56	U	101	EHZ	C9-S1	2.35	1.81	1.76
45	M	501	3PE	O31-C31	2.34	1.40	1.33
46	q	701	PC1	O31-C31	2.34	1.40	1.33
51	d	203	CDL	OB6-CB5	2.34	1.40	1.34
45	d	201	3PE	O31-C31	2.32	1.40	1.33
46	H	401	PC1	O31-C31	2.32	1.40	1.33
45	O	401	3PE	O31-C31	2.32	1.40	1.33
51	d	203	CDL	OB6-CB4	-2.32	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	U	101	EHZ	O4-C15	-2.31	1.19	1.23
45	J	201	3PE	O31-C3	-2.30	1.40	1.45
51	X	201	CDL	OA8-CA6	-2.29	1.40	1.45
51	X	201	CDL	OA8-CA7	2.29	1.40	1.33
46	q	701	PC1	O21-C21	2.28	1.40	1.34
51	N	401	CDL	OA8-CA7	2.28	1.40	1.33
52	O	402	DGT	C4-N3	2.28	1.39	1.34
54	P	501	NDP	P2B-O1X	2.28	1.57	1.50
51	d	203	CDL	OA8-CA7	2.27	1.40	1.33
45	M	502	3PE	O31-C31	2.27	1.40	1.33
45	I	204	3PE	O31-C31	2.26	1.40	1.33
52	O	402	DGT	PG-O1G	-2.26	1.46	1.54
45	M	502	3PE	O31-C3	-2.25	1.40	1.45
56	U	101	EHZ	O3-C12	-2.25	1.18	1.23
52	O	402	DGT	PG-O2G	-2.24	1.46	1.54
46	H	401	PC1	O31-C3	-2.23	1.40	1.45
51	d	203	CDL	OA8-CA6	-2.23	1.40	1.45
46	q	701	PC1	O31-C3	-2.23	1.40	1.45
56	T	101	EHZ	O3-C12	-2.23	1.18	1.23
46	B	201	PC1	O31-C3	-2.22	1.40	1.45
46	d	202	PC1	O31-C3	-2.22	1.40	1.45
45	O	401	3PE	O31-C3	-2.22	1.40	1.45
45	h	201	3PE	O31-C3	-2.21	1.40	1.45
54	P	501	NDP	C5B-C4B	2.21	1.58	1.51
45	I	204	3PE	O21-C21	2.19	1.40	1.34
51	N	401	CDL	OA8-CA6	-2.18	1.40	1.45
45	d	201	3PE	O31-C3	-2.17	1.40	1.45
45	M	501	3PE	O21-C21	2.17	1.40	1.34
56	T	101	EHZ	C9-S1	2.16	1.81	1.76
46	B	201	PC1	O21-C21	2.13	1.40	1.34
51	N	401	CDL	OB8-CB6	-2.13	1.40	1.45
51	q	702	CDL	OB8-CB6	-2.13	1.40	1.45
45	A	201	3PE	O31-C31	2.12	1.39	1.33
45	M	501	3PE	O31-C3	-2.12	1.40	1.45
51	N	401	CDL	OA6-CA5	2.11	1.40	1.34
45	J	201	3PE	O21-C21	2.11	1.40	1.34
51	q	702	CDL	OA8-CA7	2.11	1.39	1.33
45	O	401	3PE	O21-C21	2.10	1.40	1.34
51	N	401	CDL	OB6-CB5	2.10	1.40	1.34
45	Z	201	3PE	O31-C3	-2.08	1.40	1.45
45	h	201	3PE	O21-C21	2.07	1.40	1.34
51	X	201	CDL	OB8-CB6	-2.07	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H	401	PC1	O21-C21	2.05	1.40	1.34
46	A	202	PC1	O21-C21	2.05	1.40	1.34
45	Z	201	3PE	O21-C21	2.04	1.40	1.34
51	X	201	CDL	OB6-CB5	2.03	1.40	1.34
45	M	502	3PE	O21-C21	2.03	1.40	1.34
46	A	202	PC1	O31-C3	-2.03	1.40	1.45
45	d	201	3PE	O21-C21	2.03	1.40	1.34
51	d	203	CDL	OB8-CB6	-2.01	1.40	1.45
46	d	202	PC1	O21-C21	2.01	1.39	1.34
45	A	201	3PE	O21-C21	2.00	1.39	1.34

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	O	402	DGT	C8-N9-C4	7.47	120.02	106.03
57	i	201	CHD	C17-C13-C12	6.59	123.60	117.67
54	P	501	NDP	C4A-N9A-C1B	-5.74	113.22	126.63
54	P	501	NDP	N6A-C6A-N1A	-5.71	105.66	118.38
56	U	101	EHZ	C8-C9-S1	5.71	120.76	113.56
54	P	501	NDP	N3A-C2A-N1A	-5.57	120.15	128.58
56	T	101	EHZ	C8-C9-S1	5.36	120.32	113.56
54	P	501	NDP	C1B-N9A-C8A	5.16	138.54	127.09
54	P	501	NDP	C5A-C4A-N3A	-5.09	119.71	126.72
45	M	501	3PE	O21-C21-C22	4.76	121.77	111.48
56	T	101	EHZ	C16-C15-N2	4.66	125.33	116.48
51	X	201	CDL	OB6-CB5-C51	4.53	121.28	111.48
49	F	501	FMN	C7M-C7-C6	4.52	127.54	119.57
57	i	201	CHD	C17-C13-C14	4.41	104.54	100.11
45	h	201	3PE	O21-C21-C22	4.39	120.97	111.48
49	F	501	FMN	C9-C8-C7	4.34	126.06	119.69
54	P	501	NDP	N9A-C8A-N7A	-4.21	107.96	113.94
45	d	201	3PE	O21-C21-C22	4.16	120.48	111.48
54	P	501	NDP	C5A-C6A-N6A	4.15	133.55	123.29
46	H	401	PC1	O21-C21-C22	4.10	120.34	111.48
45	I	201	3PE	O21-C21-C22	4.08	120.31	111.48
57	i	201	CHD	C14-C8-C9	4.08	115.45	109.75
51	X	201	CDL	OA6-CA5-C11	4.06	120.26	111.48
46	q	701	PC1	O21-C21-C22	4.04	120.21	111.48
45	M	502	3PE	O21-C21-C22	4.03	120.21	111.48
45	Z	201	3PE	O21-C21-C22	4.00	120.13	111.48
51	N	401	CDL	OA6-CA5-C11	3.99	120.11	111.48
45	O	401	3PE	O21-C21-C22	3.97	120.08	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A	201	3PE	O21-C21-C22	3.95	120.02	111.48
45	I	204	3PE	O21-C21-C22	3.90	119.92	111.48
46	d	202	PC1	O21-C21-C22	3.89	119.89	111.48
46	B	201	PC1	O21-C21-C22	3.88	119.88	111.48
46	A	202	PC1	O21-C21-C22	3.88	119.88	111.48
51	d	203	CDL	OA6-CA5-C11	3.87	119.84	111.48
51	q	702	CDL	OA6-CA5-C11	3.84	119.79	111.48
57	i	201	CHD	C18-C13-C12	-3.83	105.23	109.06
45	J	201	3PE	O21-C21-C22	3.80	119.69	111.48
54	P	501	NDP	C2B-C1B-N9A	-3.71	107.64	113.75
51	N	401	CDL	OB6-CB5-C51	3.56	119.19	111.48
51	q	702	CDL	OB6-CB5-C51	3.54	119.15	111.48
54	P	501	NDP	C2A-N3A-C4A	3.54	120.48	111.83
52	O	402	DGT	C1'-N9-C8	-3.52	120.02	127.91
57	i	201	CHD	C18-C13-C17	-3.49	105.74	111.20
49	F	501	FMN	C8M-C8-C7	-3.46	113.69	120.76
49	F	501	FMN	C4-N3-C2	-3.45	119.51	125.64
57	i	201	CHD	C13-C17-C20	-3.42	115.34	119.48
57	i	201	CHD	C15-C14-C13	3.31	106.75	103.54
52	O	402	DGT	C2-N1-C6	-3.10	119.49	125.11
54	P	501	NDP	N3A-C4A-N9A	3.07	132.39	127.17
49	F	501	FMN	C4A-C10-N10	3.03	120.82	116.48
57	i	201	CHD	C1-C10-C5	3.00	112.05	107.75
56	U	101	EHZ	O2-C9-S1	-2.95	118.93	122.68
46	H	401	PC1	O31-C31-C32	2.87	120.59	111.83
52	O	402	DGT	O2G-PG-O3B	2.87	114.24	104.64
54	P	501	NDP	C5A-N7A-C8A	2.85	107.93	103.45
45	A	201	3PE	O31-C31-C32	2.85	120.52	111.83
45	M	502	3PE	O31-C31-C32	2.84	120.51	111.83
57	i	201	CHD	C6-C5-C4	-2.83	107.99	111.23
45	I	201	3PE	O31-C31-C32	2.81	120.42	111.83
45	J	201	3PE	O31-C31-C32	2.79	120.35	111.83
56	U	101	EHZ	C16-C15-N2	2.76	121.72	116.48
46	B	201	PC1	O31-C31-C32	2.76	120.24	111.83
51	d	203	CDL	OB8-CB7-C71	2.76	120.24	111.83
46	d	202	PC1	O31-C31-C32	2.75	120.23	111.83
51	d	203	CDL	OA8-CA7-C31	2.75	120.22	111.83
52	O	402	DGT	O1G-PG-O3B	2.71	113.72	104.64
51	q	702	CDL	OB8-CB7-C71	2.71	120.09	111.83
45	M	501	3PE	O31-C31-C32	2.70	120.06	111.83
51	q	702	CDL	OA8-CA7-C31	2.69	120.04	111.83
56	U	101	EHZ	C10-S1-C9	2.69	109.78	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	T	101	EHZ	C14-C13-C12	-2.67	107.94	112.39
57	i	201	CHD	C5-C6-C7	-2.67	111.22	114.40
45	d	201	3PE	O31-C31-C32	2.67	119.98	111.83
52	O	402	DGT	C2'-C3'-C4'	2.66	108.20	102.80
51	X	201	CDL	OA8-CA7-C31	2.65	119.92	111.83
45	Z	201	3PE	O31-C31-C32	2.64	119.87	111.83
56	T	101	EHZ	O4-C15-N2	-2.63	117.41	122.98
45	h	201	3PE	O31-C31-C32	2.63	119.84	111.83
56	T	101	EHZ	C19-C17-C16	2.59	113.19	108.77
54	P	501	NDP	P2B-O2B-C2B	-2.59	116.51	123.43
46	q	701	PC1	O31-C31-C32	2.58	119.71	111.83
51	d	203	CDL	OB6-CB5-C51	2.55	120.30	110.93
51	N	401	CDL	OB8-CB7-C71	2.55	119.61	111.83
45	O	401	3PE	O31-C31-C32	2.54	119.59	111.83
46	A	202	PC1	O31-C31-C32	2.53	119.55	111.83
57	i	201	CHD	C11-C9-C8	2.53	114.64	110.89
49	F	501	FMN	C4A-C4-N3	2.52	119.66	113.25
51	N	401	CDL	OA8-CA7-C31	2.50	119.45	111.83
45	I	204	3PE	O31-C31-C32	2.48	119.40	111.83
57	i	201	CHD	C23-C22-C20	-2.48	109.83	114.46
49	F	501	FMN	C6-C7-C8	-2.48	116.05	119.69
45	I	201	3PE	C2-O21-C21	-2.47	111.88	117.80
52	O	402	DGT	C5-C6-N1	2.46	119.52	113.25
49	F	501	FMN	C10-C4A-N5	-2.45	119.81	124.81
56	T	101	EHZ	O2-C9-S1	-2.45	119.57	122.68
49	F	501	FMN	O4-C4-C4A	-2.44	120.09	126.53
51	X	201	CDL	OB8-CB7-C71	2.42	119.20	111.83
52	O	402	DGT	O6-C6-C5	-2.42	120.16	126.53
56	T	101	EHZ	C7-C8-C9	-2.38	108.56	113.86
54	P	501	NDP	C4A-N9A-C8A	2.38	108.23	105.74
52	O	402	DGT	O1A-PA-O2A	-2.33	101.60	112.44
57	i	201	CHD	C19-C10-C5	-2.32	106.57	110.44
56	T	101	EHZ	O2-C9-C8	-2.31	120.10	123.74
56	U	101	EHZ	C13-C12-N1	2.31	120.55	116.34
52	O	402	DGT	O1B-PB-O2B	-2.30	101.75	112.44
57	i	201	CHD	C11-C9-C10	2.29	116.03	113.70
57	i	201	CHD	C4-C3-C2	2.28	113.40	110.62
54	P	501	NDP	C4A-C5A-N7A	-2.28	107.98	110.58
57	i	201	CHD	C4-C5-C10	2.23	115.04	112.66
52	O	402	DGT	C5-C4-N9	-2.19	101.74	105.66
56	U	101	EHZ	O2-C9-C8	-2.18	120.31	123.74
56	U	101	EHZ	C11-N1-C12	-2.15	118.82	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	O	402	DGT	N9-C4-N3	2.14	130.23	125.95
57	i	201	CHD	C10-C9-C8	-2.14	109.45	111.84
49	F	501	FMN	C7M-C7-C8	-2.13	116.40	120.76
49	F	501	FMN	C5'-C4'-C3'	-2.12	108.22	112.22
51	X	201	CDL	OB6-CB5-OB7	-2.10	118.79	123.70
57	i	201	CHD	C1-C10-C9	-2.10	108.07	111.34
56	U	101	EHZ	C7-C8-C9	-2.10	109.17	113.86
52	O	402	DGT	N9-C8-N7	-2.09	109.53	113.40
51	X	201	CDL	CA4-OA6-CA5	-2.08	112.81	117.80
56	T	101	EHZ	C13-C12-N1	2.07	120.12	116.34
51	d	203	CDL	CA4-OA6-CA5	-2.07	112.85	117.80
52	O	402	DGT	C1'-N9-C4	-2.06	119.95	125.50
56	T	101	EHZ	C10-S1-C9	2.03	107.84	101.84
45	M	501	3PE	O21-C21-O22	-2.02	118.99	123.70

There are no chirality outliers.

All (479) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C11-O13-P-O11
45	A	201	3PE	C11-O13-P-O14
45	A	201	3PE	C12-C11-O13-P
45	A	201	3PE	O21-C2-C3-O31
45	I	201	3PE	C1-O11-P-O14
45	I	204	3PE	C1-O11-P-O12
45	I	204	3PE	C11-O13-P-O11
45	I	204	3PE	C11-O13-P-O12
45	I	204	3PE	C11-O13-P-O14
45	J	201	3PE	C1-O11-P-O12
45	J	201	3PE	C1-O11-P-O13
45	J	201	3PE	C22-C21-O21-C2
45	M	501	3PE	C1-O11-P-O12
45	M	501	3PE	C1-O11-P-O13
45	M	501	3PE	O22-C21-O21-C2
45	M	501	3PE	C22-C21-O21-C2
45	M	502	3PE	C1-O11-P-O12
45	M	502	3PE	C1-O11-P-O13
45	M	502	3PE	C1-O11-P-O14
45	M	502	3PE	C12-C11-O13-P
45	M	502	3PE	O13-C11-C12-N
45	M	502	3PE	O21-C2-C3-O31
45	O	401	3PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
45	O	401	3PE	C11-O13-P-O12
45	O	401	3PE	O22-C21-O21-C2
45	Z	201	3PE	C11-O13-P-O11
45	Z	201	3PE	C11-O13-P-O12
45	Z	201	3PE	C11-O13-P-O14
45	Z	201	3PE	O13-C11-C12-N
45	Z	201	3PE	C22-C21-O21-C2
45	d	201	3PE	C11-O13-P-O14
45	d	201	3PE	O13-C11-C12-N
45	h	201	3PE	C1-O11-P-O12
45	h	201	3PE	C1-O11-P-O13
45	h	201	3PE	C1-O11-P-O14
46	A	202	PC1	C11-O13-P-O14
46	A	202	PC1	C11-O13-P-O11
46	A	202	PC1	O13-C11-C12-N
46	B	201	PC1	C11-O13-P-O12
46	B	201	PC1	C11-O13-P-O11
46	q	701	PC1	C11-O13-P-O14
46	q	701	PC1	C11-O13-P-O11
46	q	701	PC1	C1-O11-P-O12
46	q	701	PC1	C1-O11-P-O13
49	F	501	FMN	N10-C1'-C2'-O2'
49	F	501	FMN	C1'-C2'-C3'-C4'
49	F	501	FMN	C5'-O5'-P-O2P
49	F	501	FMN	C5'-O5'-P-O3P
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-OB5
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	OA7-CA5-OA6-CA4
51	X	201	CDL	C11-CA5-OA6-CA4
51	X	201	CDL	OB7-CB5-OB6-CB4
51	d	203	CDL	CA3-OA5-PA1-OA2
51	d	203	CDL	CA3-OA5-PA1-OA3
51	d	203	CDL	CA3-OA5-PA1-OA4
51	d	203	CDL	C51-CB5-OB6-CB4
51	q	702	CDL	C11-CA5-OA6-CA4
51	q	702	CDL	CB3-OB5-PB2-OB2
51	q	702	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
51	q	702	CDL	CB3-OB5-PB2-OB4
51	q	702	CDL	OB5-CB3-CB4-OB6
52	O	402	DGT	C5'-O5'-PA-O3A
52	O	402	DGT	C5'-O5'-PA-O1A
52	O	402	DGT	C5'-O5'-PA-O2A
54	P	501	NDP	C5D-O5D-PN-O1N
56	T	101	EHZ	C16-C15-N2-C14
56	T	101	EHZ	C16-C17-C20-O6
56	T	101	EHZ	C18-C17-C20-O6
56	T	101	EHZ	C19-C17-C20-O6
56	U	101	EHZ	S1-C10-C11-N1
56	U	101	EHZ	C11-C10-S1-C9
56	U	101	EHZ	N2-C15-C16-C17
56	U	101	EHZ	N2-C15-C16-O5
56	U	101	EHZ	O4-C15-C16-C17
56	U	101	EHZ	C15-C16-C17-C18
56	U	101	EHZ	C15-C16-C17-C19
56	U	101	EHZ	C15-C16-C17-C20
56	U	101	EHZ	O5-C16-C17-C18
56	U	101	EHZ	O2-C9-S1-C10
56	U	101	EHZ	C8-C9-S1-C10
45	J	201	3PE	O32-C31-O31-C3
45	h	201	3PE	O32-C31-O31-C3
46	d	202	PC1	O32-C31-O31-C3
51	N	401	CDL	OA9-CA7-OA8-CA6
45	I	201	3PE	O22-C21-O21-C2
45	J	201	3PE	O22-C21-O21-C2
45	Z	201	3PE	O22-C21-O21-C2
51	d	203	CDL	OB7-CB5-OB6-CB4
51	q	702	CDL	OA7-CA5-OA6-CA4
45	J	201	3PE	C32-C31-O31-C3
45	h	201	3PE	C32-C31-O31-C3
51	N	401	CDL	C31-CA7-OA8-CA6
45	I	201	3PE	C22-C21-O21-C2
45	O	401	3PE	C22-C21-O21-C2
51	X	201	CDL	C51-CB5-OB6-CB4
46	d	202	PC1	C32-C31-O31-C3
51	q	702	CDL	O1-C1-CA2-OA2
45	M	501	3PE	C32-C31-O31-C3
46	B	201	PC1	C32-C31-O31-C3
46	B	201	PC1	O32-C31-O31-C3
56	T	101	EHZ	O4-C15-N2-C14

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Mol	Chain	Res	Type	Atoms
45	M	501	3PE	O32-C31-O31-C3
46	H	401	PC1	C26-C27-C28-C29
45	I	204	3PE	C32-C31-O31-C3
51	X	201	CDL	C31-CA7-OA8-CA6
51	X	201	CDL	OA9-CA7-OA8-CA6
46	B	201	PC1	O21-C2-C3-O31
46	d	202	PC1	C35-C36-C37-C38
57	i	201	CHD	C17-C20-C22-C23
51	X	201	CDL	CA5-C11-C12-C13
57	i	201	CHD	C21-C20-C22-C23
51	q	702	CDL	CB7-C71-C72-C73
45	I	204	3PE	C26-C27-C28-C29
51	d	203	CDL	O1-C1-CB2-OB2
46	d	202	PC1	C21-C22-C23-C24
46	q	701	PC1	C32-C33-C34-C35
45	I	204	3PE	O32-C31-O31-C3
51	d	203	CDL	C31-CA7-OA8-CA6
46	A	202	PC1	C31-C32-C33-C34
51	d	203	CDL	CA2-C1-CB2-OB2
46	H	401	PC1	C32-C31-O31-C3
51	d	203	CDL	C11-CA5-OA6-CA4
51	d	203	CDL	OA7-CA5-OA6-CA4
51	N	401	CDL	OA6-CA4-CA6-OA8
51	N	401	CDL	C71-CB7-OB8-CB6
46	H	401	PC1	O32-C31-O31-C3
45	Z	201	3PE	C39-C3A-C3B-C3C
46	B	201	PC1	C39-C3A-C3B-C3C
51	d	203	CDL	CA5-C11-C12-C13
46	A	202	PC1	C33-C34-C35-C36
51	d	203	CDL	OA9-CA7-OA8-CA6
51	X	201	CDL	C19-C20-C21-C22
45	d	201	3PE	C32-C33-C34-C35
51	X	201	CDL	C14-C15-C16-C17
46	q	701	PC1	C22-C23-C24-C25
51	N	401	CDL	O1-C1-CA2-OA2
45	O	401	3PE	C32-C31-O31-C3
51	q	702	CDL	C71-CB7-OB8-CB6
45	h	201	3PE	C1-C2-C3-O31
45	Z	201	3PE	C35-C36-C37-C38
45	d	201	3PE	C26-C27-C28-C29
51	d	203	CDL	C33-C34-C35-C36
45	Z	201	3PE	C29-C2A-C2B-C2C

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Mol	Chain	Res	Type	Atoms
51	X	201	CDL	C54-C55-C56-C57
45	O	401	3PE	C26-C27-C28-C29
51	N	401	CDL	C19-C20-C21-C22
51	q	702	CDL	C51-CB5-OB6-CB4
45	Z	201	3PE	C32-C31-O31-C3
51	N	401	CDL	C11-C12-C13-C14
51	X	201	CDL	C52-C53-C54-C55
51	N	401	CDL	OB9-CB7-OB8-CB6
51	q	702	CDL	OB9-CB7-OB8-CB6
46	A	202	PC1	C28-C29-C2A-C2B
45	A	201	3PE	C2E-C2F-C2G-C2H
46	B	201	PC1	C37-C38-C39-C3A
51	X	201	CDL	C61-C62-C63-C64
56	U	101	EHZ	C1-C2-C3-C4
45	Z	201	3PE	C36-C37-C38-C39
45	A	201	3PE	C32-C31-O31-C3
46	A	202	PC1	C22-C21-O21-C2
51	N	401	CDL	C11-CA5-OA6-CA4
56	T	101	EHZ	C12-C13-C14-N2
45	I	201	3PE	C3A-C3B-C3C-C3D
46	H	401	PC1	C24-C25-C26-C27
45	A	201	3PE	C32-C33-C34-C35
45	Z	201	3PE	C3C-C3D-C3E-C3F
45	M	501	3PE	C26-C27-C28-C29
45	A	201	3PE	C26-C27-C28-C29
46	q	701	PC1	C23-C24-C25-C26
45	O	401	3PE	O32-C31-O31-C3
46	A	202	PC1	O22-C21-O21-C2
45	J	201	3PE	C35-C36-C37-C38
45	Z	201	3PE	O32-C31-O31-C3
45	I	204	3PE	C31-C32-C33-C34
51	N	401	CDL	CA7-C31-C32-C33
45	h	201	3PE	C2-C1-O11-P
45	A	201	3PE	C2B-C2C-C2D-C2E
51	q	702	CDL	OB7-CB5-OB6-CB4
51	q	702	CDL	CB2-C1-CA2-OA2
45	d	201	3PE	C22-C23-C24-C25
51	X	201	CDL	C71-C72-C73-C74
56	U	101	EHZ	O4-C15-C16-O5
45	J	201	3PE	C26-C27-C28-C29
45	I	201	3PE	C33-C34-C35-C36
51	N	401	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
51	q	702	CDL	OB5-CB3-CB4-CB6
51	X	201	CDL	C62-C63-C64-C65
45	J	201	3PE	C25-C26-C27-C28
51	d	203	CDL	C34-C35-C36-C37
51	d	203	CDL	C72-C73-C74-C75
45	A	201	3PE	C1-C2-C3-O31
46	B	201	PC1	C1-C2-C3-O31
51	N	401	CDL	CB3-CB4-CB6-OB8
51	q	702	CDL	C16-C17-C18-C19
51	X	201	CDL	C63-C64-C65-C66
51	N	401	CDL	C34-C35-C36-C37
51	X	201	CDL	C74-C75-C76-C77
51	X	201	CDL	C59-C60-C61-C62
46	B	201	PC1	C2-C1-O11-P
45	A	201	3PE	O32-C31-O31-C3
51	q	702	CDL	CA5-C11-C12-C13
45	Z	201	3PE	C1-C2-O21-C21
45	M	502	3PE	C26-C27-C28-C29
46	A	202	PC1	C36-C37-C38-C39
45	M	502	3PE	C2E-C2F-C2G-C2H
45	Z	201	3PE	C23-C24-C25-C26
51	N	401	CDL	C15-C16-C17-C18
45	J	201	3PE	C32-C33-C34-C35
56	U	101	EHZ	C2-C1-C21-C22
51	d	203	CDL	C77-C78-C79-C80
51	q	702	CDL	C73-C74-C75-C76
56	U	101	EHZ	O5-C16-C17-C19
45	d	201	3PE	C2D-C2E-C2F-C2G
46	d	202	PC1	C22-C21-O21-C2
45	I	201	3PE	C29-C2A-C2B-C2C
45	h	201	3PE	C23-C24-C25-C26
46	d	202	PC1	C37-C38-C39-C3A
46	q	701	PC1	C32-C31-O31-C3
45	M	501	3PE	C28-C29-C2A-C2B
51	N	401	CDL	OA7-CA5-OA6-CA4
45	M	501	3PE	C2-C1-O11-P
45	Z	201	3PE	C2-C1-O11-P
45	A	201	3PE	C2C-C2D-C2E-C2F
58	o	201	MYR	C3-C4-C5-C6
52	O	402	DGT	O4'-C4'-C5'-O5'
46	q	701	PC1	C24-C25-C26-C27
45	A	201	3PE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
46	q	701	PC1	C37-C38-C39-C3A
46	B	201	PC1	C3E-C3F-C3G-C3H
45	d	201	3PE	C3D-C3E-C3F-C3G
45	M	501	3PE	C1-C2-C3-O31
45	M	502	3PE	C1-C2-C3-O31
45	Z	201	3PE	C1-C2-C3-O31
46	H	401	PC1	C1-C2-C3-O31
51	N	401	CDL	CA3-CA4-CA6-OA8
51	q	702	CDL	CA3-CA4-CA6-OA8
45	A	201	3PE	C35-C36-C37-C38
51	N	401	CDL	C16-C17-C18-C19
45	M	501	3PE	C34-C35-C36-C37
46	B	201	PC1	C23-C24-C25-C26
45	I	204	3PE	O11-C1-C2-O21
56	T	101	EHZ	O1-C7-C8-C9
56	U	101	EHZ	O1-C7-C8-C9
51	N	401	CDL	C71-C72-C73-C74
45	h	201	3PE	C26-C27-C28-C29
51	N	401	CDL	C55-C56-C57-C58
46	A	202	PC1	O21-C2-C3-O31
46	H	401	PC1	O21-C2-C3-O31
51	N	401	CDL	OB6-CB4-CB6-OB8
51	N	401	CDL	CA5-C11-C12-C13
56	T	101	EHZ	C6-C7-C8-C9
56	U	101	EHZ	C6-C7-C8-C9
45	M	501	3PE	C36-C37-C38-C39
45	I	201	3PE	C21-C22-C23-C24
45	M	502	3PE	O11-C1-C2-C3
51	d	203	CDL	OA5-CA3-CA4-CA6
46	d	202	PC1	C33-C34-C35-C36
46	q	701	PC1	O32-C31-O31-C3
56	T	101	EHZ	O3-C12-C13-C14
51	X	201	CDL	C60-C61-C62-C63
56	T	101	EHZ	C2-C1-C21-C22
46	d	202	PC1	O22-C21-O21-C2
45	I	201	3PE	O11-C1-C2-O21
45	h	201	3PE	O11-C1-C2-O21
51	d	203	CDL	OA5-CA3-CA4-OA6
45	I	201	3PE	C27-C28-C29-C2A
46	B	201	PC1	C32-C33-C34-C35
45	d	201	3PE	C12-C11-O13-P
46	A	202	PC1	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
45	M	501	3PE	O21-C2-C3-O31
51	q	702	CDL	OA6-CA4-CA6-OA8
51	N	401	CDL	C36-C37-C38-C39
56	U	101	EHZ	C3-C4-C5-C6
46	q	701	PC1	O13-C11-C12-N
45	h	201	3PE	C27-C28-C29-C2A
51	q	702	CDL	C19-C20-C21-C22
46	q	701	PC1	C34-C35-C36-C37
54	P	501	NDP	C2D-C1D-N1N-C2N
54	P	501	NDP	C2D-C1D-N1N-C6N
45	I	204	3PE	O11-C1-C2-C3
56	U	101	EHZ	C18-C17-C20-O6
56	U	101	EHZ	C19-C17-C20-O6
56	T	101	EHZ	N1-C12-C13-C14
51	d	203	CDL	CB4-CB3-OB5-PB2
54	P	501	NDP	C2B-O2B-P2B-O1X
56	T	101	EHZ	C11-C10-S1-C9
45	M	502	3PE	C25-C26-C27-C28
45	M	502	3PE	O11-C1-C2-O21
45	O	401	3PE	O11-C1-C2-O21
51	N	401	CDL	OA5-CA3-CA4-OA6
51	N	401	CDL	OB5-CB3-CB4-OB6
46	A	202	PC1	C23-C24-C25-C26
45	O	401	3PE	C27-C28-C29-C2A
45	Z	201	3PE	O21-C2-C3-O31
45	h	201	3PE	O21-C2-C3-O31
51	q	702	CDL	C31-C32-C33-C34
46	H	401	PC1	C29-C2A-C2B-C2C
46	A	202	PC1	C1-C2-C3-O31
46	q	701	PC1	C31-C32-C33-C34
45	I	201	3PE	C35-C36-C37-C38
56	U	101	EHZ	C16-C17-C20-O6
45	h	201	3PE	C32-C33-C34-C35
45	M	502	3PE	C23-C24-C25-C26
45	O	401	3PE	C25-C26-C27-C28
45	A	201	3PE	O13-C11-C12-N
45	I	201	3PE	C1-O11-P-O13
45	I	201	3PE	C11-O13-P-O11
45	I	201	3PE	C11-O13-P-O14
45	I	204	3PE	C1-O11-P-O13
45	I	204	3PE	C1-O11-P-O14
45	J	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
45	M	501	3PE	C1-O11-P-O14
45	M	501	3PE	C11-O13-P-O14
45	M	502	3PE	C11-O13-P-O11
45	M	502	3PE	C11-O13-P-O12
45	M	502	3PE	C11-O13-P-O14
45	d	201	3PE	C11-O13-P-O11
45	d	201	3PE	C11-O13-P-O12
46	A	202	PC1	C1-O11-P-O14
46	B	201	PC1	C11-O13-P-O14
46	B	201	PC1	C1-O11-P-O14
46	H	401	PC1	C1-O11-P-O13
46	d	202	PC1	C11-O13-P-O12
46	d	202	PC1	C11-O13-P-O14
46	d	202	PC1	C11-O13-P-O11
46	d	202	PC1	C1-O11-P-O12
51	d	203	CDL	CA2-OA2-PA1-OA5
51	d	203	CDL	CB2-OB2-PB2-OB3
51	q	702	CDL	CA3-OA5-PA1-OA3
51	q	702	CDL	CB2-OB2-PB2-OB3
54	P	501	NDP	C5D-O5D-PN-O3
56	U	101	EHZ	O5-C16-C17-C20
49	F	501	FMN	O2'-C2'-C3'-C4'
46	q	701	PC1	C2-C1-O11-P
49	F	501	FMN	C4'-C5'-O5'-P
51	X	201	CDL	CA4-CA3-OA5-PA1
51	X	201	CDL	C32-C33-C34-C35
45	I	204	3PE	C34-C35-C36-C37
51	d	203	CDL	CB3-CB4-OB6-CB5
45	I	201	3PE	O11-C1-C2-C3
45	h	201	3PE	O11-C1-C2-C3
51	X	201	CDL	OA5-CA3-CA4-CA6
46	A	202	PC1	C21-C22-C23-C24
51	X	201	CDL	CA2-C1-CB2-OB2
45	I	201	3PE	C24-C25-C26-C27
45	d	201	3PE	C32-C31-O31-C3
54	P	501	NDP	O4D-C1D-N1N-C6N
51	q	702	CDL	OB6-CB4-CB6-OB8
46	B	201	PC1	C3F-C3G-C3H-C3I
51	X	201	CDL	C33-C34-C35-C36
52	O	402	DGT	PA-O3A-PB-O1B
51	q	702	CDL	C32-C31-CA7-OA8
51	d	203	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
45	I	201	3PE	C34-C35-C36-C37
52	O	402	DGT	C3'-C4'-C5'-O5'
45	h	201	3PE	C28-C29-C2A-C2B
45	J	201	3PE	C34-C35-C36-C37
45	d	201	3PE	C37-C38-C39-C3A
45	J	201	3PE	C29-C2A-C2B-C2C
46	B	201	PC1	C21-C22-C23-C24
51	N	401	CDL	CB2-C1-CA2-OA2
46	B	201	PC1	C35-C36-C37-C38
56	T	101	EHZ	S1-C10-C11-N1
45	M	502	3PE	C24-C25-C26-C27
45	d	201	3PE	O32-C31-O31-C3
58	o	201	MYR	C4-C5-C6-C7
46	q	701	PC1	C36-C37-C38-C39
56	T	101	EHZ	C1-C2-C3-C4
58	o	201	MYR	C5-C6-C7-C8
46	B	201	PC1	C22-C23-C24-C25
46	A	202	PC1	C25-C26-C27-C28
45	A	201	3PE	O21-C21-C22-C23
51	q	702	CDL	C1-CB2-OB2-PB2
45	d	201	3PE	C1-C2-C3-O31
51	X	201	CDL	C76-C77-C78-C79
49	F	501	FMN	O2'-C2'-C3'-O3'
45	I	201	3PE	C2D-C2E-C2F-C2G
45	J	201	3PE	C33-C34-C35-C36
46	B	201	PC1	C25-C26-C27-C28
45	M	501	3PE	C3-C2-O21-C21
51	X	201	CDL	C17-C18-C19-C20
46	B	201	PC1	C27-C28-C29-C2A
58	o	201	MYR	C6-C7-C8-C9
51	q	702	CDL	C18-C19-C20-C21
45	O	401	3PE	O11-C1-C2-C3
54	P	501	NDP	O4D-C1D-N1N-C2N
45	M	502	3PE	C2B-C2C-C2D-C2E
45	O	401	3PE	C34-C35-C36-C37
45	d	201	3PE	O31-C31-C32-C33
45	M	502	3PE	C2D-C2E-C2F-C2G
51	q	702	CDL	C51-C52-C53-C54
51	q	702	CDL	CB3-CB4-CB6-OB8
51	N	401	CDL	C32-C33-C34-C35
51	X	201	CDL	C16-C17-C18-C19
58	o	201	MYR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
46	d	202	PC1	O11-C1-C2-O21
51	X	201	CDL	OA5-CA3-CA4-OA6
51	q	702	CDL	C11-C12-C13-C14
51	N	401	CDL	C52-C51-CB5-OB6
45	M	501	3PE	C21-C22-C23-C24
49	F	501	FMN	C1'-C2'-C3'-O3'
51	N	401	CDL	OA5-CA3-CA4-CA6
46	d	202	PC1	O21-C2-C3-O31
51	N	401	CDL	C14-C15-C16-C17
51	X	201	CDL	C11-C12-C13-C14
46	A	202	PC1	C3F-C3G-C3H-C3I
46	A	202	PC1	C3B-C3C-C3D-C3E
45	M	502	3PE	O21-C21-C22-C23
45	M	501	3PE	C1-C2-O21-C21
45	h	201	3PE	C1-C2-O21-C21
45	h	201	3PE	C3-C2-O21-C21
51	q	702	CDL	OA9-CA7-OA8-CA6
46	d	202	PC1	C32-C33-C34-C35
45	I	201	3PE	C2-C1-O11-P
46	H	401	PC1	C32-C33-C34-C35
56	U	101	EHZ	C10-C11-N1-C12
46	H	401	PC1	C22-C23-C24-C25
58	o	201	MYR	C11-C10-C9-C8
51	X	201	CDL	C52-C51-CB5-OB6
45	M	501	3PE	C32-C33-C34-C35
45	I	201	3PE	C32-C33-C34-C35
45	d	201	3PE	C3C-C3D-C3E-C3F
45	h	201	3PE	C25-C26-C27-C28
45	A	201	3PE	C33-C34-C35-C36
45	I	204	3PE	O22-C21-O21-C2
51	q	702	CDL	C13-C14-C15-C16
45	d	201	3PE	C35-C36-C37-C38
54	P	501	NDP	PN-O3-PA-O2A
51	q	702	CDL	C31-CA7-OA8-CA6
45	I	204	3PE	O21-C21-C22-C23
51	N	401	CDL	C72-C71-CB7-OB8
45	Z	201	3PE	C34-C35-C36-C37
45	Z	201	3PE	C22-C23-C24-C25
45	J	201	3PE	O31-C31-C32-C33
46	d	202	PC1	O31-C31-C32-C33
51	N	401	CDL	C32-C31-CA7-OA8
46	d	202	PC1	C1-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
45	I	204	3PE	C24-C25-C26-C27
45	Z	201	3PE	O31-C31-C32-C33
46	d	202	PC1	O21-C21-C22-C23
46	q	701	PC1	O21-C21-C22-C23
46	A	202	PC1	C3E-C3F-C3G-C3H
45	J	201	3PE	O11-C1-C2-C3
46	H	401	PC1	O21-C21-C22-C23
45	I	204	3PE	C22-C21-O21-C2
49	F	501	FMN	N10-C1'-C2'-C3'
51	N	401	CDL	C35-C36-C37-C38
45	M	502	3PE	C28-C29-C2A-C2B
46	q	701	PC1	C25-C26-C27-C28
45	I	204	3PE	O22-C21-C22-C23
51	N	401	CDL	C32-C31-CA7-OA9
51	d	203	CDL	OB5-CB3-CB4-OB6
45	J	201	3PE	O21-C21-C22-C23
46	d	202	PC1	O32-C31-C32-C33
51	X	201	CDL	C57-C58-C59-C60
57	i	201	CHD	C20-C22-C23-C24
45	Z	201	3PE	O32-C31-C32-C33
51	X	201	CDL	C12-C13-C14-C15
51	X	201	CDL	O1-C1-CB2-OB2
51	N	401	CDL	C72-C71-CB7-OB9
45	A	201	3PE	C28-C29-C2A-C2B
51	X	201	CDL	C52-C51-CB5-OB7
51	d	203	CDL	CA3-CA4-CA6-OA8
45	J	201	3PE	O32-C31-C32-C33
46	H	401	PC1	O22-C21-C22-C23
46	d	202	PC1	O22-C21-C22-C23
46	q	701	PC1	O22-C21-C22-C23
51	d	203	CDL	OB5-CB3-CB4-CB6
51	q	702	CDL	C72-C71-CB7-OB8
46	H	401	PC1	C23-C24-C25-C26
45	J	201	3PE	O22-C21-C22-C23
51	q	702	CDL	C52-C53-C54-C55
45	d	201	3PE	C2B-C2C-C2D-C2E

There are no ring outliers.

24 monomers are involved in 49 short contacts:

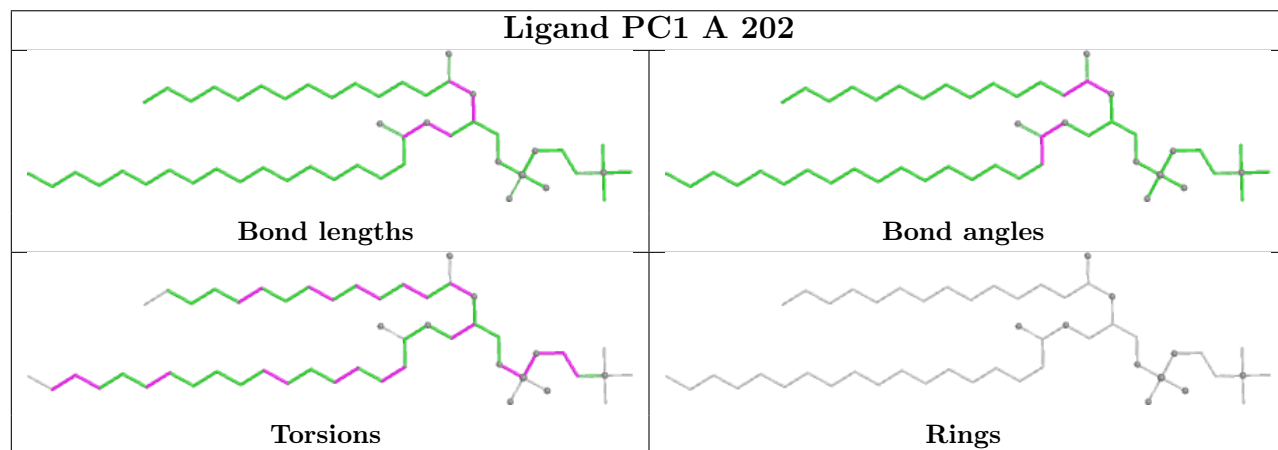
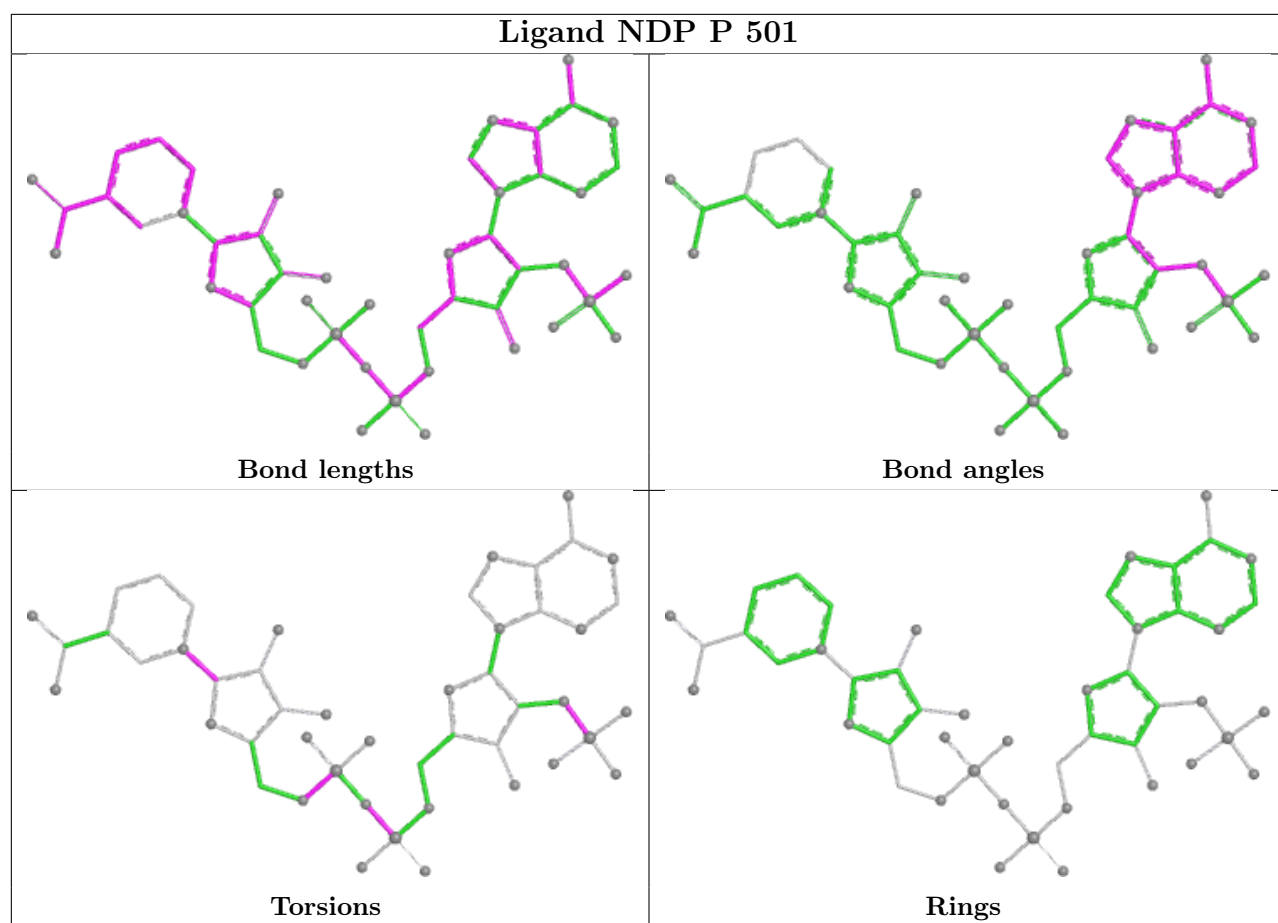
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	P	501	NDP	2	0

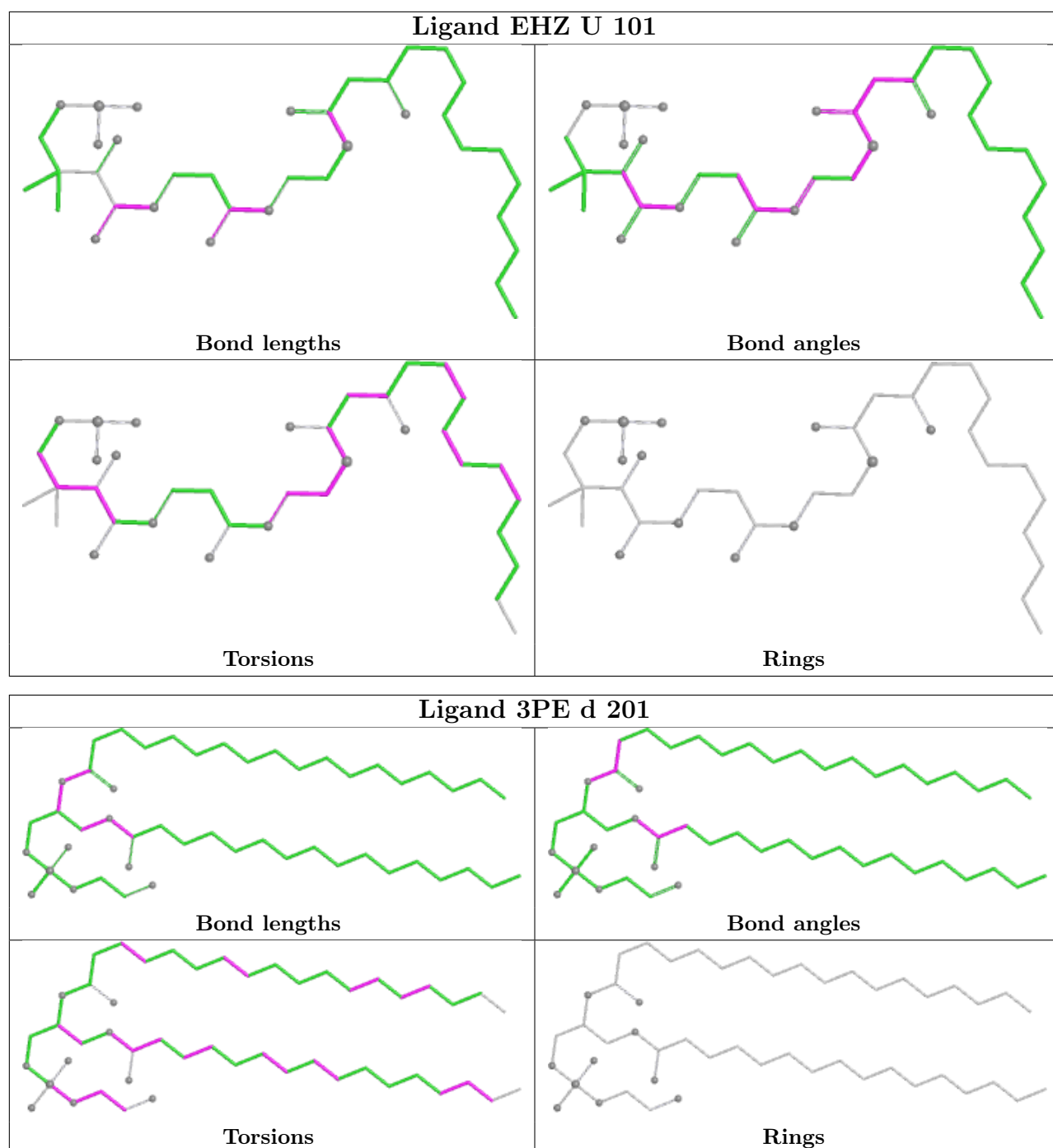
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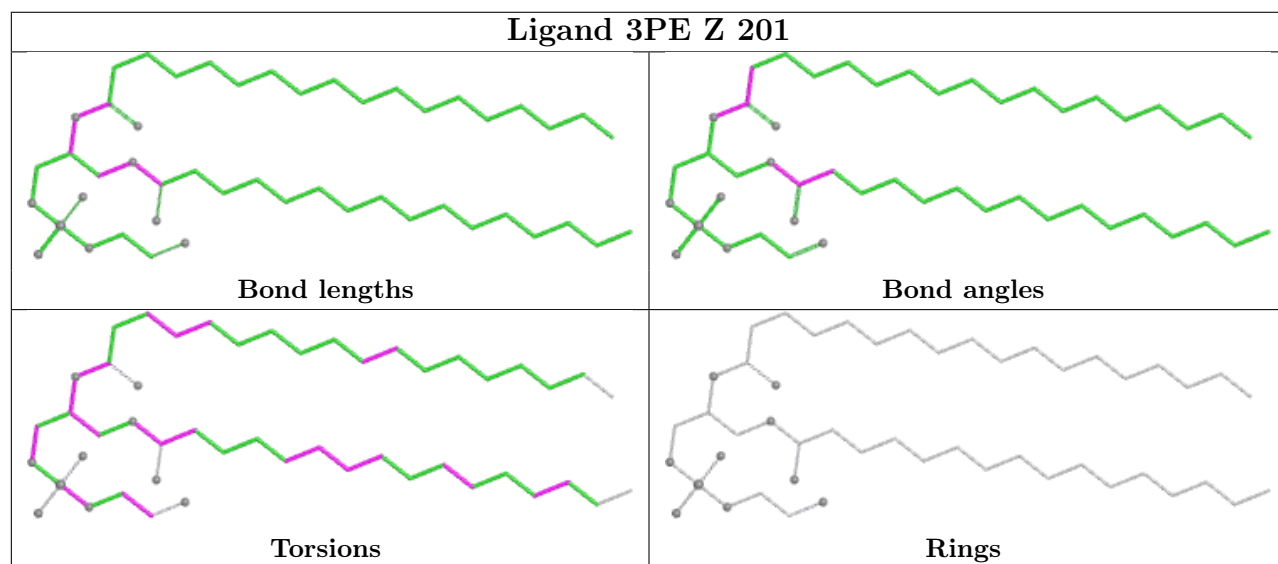
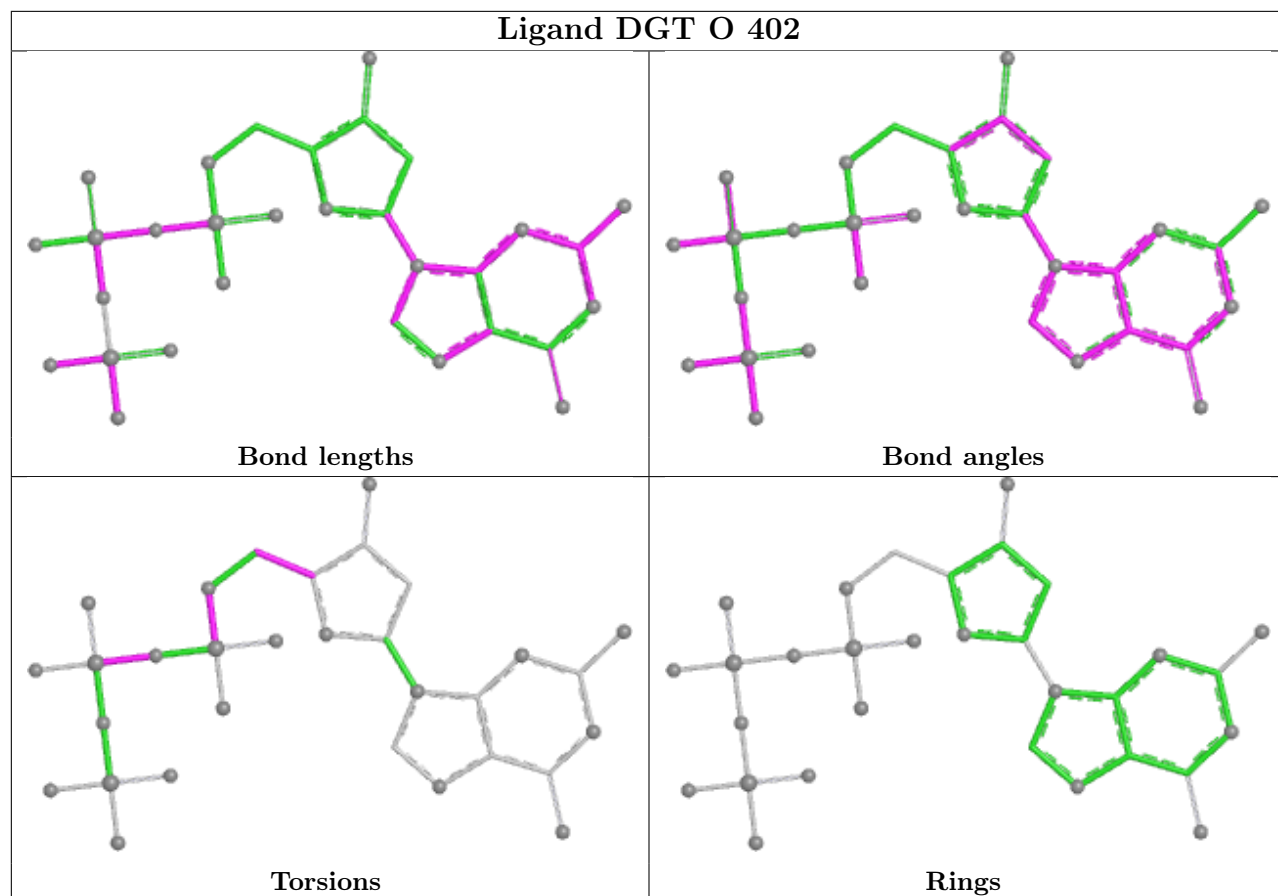
Continued from previous page...

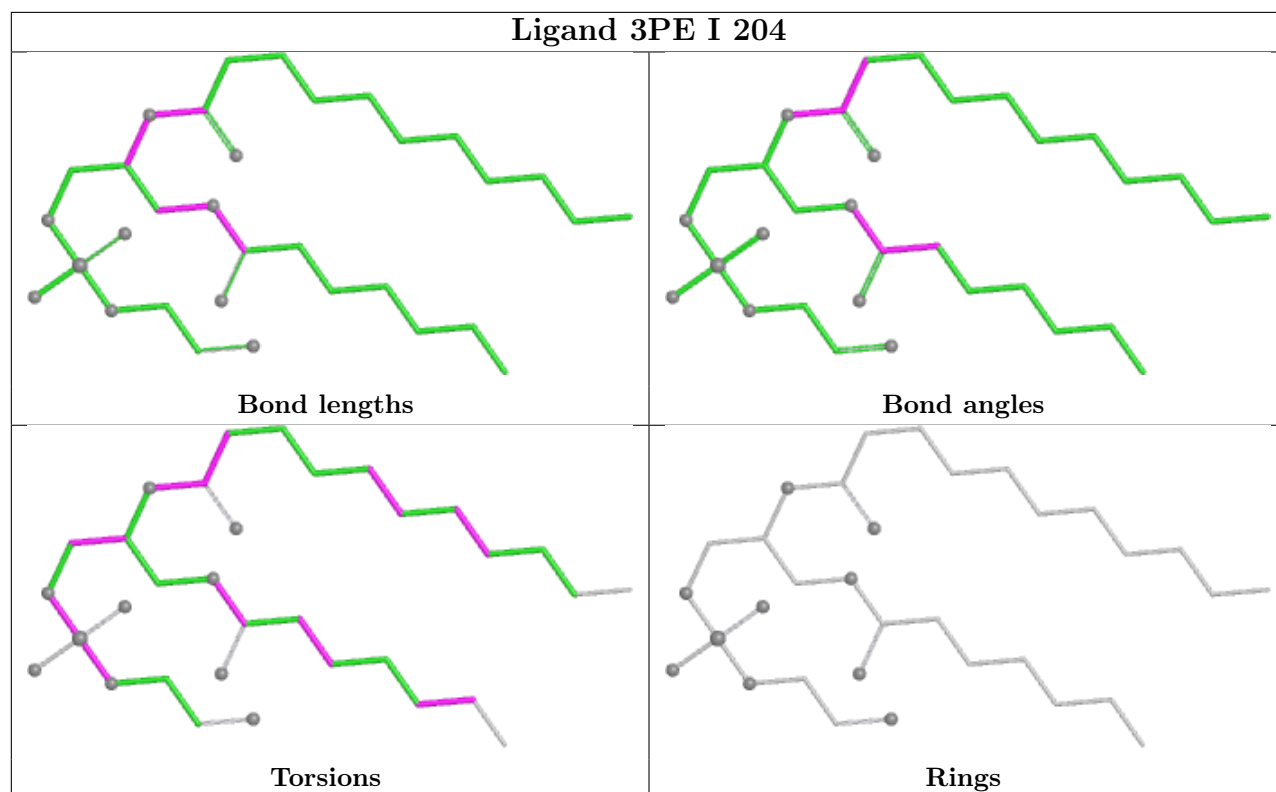
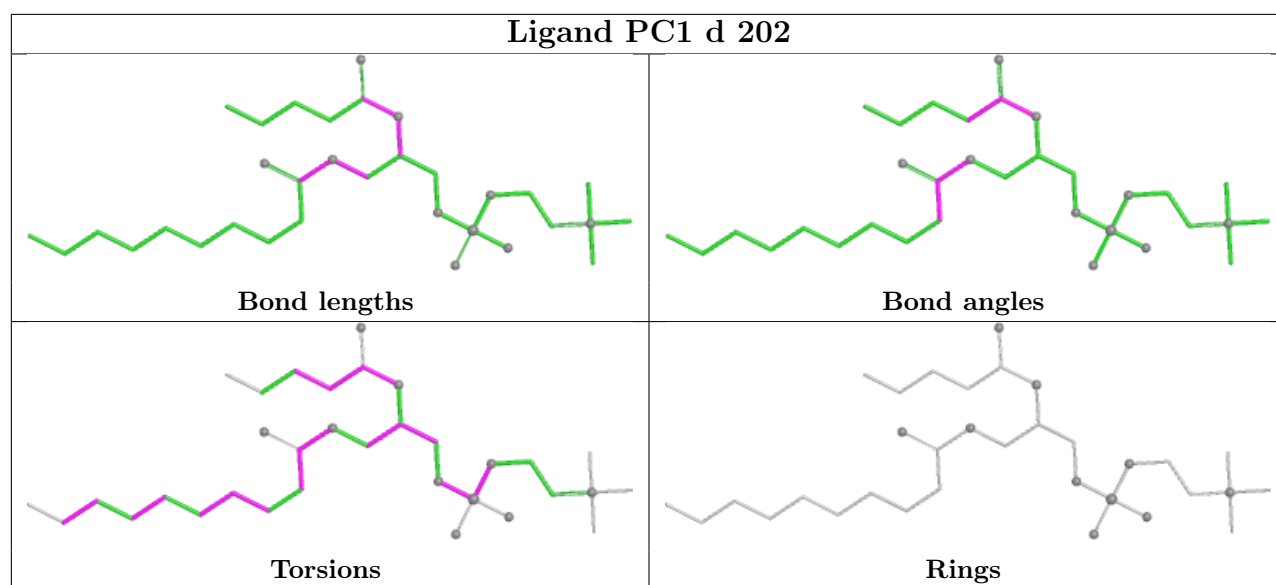
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	202	PC1	2	0
45	d	201	3PE	1	0
48	G	803	FES	1	0
52	O	402	DGT	2	0
47	F	502	SF4	1	0
45	Z	201	3PE	1	0
47	B	202	SF4	2	0
46	d	202	PC1	5	0
45	I	204	3PE	1	0
57	i	201	CHD	2	0
45	O	401	3PE	2	0
49	F	501	FMN	2	0
46	B	201	PC1	2	0
56	T	101	EHZ	1	0
47	I	202	SF4	1	0
51	N	401	CDL	2	0
51	X	201	CDL	1	0
45	h	201	3PE	4	0
45	I	201	3PE	6	0
45	M	502	3PE	3	0
45	A	201	3PE	4	0
45	M	501	3PE	2	0
51	d	203	CDL	1	0

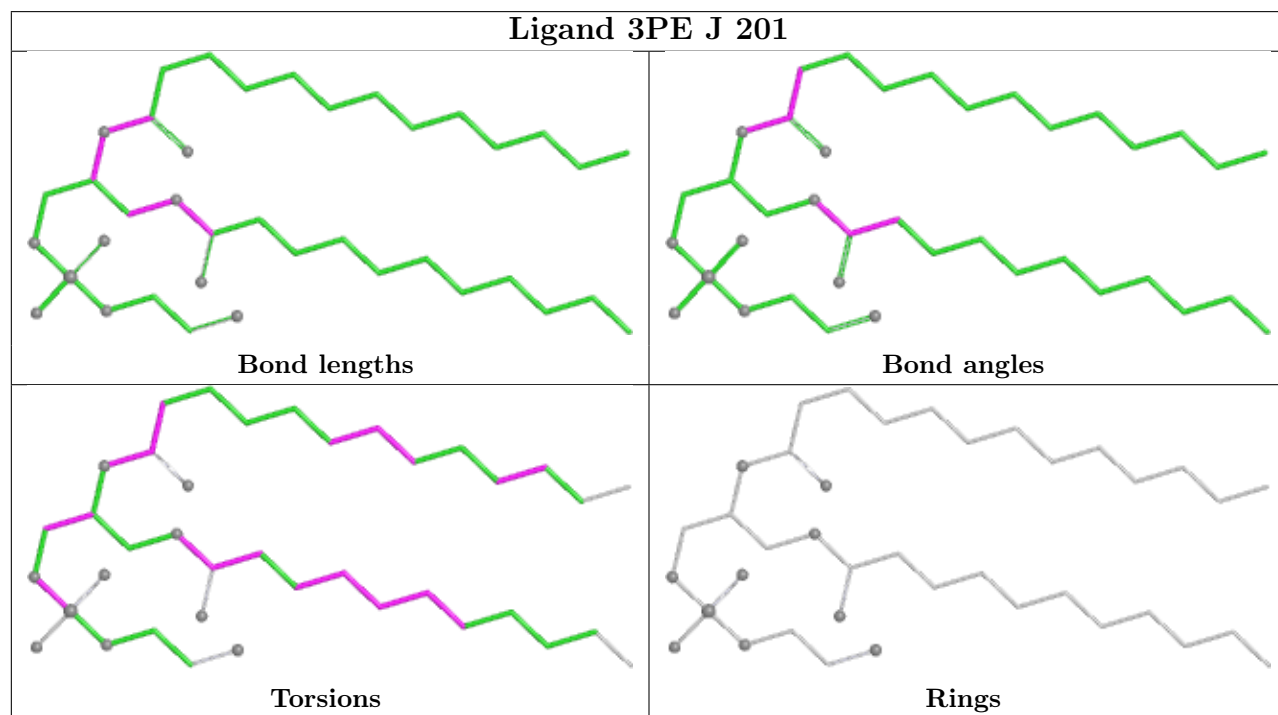
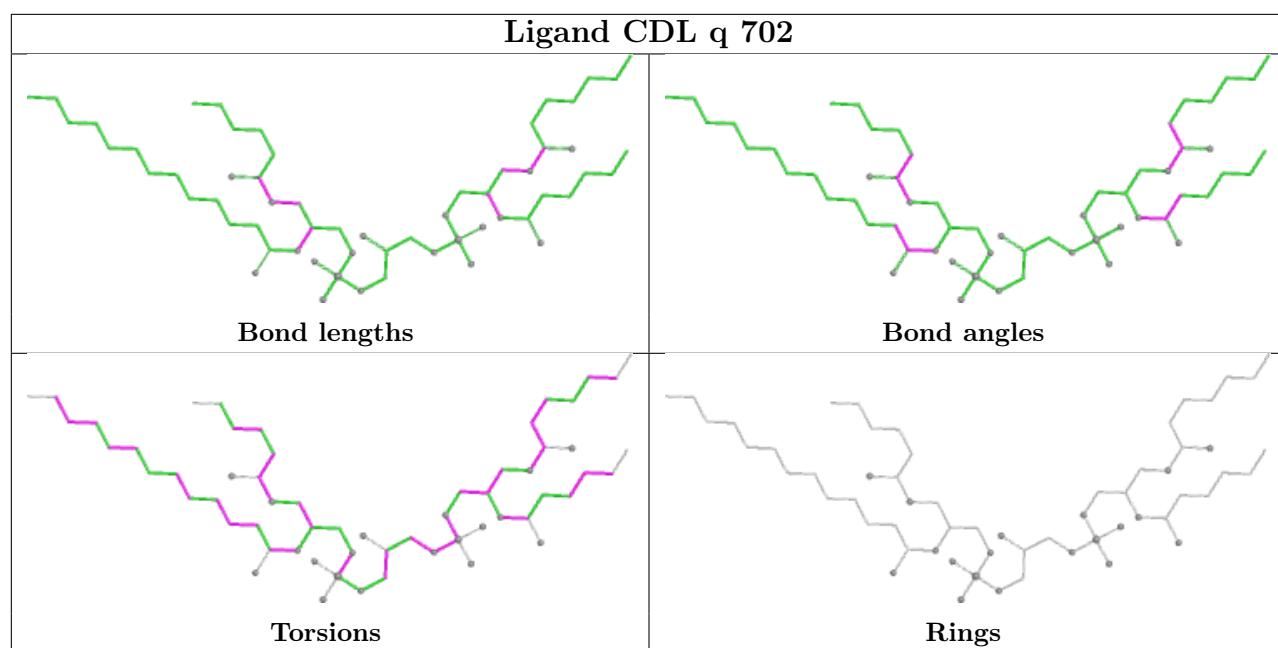
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

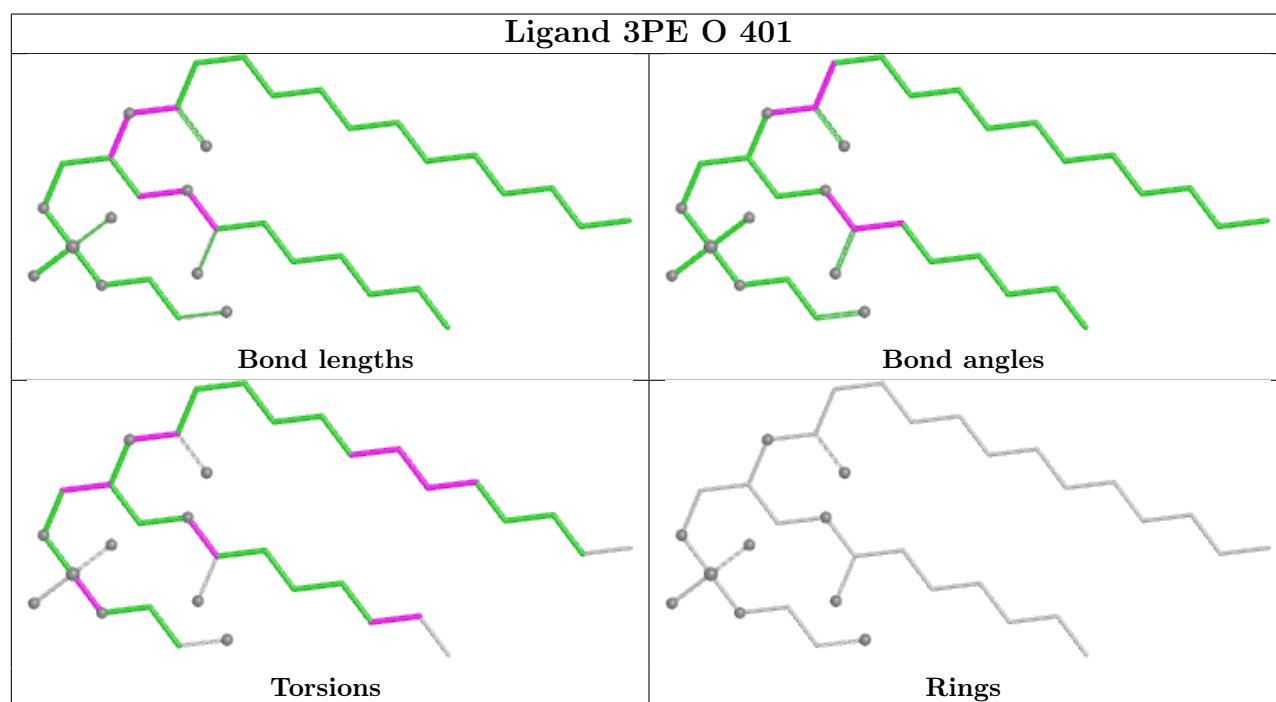
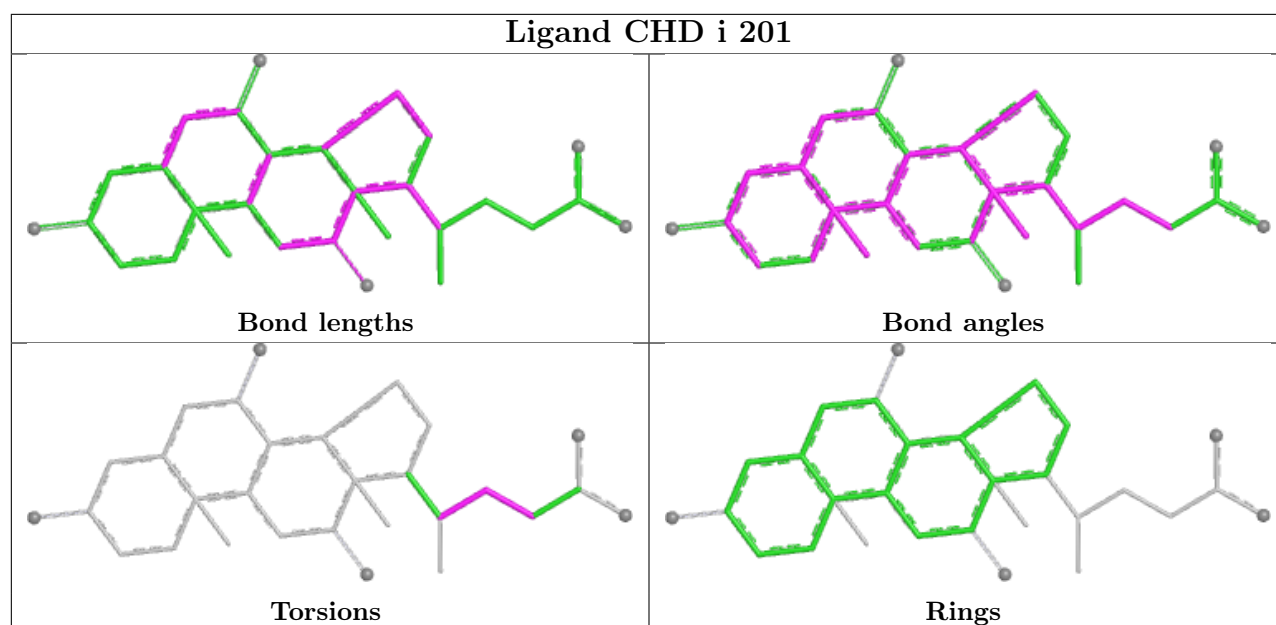


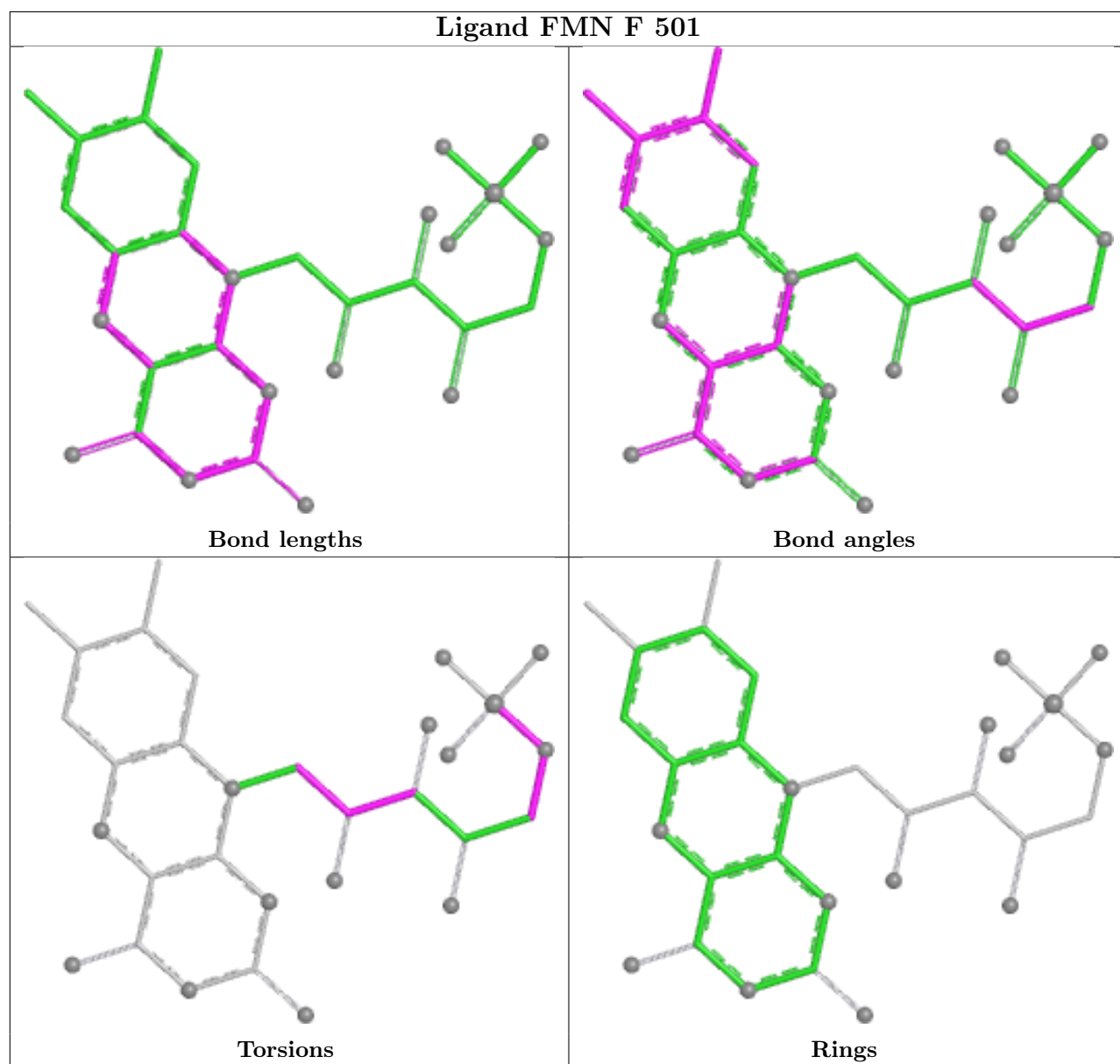
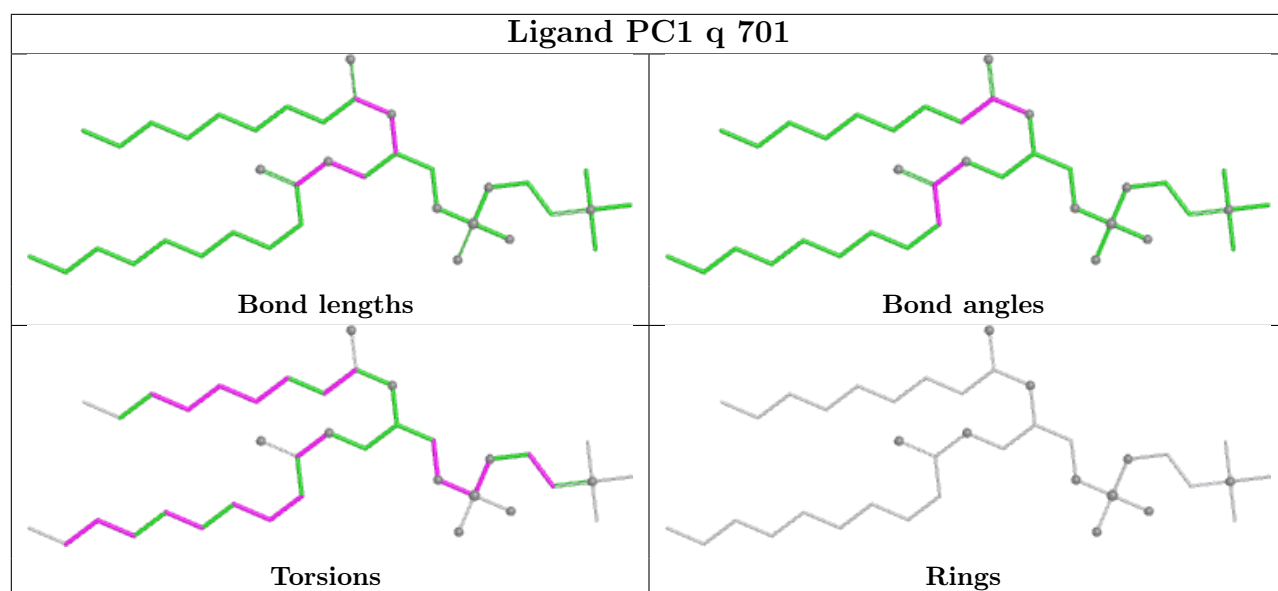


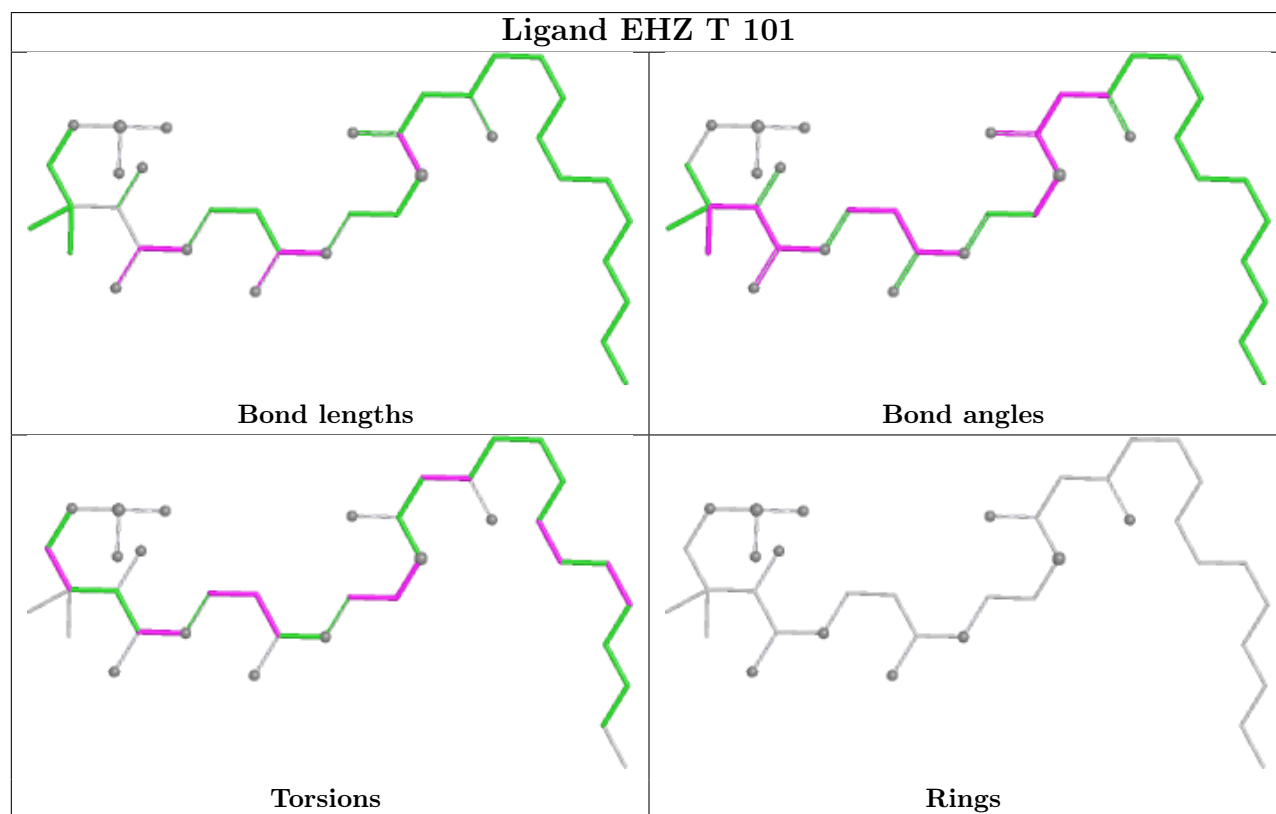
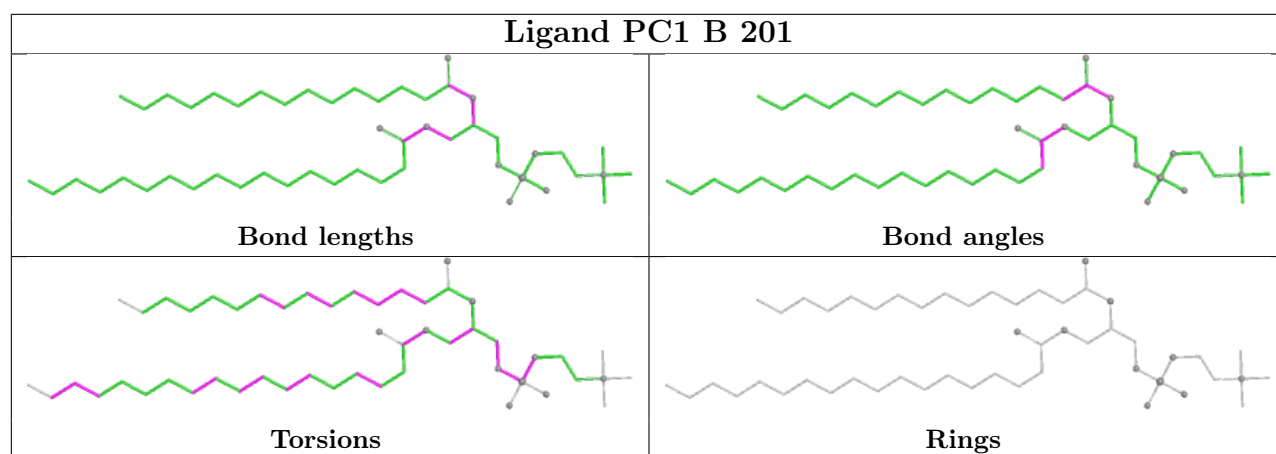


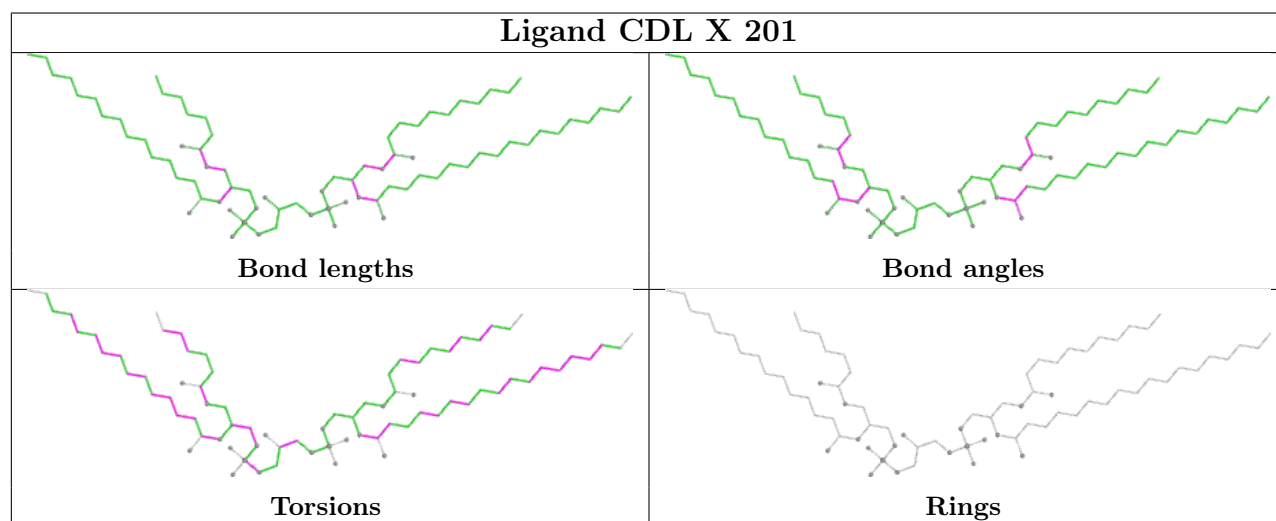
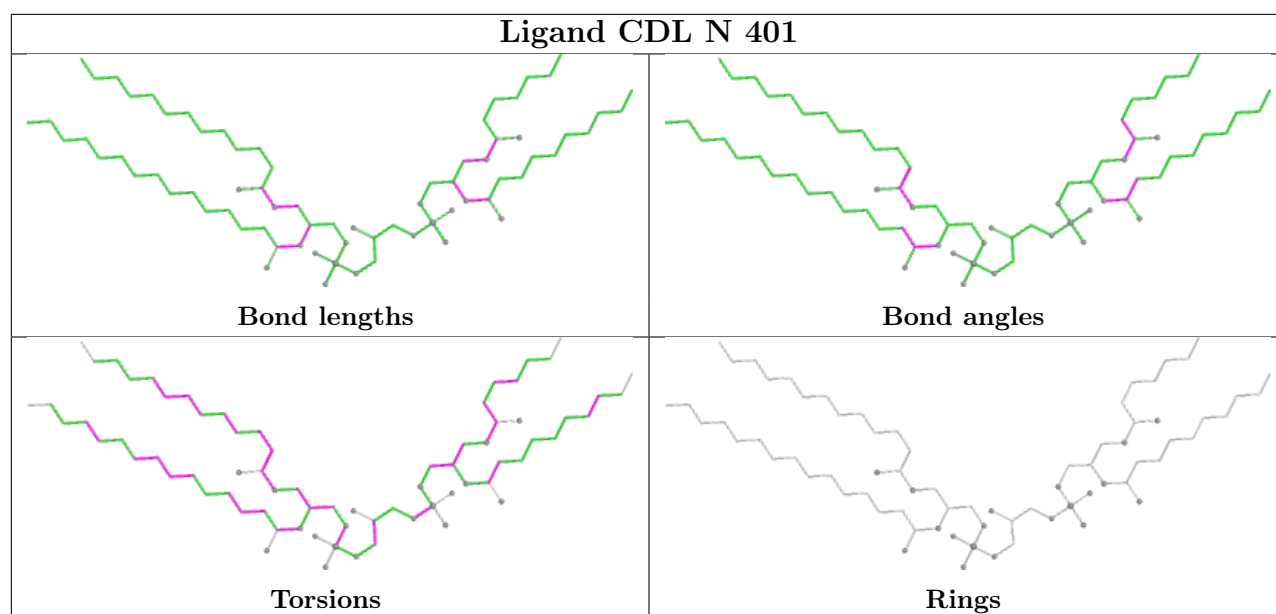


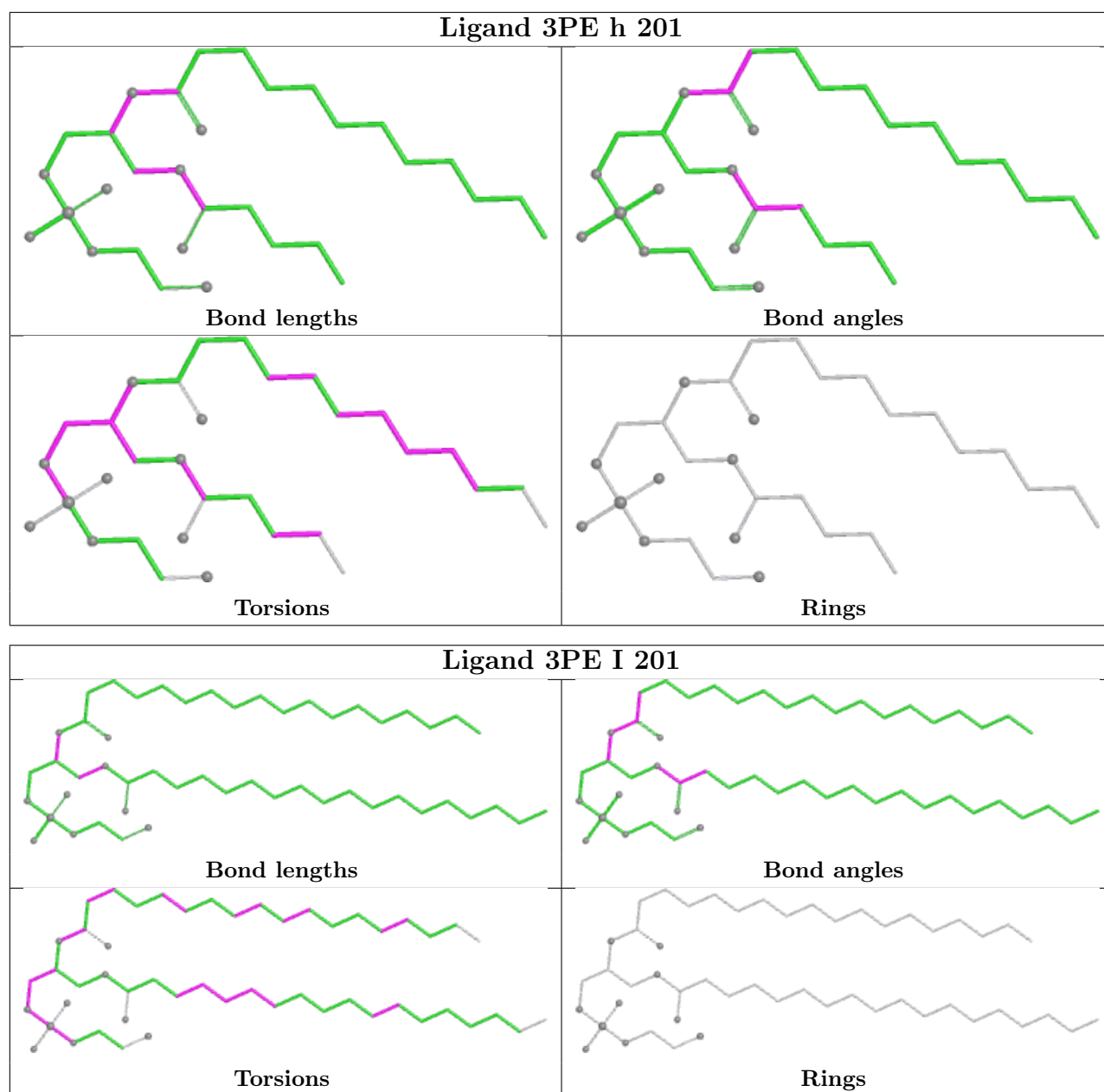


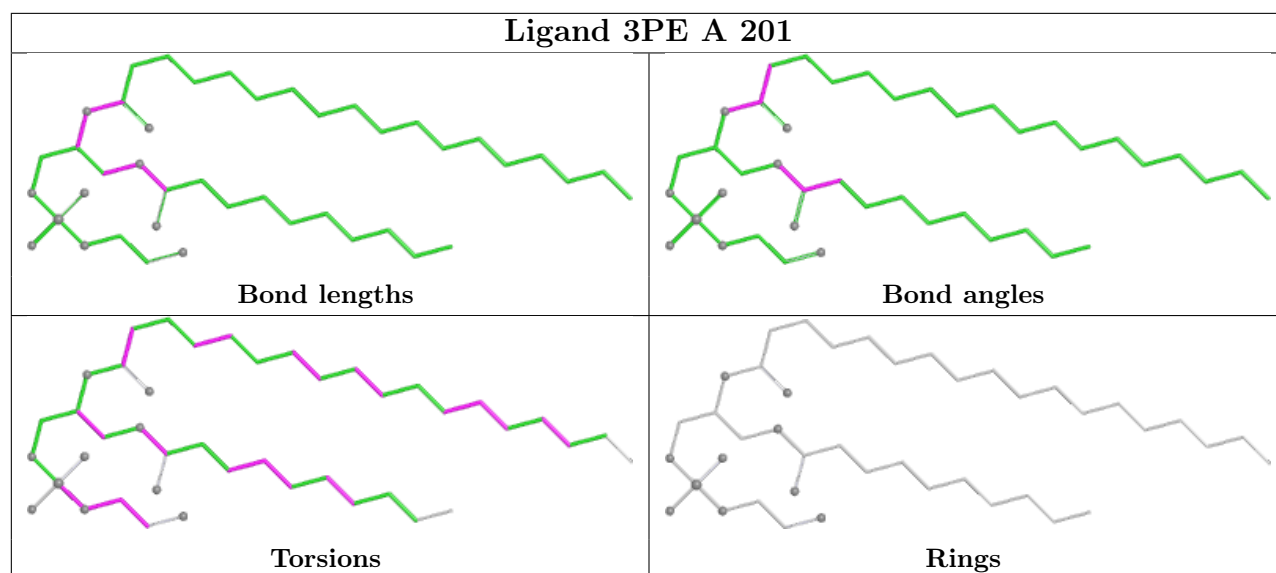
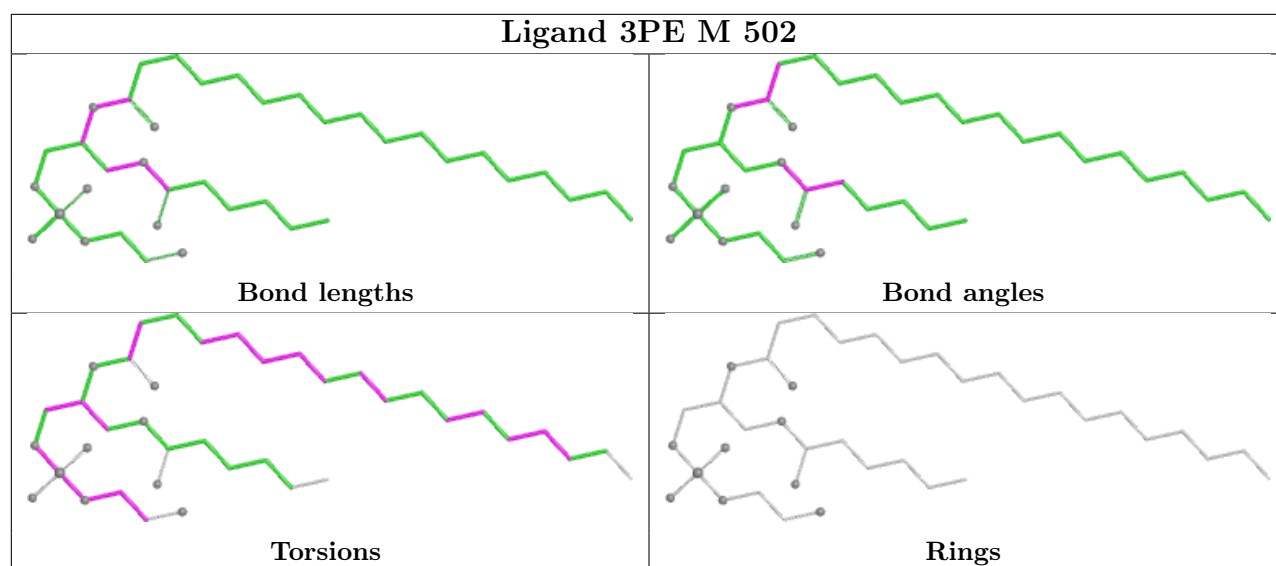


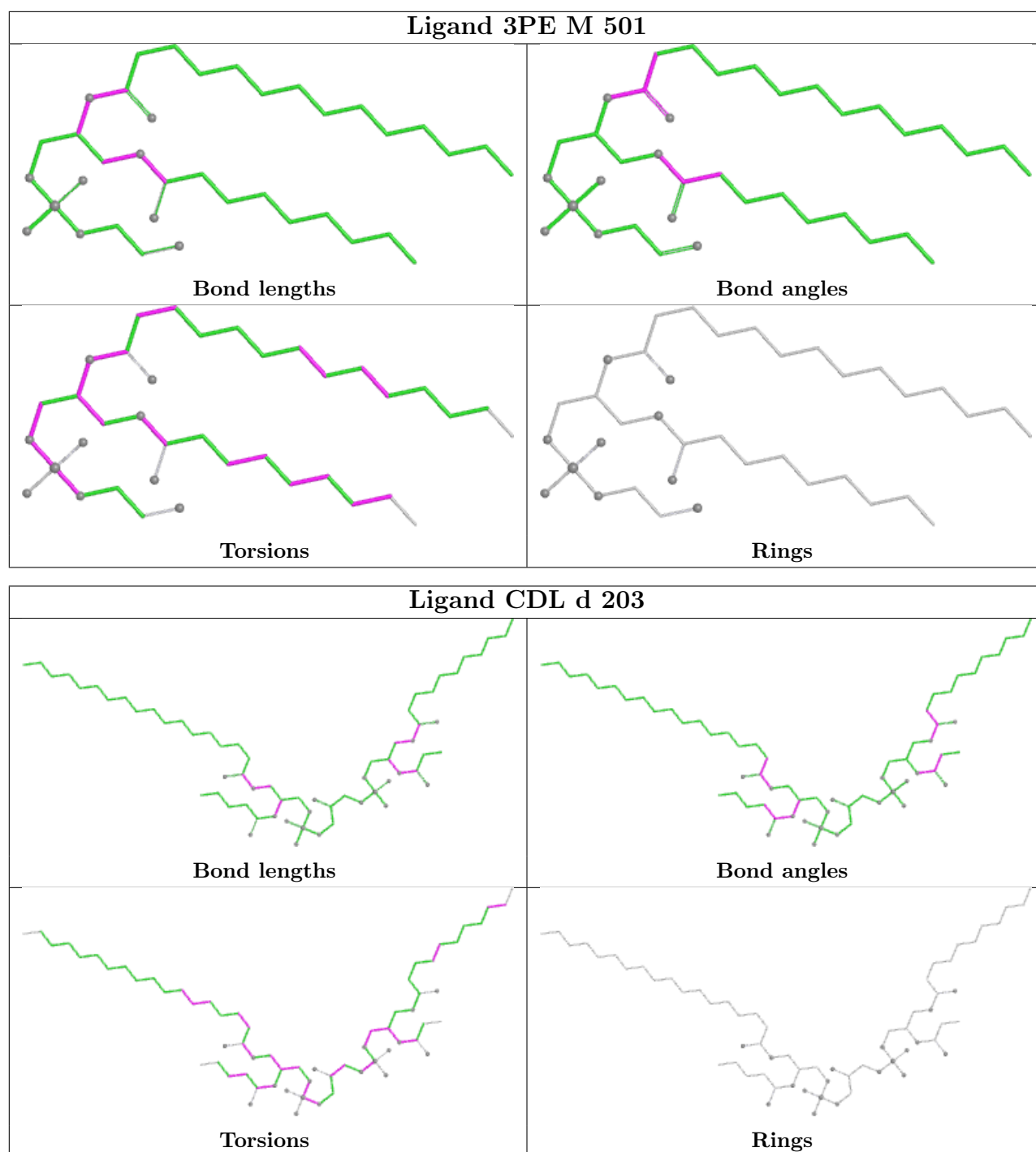


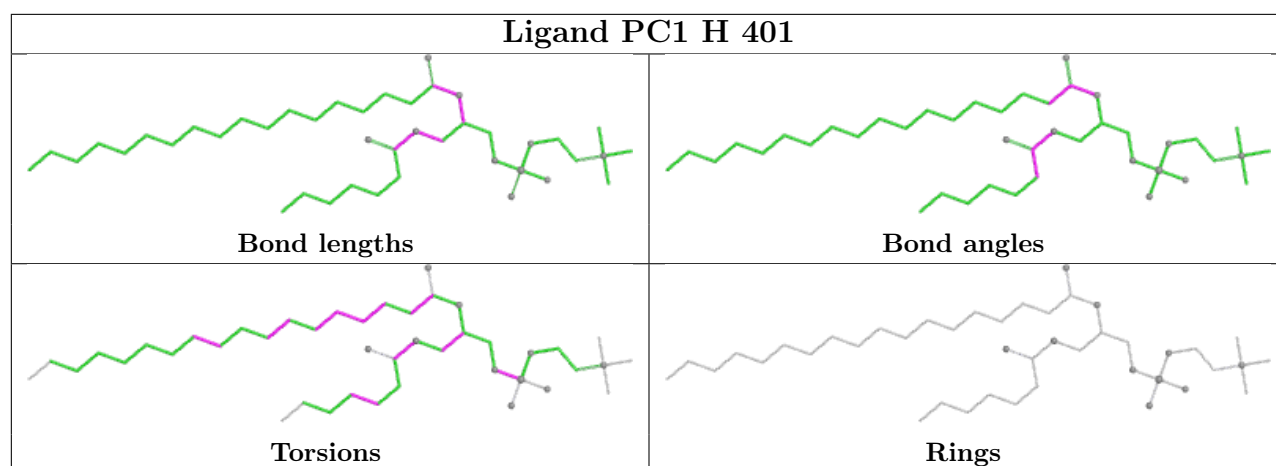












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

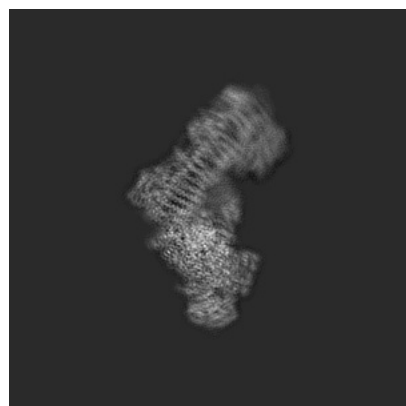
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18059. These allow visual inspection of the internal detail of the map and identification of artifacts.

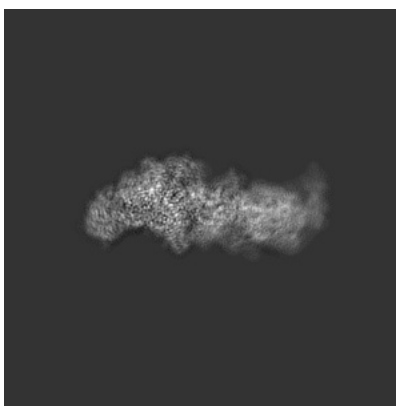
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

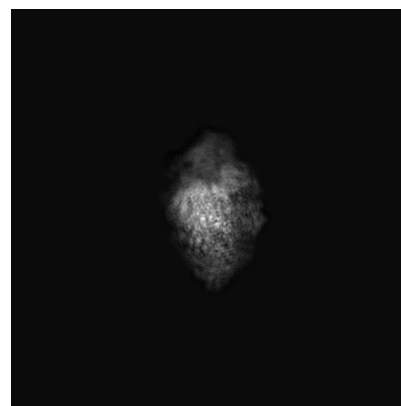
6.1.1 Primary map



X

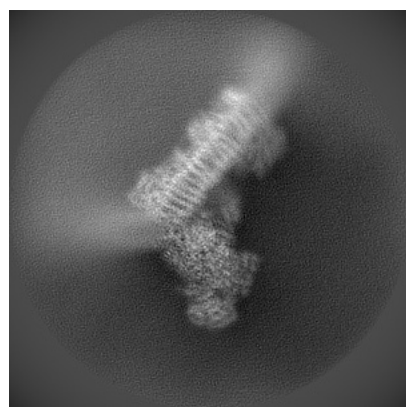


Y

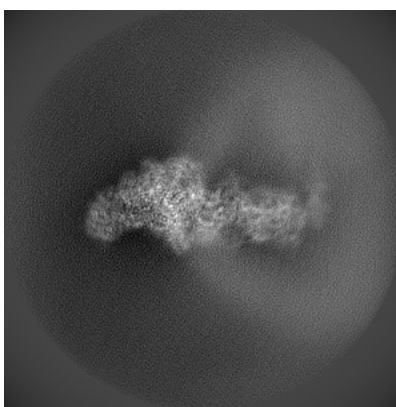


Z

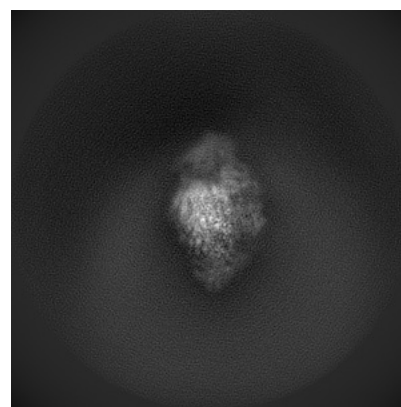
6.1.2 Raw map



X



Y

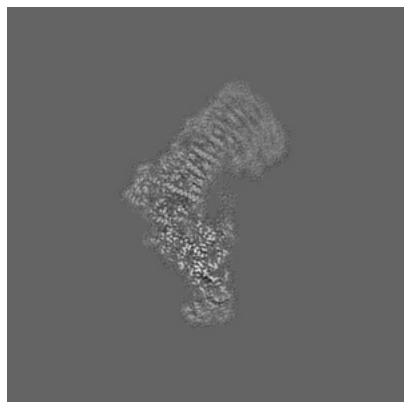


Z

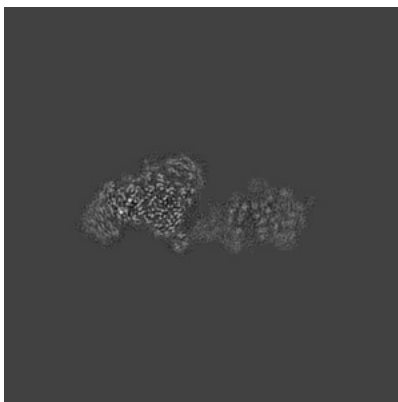
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

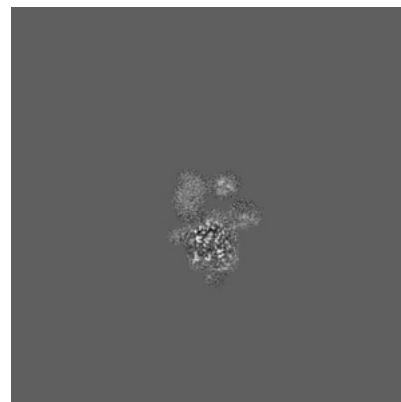
6.2.1 Primary map



X Index: 180

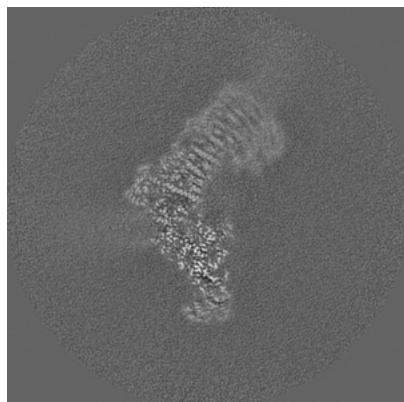


Y Index: 180

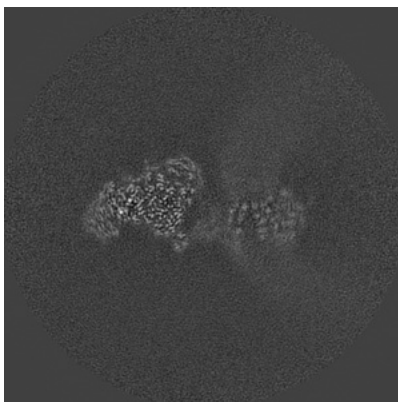


Z Index: 180

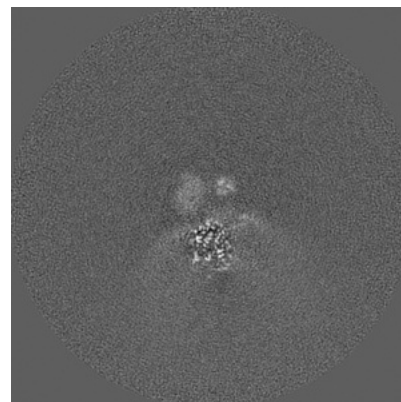
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

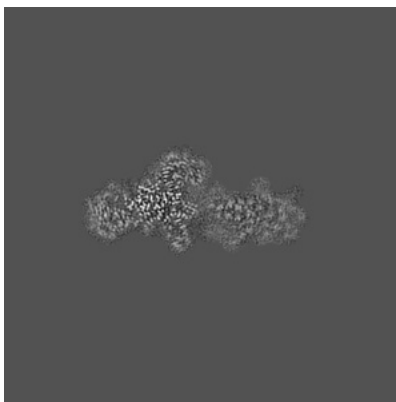
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

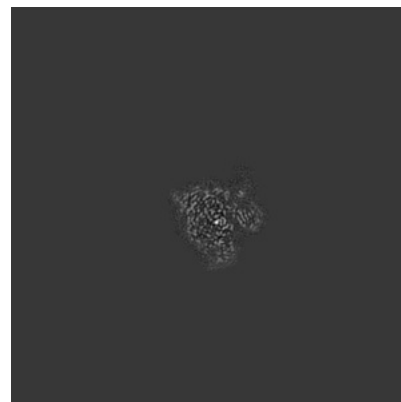
6.3.1 Primary map



X Index: 186

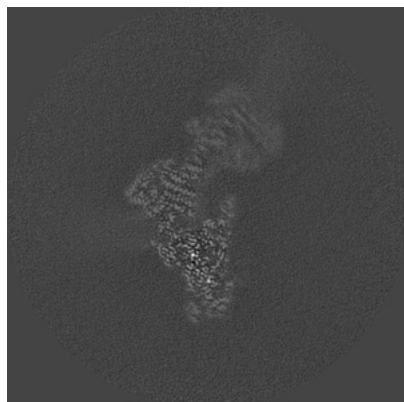


Y Index: 172

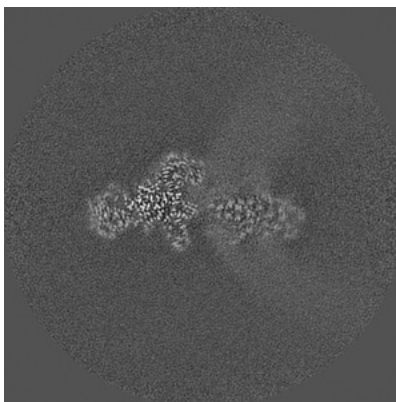


Z Index: 146

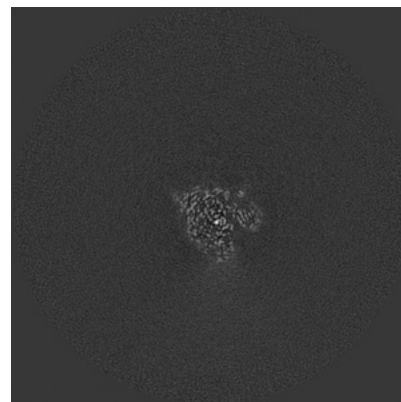
6.3.2 Raw map



X Index: 186



Y Index: 172

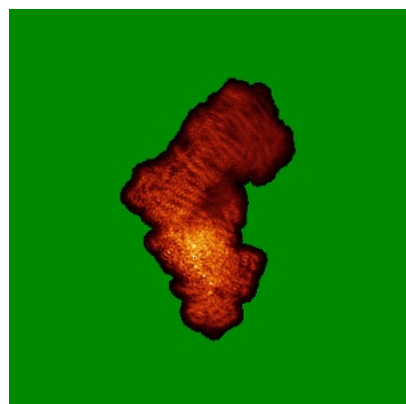


Z Index: 146

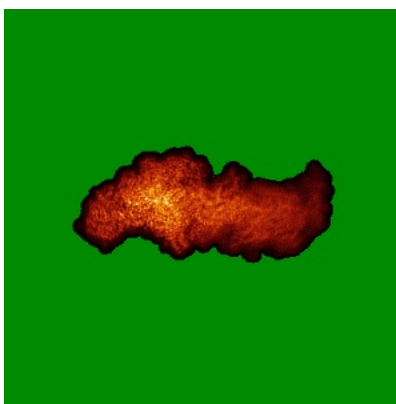
The images above show the largest variance slices of the map in three orthogonal directions.

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

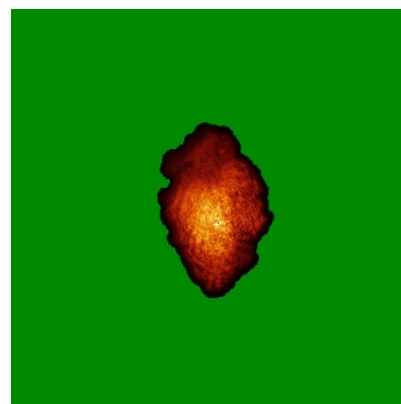
6.4.1 Primary map



X

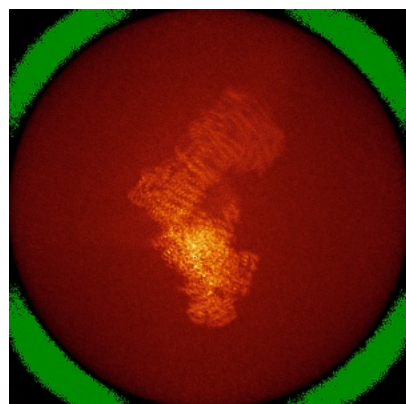


Y

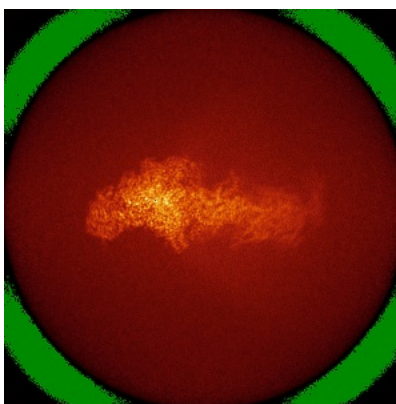


Z

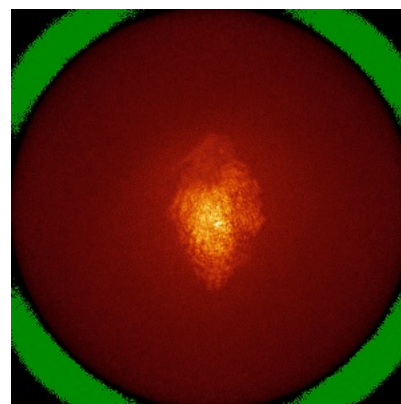
6.4.2 Raw map



X



Y

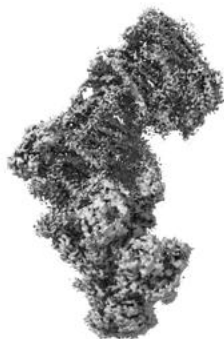


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



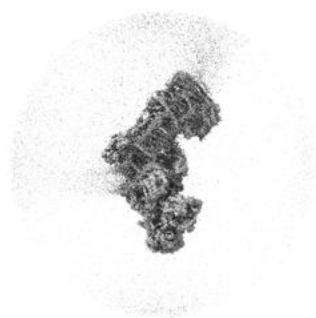
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

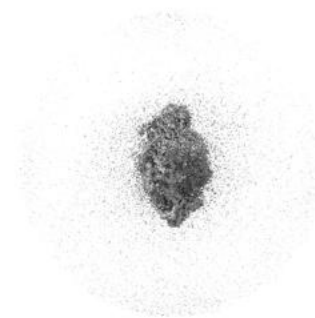
6.5.2 Raw map



X



Y



Z

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

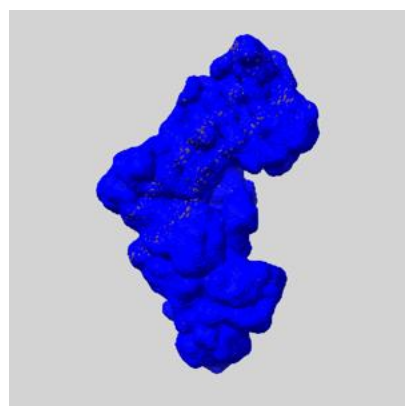
6.6 Mask visualisation [i](#)

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

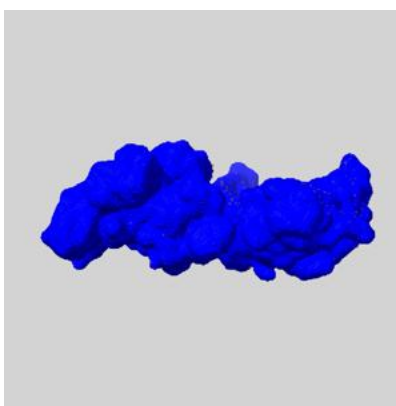
A mask typically either:

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

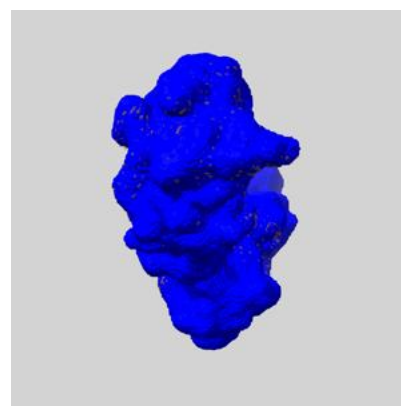
6.6.1 emd_18059_msk_1.map [i](#)



X



Y

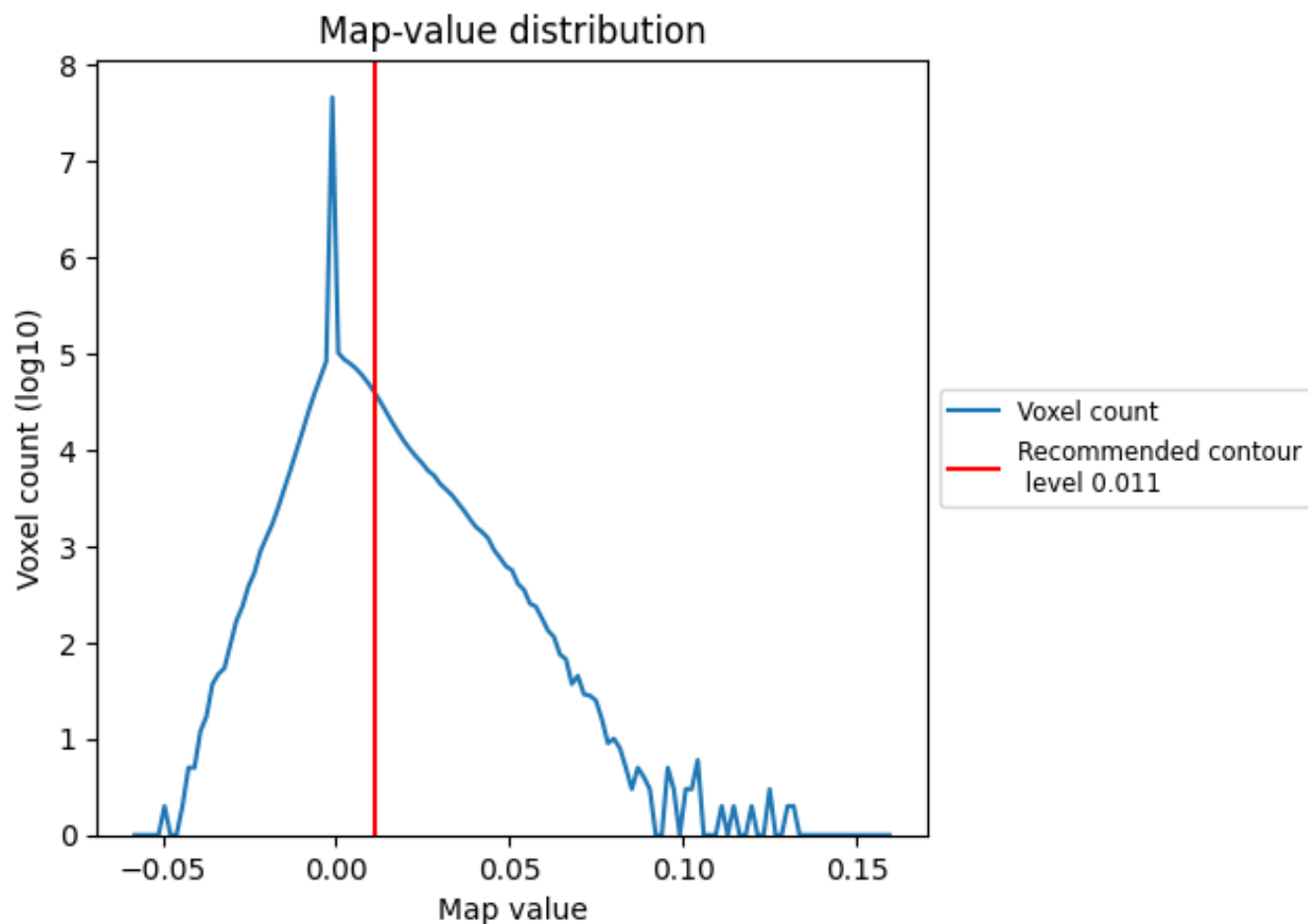


Z

7 Map analysis [i](#)

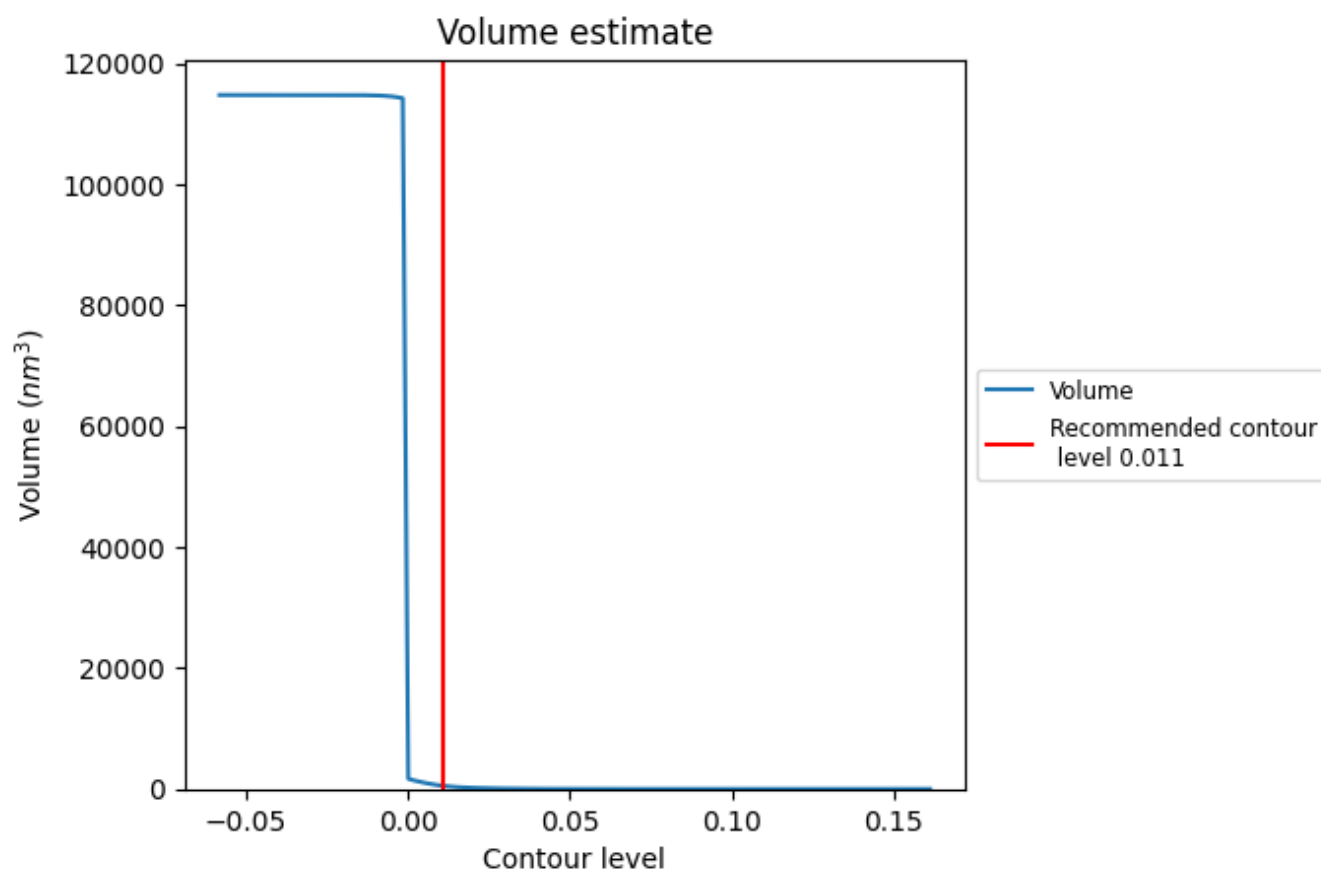
This section contains the results of statistical analysis of the map.

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.

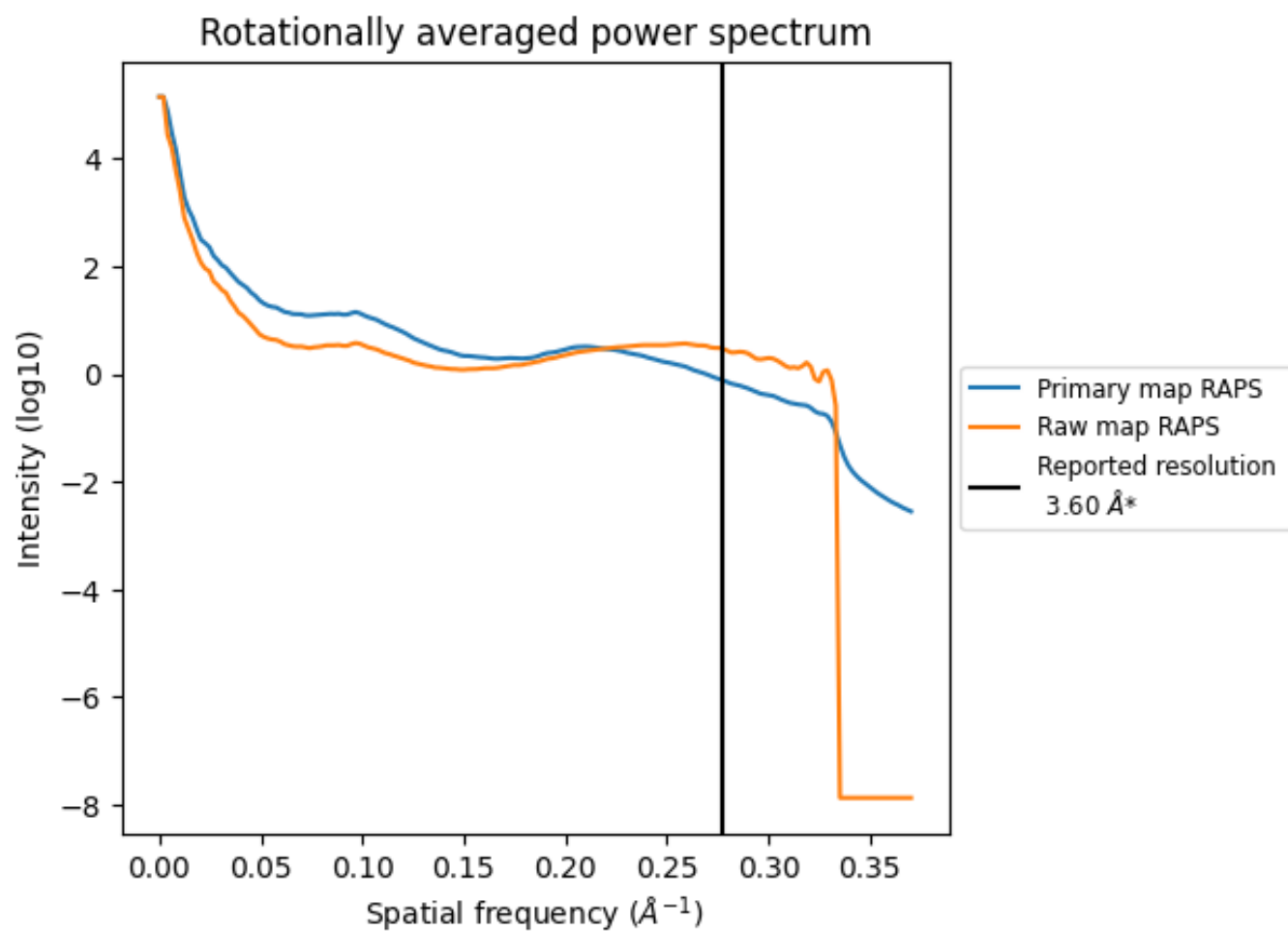
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 515 nm^3 ; this corresponds to an approximate mass of 466 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

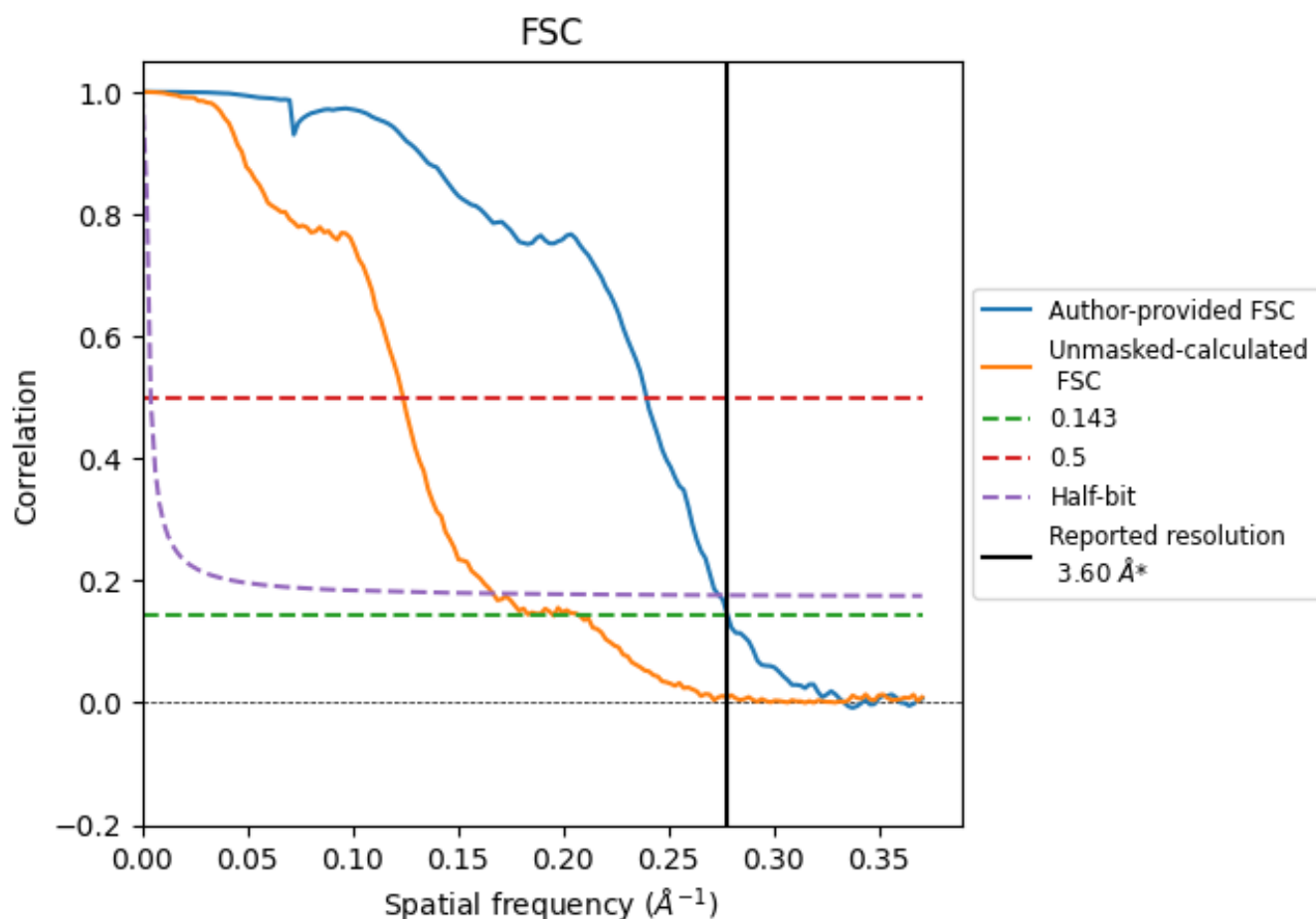


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

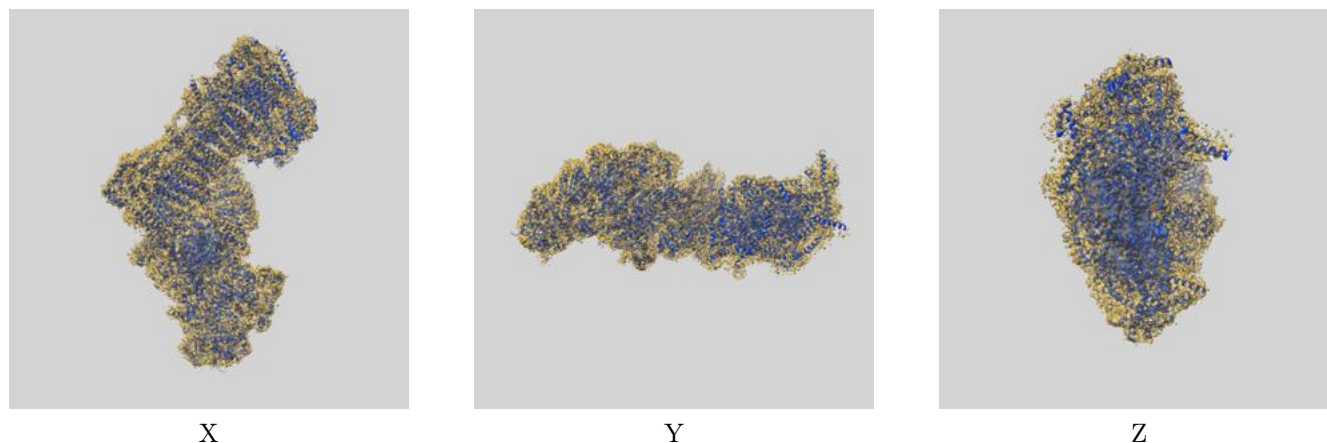
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.60	4.18	3.65
Unmasked-calculated*	5.12	8.08	6.01

*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 5.12 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

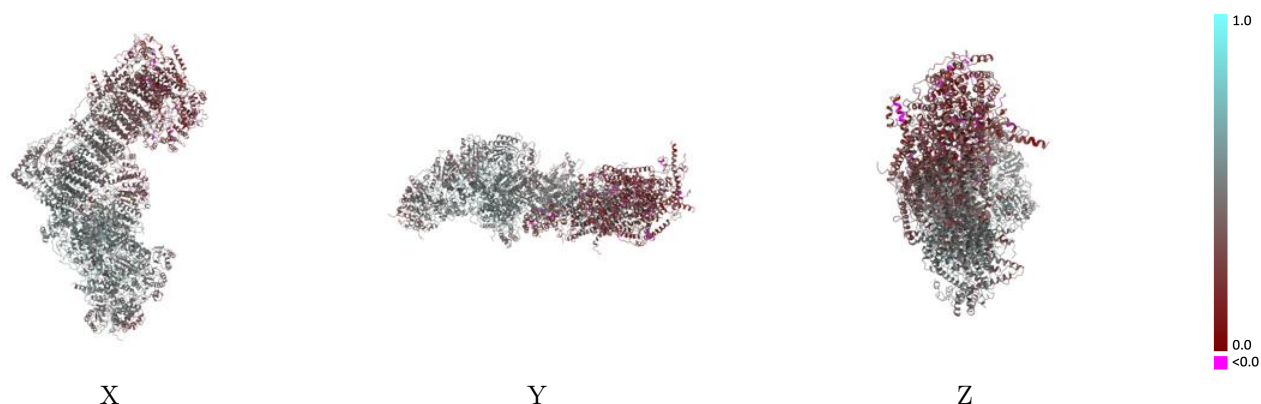
This section contains information regarding the fit between EMDB map EMD-18059 and PDB model 8Q0Q. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)



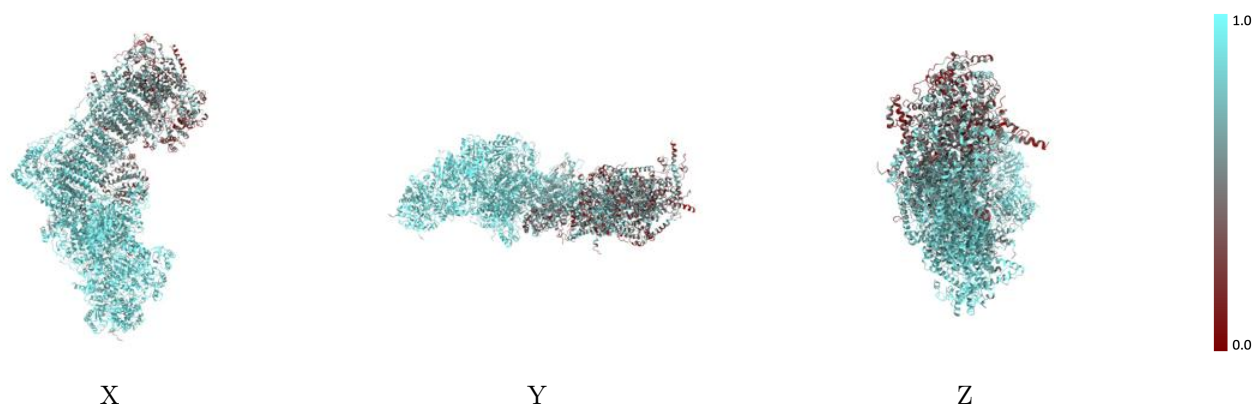
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



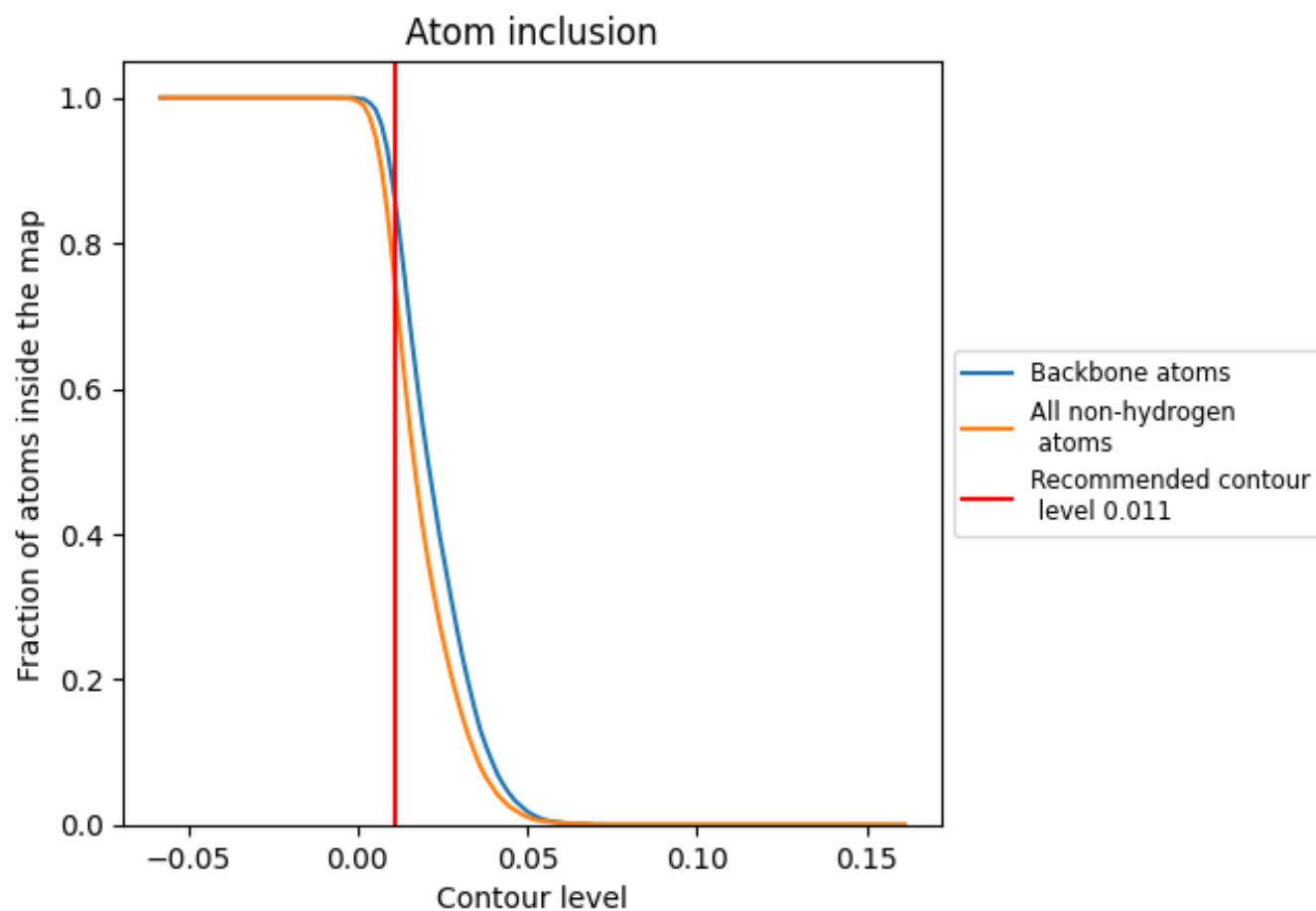
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.011).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 74% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7450	 0.4190
A	 0.7840	 0.4890
B	 0.9070	 0.5450
C	 0.9380	 0.5450
D	 0.9240	 0.5490
E	 0.8980	 0.4510
F	 0.8820	 0.4490
G	 0.9040	 0.5050
H	 0.8850	 0.5170
I	 0.9360	 0.5500
J	 0.7610	 0.4460
K	 0.8240	 0.4900
L	 0.5030	 0.2710
M	 0.6710	 0.3620
N	 0.7890	 0.4510
O	 0.4490	 0.2780
P	 0.8620	 0.4830
Q	 0.9010	 0.5330
R	 0.8520	 0.5080
S	 0.8500	 0.4300
T	 0.8270	 0.4090
U	 0.3510	 0.2220
V	 0.8960	 0.4670
W	 0.8900	 0.4970
X	 0.8190	 0.4580
Y	 0.3860	 0.3270
Z	 0.8290	 0.4700
a	 0.9000	 0.5080
b	 0.8560	 0.4630
c	 0.5760	 0.3200
d	 0.7090	 0.4010
e	 0.8250	 0.4600
f	 0.6080	 0.3670
g	 0.6120	 0.3190
h	 0.6800	 0.3480



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Chain	Atom inclusion	Q-score
i	 0.3950	 0.2140
j	 0.4060	 0.2610
k	 0.3420	 0.2420
l	 0.4780	 0.2620
m	 0.4520	 0.2890
n	 0.4760	 0.2440
o	 0.4790	 0.2640
p	 0.6400	 0.3360
q	 0.8930	 0.5280
r	 0.9050	 0.5190
s	 0.6680	 0.3900