



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:45 AM UTC

PDB ID : 8Q0J / pdb_00008q0j
EMDB ID : EMD-18054
Title : Inward-facing, slack proteoliposome complex I at 3.8 Å. Initially purified in DDM.
Authors : Grba, D.N.; Hirst, J.
Deposited on : 2023-07-28
Resolution : 3.80 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:

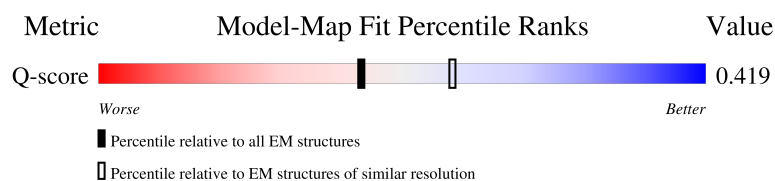
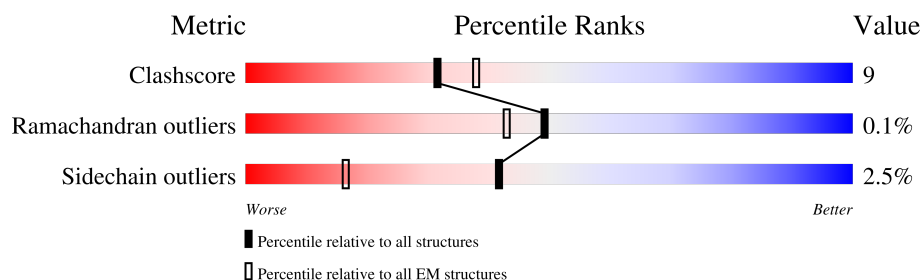
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.80 Å.

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



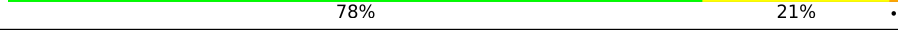
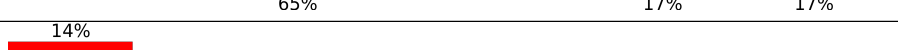
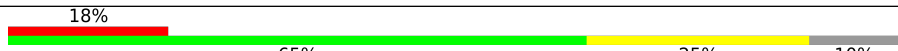
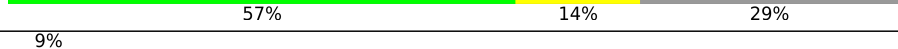
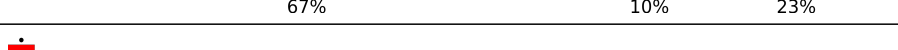
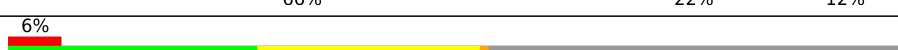
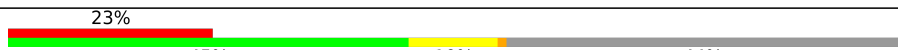
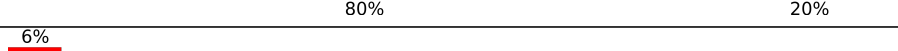
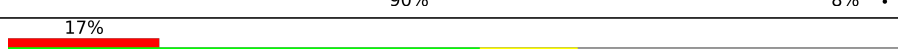
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	
2	B	216	
3	C	266	
4	D	463	

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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	

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		

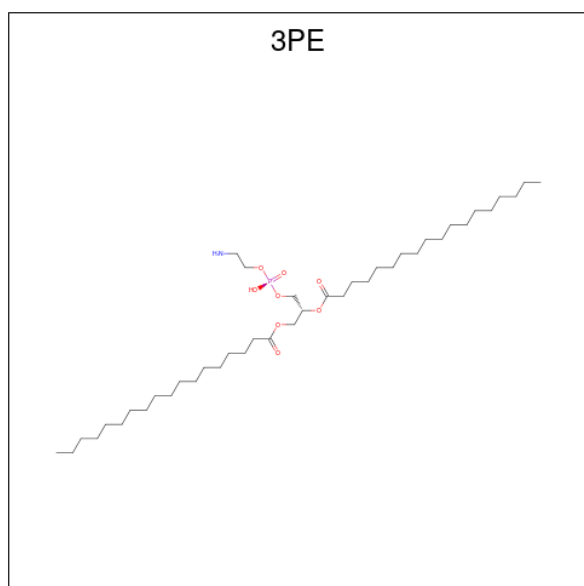
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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: $C_{41}H_{82}NO_8P$).



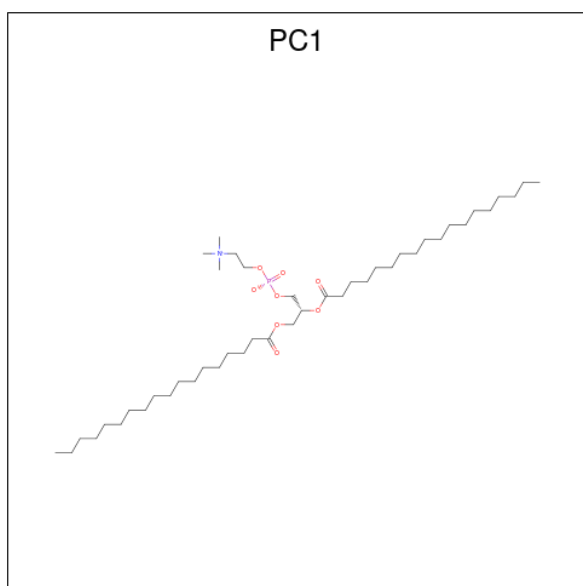
Mol	Chain	Residues	Atoms					AltConf
45	A	1	Total	C	N	O	P	0
			43	33	1	8	1	
45	D	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	I	1	Total	C	N	O	P	0
			33	23	1	8	1	
45	J	1	Total	C	N	O	P	0
			39	29	1	8	1	
45	M	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	N	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	Y	1	Total	C	N	O	P	0
			39	29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

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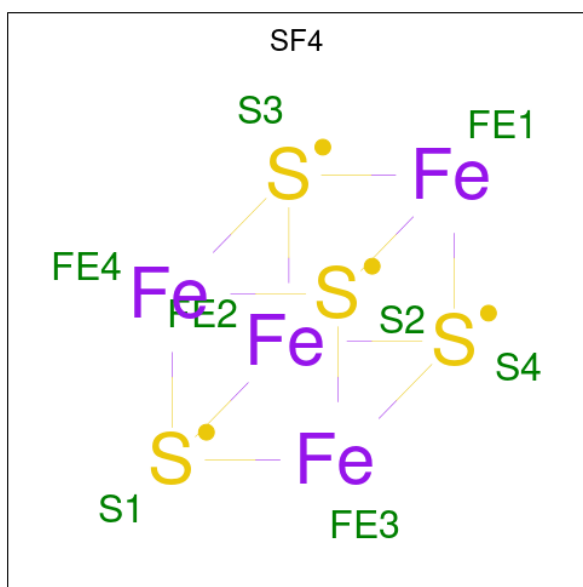
Mol	Chain	Residues	Atoms					AltConf
45	Z	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	d	1	Total	C	N	O	P	0
			49	39	1	8	1	
45	h	1	Total	C	N	O	P	0
			32	22	1	8	1	

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



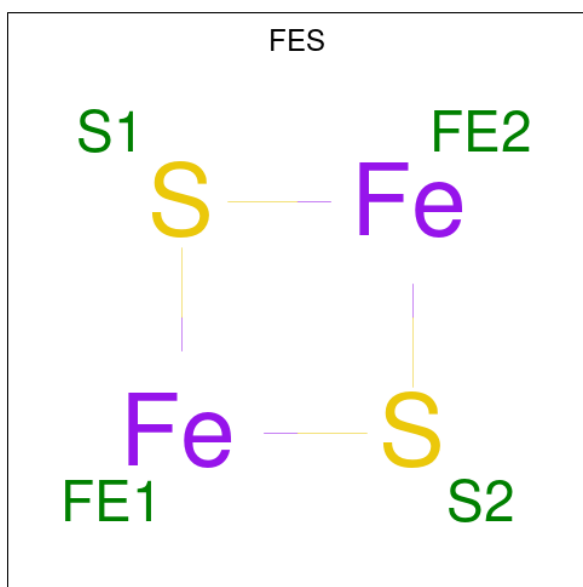
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
46	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	H	1	Total	C	N	O	P	0
			43	33	1	8	1	
46	H	1	Total	C	N	O	P	0
			37	27	1	8	1	
46	d	1	Total	C	N	O	P	0
			33	23	1	8	1	

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



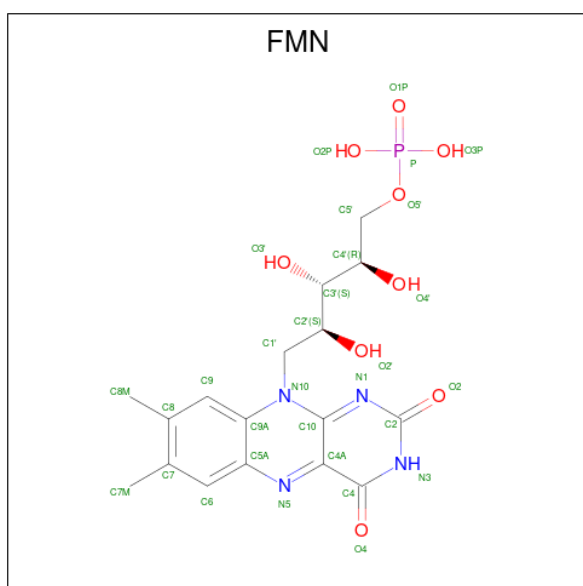
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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: $C_{17}H_{21}N_4O_9P$).

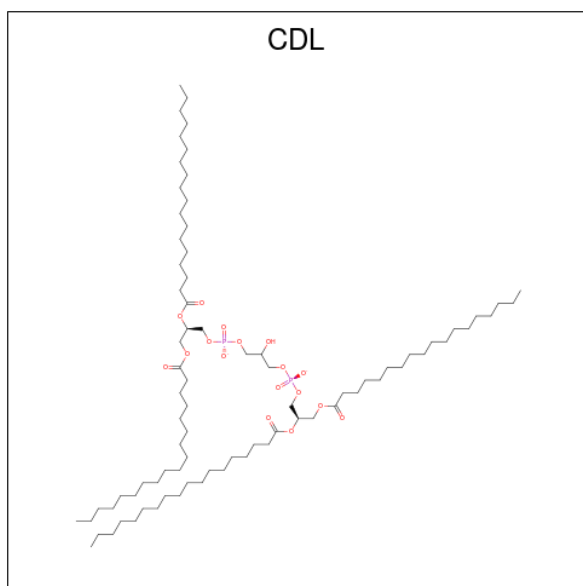


Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

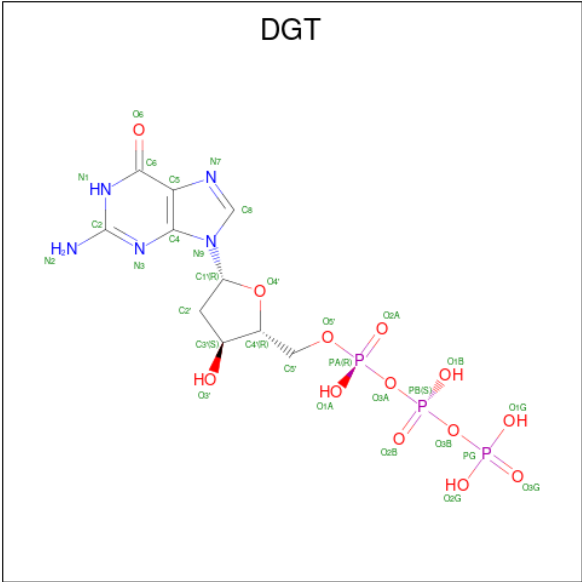
Mol	Chain	Residues	Atoms		AltConf
50	G	1	Total	K	0
			1	1	

- 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: $C_{10}H_{16}N_5O_{13}P_3$).

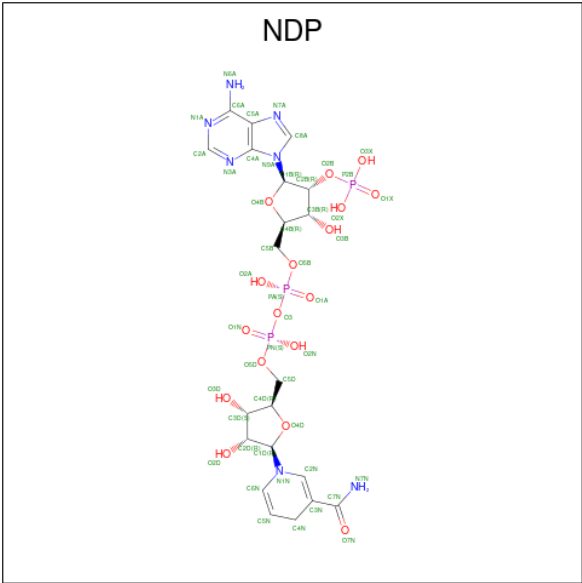


Mol	Chain	Residues	Atoms					AltConf
52	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

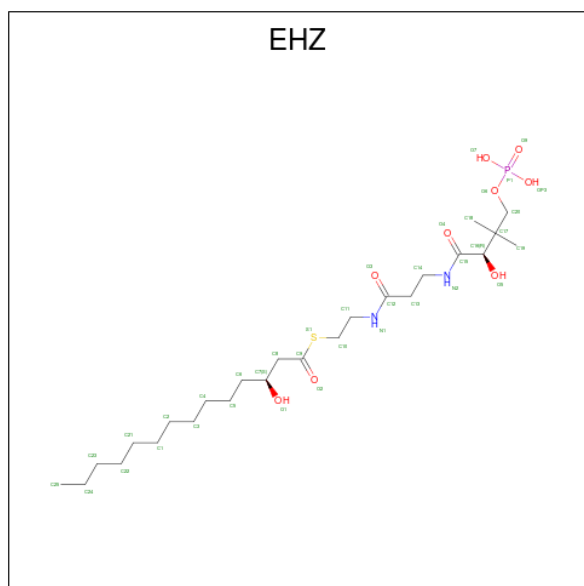


Mol	Chain	Residues	Atoms					AltConf
54	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

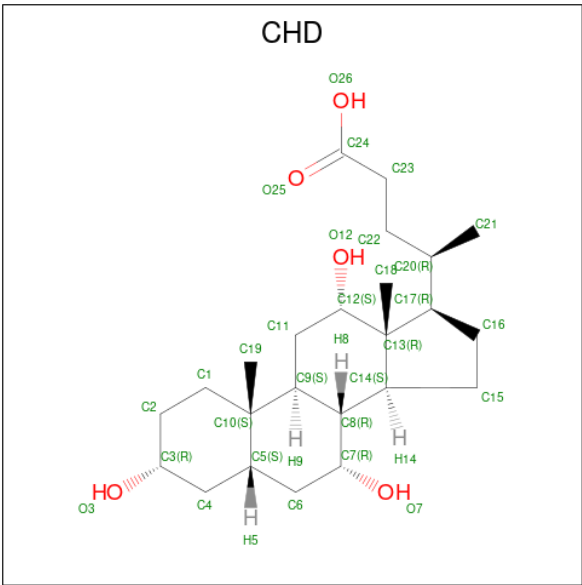
Mol	Chain	Residues	Atoms		AltConf
55	R	1	Total	Zn	0
			1	1	

- 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).



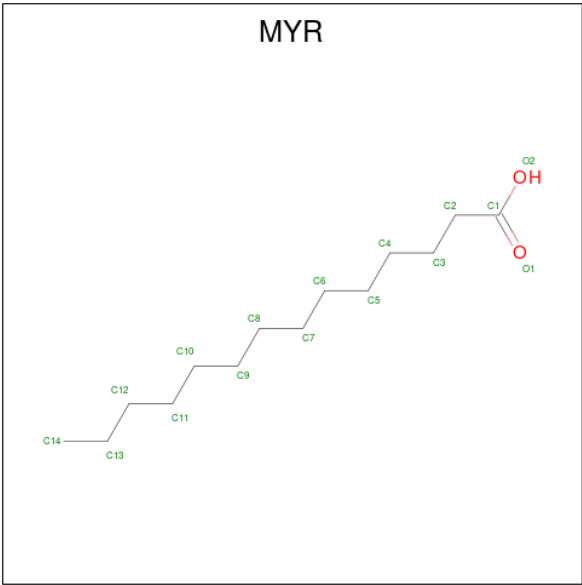
Mol	Chain	Residues	Atoms						AltConf
56	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
56	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- 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).

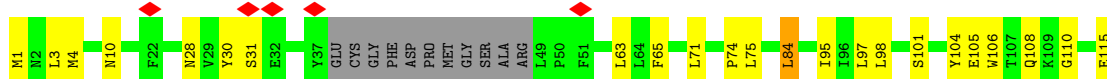


Mol	Chain	Residues	Atoms			AltConf
58	o	1	Total	C	O	0
			15	14	1	

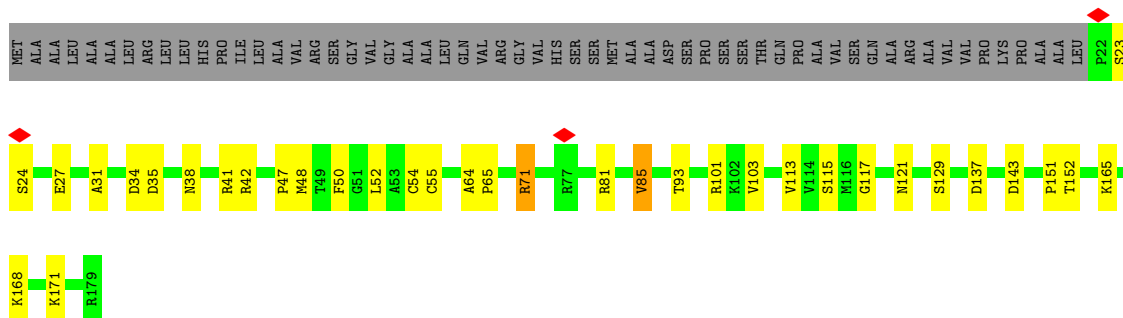
3 Residue-property plots [i](#)

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.

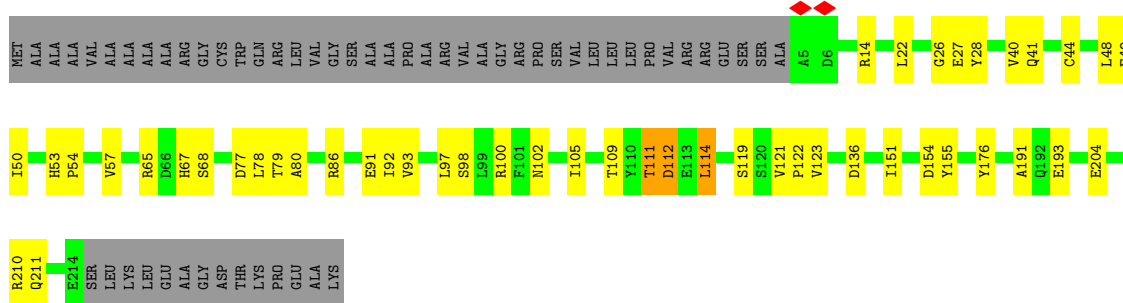
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



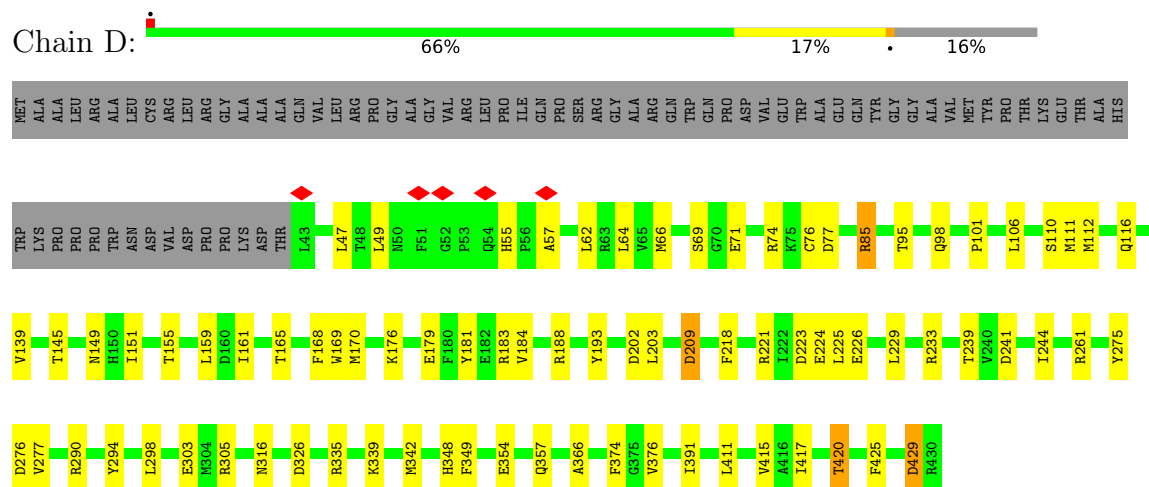
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



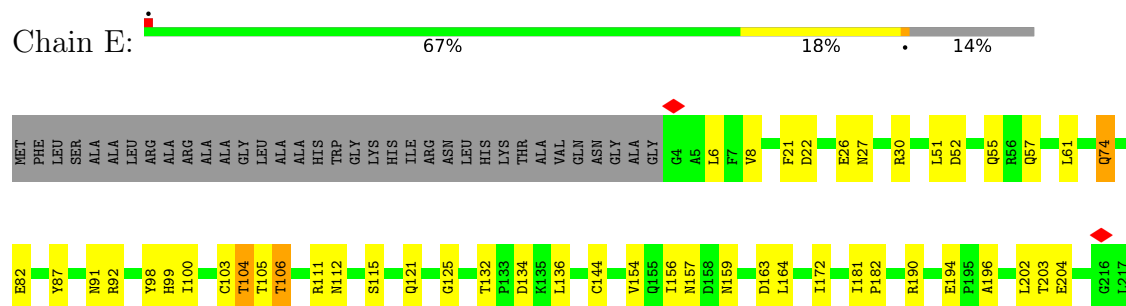
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



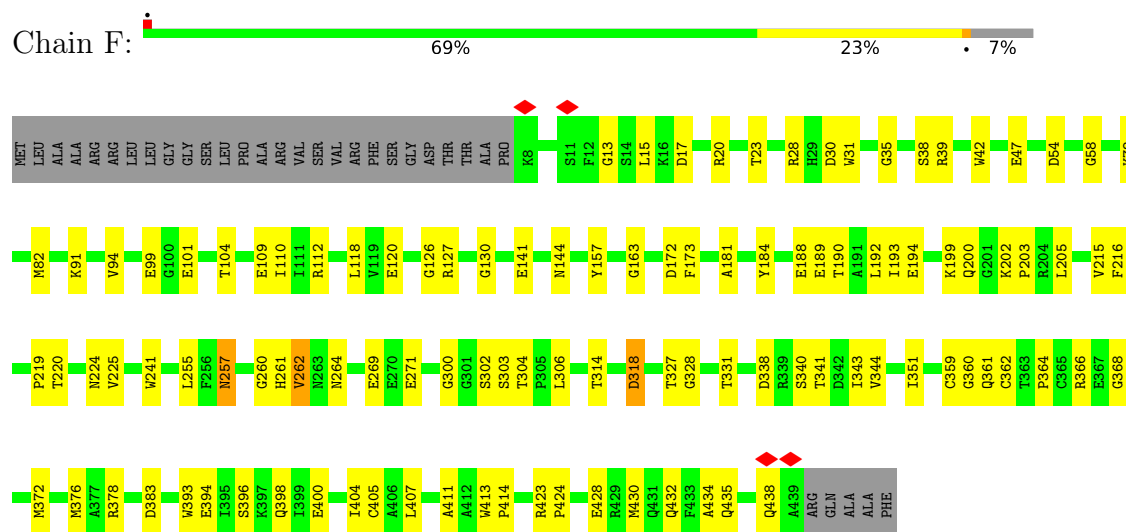
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



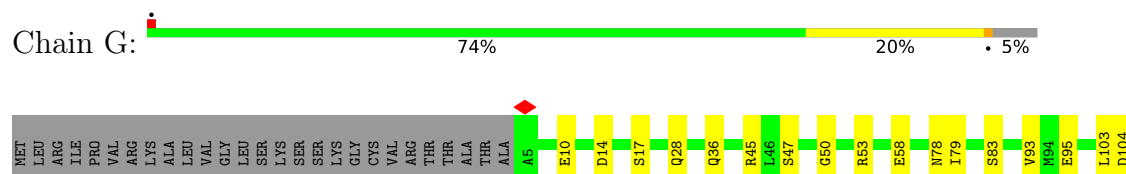
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

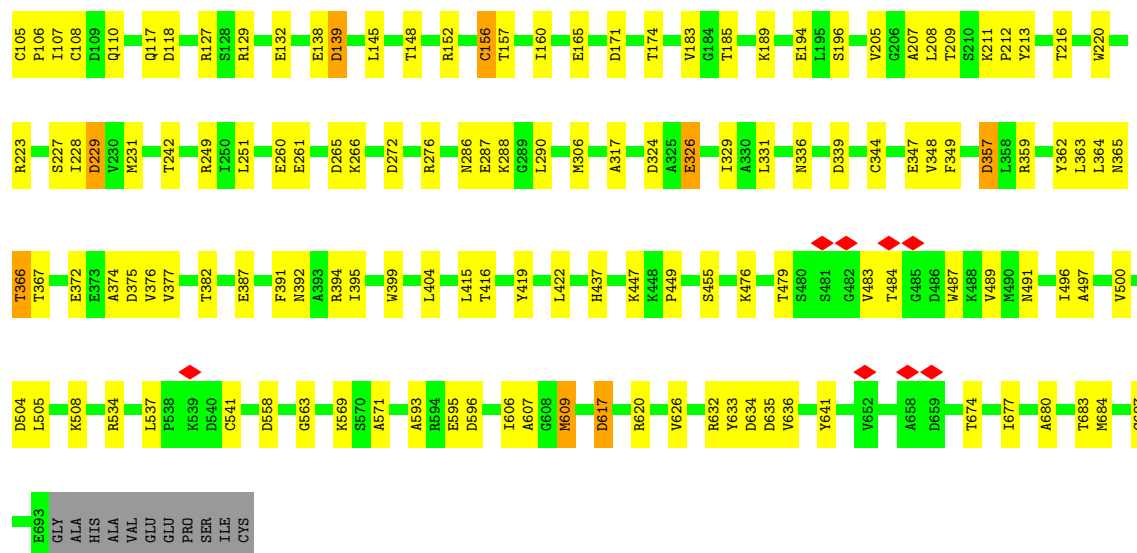


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

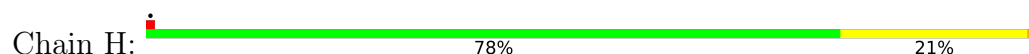


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

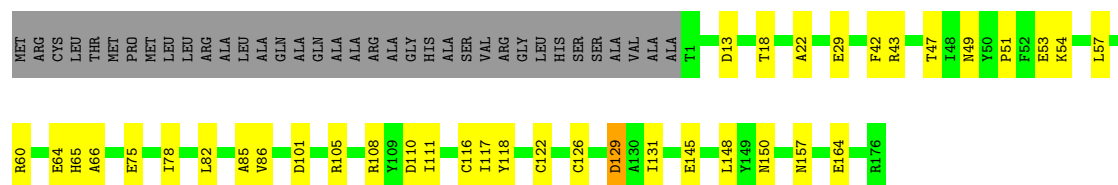




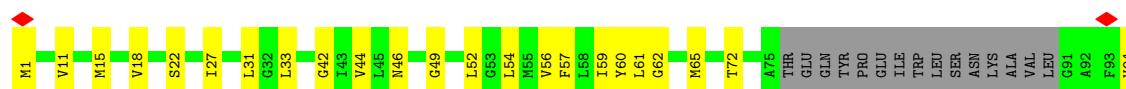
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

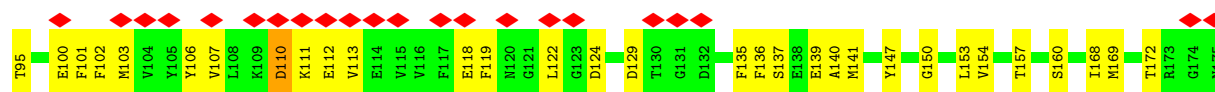


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

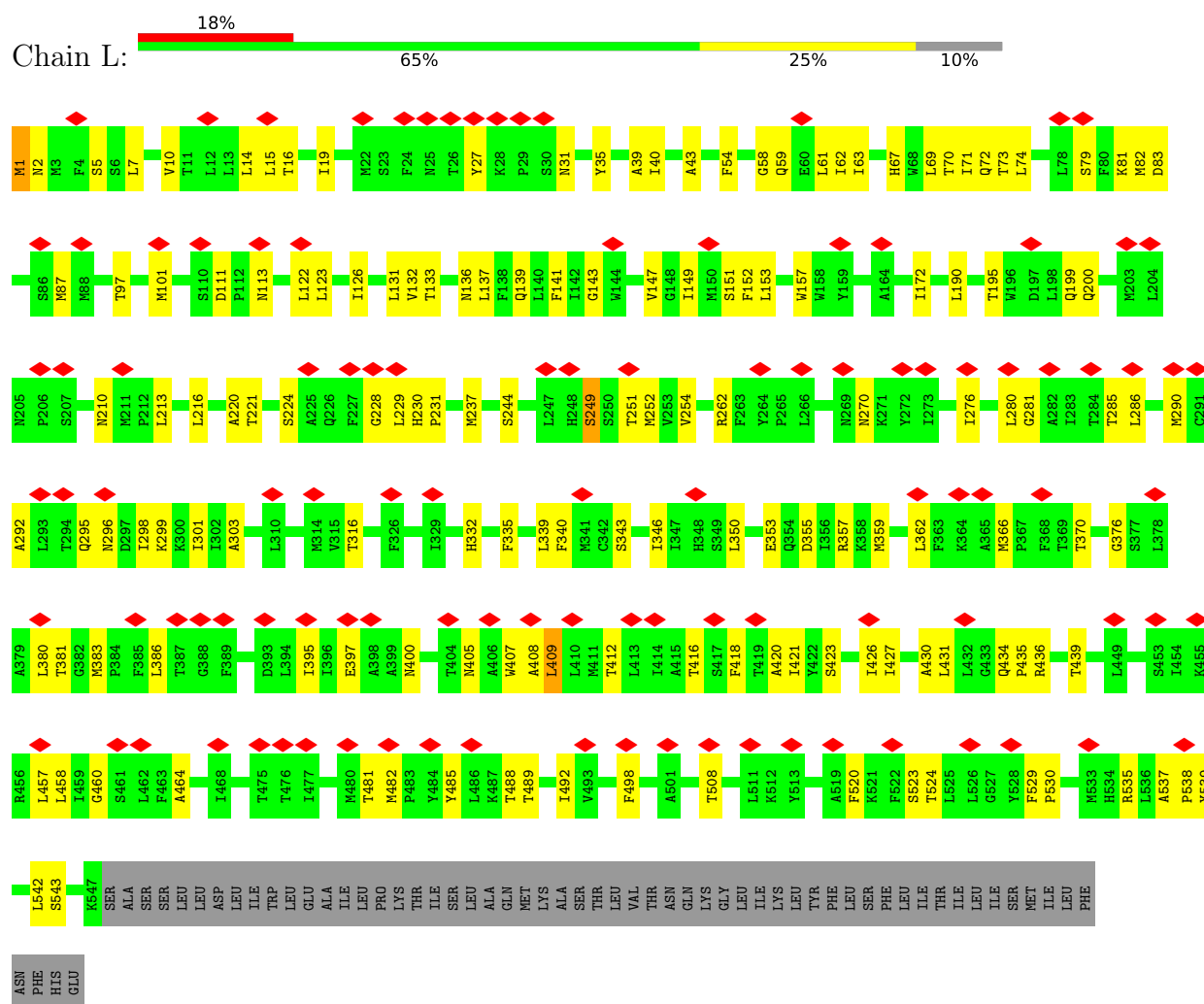




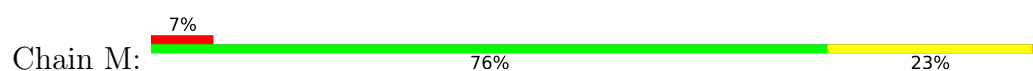
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

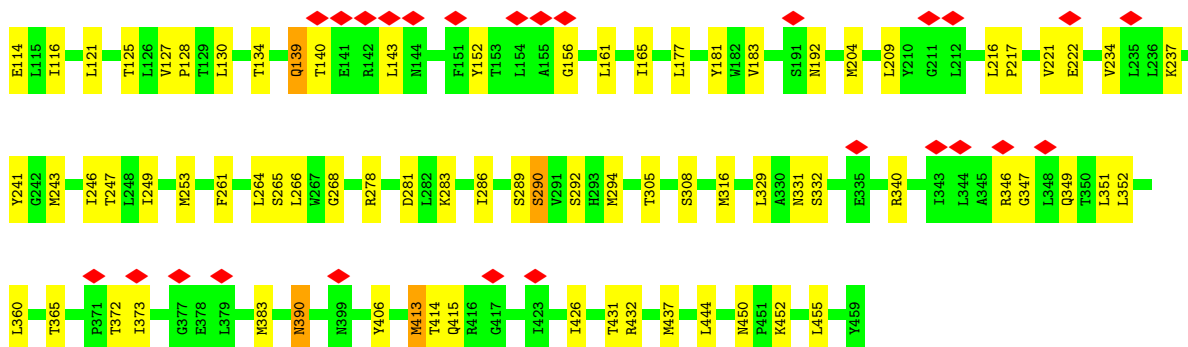


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

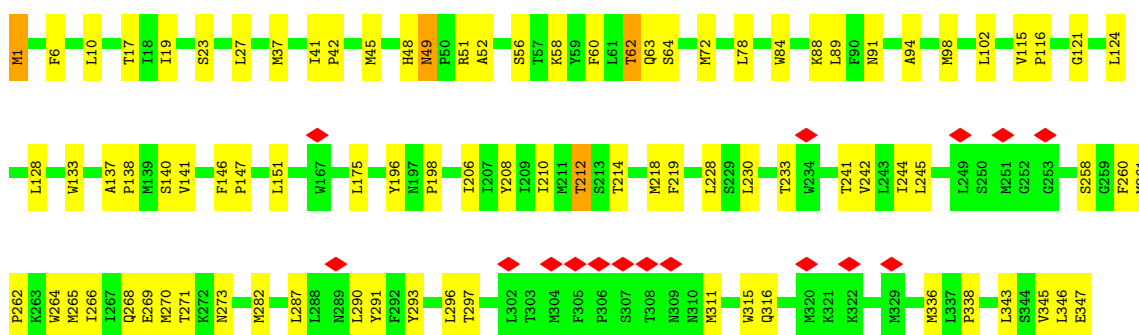
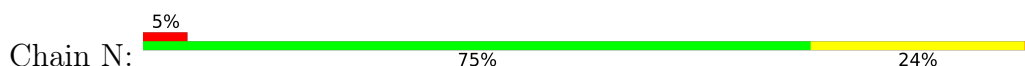


- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

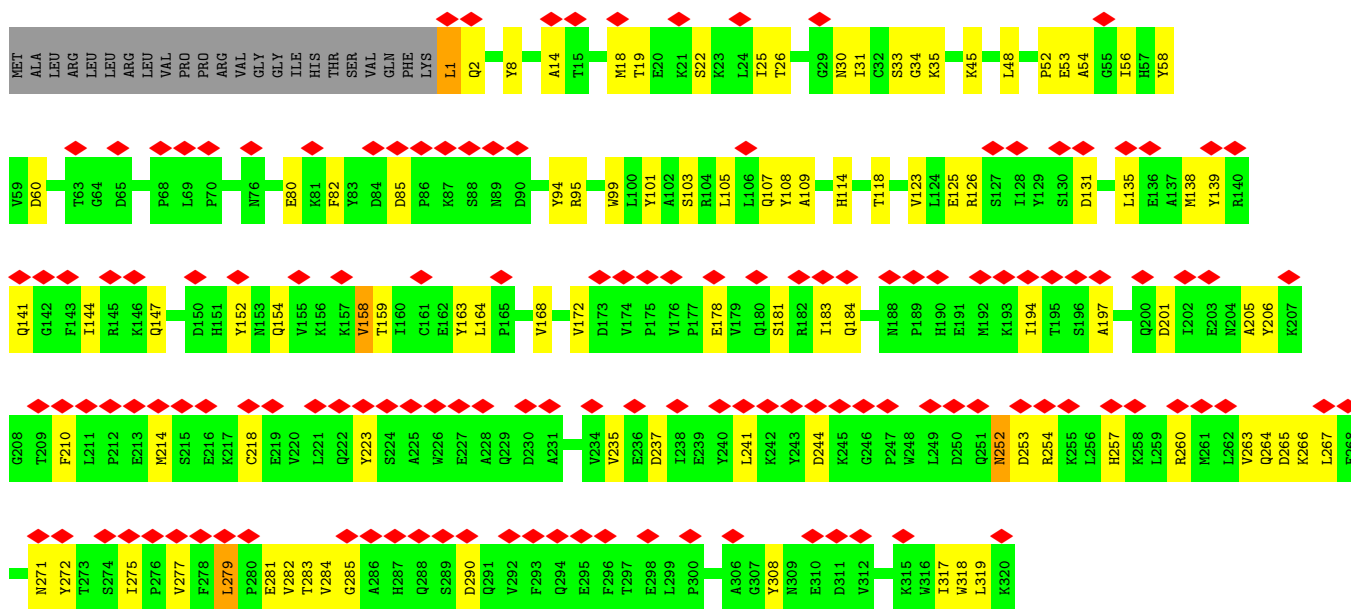
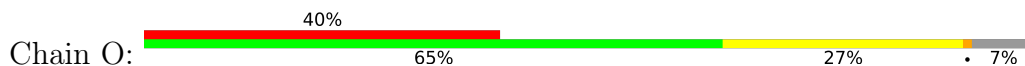




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

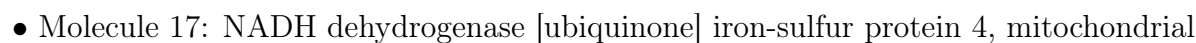


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

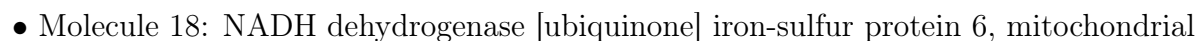


• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

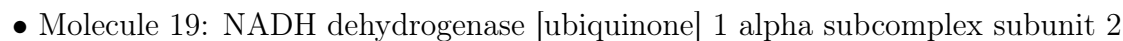
Frequency	Percentage
Daily	68%
Weekly	16%
Monthly	16%
Other	0%



Response	Percentage
Yes	57%
No	14%
Don't know	29%



Response	Percentage
Current government	9%
Opposition	67%
Don't know	10%
No answer	23%

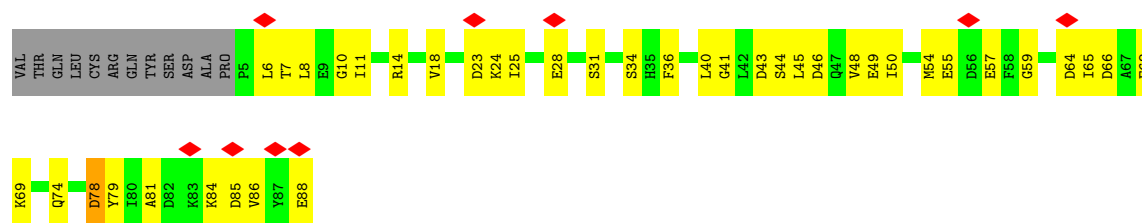


Frequency	Percentage
Daily	66%
Weekly	22%
Monthly	12%

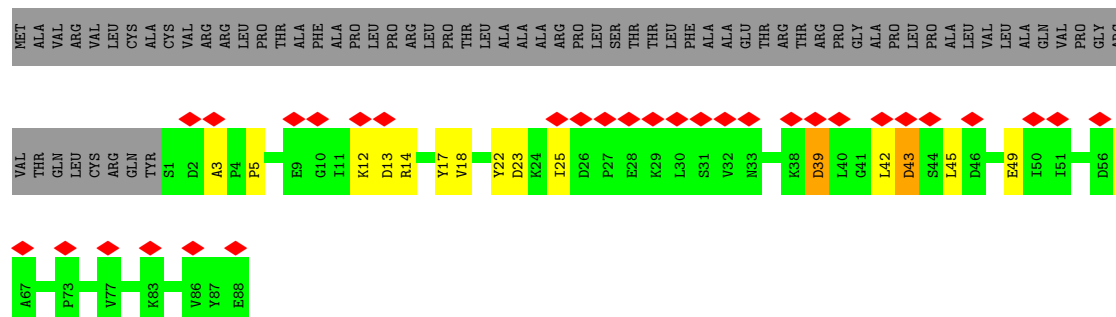


Frequency	Percentage
Very often	6%
Often	28%
Sometimes	25%
Never	46%

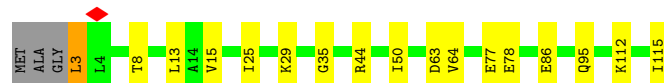
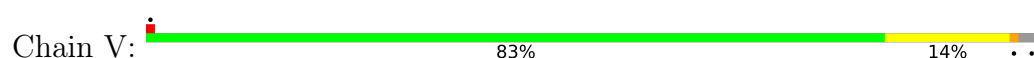




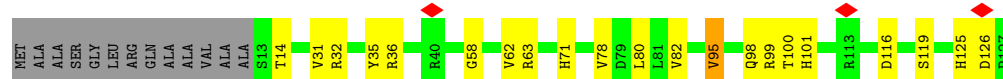
- Molecule 20: Acyl carrier protein, mitochondrial



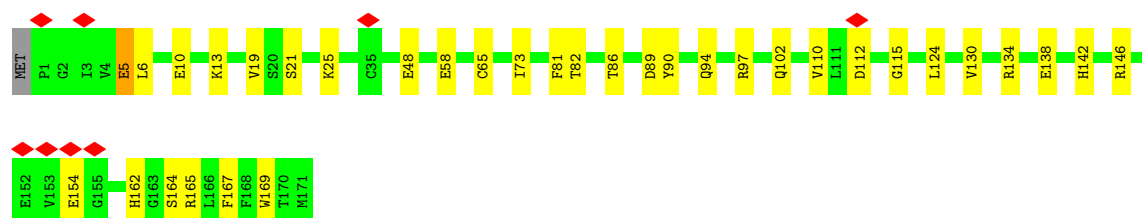
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



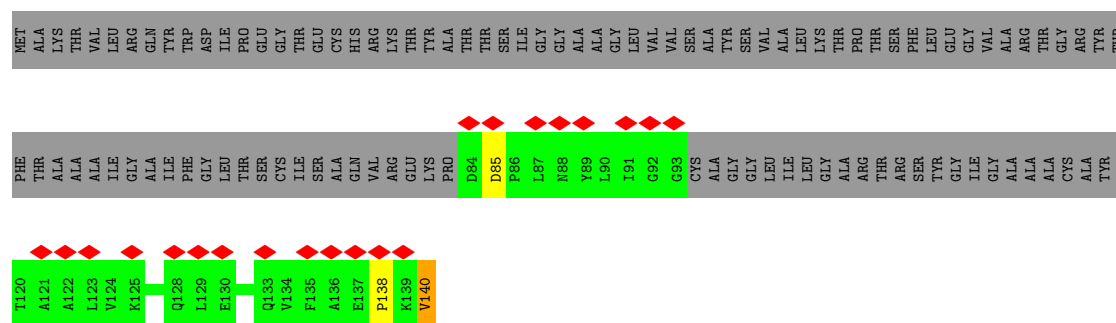
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



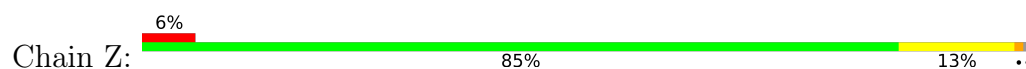
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



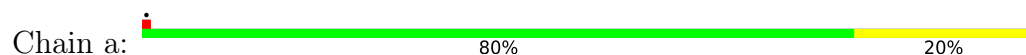
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



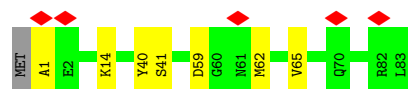
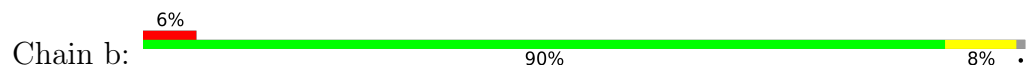
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



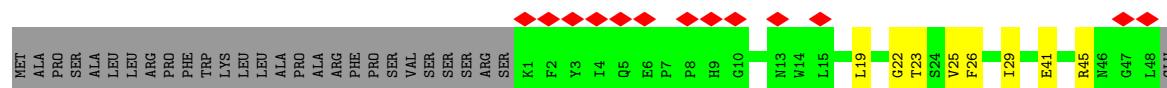
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



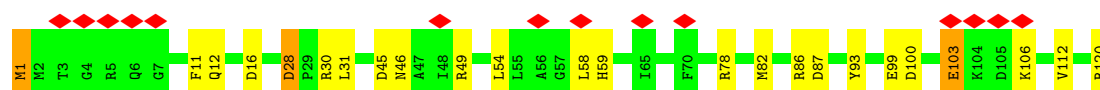
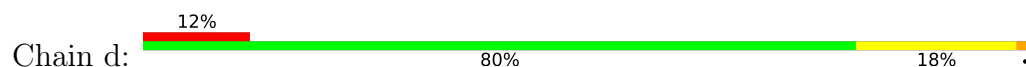
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



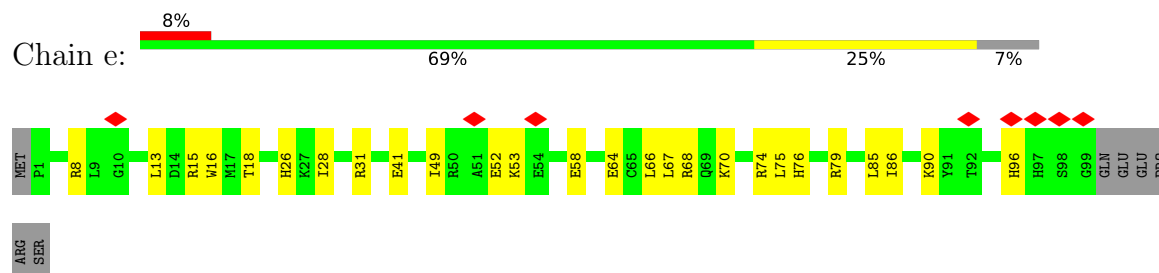
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



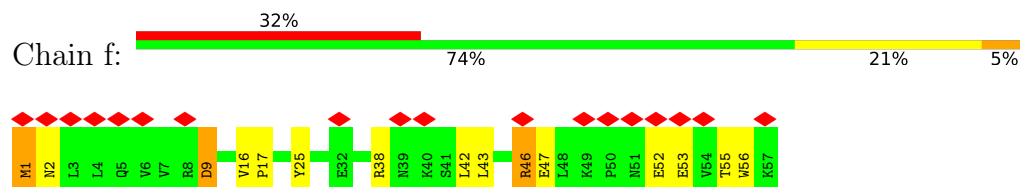
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



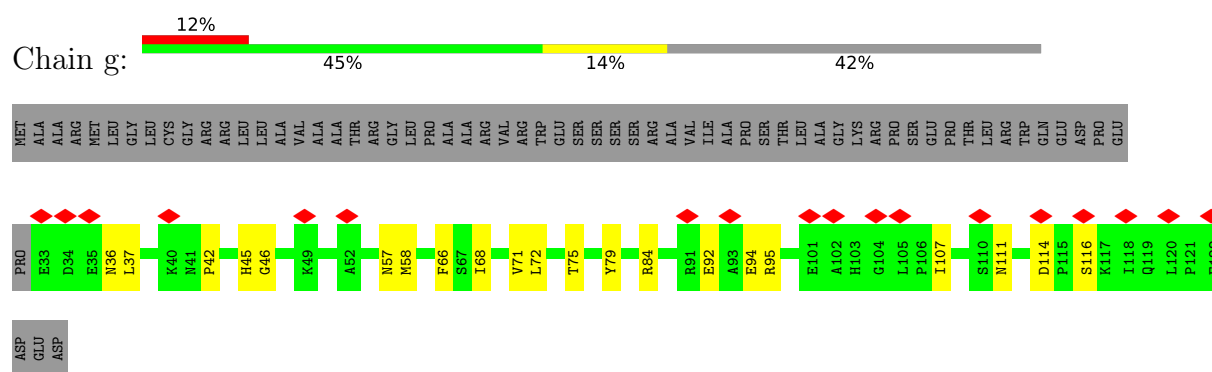
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



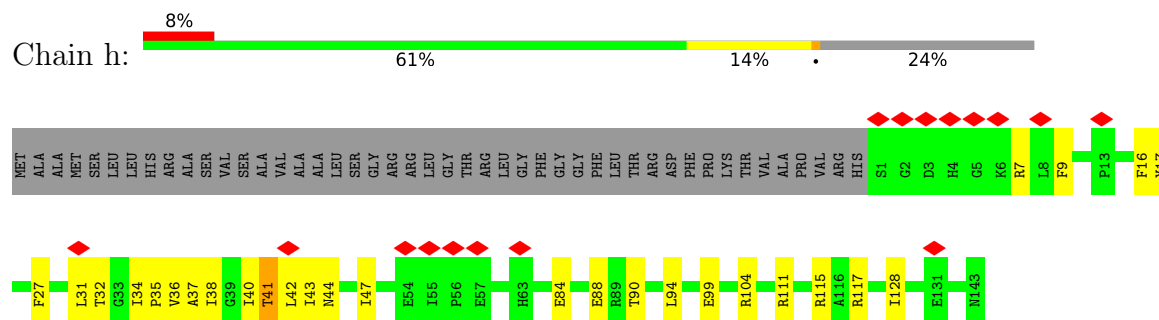
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



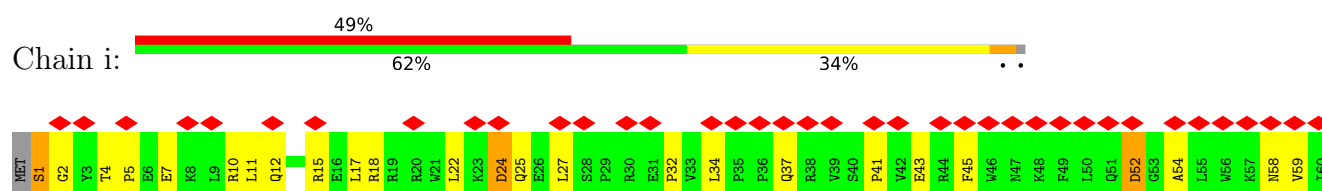
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

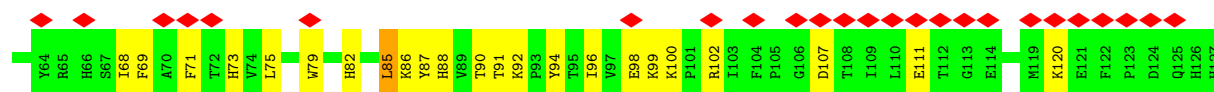


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

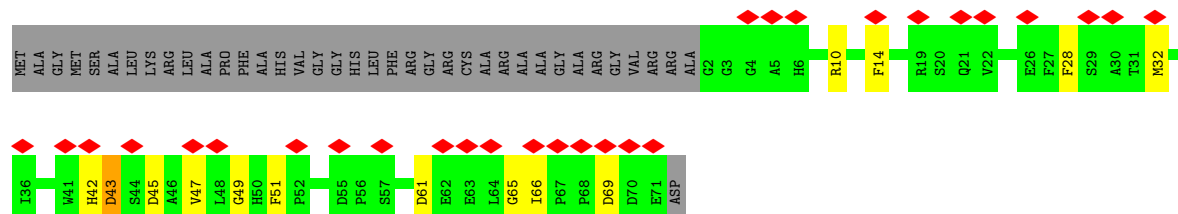


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

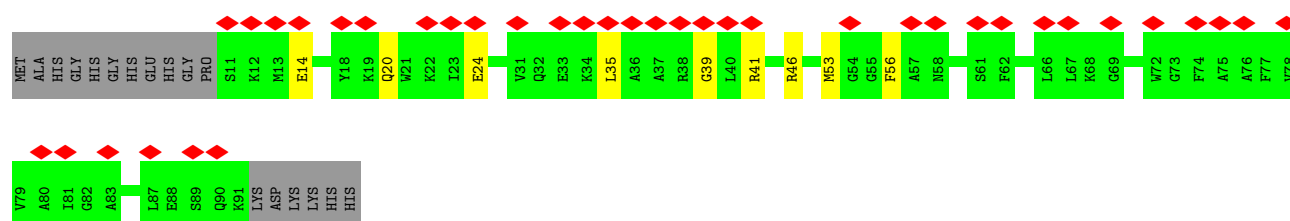
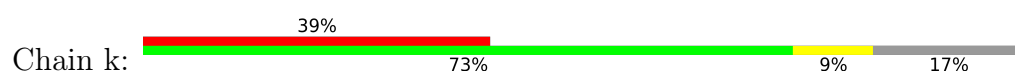




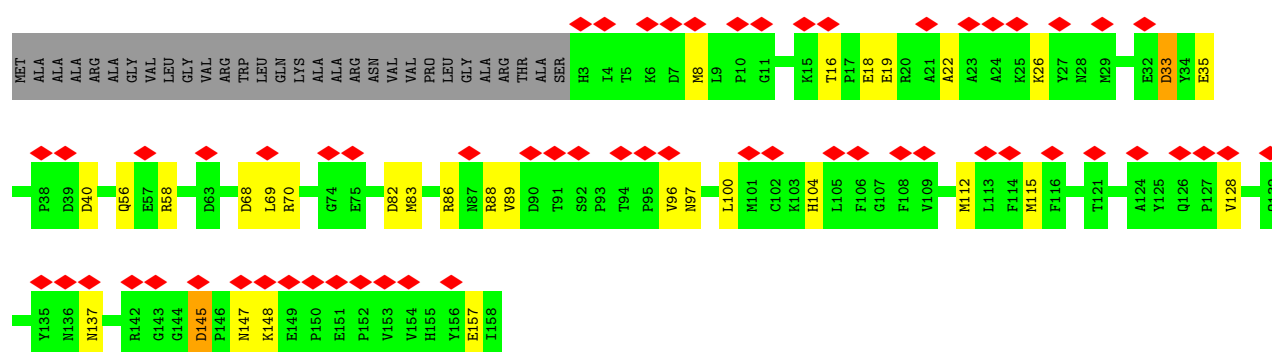
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



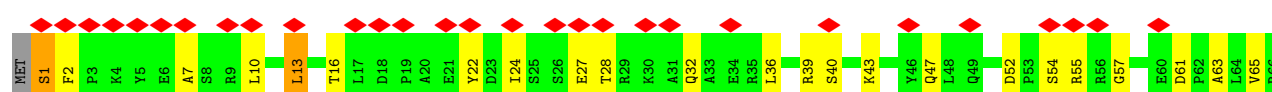
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

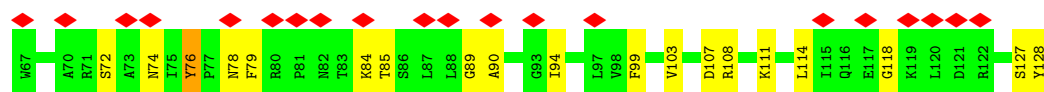


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

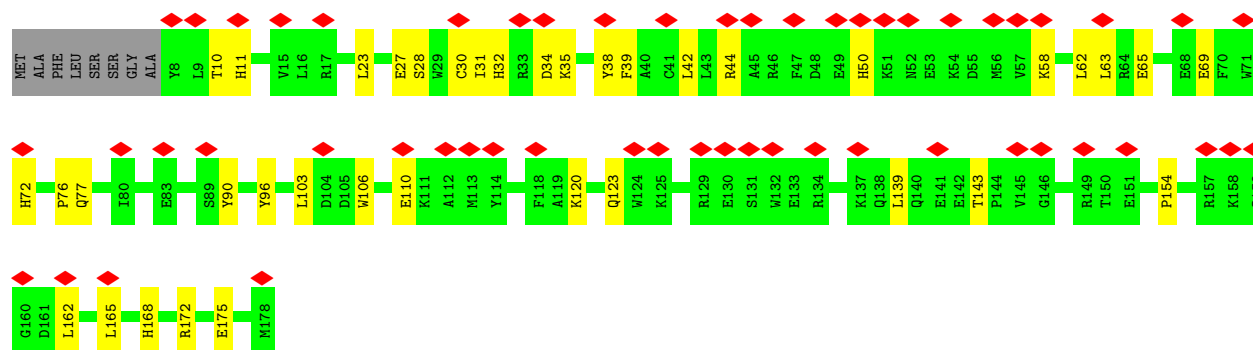
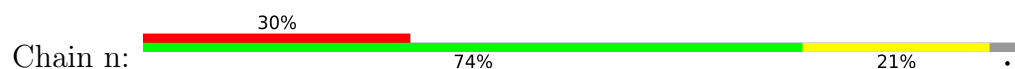


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

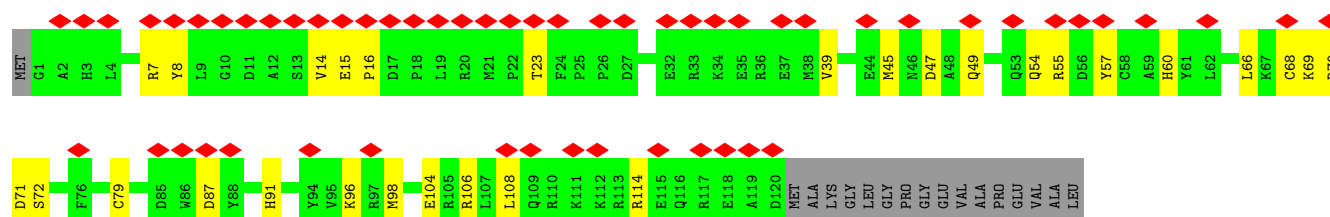
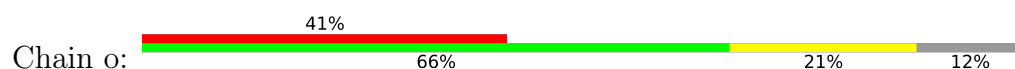




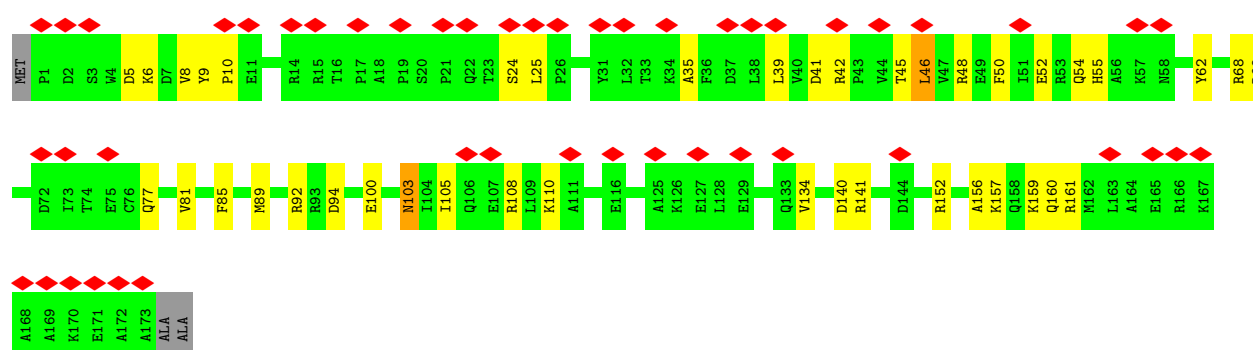
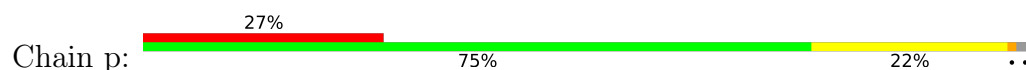
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



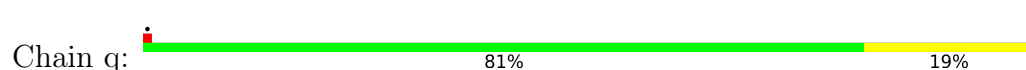
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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



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

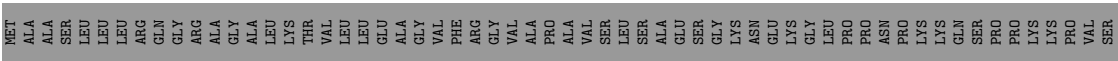




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45661	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	0.120	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, SAC, AYA, AME, 2MR, MG, FME, CHD, CDL, PC1, SF4, EHZ, DGT, MYR, FES, ZN, 3PE, K, FMN

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	0.18	0/854	0.25	0/1170
2	B	0.25	0/1292	0.29	0/1747
3	C	0.22	0/1794	0.26	0/2443
4	D	0.24	0/3170	0.28	0/4285
5	E	0.16	0/1699	0.28	0/2312
6	F	0.17	0/3398	0.25	0/4591
7	G	0.20	0/5372	0.27	0/7281
8	H	0.21	0/2571	0.28	0/3513
9	I	0.26	0/1445	0.29	0/1956
10	J	0.18	0/1239	0.26	0/1677
11	K	0.18	0/646	0.25	0/872
12	L	0.13	0/4443	0.26	0/6047
13	M	0.15	0/3738	0.24	0/5097
14	N	0.17	0/2792	0.26	0/3800
15	O	0.11	0/2651	0.24	0/3587
16	P	0.17	0/2626	0.25	0/3557
17	Q	0.21	0/1039	0.25	0/1404
18	R	0.20	0/753	0.25	0/1014
19	S	0.14	0/712	0.25	0/957
20	T	0.13	0/692	0.26	0/932
20	U	0.12	0/719	0.23	0/971
21	V	0.17	0/939	0.22	0/1272
22	W	0.18	0/1001	0.25	0/1345
23	X	0.17	0/1439	0.26	0/1942
24	Y	0.11	0/252	0.22	0/340
25	Z	0.17	0/1186	0.24	0/1599
26	a	0.20	0/584	0.26	0/786
27	b	0.16	0/667	0.25	0/916
28	c	0.15	0/418	0.22	0/567
29	d	0.15	0/1018	0.24	0/1375
30	e	0.15	0/850	0.28	0/1136

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	f	0.14	0/505	0.27	0/681
32	g	0.13	0/772	0.26	0/1046
33	h	0.15	0/1221	0.25	0/1651
34	i	0.13	0/1127	0.26	0/1534
35	j	0.11	0/619	0.25	0/848
36	k	0.10	0/672	0.22	0/906
37	l	0.11	0/1369	0.25	0/1873
38	m	0.12	0/1088	0.25	0/1472
39	n	0.11	0/1540	0.24	0/2085
40	o	0.11	0/1060	0.23	0/1420
41	p	0.11	0/1489	0.23	0/2008
42	q	0.21	0/1242	0.24	0/1688
43	r	0.19	0/798	0.25	0/1079
44	s	0.13	0/392	0.23	0/531
All	All	0.17	0/65893	0.26	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	15	0
2	B	1260	0	1269	23	0
3	C	1743	0	1690	35	0
4	D	3110	0	3089	56	0
5	E	1659	0	1664	38	0
6	F	3324	0	3279	79	0
7	G	5284	0	5306	110	0
8	H	2509	0	2621	51	0
9	I	1414	0	1370	32	0
10	J	1219	0	1227	38	0
11	K	647	0	690	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	4334	0	4451	104	0
13	M	3654	0	3852	70	0
14	N	2733	0	2912	60	0
15	O	2589	0	2565	64	0
16	P	2560	0	2581	40	0
17	Q	1016	0	1014	18	0
18	R	740	0	714	6	0
19	S	701	0	717	18	0
20	T	681	0	677	29	0
20	U	707	0	700	13	0
21	V	919	0	961	12	0
22	W	977	0	994	19	0
23	X	1402	0	1379	29	0
24	Y	248	0	247	3	0
25	Z	1157	0	1156	15	0
26	a	569	0	568	13	0
27	b	654	0	663	3	0
28	c	405	0	409	4	0
29	d	999	0	988	23	0
30	e	829	0	829	17	0
31	f	492	0	501	10	0
32	g	750	0	711	18	0
33	h	1186	0	1193	28	0
34	i	1097	0	1108	38	0
35	j	592	0	528	9	0
36	k	653	0	639	7	0
37	l	1314	0	1210	21	0
38	m	1070	0	1068	26	0
39	n	1487	0	1433	30	0
40	o	1035	0	1002	23	0
41	p	1455	0	1430	29	0
42	q	1212	0	1183	21	0
43	r	785	0	795	12	0
44	s	380	0	349	8	0
45	A	43	0	63	1	0
45	D	51	0	82	1	0
45	I	33	0	40	1	0
45	J	39	0	52	0	0
45	M	38	0	50	1	0
45	N	35	0	44	1	0
45	Y	39	0	55	0	0
45	Z	49	0	75	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	d	49	0	75	0	0
45	h	32	0	38	0	0
46	A	50	0	77	0	0
46	B	51	0	79	2	0
46	H	80	0	111	4	0
46	d	33	0	40	1	0
47	B	8	0	0	1	0
47	F	8	0	0	1	0
47	G	16	0	0	2	0
47	I	16	0	0	1	0
48	E	4	0	0	1	0
48	G	4	0	0	0	0
49	F	31	0	19	3	0
50	G	1	0	0	0	0
51	N	73	0	90	0	0
51	X	79	0	105	0	0
51	d	65	0	77	0	0
51	q	60	0	64	2	0
52	O	31	0	12	3	0
53	O	1	0	0	0	0
54	P	48	0	25	1	0
55	R	1	0	0	0	0
56	T	37	0	0	2	0
56	U	37	0	0	3	0
57	i	29	0	38	5	0
58	o	15	0	27	0	0
All	All	65579	0	65952	1141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1141) 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)
2:B:55:CYS:N	47:B:201:SF4:S1	2.40	0.95
4:D:139:VAL:HG21	4:D:277:VAL:HG22	1.50	0.93
9:I:108:ARG:NH1	9:I:110:ASP:OD2	2.01	0.93
7:G:362:TYR:OH	7:G:504:ASP:OD1	1.87	0.91
38:m:52:ASP:OD2	38:m:54:SER:OG	1.88	0.91
6:F:338:ASP:OD2	6:F:340:SER:OG	1.91	0.89
2:B:115:SER:OG	2:B:121:ASN:OD1	1.89	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:195:THR:OG1	12:L:200:GLN:OE1	1.91	0.88
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.06	0.88
4:D:151:ILE:O	4:D:155:THR:OG1	1.90	0.88
15:O:52:PRO:O	15:O:107:GLN:NE2	2.07	0.87
6:F:78:LYS:NZ	49:F:502:FMN:O3P	2.08	0.86
12:L:290:MET:O	12:L:523:SER:OG	1.94	0.86
19:S:61:GLN:OE1	19:S:79:ASN:ND2	2.09	0.85
17:Q:28:GLU:O	17:Q:32:THR:OG1	1.93	0.85
41:p:140:ASP:O	41:p:157:LYS:NZ	2.10	0.85
7:G:287:GLU:OE2	7:G:288:LYS:NZ	2.11	0.84
16:P:27:THR:OG1	54:P:501:NDP:O3B	1.94	0.84
16:P:220:ASP:OD2	16:P:223:ALA:N	2.11	0.84
13:M:35:SER:O	13:M:38:SER:OG	1.94	0.84
5:E:98:TYR:N	5:E:136:LEU:O	2.11	0.83
6:F:94:VAL:HG23	6:F:220:THR:HG21	1.60	0.83
7:G:347:GLU:OE2	7:G:455:SER:OG	1.96	0.83
4:D:69:SER:OG	4:D:74:ARG:NE	2.11	0.83
7:G:382:THR:OG1	7:G:387:GLU:OE1	1.96	0.83
23:X:146:ARG:NH2	30:e:41:GLU:OE1	2.11	0.83
7:G:45:ARG:NH1	7:G:260:GLU:OE1	2.12	0.83
32:g:111:ASN:OD1	41:p:161:ARG:NH2	2.12	0.82
8:H:266:LEU:O	8:H:269:SER:OG	1.96	0.82
10:J:153:LEU:O	10:J:157:THR:OG1	1.96	0.82
12:L:59:GLN:NE2	34:i:98:GLU:OE1	2.12	0.82
29:d:120:ARG:O	38:m:108:ARG:NH2	2.12	0.82
8:H:107:ALA:O	8:H:110:SER:OG	1.97	0.82
14:N:19:ILE:O	14:N:23:SER:OG	1.96	0.82
15:O:201:ASP:O	15:O:205:ALA:N	2.13	0.82
34:i:107:ASP:OD2	40:o:70:ARG:NH2	2.13	0.82
7:G:326:GLU:N	7:G:326:GLU:OE1	2.12	0.82
12:L:370:THR:HG23	12:L:431:LEU:HD13	1.61	0.82
4:D:176:LYS:NZ	43:r:24:GLN:O	2.13	0.82
6:F:338:ASP:OD1	6:F:341:THR:OG1	1.98	0.82
37:l:157:GLU:OE1	40:o:96:LYS:NZ	2.12	0.82
20:U:49:GLU:OE2	39:n:44:ARG:NH1	2.13	0.81
20:T:14:ARG:NH2	20:T:57:GLU:O	2.12	0.81
14:N:88:LYS:NZ	30:e:52:GLU:OE2	2.13	0.81
15:O:95:ARG:NH1	15:O:281:GLU:O	2.13	0.81
38:m:72:SER:O	38:m:76:TYR:OH	1.98	0.81
8:H:170:GLU:OE1	23:X:97:ARG:NH2	2.13	0.81
16:P:76:ARG:NH2	16:P:103:ASN:O	2.13	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:289:SER:O	13:M:292:SER:OG	1.99	0.80
15:O:114:HIS:O	15:O:118:THR:OG1	1.99	0.80
6:F:141:GLU:OE1	6:F:141:GLU:N	2.13	0.80
9:I:150:ASN:OD1	42:q:124:TYR:OH	1.99	0.80
7:G:103:LEU:O	18:R:86:TYR:OH	1.98	0.80
7:G:194:GLU:N	7:G:194:GLU:OE1	2.15	0.79
7:G:287:GLU:OE1	7:G:287:GLU:N	2.14	0.79
7:G:10:GLU:OE2	7:G:17:SER:OG	2.01	0.79
23:X:25:LYS:NZ	23:X:94:GLN:O	2.13	0.79
20:T:6:LEU:HD22	20:T:86:VAL:HG12	1.63	0.78
37:l:18:GLU:N	37:l:18:GLU:OE1	2.16	0.78
7:G:117:GLN:NE2	47:G:803:SF4:S3	2.56	0.78
12:L:434:GLN:NE2	36:k:56:PHE:O	2.16	0.78
15:O:168:VAL:HG21	15:O:241:LEU:HD13	1.65	0.78
11:K:50:ASN:O	30:e:31:ARG:NH2	2.15	0.78
15:O:264:GLN:O	15:O:266:LYS:NZ	2.16	0.78
14:N:269:GLU:O	14:N:273:ASN:ND2	2.16	0.78
44:s:71:GLU:OE1	44:s:71:GLU:N	2.16	0.78
36:k:14:GLU:N	36:k:14:GLU:OE1	2.15	0.78
15:O:131:ASP:OD1	15:O:152:TYR:OH	2.01	0.78
2:B:129:SER:OG	4:D:85:2MR:O	2.00	0.78
5:E:6:LEU:O	5:E:92:ARG:NH2	2.16	0.78
5:E:82:GLU:OE2	7:G:174:THR:N	2.16	0.78
15:O:267:LEU:O	15:O:271:ASN:N	2.17	0.78
17:Q:90:GLU:OE1	17:Q:90:GLU:N	2.17	0.78
3:C:191:ALA:O	17:Q:74:SER:OG	2.02	0.77
8:H:169:GLN:NE2	8:H:241:LEU:O	2.17	0.77
29:d:103:GLU:OE1	29:d:103:GLU:N	2.18	0.77
4:D:335:ARG:NH2	9:I:126:CYS:O	2.18	0.77
13:M:237:LYS:NZ	13:M:316:MET:O	2.18	0.77
4:D:326:ASP:OD1	7:G:127:ARG:NH2	2.17	0.77
41:p:42:ARG:O	41:p:46:LEU:N	2.18	0.77
7:G:489:VAL:O	7:G:491:ASN:ND2	2.18	0.77
26:a:40:HIS:N	26:a:44:GLN:OE1	2.18	0.77
28:c:41:GLU:OE2	28:c:45:ARG:NE	2.19	0.76
42:q:78:ASP:OD2	42:q:80:SER:OG	2.04	0.76
19:S:44:LYS:NZ	19:S:50:LEU:O	2.16	0.76
9:I:29:GLU:N	9:I:29:GLU:OE1	2.19	0.76
44:s:70:ARG:NH1	44:s:75:HIS:O	2.18	0.76
5:E:194:GLU:N	5:E:194:GLU:OE1	2.17	0.76
34:i:99:LYS:NZ	40:o:49:GLN:OE1	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:256:THR:O	8:H:260:THR:OG1	2.03	0.76
10:J:22:SER:O	11:K:22:TYR:OH	2.03	0.76
12:L:31:ASN:ND2	57:i:201:CHD:H62	2.01	0.76
12:L:485:TYR:O	12:L:489:THR:N	2.19	0.76
13:M:51:ASN:OD1	33:h:90:THR:OG1	2.01	0.76
15:O:214:MET:O	15:O:218:CYS:N	2.19	0.76
14:N:208:TYR:O	14:N:212:THR:OG1	2.02	0.76
15:O:319:LEU:O	29:d:59:HIS:ND1	2.17	0.75
16:P:311:GLU:OE1	16:P:311:GLU:N	2.18	0.75
25:Z:20:TYR:OH	43:r:108:ASP:OD2	2.04	0.75
12:L:383:MET:HB3	12:L:386:LEU:HD12	1.69	0.75
39:n:58:LYS:O	39:n:62:LEU:N	2.19	0.75
4:D:348:HIS:O	4:D:348:HIS:ND1	2.18	0.75
14:N:51:ARG:NH2	14:N:121:GLY:O	2.19	0.75
12:L:35:TYR:OH	34:i:73:HIS:NE2	2.19	0.75
18:R:81:THR:OG1	18:R:90:GLN:OE1	2.03	0.75
10:J:18:VAL:O	10:J:22:SER:OG	2.02	0.75
31:f:56:TRP:NE1	33:h:88:GLU:OE1	2.19	0.75
7:G:372:GLU:OE2	7:G:394:ARG:NH1	2.21	0.74
12:L:147:VAL:O	12:L:151:SER:OG	2.05	0.74
20:T:46:ASP:OD1	22:W:63:ARG:NH2	2.20	0.74
7:G:534:ARG:NH2	7:G:558:ASP:OD1	2.20	0.74
21:V:112:LYS:NZ	21:V:115:ILE:O	2.20	0.74
5:E:112:ASN:OD1	5:E:115:SER:OG	2.00	0.74
34:i:86:LYS:O	34:i:90:THR:OG1	2.06	0.74
39:n:11:HIS:ND1	39:n:63:LEU:HD22	2.02	0.74
5:E:196:ALA:N	6:F:264:ASN:OD1	2.21	0.74
34:i:12:GLN:OE1	34:i:15:ARG:NH2	2.20	0.74
40:o:70:ARG:NH1	40:o:71:ASP:OD1	2.20	0.74
7:G:339:ASP:OD1	19:S:16:ARG:NH2	2.19	0.74
12:L:542:LEU:O	13:M:278:ARG:NH1	2.20	0.74
7:G:569:LYS:NZ	7:G:596:ASP:OD2	2.21	0.73
8:H:287:HIS:O	8:H:292:ASN:ND2	2.20	0.73
16:P:301:GLU:N	16:P:301:GLU:OE1	2.19	0.73
6:F:224:ASN:ND2	49:F:502:FMN:O2	2.21	0.73
12:L:111:ASP:OD2	39:n:96:TYR:OH	2.06	0.73
29:d:28:ASP:OD1	29:d:30:ARG:N	2.20	0.73
5:E:132:THR:OG1	5:E:134:ASP:OD1	2.01	0.73
33:h:37:ALA:O	33:h:41:THR:OG1	2.06	0.73
41:p:105:ILE:HG13	41:p:134:VAL:HG21	1.71	0.73
5:E:27:ASN:ND2	5:E:57:GLN:OE1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:102:VAL:HG13	8:H:150:LEU:HD21	1.68	0.73
9:I:108:ARG:NH2	17:Q:70:MET:O	2.22	0.73
16:P:299:GLY:N	16:P:302:ASP:OD2	2.22	0.73
16:P:22:THR:HG1	16:P:88:SER:HG	1.30	0.73
7:G:365:ASN:N	7:G:491:ASN:OD1	2.22	0.73
14:N:91:ASN:OD1	14:N:94:ALA:N	2.22	0.72
7:G:364:LEU:HD12	7:G:491:ASN:HB3	1.71	0.72
30:e:64:GLU:OE2	30:e:70:LYS:N	2.22	0.72
34:i:1:SAC:OG	34:i:2:GLY:N	2.20	0.72
39:n:139:LEU:O	39:n:143:THR:OG1	2.05	0.72
2:B:34:ASP:OD1	2:B:38:ASN:ND2	2.22	0.72
5:E:30:ARG:NH1	44:s:53:ASP:OD1	2.22	0.72
10:J:94:VAL:O	10:J:95:THR:OG1	2.05	0.72
19:S:24:GLN:OE1	19:S:24:GLN:N	2.21	0.72
10:J:42:GLY:O	10:J:46:ASN:ND2	2.23	0.72
14:N:52:ALA:O	14:N:56:SER:OG	2.01	0.72
23:X:102:GLN:N	23:X:102:GLN:OE1	2.22	0.72
37:l:100:LEU:O	37:l:104:HIS:N	2.22	0.72
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.18	0.72
41:p:35:ALA:HB1	41:p:39:LEU:HD12	1.71	0.72
5:E:111:ARG:NH1	6:F:260:GLY:O	2.22	0.72
13:M:347:GLY:N	13:M:414:THR:O	2.22	0.72
30:e:58:GLU:N	30:e:58:GLU:OE1	2.23	0.72
6:F:17:ASP:OD1	6:F:20:ARG:NH1	2.22	0.71
34:i:87:TYR:O	34:i:91:THR:OG1	2.03	0.71
14:N:58:LYS:O	14:N:62:THR:OG1	2.08	0.71
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.23	0.71
3:C:41:GLN:NE2	3:C:49:GLU:OE1	2.23	0.71
29:d:99:GLU:OE1	29:d:99:GLU:N	2.22	0.71
23:X:58:GLU:N	23:X:58:GLU:OE1	2.24	0.71
1:A:71:LEU:O	10:J:147:TYR:OH	2.09	0.71
7:G:366:THR:O	7:G:367:THR:OG1	2.09	0.70
38:m:84:LYS:NZ	38:m:84:LYS:O	2.24	0.70
15:O:80:GLU:N	15:O:80:GLU:OE1	2.24	0.70
12:L:132:VAL:O	12:L:262:ARG:NH2	2.25	0.70
39:n:23:LEU:O	39:n:27:GLU:N	2.25	0.70
9:I:57:LEU:HD12	42:q:93:MET:HE2	1.73	0.70
7:G:45:ARG:NE	7:G:261:GLU:OE2	2.22	0.70
14:N:137:ALA:O	14:N:140:SER:OG	2.10	0.70
13:M:181:TYR:O	41:p:152:ARG:NH1	2.25	0.70
16:P:162:GLU:OE1	16:P:162:GLU:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:145:THR:HG1	4:D:181:TYR:HH	1.39	0.69
4:D:223:ASP:OD1	4:D:305:ARG:NH2	2.25	0.69
12:L:199:GLN:NE2	41:p:110:LYS:O	2.25	0.69
16:P:237:LEU:HB2	16:P:340:ILE:HD12	1.74	0.69
34:i:18:ARG:NH2	39:n:172:ARG:O	2.25	0.69
12:L:71:ILE:O	12:L:73:THR:N	2.25	0.69
12:L:508:THR:O	39:n:35:LYS:NZ	2.24	0.69
34:i:58:ASN:OD1	34:i:59:VAL:N	2.25	0.69
7:G:58:GLU:OE1	7:G:83:SER:OG	2.06	0.69
23:X:110:VAL:O	23:X:115:GLY:N	2.26	0.69
15:O:126:ARG:NH2	52:O:401:DGT:O2A	2.24	0.69
23:X:154:GLU:N	23:X:154:GLU:OE1	2.25	0.69
15:O:279:LEU:O	15:O:283:THR:OG1	2.08	0.69
3:C:54:PRO:O	3:C:57:VAL:HG23	1.93	0.68
31:f:46:ARG:NH2	31:f:52:GLU:OE1	2.26	0.68
4:D:429:ASP:N	4:D:429:ASP:OD1	2.22	0.68
6:F:188:GLU:OE1	6:F:189:GLU:N	2.25	0.68
7:G:145:LEU:HD21	7:G:687:CYS:SG	2.33	0.68
15:O:56:ILE:O	15:O:99:TRP:NE1	2.26	0.68
6:F:28:ARG:NH1	44:s:35:ASN:O	2.27	0.68
7:G:276:ARG:NH1	7:G:680:ALA:O	2.27	0.68
23:X:124:LEU:N	25:Z:65:GLU:OE2	2.27	0.68
6:F:82:MET:O	6:F:91:LYS:NZ	2.19	0.68
20:T:8:LEU:HD23	20:T:8:LEU:O	1.93	0.68
34:i:111:GLU:OE1	34:i:111:GLU:N	2.25	0.68
7:G:329:ILE:HD11	7:G:626:VAL:HG21	1.75	0.68
7:G:609:MET:SD	7:G:609:MET:N	2.67	0.68
7:G:632:ARG:NH2	19:S:58:SER:O	2.26	0.68
12:L:295:GLN:NE2	12:L:523:SER:O	2.27	0.68
20:T:28:GLU:N	20:T:28:GLU:OE1	2.25	0.68
8:H:301:CYS:O	8:H:305:VAL:HG23	1.93	0.68
16:P:10:LYS:NZ	22:W:126:ASP:OD2	2.27	0.68
23:X:10:GLU:N	23:X:10:GLU:OE1	2.27	0.68
16:P:285:GLU:O	16:P:289:THR:OG1	2.02	0.68
38:m:114:LEU:O	38:m:118:GLY:N	2.27	0.68
40:o:45:MET:O	40:o:55:ARG:NH2	2.27	0.68
7:G:317:ALA:HB1	7:G:331:LEU:HD21	1.75	0.68
7:G:374:ALA:O	7:G:404:LEU:HD13	1.94	0.67
9:I:53:GLU:OE2	42:q:34:ARG:NH2	2.27	0.67
9:I:75:GLU:O	9:I:105:ARG:NH1	2.27	0.67
16:P:133:SER:N	16:P:166:ILE:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:q:95:ASP:OD2	43:r:34:THR:N	2.26	0.67
15:O:265:ASP:OD1	15:O:266:LYS:N	2.28	0.67
15:O:252:ASN:N	15:O:252:ASN:OD1	2.26	0.67
8:H:120:GLY:O	8:H:123:SER:OG	2.06	0.67
12:L:220:ALA:O	12:L:224:SER:OG	2.12	0.67
10:J:129:ASP:OD2	11:K:52:HIS:NE2	2.28	0.67
14:N:175:LEU:HD13	14:N:219:PHE:CZ	2.28	0.67
33:h:84:GLU:N	33:h:84:GLU:OE1	2.28	0.67
20:T:36:PHE:CD1	20:T:40:LEU:HD12	2.30	0.67
12:L:137:LEU:O	12:L:141:PHE:N	2.26	0.67
15:O:147:GLN:N	15:O:147:GLN:OE1	2.28	0.67
20:T:66:ASP:OD2	20:T:79:TYR:OH	2.13	0.67
35:j:61:ASP:O	35:j:65:GLY:N	2.28	0.66
15:O:53:GLU:N	15:O:125:GLU:OE1	2.28	0.66
23:X:162:HIS:NE2	33:h:99:GLU:OE1	2.28	0.66
10:J:141:MET:HA	10:J:141:MET:HE2	1.77	0.66
20:T:45:LEU:HD11	22:W:35:TYR:CD2	2.31	0.66
37:l:22:ALA:O	37:l:26:LYS:N	2.29	0.66
38:m:107:ASP:O	38:m:111:LYS:N	2.25	0.66
40:o:57:TYR:O	40:o:60:HIS:ND1	2.28	0.66
10:J:168:ILE:O	10:J:172:THR:HG23	1.96	0.66
4:D:112:MET:HE2	4:D:193:TYR:HB3	1.78	0.66
15:O:223:TYR:OH	15:O:237:ASP:OD2	2.13	0.66
32:g:36:ASN:OD1	32:g:37:LEU:N	2.28	0.66
3:C:111:THR:OG1	3:C:112:ASP:N	2.26	0.66
4:D:261:ARG:NH2	4:D:303:GLU:OE2	2.28	0.66
7:G:118:ASP:OD2	17:Q:46:GLN:NE2	2.29	0.66
38:m:55:ARG:NH1	38:m:57:GLY:O	2.29	0.66
3:C:27:GLU:OE1	3:C:27:GLU:N	2.28	0.65
7:G:537:LEU:HD13	7:G:541:CYS:SG	2.37	0.65
2:B:71:ARG:NH1	8:H:38:ASN:OD1	2.29	0.65
14:N:347:GLU:HB2	29:d:82:MET:HE2	1.78	0.65
5:E:163:ASP:OD2	5:E:190:ARG:NH2	2.30	0.65
12:L:27:TYR:CD1	57:i:201:CHD:H151	2.31	0.65
20:T:8:LEU:N	20:T:88:GLU:OE2	2.29	0.65
6:F:42:TRP:N	6:F:120:GLU:OE1	2.28	0.65
36:k:24:GLU:OE1	36:k:24:GLU:N	2.30	0.65
6:F:35:GLY:O	6:F:38:SER:OG	2.08	0.65
6:F:205:LEU:HD11	6:F:404:ILE:HD13	1.79	0.65
16:P:134:HIS:O	16:P:167:LYS:NZ	2.29	0.65
22:W:58:GLY:O	22:W:62:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:LEU:N	10:J:139:GLU:OE2	2.28	0.65
7:G:375:ASP:OD1	7:G:376:VAL:N	2.30	0.64
8:H:245:THR:OG1	8:H:262:LYS:NZ	2.23	0.64
34:i:43:GLU:N	34:i:43:GLU:OE1	2.29	0.64
40:o:68:CYS:O	40:o:72:SER:OG	2.10	0.64
43:r:32:LYS:O	43:r:35:GLN:NE2	2.31	0.64
12:L:407:TRP:NE1	37:l:112:MET:SD	2.70	0.64
13:M:121:LEU:O	13:M:125:THR:HG23	1.98	0.64
7:G:377:VAL:HG23	7:G:404:LEU:HD11	1.80	0.64
12:L:31:ASN:HD21	57:i:201:CHD:H41	1.62	0.64
12:L:412:THR:O	12:L:416:THR:OG1	2.15	0.64
33:h:44:ASN:O	41:p:55:HIS:NE2	2.28	0.64
34:i:94:TYR:OH	41:p:10:PRO:O	2.14	0.64
39:n:38:TYR:CE1	39:n:42:LEU:HD11	2.33	0.64
39:n:65:GLU:O	39:n:69:GLU:N	2.31	0.64
4:D:226:GLU:OE1	25:Z:22:ARG:NE	2.31	0.64
32:g:94:GLU:OE2	41:p:9:TYR:OH	2.16	0.64
33:h:9:PHE:N	34:i:25:GLN:O	2.27	0.64
41:p:50:PHE:O	41:p:54:GLN:NE2	2.30	0.64
18:R:27:ARG:O	18:R:31:ARG:NH2	2.31	0.63
20:U:14:ARG:NH2	20:U:57:GLU:OE2	2.31	0.63
4:D:241:ASP:OD1	4:D:290:ARG:NH2	2.30	0.63
7:G:336:ASN:O	19:S:71:GLY:N	2.31	0.63
7:G:357:ASP:OD2	19:S:40:TYR:OH	2.15	0.63
12:L:54:PHE:O	12:L:58:GLY:N	2.29	0.63
31:f:9:ASP:N	31:f:9:ASP:OD1	2.30	0.63
3:C:204:GLU:OE2	3:C:210:ARG:NE	2.29	0.63
7:G:53:ARG:O	7:G:93:VAL:HG21	1.98	0.63
12:L:61:LEU:N	12:L:82:MET:O	2.31	0.63
20:T:68:GLU:OE2	22:W:32:ARG:NE	2.32	0.63
10:J:141:MET:SD	30:e:26:HIS:NE2	2.70	0.63
16:P:77:ASP:OD1	16:P:78:LYS:N	2.32	0.63
56:U:101:EHZ:O5	56:U:101:EHZ:O6	2.13	0.63
7:G:36:GLN:NE2	17:Q:47:SER:O	2.32	0.62
7:G:95:GLU:OE2	7:G:129:ARG:NE	2.28	0.62
15:O:178:GLU:O	15:O:181:SER:OG	2.15	0.62
39:n:11:HIS:CE1	39:n:63:LEU:HD22	2.33	0.62
10:J:112:GLU:OE2	30:e:76:HIS:ND1	2.31	0.62
19:S:87:THR:HG22	19:S:91:GLU:OE2	1.99	0.62
34:i:17:LEU:HD11	39:n:162:LEU:HD22	1.81	0.62
13:M:45:PHE:O	32:g:84:ARG:NH2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:43:ASP:N	20:U:43:ASP:OD1	2.32	0.62
32:g:92:GLU:OE2	32:g:95:ARG:NH2	2.31	0.62
12:L:535:ARG:NH1	38:m:10:LEU:O	2.32	0.62
6:F:372:MET:HE1	6:F:411:ALA:O	1.99	0.62
7:G:272:ASP:OD2	7:G:683:THR:OG1	2.09	0.62
31:f:55:THR:HG1	31:f:56:TRP:CD1	2.17	0.62
29:d:12:GLN:OE1	30:e:8:ARG:NH1	2.31	0.62
34:i:10:ARG:NH1	39:n:154:PRO:O	2.32	0.62
2:B:81:ARG:NH1	8:H:213:VAL:O	2.33	0.62
5:E:104:THR:O	5:E:104:THR:OG1	2.12	0.62
7:G:620:ARG:NH1	7:G:633:TYR:OH	2.33	0.62
6:F:435:GLN:O	6:F:438:GLN:NE2	2.34	0.61
7:G:227:SER:OG	7:G:228:ILE:N	2.34	0.61
6:F:318:ASP:N	6:F:318:ASP:OD1	2.34	0.61
12:L:485:TYR:O	12:L:489:THR:OG1	2.13	0.61
29:d:112:VAL:O	41:p:159:LYS:NZ	2.33	0.61
6:F:47:GLU:N	6:F:47:GLU:OE1	2.32	0.61
15:O:141:GLN:NE2	15:O:197:ALA:O	2.33	0.61
2:B:117:GLY:O	2:B:121:ASN:ND2	2.34	0.61
12:L:81:LYS:N	12:L:133:THR:O	2.33	0.61
56:U:101:EHZ:O1	39:n:50:HIS:ND1	2.33	0.61
3:C:65:ARG:NH1	3:C:123:VAL:O	2.34	0.61
37:l:137:ASN:O	37:l:137:ASN:ND2	2.34	0.61
29:d:93:TYR:OH	33:h:117:ARG:NH2	2.32	0.61
7:G:213:TYR:O	7:G:216:THR:OG1	2.13	0.61
9:I:129:ASP:N	9:I:129:ASP:OD1	2.32	0.60
10:J:59:ILE:HB	11:K:64:LEU:HD21	1.83	0.60
15:O:30:ASN:OD1	15:O:31:ILE:N	2.33	0.60
20:U:13:ASP:O	20:U:17:TYR:N	2.26	0.60
36:k:35:LEU:HD13	36:k:41:ARG:HA	1.82	0.60
16:P:122:LYS:NZ	16:P:159:THR:O	2.33	0.60
17:Q:20:THR:HG22	17:Q:99:ASN:C	2.26	0.60
23:X:142:HIS:ND1	25:Z:113:THR:OG1	2.28	0.60
31:f:46:ARG:NH1	31:f:47:GLU:O	2.34	0.60
34:i:68:ILE:HG21	57:i:201:CHD:H111	1.82	0.60
36:k:20:GLN:O	36:k:53:MET:HE1	2.02	0.60
7:G:684:MET:HA	7:G:684:MET:HE2	1.83	0.60
20:U:25:ILE:HD11	20:U:42:LEU:HD11	1.82	0.60
2:B:113:VAL:N	2:B:143:ASP:OD2	2.33	0.60
1:A:3:LEU:HD23	46:H:401:PC1:H231	1.84	0.60
14:N:78:LEU:HD22	14:N:84:TRP:CZ2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:69:ASP:O	40:o:114:ARG:NH1	2.34	0.60
38:m:16:THR:O	38:m:22:TYR:OH	2.19	0.60
23:X:19:VAL:O	26:a:50:ARG:NH1	2.35	0.60
14:N:311:MET:O	14:N:315:TRP:NE1	2.35	0.60
38:m:99:PHE:O	38:m:103:VAL:HG23	2.02	0.60
38:m:61:ASP:OD1	38:m:63:ALA:N	2.35	0.60
12:L:524:THR:HG21	39:n:76:PRO:HB2	1.83	0.59
40:o:7:ARG:NH1	40:o:8:TYR:OH	2.35	0.59
12:L:420:ALA:O	12:L:423:SER:OG	2.20	0.59
15:O:154:GLN:OE1	15:O:277:VAL:HG21	2.01	0.59
3:C:14:ARG:NH1	3:C:44:CYS:O	2.35	0.59
21:V:35:GLY:O	21:V:44:ARG:NH1	2.36	0.59
10:J:103:MET:O	10:J:107:VAL:HG23	2.02	0.59
10:J:111:LYS:O	10:J:113:VAL:HG13	2.02	0.59
20:U:39:ASP:OD1	20:U:39:ASP:N	2.35	0.59
31:f:43:LEU:O	41:p:68:ARG:NH2	2.36	0.59
9:I:65:HIS:CE1	47:I:201:SF4:S2	2.96	0.59
14:N:60:PHE:O	14:N:64:SER:OG	2.10	0.59
33:h:32:THR:O	33:h:36:VAL:HG23	2.03	0.59
3:C:102:ASN:ND2	3:C:102:ASN:O	2.35	0.58
6:F:364:PRO:O	6:F:368:GLY:N	2.35	0.58
12:L:296:ASN:N	39:n:77:GLN:OE1	2.35	0.58
17:Q:89:LYS:NZ	17:Q:107:GLU:OE1	2.32	0.58
12:L:405:ASN:OD1	12:L:408:ALA:N	2.36	0.58
14:N:287:LEU:O	14:N:291:TYR:N	2.36	0.58
16:P:115:GLN:O	16:P:118:ALA:N	2.35	0.58
9:I:145:GLU:OE1	9:I:145:GLU:N	2.34	0.58
12:L:190:LEU:HD23	13:M:383:MET:HB3	1.85	0.58
23:X:167:PHE:O	33:h:104:ARG:NH2	2.36	0.58
34:i:24:ASP:N	34:i:24:ASP:OD1	2.37	0.58
3:C:68:SER:OG	21:V:86:GLU:OE1	2.22	0.58
12:L:405:ASN:OD1	12:L:407:TRP:N	2.36	0.58
43:r:12:ASN:O	43:r:16:GLY:N	2.36	0.58
8:H:102:VAL:CG1	8:H:150:LEU:HD21	2.33	0.58
3:C:154:ASP:OD1	3:C:155:TYR:N	2.36	0.58
6:F:127:ARG:O	6:F:127:ARG:NH1	2.36	0.58
7:G:366:THR:N	7:G:491:ASN:OD1	2.36	0.58
19:S:30:GLN:OE1	19:S:33:ARG:NH2	2.37	0.58
12:L:16:THR:HG22	12:L:126:ILE:HD13	1.86	0.58
12:L:151:SER:OG	12:L:252:MET:SD	2.62	0.58
20:T:43:ASP:OD1	20:T:44:SER:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:10:ARG:NH1	35:j:14:PHE:O	2.33	0.58
35:j:28:PHE:O	35:j:32:MET:N	2.36	0.58
36:k:35:LEU:O	36:k:39:GLY:N	2.37	0.58
4:D:111:MET:SD	4:D:111:MET:N	2.75	0.58
14:N:6:PHE:CE2	14:N:10:LEU:HD11	2.39	0.58
23:X:164:SER:O	29:d:86:ARG:NH2	2.35	0.58
12:L:111:ASP:OD2	12:L:157:TRP:NE1	2.35	0.58
12:L:439:THR:OG1	20:U:57:GLU:OE2	2.19	0.58
12:L:244:SER:O	12:L:249:SER:OG	2.22	0.58
33:h:16:PHE:N	39:n:110:GLU:OE2	2.36	0.58
3:C:112:ASP:N	3:C:112:ASP:OD1	2.36	0.57
6:F:361:GLN:O	6:F:366:ARG:NH1	2.36	0.57
7:G:635:ASP:OD1	7:G:636:VAL:N	2.36	0.57
10:J:124:ASP:OD2	11:K:4:VAL:HG21	2.04	0.57
7:G:449:PRO:O	7:G:487:TRP:NE1	2.34	0.57
14:N:210:ILE:O	14:N:214:THR:OG1	2.22	0.57
29:d:100:ASP:OD2	33:h:117:ARG:NH2	2.36	0.57
4:D:239:THR:O	4:D:294:TYR:N	2.37	0.57
6:F:101:GLU:OE2	6:F:303:SER:OG	2.19	0.57
7:G:357:ASP:N	7:G:357:ASP:OD1	2.38	0.57
42:q:42:ASP:OD2	42:q:46:ASN:ND2	2.37	0.57
7:G:317:ALA:CB	7:G:331:LEU:HD21	2.33	0.57
7:G:415:LEU:O	7:G:416:THR:OG1	2.18	0.57
15:O:34:GLY:N	52:O:401:DGT:O3G	2.35	0.57
15:O:183:ILE:HD13	15:O:194:ILE:CG2	2.34	0.57
20:T:25:ILE:HG12	20:T:40:LEU:HD13	1.86	0.57
15:O:45:LYS:CB	15:O:235:VAL:HG21	2.35	0.57
22:W:116:ASP:OD1	22:W:119:SER:OG	2.15	0.57
16:P:136:ASN:N	16:P:136:ASN:OD1	2.37	0.57
20:T:64:ASP:OD2	22:W:36:ARG:NH2	2.38	0.57
34:i:102:ARG:NH2	40:o:49:GLN:O	2.38	0.57
13:M:106:LEU:HD13	13:M:234:VAL:HG11	1.87	0.57
32:g:79:TYR:OH	33:h:40:ILE:HD13	2.05	0.57
13:M:14:LEU:O	13:M:18:SER:OG	2.06	0.57
16:P:77:ASP:OD1	16:P:79:ASP:N	2.36	0.57
2:B:171:LYS:N	16:P:52:GLU:OE2	2.34	0.57
4:D:202:ASP:OD1	4:D:203:LEU:N	2.38	0.57
7:G:229:ASP:OD1	7:G:231:MET:N	2.36	0.57
5:E:22:ASP:O	5:E:57:GLN:NE2	2.38	0.56
13:M:305:THR:HG1	13:M:308:SER:CB	2.17	0.56
17:Q:123:SER:OG	17:Q:126:LYS:N	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:43:LYS:O	38:m:47:GLN:N	2.36	0.56
4:D:415:VAL:HG21	8:H:207:LEU:HD11	1.86	0.56
10:J:56:VAL:O	10:J:60:TYR:N	2.38	0.56
12:L:69:LEU:HD11	13:M:455:LEU:HD11	1.87	0.56
12:L:152:PHE:HB2	12:L:172:ILE:HD11	1.88	0.56
17:Q:36:ARG:N	17:Q:58:GLU:O	2.37	0.56
30:e:64:GLU:O	30:e:68:ARG:N	2.28	0.56
34:i:52:ASP:OD1	34:i:52:ASP:N	2.39	0.56
34:i:54:ALA:O	34:i:58:ASN:ND2	2.37	0.56
4:D:64:LEU:HD11	4:D:76:CYS:SG	2.46	0.56
5:E:121:GLN:O	5:E:125:GLY:N	2.38	0.56
6:F:200:GLN:OE1	6:F:202:LYS:NZ	2.35	0.56
15:O:99:TRP:CD1	15:O:103:SER:HG	2.23	0.56
3:C:50:ILE:HG13	3:C:105:ILE:HD11	1.87	0.56
15:O:30:ASN:O	15:O:35:LYS:NZ	2.38	0.56
7:G:359:ARG:NE	7:G:504:ASP:OD2	2.32	0.56
11:K:44:ALA:HB1	11:K:59:MET:HE1	1.88	0.56
15:O:253:ASP:O	15:O:257:HIS:N	2.37	0.56
34:i:100:LYS:O	40:o:49:GLN:NE2	2.36	0.56
40:o:72:SER:OG	40:o:79:CYS:SG	2.64	0.56
41:p:100:GLU:O	41:p:103:ASN:N	2.39	0.56
3:C:86:ARG:NH2	21:V:112:LYS:O	2.37	0.56
3:C:136:ASP:OD2	3:C:151:ILE:N	2.33	0.56
14:N:175:LEU:HD13	14:N:219:PHE:CE1	2.41	0.56
26:a:67:GLU:N	26:a:67:GLU:OE1	2.39	0.56
34:i:71:PHE:HD1	34:i:75:LEU:HD23	1.70	0.56
11:K:41:PHE:HE2	11:K:64:LEU:HD22	1.71	0.56
14:N:49:ASN:OD1	14:N:49:ASN:N	2.39	0.56
23:X:5:GLU:OE1	23:X:6:LEU:N	2.39	0.56
34:i:86:LYS:NZ	41:p:45:THR:OG1	2.38	0.56
19:S:68:TYR:N	19:S:72:GLN:O	2.36	0.56
3:C:114:LEU:HD23	22:W:80:LEU:HD12	1.88	0.55
8:H:5:ASN:O	8:H:9:LEU:N	2.39	0.55
13:M:217:PRO:O	13:M:221:VAL:HG23	2.06	0.55
15:O:108:TYR:OH	15:O:164:LEU:O	2.24	0.55
16:P:276:GLU:N	16:P:276:GLU:OE1	2.39	0.55
15:O:101:TYR:OH	15:O:159:THR:OG1	2.23	0.55
30:e:13:LEU:O	30:e:16:TRP:NE1	2.36	0.55
31:f:38:ARG:NH1	31:f:56:TRP:O	2.40	0.55
8:H:173:TRP:HB3	8:H:175:ILE:HG22	1.88	0.55
3:C:50:ILE:CG1	3:C:105:ILE:HD11	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:249:ARG:NE	7:G:251:LEU:HD11	2.22	0.55
12:L:362:LEU:HD13	12:L:366:MET:SD	2.47	0.55
7:G:391:PHE:CE2	7:G:395:ILE:HD11	2.41	0.55
12:L:1:FME:SD	12:L:2:ASN:N	2.80	0.55
20:U:14:ARG:O	20:U:18:VAL:HG23	2.07	0.55
9:I:64:GLU:OE2	9:I:157:ASN:ND2	2.39	0.55
12:L:136:ASN:OD1	12:L:139:GLN:N	2.33	0.55
12:L:427:ILE:HG23	12:L:431:LEU:HD12	1.89	0.55
15:O:260:ARG:HA	15:O:263:VAL:HG22	1.88	0.55
23:X:19:VAL:CG1	26:a:69:ILE:HD11	2.37	0.55
34:i:85:LEU:O	34:i:90:THR:HG23	2.07	0.55
1:A:106:TRP:NE1	45:A:201:3PE:O12	2.39	0.55
7:G:324:ASP:CB	7:G:571:ALA:HB1	2.37	0.55
8:H:70:MET:HE3	8:H:118:TRP:CD1	2.42	0.55
38:m:28:THR:HG22	38:m:32:GLN:NE2	2.22	0.55
7:G:107:ILE:CG2	9:I:78:ILE:HD12	2.37	0.55
12:L:276:ILE:O	12:L:280:LEU:N	2.35	0.55
13:M:114:GLU:OE1	13:M:116:ILE:N	2.40	0.55
13:M:349:GLN:N	13:M:415:GLN:OE1	2.40	0.55
41:p:8:VAL:O	41:p:108:ARG:NH2	2.40	0.55
6:F:31:TRP:NE1	44:s:42:GLN:OE1	2.39	0.54
6:F:304:THR:HG21	6:F:328:GLY:O	2.07	0.54
13:M:110:PHE:O	13:M:241:TYR:OH	2.04	0.54
39:n:168:HIS:O	39:n:172:ARG:N	2.41	0.54
2:B:50:PHE:HD1	2:B:52:LEU:HD21	1.72	0.54
7:G:139:ASP:N	7:G:139:ASP:OD1	2.40	0.54
7:G:329:ILE:CD1	7:G:626:VAL:HG21	2.37	0.54
13:M:16:TRP:O	13:M:93:LYS:NZ	2.33	0.54
9:I:65:HIS:CD2	9:I:122:CYS:SG	3.00	0.54
3:C:28:TYR:OH	3:C:67:HIS:NE2	2.36	0.54
4:D:184:VAL:O	9:I:60:ARG:NH1	2.41	0.54
7:G:174:THR:HG22	7:G:183:VAL:HG22	1.88	0.54
14:N:290:LEU:HD12	14:N:293:TYR:HB2	1.90	0.54
32:g:42:PRO:O	33:h:17:TYR:OH	2.22	0.54
13:M:289:SER:OG	13:M:406:TYR:OH	2.24	0.54
13:M:305:THR:O	13:M:308:SER:OG	2.25	0.54
15:O:318:TRP:O	29:d:58:LEU:N	2.37	0.54
12:L:520:PHE:O	12:L:524:THR:OG1	2.22	0.54
13:M:265:SER:O	13:M:268:GLY:N	2.41	0.54
14:N:37:MET:HE2	14:N:63:GLN:HB3	1.89	0.54
15:O:135:LEU:HD22	15:O:152:TYR:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:7:THR:O	20:T:10:GLY:N	2.41	0.54
4:D:66:MET:HE1	4:D:411:LEU:HD11	1.90	0.54
4:D:342:MET:HE3	4:D:342:MET:HA	1.88	0.54
12:L:251:THR:O	12:L:254:VAL:HG22	2.08	0.54
13:M:139:GLN:OE1	13:M:340:ARG:NH2	2.41	0.54
4:D:112:MET:HE2	4:D:193:TYR:CB	2.37	0.54
16:P:202:LYS:NZ	16:P:286:ARG:O	2.34	0.54
21:V:63:ASP:OD1	21:V:64:VAL:N	2.40	0.54
5:E:51:LEU:HD21	5:E:61:LEU:HD13	1.89	0.54
13:M:57:PHE:HB3	13:M:113:MET:HE3	1.90	0.54
14:N:343:LEU:C	14:N:343:LEU:HD12	2.33	0.54
3:C:40:VAL:HG13	3:C:50:ILE:HD13	1.90	0.53
16:P:176:ASP:O	16:P:180:ASN:ND2	2.40	0.53
23:X:21:SER:N	26:a:51:ASP:OD2	2.35	0.53
35:j:66:ILE:HG21	40:o:106:ARG:HB3	1.89	0.53
4:D:241:ASP:HA	4:D:244:ILE:HD11	1.90	0.53
33:h:7:ARG:NH1	34:i:27:LEU:HD12	2.23	0.53
34:i:18:ARG:CZ	34:i:22:LEU:HD21	2.39	0.53
37:l:68:ASP:OD1	37:l:69:LEU:N	2.41	0.53
32:g:68:ILE:O	32:g:72:LEU:N	2.41	0.53
13:M:390:ASN:OD1	13:M:390:ASN:N	2.39	0.53
20:U:23:ASP:OD1	36:k:46:ARG:NH2	2.38	0.53
37:l:145:ASP:OD1	37:l:147:ASN:ND2	2.39	0.53
6:F:13:GLY:N	6:F:271:GLU:OE1	2.41	0.53
6:F:94:VAL:HG23	6:F:220:THR:CG2	2.36	0.53
8:H:114:TYR:OH	10:J:61:LEU:O	2.15	0.53
17:Q:18:ASP:OD1	17:Q:20:THR:HG23	2.09	0.53
12:L:111:ASP:OD1	12:L:113:ASN:N	2.42	0.53
12:L:237:MET:HE3	12:L:303:ALA:HB2	1.91	0.53
38:m:90:ALA:O	38:m:94:ILE:HG22	2.09	0.53
3:C:77:ASP:OD1	3:C:78:LEU:N	2.41	0.53
34:i:86:LYS:NZ	41:p:41:ASP:OD1	2.38	0.53
12:L:7:LEU:O	12:L:10:VAL:HG22	2.08	0.53
12:L:355:ASP:OD1	12:L:357:ARG:NE	2.40	0.53
12:L:397:GLU:CB	12:L:482:MET:HE1	2.39	0.52
42:q:76:ASP:N	42:q:76:ASP:OD1	2.42	0.52
42:q:117:LEU:O	42:q:120:THR:OG1	2.28	0.52
7:G:641:TYR:OH	19:S:56:GLU:OE2	2.20	0.52
10:J:169:MET:O	10:J:172:THR:OG1	2.23	0.52
6:F:219:PRO:O	6:F:220:THR:OG1	2.24	0.52
33:h:38:ILE:HG22	33:h:42:LEU:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:209:ASP:N	4:D:209:ASP:OD1	2.43	0.52
11:K:59:MET:HG2	14:N:27:LEU:HD22	1.92	0.52
13:M:351:LEU:O	13:M:352:LEU:HD23	2.09	0.52
33:h:47:ILE:N	33:h:47:ILE:HD12	2.25	0.52
1:A:3:LEU:HD23	46:H:401:PC1:C23	2.39	0.52
15:O:14:ALA:O	15:O:18:MET:N	2.37	0.52
4:D:165:THR:OG1	8:H:275:ALA:O	2.10	0.52
15:O:158:VAL:CG1	15:O:159:THR:HG23	2.40	0.52
5:E:154:VAL:HG22	5:E:164:LEU:HD11	1.90	0.52
7:G:148:THR:HG22	7:G:208:LEU:CD2	2.39	0.52
16:P:132:ILE:O	16:P:149:LYS:NZ	2.43	0.52
5:E:159:ASN:OD1	6:F:144:ASN:ND2	2.41	0.52
42:q:44:TYR:OH	42:q:113:HIS:N	2.42	0.52
43:r:34:THR:O	43:r:35:GLN:NE2	2.43	0.52
1:A:84:LEU:HD13	8:H:309:ILE:HG23	1.90	0.52
14:N:242:VAL:HG21	45:N:401:3PE:O32	2.09	0.52
5:E:74:GLN:N	5:E:74:GLN:OE1	2.43	0.51
7:G:160:ILE:CD1	7:G:174:THR:HG23	2.40	0.51
12:L:362:LEU:HD12	12:L:430:ALA:O	2.09	0.51
13:M:87:GLU:O	13:M:92:LYS:NZ	2.33	0.51
10:J:137:SER:O	10:J:140:ALA:N	2.41	0.51
34:i:75:LEU:HD21	34:i:79:TRP:CZ2	2.46	0.51
37:l:56:GLN:OE1	37:l:70:ARG:NH1	2.44	0.51
20:T:31:SER:N	20:T:34:SER:OG	2.44	0.51
22:W:95:VAL:HG12	22:W:95:VAL:O	2.11	0.51
32:g:111:ASN:C	41:p:141:ARG:HE	2.18	0.51
56:U:101:EHZ:C7	39:n:50:HIS:HD1	2.24	0.51
4:D:151:ILE:HG23	4:D:170:MET:HB3	1.93	0.51
43:r:8:GLN:O	43:r:12:ASN:ND2	2.44	0.51
7:G:104:ASP:OD2	7:G:152:ARG:NE	2.40	0.51
7:G:422:LEU:HD22	7:G:437:HIS:HE1	1.74	0.51
8:H:170:GLU:OE2	23:X:97:ARG:NH1	2.43	0.51
20:T:7:THR:HG22	20:T:10:GLY:H	1.75	0.51
29:d:45:ASP:OD1	29:d:49:ARG:NH1	2.42	0.51
44:s:34:ASP:OD1	44:s:36:THR:OG1	2.23	0.51
14:N:151:LEU:HD22	24:Y:138:PRO:HD3	1.93	0.51
32:g:75:THR:HG21	33:h:36:VAL:HG13	1.93	0.51
3:C:86:ARG:NH1	3:C:91:GLU:OE1	2.43	0.51
8:H:5:ASN:HD21	26:a:26:ILE:HG21	1.76	0.51
21:V:77:GLU:OE1	21:V:77:GLU:N	2.39	0.51
4:D:49:LEU:HB2	4:D:66:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:306:MET:SD	7:G:306:MET:N	2.84	0.50
14:N:258:SER:OG	14:N:336:MET:N	2.42	0.50
38:m:85:THR:O	38:m:89:GLY:N	2.41	0.50
4:D:98:GLN:O	4:D:101:PRO:HD2	2.11	0.50
7:G:156:CYS:O	7:G:157:THR:OG1	2.28	0.50
28:c:19:LEU:O	28:c:23:THR:OG1	2.15	0.50
42:q:3:LEU:HD13	51:q:201:CDL:H521	1.92	0.50
13:M:329:LEU:O	13:M:332:SER:OG	2.20	0.50
23:X:165:ARG:NH2	29:d:87:ASP:OD1	2.40	0.50
42:q:2:GLU:O	42:q:6:VAL:HG23	2.11	0.50
5:E:8:VAL:HG11	7:G:138:GLU:OE2	2.11	0.50
27:b:59:ASP:OD1	27:b:59:ASP:N	2.44	0.50
39:n:120:LYS:HA	39:n:123:GLN:NE2	2.26	0.50
8:H:8:MET:HE2	8:H:8:MET:HA	1.94	0.50
15:O:45:LYS:HB2	15:O:235:VAL:HG21	1.94	0.50
15:O:105:LEU:O	15:O:109:ALA:N	2.33	0.50
24:Y:140:VAL:O	33:h:111:ARG:NH2	2.45	0.50
32:g:107:ILE:HG21	41:p:134:VAL:HG22	1.94	0.50
3:C:79:THR:OG1	3:C:80:ALA:N	2.43	0.50
4:D:354:GLU:OE2	4:D:357:GLN:NE2	2.45	0.50
7:G:205:VAL:HG23	7:G:207:ALA:H	1.75	0.50
12:L:39:ALA:O	12:L:43:ALA:N	2.37	0.50
12:L:488:THR:O	12:L:492:ILE:N	2.44	0.50
13:M:152:TYR:O	13:M:156:GLY:N	2.44	0.50
14:N:45:MET:O	14:N:48:HIS:N	2.42	0.50
41:p:24:SER:O	41:p:25:LEU:HD12	2.11	0.50
7:G:171:ASP:OD2	7:G:189:LYS:NZ	2.35	0.50
13:M:373:ILE:HD11	13:M:444:LEU:HD12	1.93	0.50
7:G:196:SER:OG	7:G:265:ASP:OD2	2.29	0.50
12:L:397:GLU:HB3	12:L:482:MET:HE1	1.93	0.50
3:C:22:LEU:O	3:C:26:GLY:N	2.45	0.50
8:H:297:THR:O	8:H:301:CYS:N	2.40	0.50
10:J:150:GLY:O	10:J:154:VAL:HG23	2.12	0.50
12:L:346:ILE:O	12:L:350:LEU:HD13	2.12	0.50
14:N:338:PRO:O	23:X:169:TRP:NE1	2.44	0.50
15:O:33:SER:O	15:O:33:SER:OG	2.30	0.50
5:E:87:TYR:CG	6:F:181:ALA:HB3	2.47	0.49
41:p:69:ARG:NH2	41:p:94:ASP:OD2	2.40	0.49
42:q:4:LEU:HD23	42:q:4:LEU:O	2.12	0.49
6:F:192:LEU:C	6:F:192:LEU:HD23	2.37	0.49
12:L:335:PHE:O	12:L:339:LEU:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:18:ILE:HD12	19:S:50:LEU:HD21	1.94	0.49
22:W:78:VAL:O	22:W:82:VAL:HG23	2.12	0.49
39:n:30:CYS:O	39:n:32:HIS:N	2.45	0.49
6:F:15:LEU:O	6:F:20:ARG:NH2	2.44	0.49
9:I:13:ASP:OD1	9:I:13:ASP:N	2.45	0.49
11:K:34:GLU:HA	11:K:37:MET:HE3	1.94	0.49
7:G:266:LYS:NZ	7:G:674:THR:OG1	2.26	0.49
7:G:357:ASP:O	19:S:55:ARG:NH1	2.45	0.49
35:j:43:ASP:OD1	35:j:43:ASP:N	2.45	0.49
5:E:51:LEU:HD23	5:E:51:LEU:O	2.13	0.49
7:G:104:ASP:O	7:G:108:CYS:N	2.42	0.49
10:J:103:MET:HA	10:J:106:TYR:CD1	2.48	0.49
11:K:40:LEU:CD2	14:N:72:MET:HE2	2.42	0.49
12:L:15:LEU:O	12:L:122:LEU:HD21	2.12	0.49
34:i:88:HIS:O	34:i:92:LYS:NZ	2.44	0.49
12:L:458:LEU:HD23	12:L:458:LEU:O	2.12	0.49
13:M:47:ASP:OD1	13:M:48:ASN:N	2.45	0.49
13:M:143:LEU:HD12	13:M:143:LEU:H	1.77	0.49
23:X:48:GLU:OE1	23:X:134:ARG:NH2	2.43	0.49
3:C:68:SER:HB2	21:V:50:ILE:HD12	1.95	0.49
9:I:164:GLU:OE2	42:q:88:ARG:N	2.46	0.49
13:M:431:THR:N	32:g:45:HIS:O	2.45	0.49
29:d:11:PHE:N	46:d:202:PC1:O12	2.44	0.49
34:i:120:LYS:HB2	40:o:39:VAL:HG13	1.94	0.49
8:H:77:MET:HE2	46:H:401:PC1:H2I3	1.95	0.49
8:H:281:ARG:NH1	8:H:284:GLN:OE1	2.46	0.49
37:l:58:ARG:NH2	37:l:70:ARG:O	2.42	0.49
13:M:281:ASP:OD1	13:M:283:LYS:N	2.45	0.49
15:O:139:TYR:HB2	15:O:144:ILE:HD11	1.95	0.49
15:O:184:GLN:OE1	15:O:184:GLN:N	2.46	0.49
34:i:4:THR:O	34:i:7:GLU:N	2.46	0.49
10:J:110:ASP:OD2	30:e:79:ARG:NH2	2.46	0.48
12:L:97:THR:O	12:L:101:MET:N	2.44	0.48
13:M:204:MET:HE3	13:M:261:PHE:CD1	2.48	0.48
12:L:79:SER:O	12:L:139:GLN:NE2	2.44	0.48
16:P:17:SER:HG	16:P:43:SER:HG	1.52	0.48
38:m:7:ALA:HB2	38:m:13:LEU:HD13	1.96	0.48
4:D:339:LYS:NZ	18:R:65:ALA:O	2.36	0.48
34:i:82:HIS:O	34:i:86:LYS:N	2.41	0.48
7:G:617:ASP:OD1	7:G:617:ASP:N	2.44	0.48
8:H:179:TRP:N	8:H:180:PRO:CD	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:44:VAL:HG12	10:J:49:GLY:HA3	1.95	0.48
20:T:23:ASP:OD1	20:T:24:LYS:N	2.46	0.48
6:F:327:THR:OG1	6:F:328:GLY:N	2.46	0.48
12:L:71:ILE:O	12:L:74:LEU:N	2.46	0.48
12:L:281:GLY:O	12:L:285:THR:HG22	2.14	0.48
13:M:289:SER:HG	13:M:406:TYR:HH	1.59	0.48
5:E:55:GLN:OE1	5:E:91:ASN:N	2.45	0.48
5:E:202:LEU:HD22	6:F:23:THR:HA	1.95	0.48
15:O:244:ASP:OD1	15:O:244:ASP:N	2.43	0.48
20:T:81:ALA:O	20:T:85:ASP:N	2.42	0.48
13:M:243:MET:HA	13:M:246:ILE:HG22	1.95	0.48
5:E:51:LEU:HD23	5:E:51:LEU:C	2.38	0.48
12:L:213:LEU:HD23	12:L:216:LEU:HD12	1.94	0.48
32:g:114:ASP:OD1	32:g:116:SER:OG	2.30	0.48
4:D:159:LEU:HD23	4:D:159:LEU:O	2.14	0.48
11:K:1:FME:O	11:K:3:MET:N	2.47	0.48
13:M:143:LEU:HD13	13:M:222:GLU:OE2	2.14	0.48
33:h:128:ILE:HD12	33:h:128:ILE:H	1.79	0.48
8:H:219:PRO:O	8:H:222:LEU:N	2.47	0.47
13:M:450:ASN:OD1	13:M:452:LYS:NZ	2.39	0.47
23:X:138:GLU:N	23:X:138:GLU:OE1	2.47	0.47
11:K:10:MET:O	11:K:14:VAL:HG23	2.15	0.47
13:M:34:ILE:O	13:M:37:THR:OG1	2.28	0.47
41:p:89:MET:HE2	41:p:89:MET:HA	1.96	0.47
6:F:398:GLN:NE2	7:G:95:GLU:OE1	2.42	0.47
9:I:66:ALA:O	9:I:131:ILE:HD12	2.15	0.47
9:I:145:GLU:OE2	16:P:66:GLY:N	2.46	0.47
10:J:57:PHE:O	10:J:62:GLY:N	2.45	0.47
14:N:265:MET:HA	14:N:265:MET:HE2	1.95	0.47
16:P:143:SER:O	16:P:146:LEU:N	2.47	0.47
19:S:90:LEU:O	19:S:90:LEU:HD23	2.14	0.47
20:T:48:VAL:HG13	22:W:36:ARG:HE	1.79	0.47
30:e:49:ILE:O	30:e:53:LYS:NZ	2.45	0.47
35:j:66:ILE:HG21	40:o:106:ARG:CB	2.44	0.47
37:l:86:ARG:NH2	39:n:90:TYR:OH	2.48	0.47
6:F:194:GLU:OE2	6:F:199:LYS:NZ	2.36	0.47
7:G:47:SER:OG	7:G:165:GLU:OE2	2.32	0.47
12:L:418:PHE:CD1	12:L:421:ILE:HD12	2.49	0.47
28:c:22:GLY:O	28:c:26:PHE:N	2.33	0.47
16:P:119:GLN:NE2	16:P:123:GLU:OE2	2.44	0.47
5:E:100:ILE:HG23	5:E:156:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:189:GLU:HG3	6:F:190:THR:HG23	1.97	0.47
18:R:94:GLN:O	18:R:95:HIS:ND1	2.47	0.47
20:T:50:ILE:HG23	20:T:54:MET:HE2	1.95	0.47
38:m:27:GLU:OE1	38:m:27:GLU:N	2.45	0.47
38:m:47:GLN:CD	39:n:165:LEU:HD13	2.39	0.47
2:B:23:SER:O	2:B:24:SER:OG	2.27	0.47
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.96	0.47
15:O:138:MET:HE2	15:O:144:ILE:HG23	1.97	0.47
16:P:157:ARG:NH1	16:P:225:GLY:O	2.48	0.47
56:T:101:EHZ:O2	56:T:101:EHZ:O1	2.32	0.47
23:X:19:VAL:HG13	26:a:69:ILE:HD11	1.95	0.47
25:Z:34:MET:O	25:Z:38:GLY:N	2.43	0.47
7:G:476:LYS:O	7:G:479:THR:OG1	2.33	0.47
8:H:87:ILE:N	8:H:88:PRO:CD	2.78	0.47
8:H:318:THR:N	25:Z:60:GLN:OE1	2.48	0.47
10:J:122:LEU:HD23	10:J:122:LEU:C	2.39	0.47
12:L:381:THR:HG22	12:L:420:ALA:HA	1.97	0.47
4:D:218:PHE:O	4:D:221:ARG:N	2.45	0.47
7:G:160:ILE:HD11	7:G:174:THR:HG23	1.97	0.47
7:G:286:ASN:OD1	7:G:290:LEU:N	2.44	0.47
10:J:103:MET:O	10:J:107:VAL:N	2.43	0.47
14:N:52:ALA:O	14:N:56:SER:N	2.38	0.47
6:F:99:GLU:OE2	6:F:104:THR:HG22	2.15	0.47
6:F:300:GLY:O	6:F:331:THR:OG1	2.33	0.47
9:I:148:LEU:HD12	9:I:148:LEU:N	2.29	0.47
20:U:12:LYS:NZ	20:U:13:ASP:OD1	2.48	0.47
24:Y:85:ASP:OD1	24:Y:85:ASP:N	2.48	0.47
4:D:225:LEU:HD11	4:D:229:LEU:CD1	2.44	0.46
6:F:362:CYS:SG	6:F:404:ILE:HD12	2.55	0.46
6:F:400:GLU:OE2	6:F:413:TRP:NE1	2.41	0.46
6:F:430:MET:O	6:F:434:ALA:N	2.44	0.46
11:K:40:LEU:HD21	14:N:72:MET:HE2	1.96	0.46
20:T:36:PHE:O	20:T:41:GLY:N	2.48	0.46
4:D:224:GLU:OE2	9:I:43:ARG:NH2	2.43	0.46
6:F:360:GLY:O	6:F:366:ARG:NH1	2.37	0.46
12:L:61:LEU:O	12:L:82:MET:N	2.48	0.46
13:M:346:ARG:HG2	13:M:413:MET:HE1	1.97	0.46
15:O:114:HIS:ND1	15:O:118:THR:HG21	2.30	0.46
20:U:22:TYR:HD2	20:U:25:ILE:HD12	1.79	0.46
6:F:394:GLU:OE2	43:r:50:ASN:N	2.41	0.46
7:G:171:ASP:O	7:G:185:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:563:GLY:O	7:G:593:ALA:HB1	2.15	0.46
9:I:42:PHE:CD2	43:r:7:ILE:HD12	2.50	0.46
17:Q:14:ASP:OD1	17:Q:14:ASP:N	2.47	0.46
42:q:3:LEU:HD13	51:q:201:CDL:C52	2.46	0.46
2:B:42:ARG:NH1	46:B:202:PC1:O14	2.41	0.46
4:D:349:PHE:CD1	9:I:82:LEU:HD11	2.50	0.46
6:F:205:LEU:HD21	7:G:50:GLY:O	2.14	0.46
6:F:261:HIS:O	6:F:262:VAL:HG13	2.15	0.46
9:I:42:PHE:HD2	43:r:7:ILE:HD12	1.79	0.46
12:L:359:MET:O	12:L:436:ARG:NH2	2.48	0.46
14:N:230:LEU:HD11	14:N:244:ILE:HD13	1.97	0.46
16:P:107:GLU:HG3	16:P:111:VAL:HG21	1.97	0.46
33:h:38:ILE:HG22	33:h:42:LEU:CD1	2.45	0.46
42:q:6:VAL:HG22	42:q:9:ARG:NH2	2.30	0.46
43:r:105:LEU:HD22	43:r:110:PRO:HB3	1.98	0.46
8:H:194:ASN:CG	8:H:201:THR:HG1	2.21	0.46
12:L:357:ARG:NH1	39:n:28:SER:OG	2.48	0.46
13:M:243:MET:O	13:M:247:THR:HG23	2.14	0.46
17:Q:20:THR:HG22	17:Q:99:ASN:O	2.14	0.46
4:D:294:TYR:HE1	4:D:298:LEU:HD11	1.81	0.46
15:O:158:VAL:HG13	15:O:159:THR:HG23	1.97	0.46
8:H:283:ASP:OD1	8:H:283:ASP:N	2.49	0.46
6:F:118:LEU:HD22	6:F:225:VAL:HG13	1.98	0.46
15:O:308:TYR:O	15:O:317:ILE:HD13	2.16	0.46
22:W:100:THR:HG23	22:W:101:HIS:N	2.30	0.46
33:h:27:PHE:O	33:h:31:LEU:N	2.49	0.46
8:H:1:FME:O	8:H:4:ILE:N	2.40	0.46
10:J:27:ILE:H	10:J:27:ILE:HD12	1.81	0.46
11:K:84:THR:HG23	11:K:85:TYR:N	2.30	0.46
12:L:298:ILE:HG23	12:L:299:LYS:N	2.31	0.46
14:N:146:PHE:N	14:N:147:PRO:CD	2.79	0.46
37:l:33:ASP:OD1	37:l:33:ASP:N	2.48	0.46
6:F:428:GLU:OE2	6:F:432:GLN:NE2	2.49	0.45
8:H:77:MET:CE	46:H:401:PC1:H2I3	2.46	0.45
12:L:19:ILE:HG12	12:L:122:LEU:HD23	1.98	0.45
12:L:407:TRP:CZ3	37:l:115:MET:HE2	2.51	0.45
13:M:209:LEU:HD21	13:M:264:LEU:HD13	1.97	0.45
14:N:316:GLN:NE2	15:O:60:ASP:OD1	2.49	0.45
7:G:329:ILE:HD13	7:G:505:LEU:HD22	1.98	0.45
13:M:305:THR:N	13:M:308:SER:OG	2.48	0.45
19:S:23:CYS:SG	19:S:24:GLN:N	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:82:THR:O	23:X:86:THR:OG1	2.23	0.45
23:X:90:TYR:OH	26:a:28:ARG:NH2	2.49	0.45
40:o:16:PRO:HG3	40:o:108:LEU:HD12	1.97	0.45
6:F:54:ASP:O	6:F:58:GLY:N	2.48	0.45
10:J:118:GLU:OE1	10:J:118:GLU:N	2.49	0.45
12:L:286:LEU:O	12:L:290:MET:N	2.33	0.45
6:F:205:LEU:HD12	6:F:205:LEU:N	2.31	0.45
8:H:98:MET:HE1	8:H:104:PHE:CD2	2.51	0.45
12:L:83:ASP:OD2	12:L:262:ARG:NH1	2.49	0.45
6:F:188:GLU:OE1	6:F:190:THR:N	2.42	0.45
8:H:176:LEU:HB3	8:H:177:PRO:CD	2.46	0.45
13:M:365:THR:HG22	13:M:372:THR:HG21	1.99	0.45
14:N:1:FME:O1	15:O:254:ARG:NH1	2.48	0.45
20:T:55:GLU:O	20:T:59:GLY:N	2.48	0.45
1:A:97:LEU:O	1:A:101:SER:OG	2.34	0.45
2:B:31:ALA:O	2:B:35:ASP:N	2.45	0.45
5:E:156:ILE:HG22	5:E:156:ILE:O	2.15	0.45
7:G:324:ASP:HB3	7:G:571:ALA:HB1	1.99	0.45
13:M:192:ASN:HB2	13:M:253:MET:HE1	1.99	0.45
34:i:85:LEU:HD21	34:i:96:ILE:HD11	1.98	0.45
37:l:8:MET:HE2	37:l:8:MET:HA	1.99	0.45
44:s:46:TYR:CD1	44:s:50:THR:HG21	2.52	0.45
5:E:105:THR:HG22	5:E:106:THR:H	1.81	0.45
6:F:407:LEU:C	6:F:407:LEU:HD23	2.41	0.45
16:P:246:PHE:O	16:P:250:HIS:N	2.50	0.45
13:M:265:SER:O	13:M:266:LEU:C	2.58	0.45
17:Q:33:ARG:NH1	17:Q:77:ASP:OD2	2.50	0.45
39:n:39:PHE:HA	39:n:42:LEU:HD12	1.98	0.45
4:D:110:SER:OG	4:D:149:ASN:OD1	2.34	0.45
7:G:78:ASN:OD1	7:G:79:ILE:N	2.50	0.45
19:S:90:LEU:HD23	19:S:90:LEU:C	2.42	0.45
22:W:98:GLN:O	22:W:101:HIS:N	2.50	0.45
4:D:168:PHE:O	4:D:169:TRP:C	2.60	0.45
11:K:41:PHE:CE2	11:K:64:LEU:HD22	2.50	0.45
12:L:190:LEU:HD11	38:m:127:SER:OG	2.17	0.45
13:M:183:VAL:HG23	13:M:249:ILE:HG22	1.98	0.45
40:o:87:ASP:O	40:o:91:HIS:N	2.42	0.45
4:D:316:ASN:OD1	25:Z:15:TYR:N	2.48	0.44
7:G:348:VAL:HG12	7:G:349:PHE:N	2.32	0.44
14:N:124:LEU:O	14:N:128:LEU:N	2.48	0.44
26:a:49:GLU:O	26:a:53:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:GLU:OE1	5:E:26:GLU:N	2.43	0.44
8:H:93:TYR:OH	26:a:35:GLU:OE1	2.34	0.44
25:Z:124:TYR:HD2	25:Z:132:VAL:HG22	1.82	0.44
1:A:65:PHE:CD2	1:A:98:LEU:HD11	2.53	0.44
5:E:203:THR:N	6:F:17:ASP:OD2	2.51	0.44
10:J:136:PHE:CE1	30:e:28:ILE:HD11	2.52	0.44
13:M:106:LEU:HD22	13:M:234:VAL:CG1	2.47	0.44
14:N:17:THR:OG1	14:N:133:TRP:NE1	2.51	0.44
6:F:163:GLY:N	6:F:173:PHE:O	2.50	0.44
9:I:49:ASN:O	9:I:53:GLU:N	2.50	0.44
9:I:101:ASP:OD1	9:I:101:ASP:N	2.51	0.44
11:K:8:ILE:HG21	11:K:43:MET:HB2	1.99	0.44
12:L:537:ALA:HB3	12:L:538:PRO:HD3	1.99	0.44
15:O:1:LEU:HD13	15:O:2:GLN:N	2.31	0.44
15:O:31:ILE:HG23	52:O:401:DGT:H3'	2.00	0.44
15:O:206:TYR:O	15:O:210:PHE:N	2.51	0.44
15:O:272:TYR:HA	15:O:275:ILE:HG23	1.99	0.44
33:h:94:LEU:HB3	41:p:81:VAL:HG21	1.99	0.44
2:B:48:MET:HE1	2:B:103:VAL:HG11	1.99	0.44
4:D:179:GLU:O	4:D:183:ARG:N	2.44	0.44
35:j:47:VAL:HG12	35:j:47:VAL:O	2.18	0.44
4:D:294:TYR:CE1	4:D:298:LEU:HD11	2.52	0.44
6:F:215:VAL:HG22	6:F:216:PHE:CE2	2.53	0.44
45:I:203:3PE:N	25:Z:34:MET:HE1	2.33	0.44
12:L:10:VAL:O	12:L:14:LEU:N	2.35	0.44
12:L:82:MET:HE3	12:L:87:MET:HE3	1.98	0.44
13:M:12:MET:HB2	13:M:13:PRO:HD3	2.00	0.44
38:m:36:LEU:O	38:m:40:SER:N	2.41	0.44
6:F:109:GLU:OE1	6:F:112:ARG:NH2	2.42	0.44
6:F:30:ASP:O	6:F:39:ARG:NH2	2.44	0.44
15:O:168:VAL:HG21	15:O:241:LEU:CD1	2.42	0.44
16:P:95:VAL:HG12	16:P:96:GLY:N	2.33	0.44
31:f:16:VAL:HB	31:f:17:PRO:HD3	1.99	0.44
33:h:34:ILE:HB	33:h:35:PRO:HD3	1.99	0.44
34:i:4:THR:O	34:i:5:PRO:C	2.61	0.44
6:F:215:VAL:HG22	6:F:216:PHE:CD2	2.53	0.44
10:J:102:PHE:O	10:J:103:MET:HB2	2.17	0.44
12:L:376:GLY:O	12:L:380:LEU:N	2.41	0.44
14:N:347:GLU:CB	29:d:82:MET:HE2	2.47	0.44
38:m:61:ASP:O	38:m:65:VAL:HG23	2.18	0.44
7:G:107:ILE:HG23	9:I:78:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:415:LEU:HD12	7:G:419:TYR:CD2	2.52	0.43
8:H:6:ILE:HG22	8:H:10:ILE:HD12	1.99	0.43
14:N:41:ILE:N	14:N:42:PRO:HD2	2.33	0.43
25:Z:141:TRP:O	25:Z:143:THR:N	2.51	0.43
42:q:34:ARG:NH1	42:q:58:ARG:O	2.42	0.43
2:B:50:PHE:CD1	2:B:52:LEU:HD21	2.53	0.43
45:D:501:3PE:H262	8:H:187:ILE:HD12	2.00	0.43
5:E:156:ILE:N	5:E:156:ILE:HD12	2.33	0.43
6:F:203:PRO:CG	47:F:501:SF4:S2	3.06	0.43
37:l:145:ASP:OD2	37:l:148:LYS:N	2.43	0.43
40:o:23:THR:N	40:o:104:GLU:OE2	2.43	0.43
46:B:202:PC1:H143	46:B:202:PC1:O13	2.18	0.43
6:F:202:LYS:O	17:Q:133:LYS:NZ	2.42	0.43
14:N:214:THR:HG22	14:N:218:MET:HE2	2.00	0.43
20:T:65:ILE:O	20:T:69:LYS:NZ	2.39	0.43
23:X:124:LEU:HD13	25:Z:69:ALA:HB2	2.00	0.43
5:E:105:THR:HB	48:E:301:FES:S2	2.58	0.43
10:J:135:PHE:CD1	10:J:135:PHE:N	2.85	0.43
13:M:59:ASP:N	13:M:62:SER:OG	2.51	0.43
34:i:27:LEU:HD13	34:i:32:PRO:HG3	2.01	0.43
1:A:10:ASN:OD1	8:H:10:ILE:HD11	2.19	0.43
6:F:190:THR:O	6:F:193:ILE:N	2.51	0.43
8:H:106:LEU:HD13	8:H:150:LEU:HD23	2.00	0.43
10:J:33:LEU:HD23	10:J:65:MET:SD	2.58	0.43
12:L:27:TYR:HD1	57:i:201:CHD:H151	1.80	0.43
12:L:508:THR:O	12:L:508:THR:HG22	2.18	0.43
13:M:104:LEU:HG	13:M:108:MET:HE2	2.00	0.43
32:g:114:ASP:OD1	32:g:116:SER:N	2.41	0.43
34:i:41:PRO:O	34:i:45:PHE:N	2.47	0.43
43:r:105:LEU:HD22	43:r:110:PRO:CB	2.49	0.43
5:E:156:ILE:O	5:E:157:ASN:ND2	2.51	0.43
7:G:220:TRP:NE1	9:I:85:ALA:HB2	2.34	0.43
7:G:231:MET:HE1	7:G:677:ILE:HG21	2.00	0.43
7:G:375:ASP:OD2	7:G:447:LYS:N	2.52	0.43
12:L:340:PHE:O	12:L:343:SER:OG	2.24	0.43
12:L:418:PHE:HA	12:L:421:ILE:HD12	1.99	0.43
14:N:206:ILE:HD12	14:N:346:LEU:HD11	2.01	0.43
15:O:82:PHE:CZ	15:O:138:MET:HE3	2.54	0.43
19:S:22:LEU:HD23	19:S:22:LEU:N	2.33	0.43
23:X:73:ILE:HG21	23:X:81:PHE:CD2	2.54	0.43
30:e:15:ARG:HA	30:e:18:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:90:THR:HG21	41:p:85:PHE:CE2	2.53	0.43
37:l:82:ASP:OD1	37:l:83:MET:N	2.52	0.43
1:A:30:TYR:OH	2:B:41:ARG:NH2	2.52	0.43
2:B:165:LYS:O	2:B:168:LYS:N	2.52	0.43
4:D:155:THR:O	4:D:159:LEU:N	2.51	0.43
6:F:255:LEU:HD23	6:F:269:GLU:HB2	2.00	0.43
6:F:394:GLU:OE1	7:G:129:ARG:NH1	2.45	0.43
7:G:194:GLU:O	7:G:265:ASP:N	2.49	0.43
15:O:284:VAL:HG12	15:O:285:GLY:N	2.33	0.43
42:q:38:LEU:HD11	42:q:40:GLY:O	2.19	0.43
2:B:64:ALA:HB1	2:B:65:PRO:CD	2.49	0.43
4:D:76:CYS:SG	4:D:77:ASP:N	2.91	0.43
6:F:126:GLY:O	6:F:130:GLY:N	2.52	0.43
7:G:324:ASP:OD1	7:G:324:ASP:N	2.52	0.43
8:H:288:LEU:HD11	8:H:293:PHE:CE1	2.53	0.43
13:M:127:VAL:HB	13:M:128:PRO:HD3	2.00	0.43
13:M:286:ILE:O	13:M:290:SER:OG	2.35	0.43
41:p:5:ASP:OD1	41:p:6:LYS:N	2.51	0.43
5:E:27:ASN:O	5:E:30:ARG:N	2.51	0.43
6:F:302:SER:O	6:F:414:PRO:HG3	2.19	0.43
9:I:116:CYS:SG	9:I:118:TYR:N	2.88	0.43
17:Q:132:THR:OG1	17:Q:133:LYS:N	2.52	0.43
38:m:1:SAC:O	38:m:2:PHE:C	2.62	0.43
6:F:360:GLY:O	6:F:366:ARG:HD3	2.19	0.42
7:G:205:VAL:HG22	47:G:804:SF4:S3	2.59	0.42
10:J:100:GLU:O	10:J:102:PHE:N	2.51	0.42
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.00	0.42
13:M:352:LEU:HD21	13:M:426:ILE:HG23	2.01	0.42
29:d:28:ASP:OD1	29:d:31:LEU:N	2.46	0.42
32:g:66:PHE:O	32:g:71:VAL:HG23	2.19	0.42
1:A:104:TYR:O	1:A:108:GLN:HG2	2.19	0.42
8:H:102:VAL:HG23	8:H:160:PHE:O	2.18	0.42
12:L:210:ASN:OD1	12:L:270:ASN:ND2	2.53	0.42
12:L:221:THR:HB	12:L:229:LEU:HD12	2.01	0.42
14:N:270:MET:HE1	14:N:282:MET:SD	2.60	0.42
15:O:33:SER:O	15:O:172:VAL:HG11	2.20	0.42
20:T:11:ILE:HD11	20:T:84:LYS:HD2	2.00	0.42
22:W:98:GLN:O	22:W:99:ARG:C	2.63	0.42
30:e:75:LEU:O	30:e:79:ARG:N	2.38	0.42
31:f:2:ASN:OD1	31:f:2:ASN:N	2.52	0.42
37:l:96:VAL:HG12	37:l:97:ASN:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:n:103:LEU:HA	39:n:106:TRP:CD1	2.54	0.42
40:o:14:VAL:HG23	40:o:15:GLU:OE2	2.20	0.42
40:o:47:ASP:OD1	40:o:47:ASP:N	2.52	0.42
1:A:105:GLU:O	1:A:110:GLY:N	2.41	0.42
12:L:381:THR:HG21	12:L:498:PHE:CZ	2.55	0.42
14:N:115:VAL:HB	14:N:116:PRO:HD3	2.00	0.42
14:N:196:TYR:O	33:h:115:ARG:NH2	2.51	0.42
15:O:48:LEU:HD12	15:O:123:VAL:CG2	2.50	0.42
2:B:101:ARG:CZ	3:C:176:TYR:CZ	3.02	0.42
2:B:137:ASP:N	2:B:137:ASP:OD1	2.51	0.42
7:G:28:GLN:NE2	17:Q:114:LYS:O	2.52	0.42
13:M:130:LEU:O	13:M:134:THR:HG23	2.20	0.42
14:N:266:ILE:HG23	14:N:270:MET:HE3	2.01	0.42
14:N:345:VAL:O	29:d:78:ARG:NH2	2.52	0.42
4:D:62:LEU:HD22	4:D:425:PHE:HZ	1.84	0.42
5:E:156:ILE:HG22	5:E:157:ASN:HD22	1.83	0.42
6:F:157:TYR:OH	44:s:62:ARG:NH1	2.51	0.42
12:L:400:ASN:HA	12:L:409:LEU:HD21	2.01	0.42
13:M:329:LEU:HD23	13:M:437:MET:SD	2.60	0.42
14:N:233:THR:HG22	14:N:241:THR:OG1	2.19	0.42
16:P:107:GLU:O	16:P:111:VAL:N	2.48	0.42
25:Z:85:MET:HE1	25:Z:124:TYR:CE1	2.54	0.42
35:j:45:ASP:O	35:j:49:GLY:N	2.53	0.42
4:D:366:ALA:HA	4:D:374:PHE:O	2.19	0.42
14:N:89:LEU:HD11	14:N:98:MET:SD	2.59	0.42
20:T:18:VAL:HG11	20:T:54:MET:SD	2.60	0.42
32:g:45:HIS:NE2	32:g:58:MET:HE2	2.35	0.42
33:h:128:ILE:HD12	33:h:128:ILE:N	2.34	0.42
38:m:24:ILE:HD11	39:n:10:THR:HA	2.01	0.42
38:m:78:ASN:OD1	38:m:79:PHE:N	2.52	0.42
41:p:41:ASP:O	41:p:45:THR:N	2.51	0.42
10:J:11:VAL:HG12	10:J:15:MET:HE2	2.02	0.42
10:J:119:PHE:CZ	30:e:67:LEU:HD22	2.55	0.42
11:K:42:VAL:O	11:K:46:LEU:HD13	2.20	0.42
12:L:539:TYR:O	12:L:543:SER:OG	2.26	0.42
14:N:102:LEU:HD11	14:N:141:VAL:CG1	2.50	0.42
14:N:268:GLN:O	14:N:271:THR:OG1	2.37	0.42
39:n:39:PHE:CD1	39:n:42:LEU:HD12	2.54	0.42
4:D:55:HIS:O	4:D:57:ALA:N	2.51	0.42
6:F:351:ILE:HG13	6:F:376:MET:HG3	2.00	0.42
10:J:57:PHE:CD1	10:J:61:LEU:HD12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:316:THR:HG23	12:L:395:ILE:HG23	2.02	0.42
13:M:331:ASN:O	13:M:331:ASN:ND2	2.52	0.42
16:P:46:ILE:N	16:P:46:ILE:HD12	2.34	0.42
20:T:49:GLU:OE2	22:W:63:ARG:NH2	2.53	0.42
1:A:95:ILE:HG21	8:H:302:MET:HG3	2.01	0.42
3:C:119:SER:OG	3:C:121:VAL:HG23	2.19	0.42
4:D:161:ILE:HG22	4:D:161:ILE:O	2.19	0.42
12:L:5:SER:HB2	12:L:63:ILE:HD11	2.01	0.42
12:L:153:LEU:HD11	13:M:360:LEU:HD21	2.00	0.42
12:L:228:GLY:O	12:L:229:LEU:HD23	2.20	0.42
21:V:8:THR:HG21	21:V:13:LEU:O	2.20	0.42
37:l:16:THR:HG23	37:l:19:GLU:H	1.85	0.42
37:l:88:ARG:O	37:l:89:VAL:C	2.63	0.42
4:D:225:LEU:HD11	4:D:229:LEU:HD12	2.02	0.42
6:F:378:ARG:NE	7:G:132:GLU:OE2	2.53	0.42
7:G:105:CYS:HB2	7:G:106:PRO:HD3	2.02	0.42
7:G:392:ASN:O	7:G:395:ILE:N	2.52	0.42
7:G:395:ILE:O	7:G:399:TRP:N	2.43	0.42
14:N:245:LEU:HD13	14:N:297:THR:HG23	2.02	0.42
15:O:31:ILE:HD12	15:O:31:ILE:H	1.84	0.42
20:T:8:LEU:HD23	20:T:8:LEU:C	2.44	0.42
33:h:40:ILE:HG22	33:h:44:ASN:OD1	2.20	0.42
1:A:74:PRO:O	1:A:75:LEU:C	2.63	0.41
6:F:343:ILE:HG23	6:F:344:VAL:N	2.35	0.41
6:F:378:ARG:NH1	6:F:383:ASP:O	2.53	0.41
7:G:104:ASP:OD2	7:G:152:ARG:NH2	2.53	0.41
15:O:94:TYR:CD2	15:O:282:VAL:HG13	2.55	0.41
16:P:97:ARG:HE	16:P:97:ARG:HA	1.85	0.41
20:U:3:ALA:O	20:U:5:PRO:HD3	2.20	0.41
29:d:1:AME:OT	29:d:1:AME:CB	2.68	0.41
29:d:46:ASN:OD1	29:d:46:ASN:N	2.52	0.41
3:C:48:LEU:HD23	3:C:105:ILE:HD12	2.00	0.41
6:F:110:ILE:HD11	6:F:255:LEU:CD1	2.50	0.41
7:G:363:LEU:HD21	7:G:500:VAL:HG13	2.01	0.41
7:G:496:ILE:HG22	7:G:497:ALA:N	2.35	0.41
8:H:103:LEU:HB3	10:J:54:LEU:HD13	2.01	0.41
13:M:113:MET:HE2	13:M:177:LEU:HD11	2.01	0.41
13:M:432:ARG:NE	32:g:46:GLY:O	2.49	0.41
27:b:40:TYR:O	27:b:41:SER:C	2.63	0.41
29:d:106:LYS:NZ	41:p:77:GLN:OE1	2.46	0.41
30:e:70:LYS:O	30:e:74:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:l:40:ASP:OD1	37:l:40:ASP:N	2.52	0.41
42:q:91:HIS:HB2	42:q:93:MET:HE3	2.02	0.41
1:A:63:LEU:HD23	11:K:72:ALA:HB2	2.01	0.41
12:L:434:GLN:HB3	12:L:435:PRO:HD2	2.01	0.41
23:X:6:LEU:O	25:Z:87:ARG:NH2	2.54	0.41
27:b:62:MET:HE2	27:b:65:VAL:HG21	2.02	0.41
42:q:7:LEU:O	42:q:10:GLY:N	2.51	0.41
3:C:121:VAL:N	3:C:122:PRO:CD	2.83	0.41
5:E:172:ILE:HG23	5:E:182:PRO:CG	2.51	0.41
7:G:483:VAL:HG12	7:G:484:THR:N	2.35	0.41
11:K:12:PHE:O	11:K:15:SER:OG	2.33	0.41
12:L:40:ILE:HA	12:L:43:ALA:HB3	2.02	0.41
12:L:131:LEU:HD13	12:L:143:GLY:C	2.46	0.41
12:L:301:ILE:CG2	12:L:426:ILE:HD11	2.50	0.41
13:M:51:ASN:HA	13:M:57:PHE:HB2	2.02	0.41
13:M:63:THR:N	13:M:64:PRO:HD2	2.36	0.41
15:O:54:ALA:HB1	15:O:58:TYR:CB	2.49	0.41
20:T:78:ASP:N	20:T:78:ASP:OD1	2.52	0.41
41:p:48:ARG:O	41:p:52:GLU:N	2.46	0.41
2:B:47:PRO:HA	2:B:85:VAL:O	2.20	0.41
4:D:415:VAL:CG2	8:H:207:LEU:HD11	2.49	0.41
6:F:257:ASN:OD1	6:F:257:ASN:N	2.53	0.41
8:H:97:ASN:OD1	26:a:40:HIS:NE2	2.52	0.41
13:M:352:LEU:HD21	13:M:426:ILE:CG2	2.51	0.41
14:N:208:TYR:CZ	14:N:212:THR:HG21	2.56	0.41
21:V:25:ILE:HG22	21:V:29:LYS:HD3	2.03	0.41
39:n:34:ASP:OD1	39:n:35:LYS:N	2.53	0.41
42:q:145:LYS:HE2	42:q:145:LYS:HA	2.02	0.41
6:F:338:ASP:OD1	6:F:338:ASP:N	2.54	0.41
7:G:211:LYS:HB3	7:G:212:PRO:HD3	2.03	0.41
8:H:245:THR:HG1	8:H:262:LYS:HZ2	1.57	0.41
12:L:230:HIS:N	12:L:231:PRO:CD	2.83	0.41
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.03	0.41
14:N:137:ALA:HB3	14:N:138:PRO:HD3	2.03	0.41
18:R:49:VAL:HG12	18:R:50:SER:N	2.35	0.41
25:Z:142:TYR:O	25:Z:143:THR:OG1	2.26	0.41
41:p:156:ALA:O	41:p:160:GLN:N	2.49	0.41
1:A:30:TYR:O	1:A:31:SER:OG	2.34	0.41
5:E:103:CYS:SG	5:E:144:CYS:HA	2.60	0.41
9:I:51:PRO:O	9:I:54:LYS:NZ	2.48	0.41
15:O:19:THR:N	15:O:22:SER:OG	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:11:PRO:HD2	25:Z:15:TYR:CE2	2.55	0.41
37:l:128:VAL:HG12	40:o:98:MET:HG2	2.02	0.41
3:C:92:ILE:HG22	3:C:93:VAL:N	2.36	0.41
4:D:233:ARG:NH2	9:I:29:GLU:OE2	2.49	0.41
6:F:423:ARG:N	6:F:424:PRO:HD2	2.35	0.41
14:N:261:MET:N	14:N:262:PRO:HD2	2.36	0.41
16:P:200:THR:O	16:P:237:LEU:HD12	2.21	0.41
19:S:18:ILE:CD1	19:S:50:LEU:HD21	2.50	0.41
21:V:3:LEU:HD13	21:V:3:LEU:O	2.21	0.41
31:f:1:MET:HE3	31:f:1:MET:N	2.36	0.41
32:g:71:VAL:O	32:g:75:THR:OG1	2.34	0.41
38:m:1:SAC:H2A1	38:m:1:SAC:HA	1.90	0.41
3:C:100:ARG:NH2	21:V:78:GLU:OE1	2.53	0.41
3:C:114:LEU:HD23	22:W:80:LEU:CD1	2.50	0.41
3:C:193:GLU:OE2	7:G:223:ARG:NH2	2.54	0.41
3:C:211:GLN:OE1	21:V:112:LYS:NZ	2.48	0.41
4:D:106:LEU:HD11	4:D:391:ILE:HD13	2.02	0.41
6:F:184:TYR:CZ	49:F:502:FMN:HM73	2.56	0.41
7:G:103:LEU:HD12	7:G:103:LEU:N	2.36	0.41
9:I:18:THR:O	9:I:22:ALA:N	2.44	0.41
12:L:481:THR:OG1	40:o:91:HIS:ND1	2.52	0.41
13:M:373:ILE:HD11	13:M:444:LEU:CD1	2.51	0.41
14:N:208:TYR:OH	14:N:212:THR:HG21	2.21	0.41
14:N:260:PHE:CZ	14:N:264:TRP:HB2	2.56	0.41
15:O:25:ILE:HG22	15:O:26:THR:N	2.36	0.41
56:T:101:EHZ:O3	22:W:31:VAL:HG11	2.19	0.41
26:a:51:ASP:OD1	26:a:51:ASP:N	2.53	0.41
28:c:25:VAL:O	28:c:29:ILE:HG12	2.21	0.41
42:q:42:ASP:OD1	42:q:46:ASN:N	2.46	0.41
5:E:21:PHE:CG	5:E:22:ASP:N	2.88	0.41
5:E:156:ILE:HG22	5:E:157:ASN:ND2	2.36	0.41
6:F:306:LEU:HD12	6:F:306:LEU:O	2.21	0.41
7:G:607:ALA:CB	7:G:609:MET:HE1	2.51	0.41
8:H:236:ILE:HG23	8:H:259:PHE:HZ	1.85	0.41
13:M:6:ILE:N	13:M:7:PRO:HD2	2.36	0.41
14:N:198:PRO:HD2	29:d:1:AME:HT22	2.03	0.41
15:O:158:VAL:HG21	15:O:272:TYR:HB3	2.03	0.41
17:Q:63:GLU:OE1	22:W:125:HIS:ND1	2.54	0.41
39:n:39:PHE:HD1	39:n:42:LEU:HD12	1.86	0.41
40:o:66:LEU:O	40:o:69:LYS:N	2.54	0.41
3:C:53:HIS:CG	3:C:54:PRO:HD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:LEU:HD12	3:C:98:SER:H	1.86	0.40
13:M:140:THR:HG22	13:M:140:THR:O	2.21	0.40
16:P:115:GLN:O	16:P:116:ALA:C	2.64	0.40
16:P:203:GLN:N	16:P:291:ASP:OD2	2.36	0.40
20:T:74:GLN:NE2	20:T:78:ASP:OD1	2.54	0.40
20:U:45:LEU:O	20:U:45:LEU:HD23	2.20	0.40
8:H:110:SER:O	8:H:113:VAL:HG22	2.21	0.40
12:L:460:GLY:O	12:L:464:ALA:N	2.54	0.40
22:W:116:ASP:OD1	22:W:116:ASP:N	2.52	0.40
38:m:2:PHE:O	38:m:2:PHE:CD2	2.73	0.40
2:B:151:PRO:O	2:B:152:THR:C	2.65	0.40
2:B:152:THR:HG22	4:D:188:ARG:HD3	2.02	0.40
6:F:393:TRP:O	6:F:396:SER:OG	2.34	0.40
13:M:73:LEU:N	13:M:74:PRO:HD2	2.36	0.40
13:M:161:LEU:HD11	13:M:165:ILE:HD11	2.02	0.40
45:M:501:3PE:H291	29:d:54:LEU:HD22	2.02	0.40
14:N:102:LEU:HD11	14:N:141:VAL:HG11	2.03	0.40
15:O:8:TYR:OH	15:O:254:ARG:N	2.54	0.40
34:i:18:ARG:NH2	34:i:22:LEU:HD21	2.35	0.40
16:P:91:VAL:HG23	16:P:126:VAL:HG11	2.02	0.40
16:P:237:LEU:HD13	16:P:340:ILE:CD1	2.51	0.40
23:X:89:ASP:OD2	26:a:34:LYS:NZ	2.45	0.40
4:D:417:ILE:O	4:D:420:THR:HG22	2.21	0.40
7:G:344:CYS:HA	7:G:508:LYS:O	2.21	0.40
12:L:292:ALA:HA	12:L:295:GLN:HG2	2.03	0.40
14:N:296:LEU:HD23	14:N:296:LEU:C	2.47	0.40
16:P:278:TRP:CD1	16:P:278:TRP:N	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	100/115 (87%)	92 (92%)	8 (8%)	0	100	100
2	B	156/216 (72%)	141 (90%)	15 (10%)	0	100	100
3	C	208/266 (78%)	194 (93%)	14 (7%)	0	100	100
4	D	385/463 (83%)	363 (94%)	22 (6%)	0	100	100
5	E	212/249 (85%)	192 (91%)	20 (9%)	0	100	100
6	F	430/464 (93%)	402 (94%)	28 (6%)	0	100	100
7	G	687/727 (94%)	627 (91%)	60 (9%)	0	100	100
8	H	316/318 (99%)	291 (92%)	25 (8%)	0	100	100
9	I	174/212 (82%)	164 (94%)	10 (6%)	0	100	100
10	J	156/175 (89%)	140 (90%)	16 (10%)	0	100	100
11	K	84/98 (86%)	81 (96%)	2 (2%)	1 (1%)	10	40
12	L	545/606 (90%)	511 (94%)	33 (6%)	1 (0%)	43	73
13	M	457/459 (100%)	429 (94%)	28 (6%)	0	100	100
14	N	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
15	O	318/343 (93%)	302 (95%)	16 (5%)	0	100	100
16	P	314/380 (83%)	292 (93%)	22 (7%)	0	100	100
17	Q	123/175 (70%)	116 (94%)	7 (6%)	0	100	100
18	R	94/124 (76%)	90 (96%)	4 (4%)	0	100	100
19	S	85/99 (86%)	79 (93%)	6 (7%)	0	100	100
20	T	82/156 (53%)	74 (90%)	8 (10%)	0	100	100
20	U	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
21	V	111/116 (96%)	108 (97%)	3 (3%)	0	100	100
22	W	113/128 (88%)	103 (91%)	9 (8%)	1 (1%)	14	45
23	X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
24	Y	29/141 (21%)	27 (93%)	2 (7%)	0	100	100
25	Z	140/144 (97%)	136 (97%)	4 (3%)	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%)	42 (91%)	4 (9%)	0	100	100
29	d	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
30	e	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
31	f	55/57 (96%)	52 (94%)	3 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	g	88/154 (57%)	79 (90%)	9 (10%)	0	100	100
33	h	141/189 (75%)	130 (92%)	11 (8%)	0	100	100
34	i	125/128 (98%)	113 (90%)	11 (9%)	1 (1%)	16	48
35	j	68/108 (63%)	62 (91%)	6 (9%)	0	100	100
36	k	79/98 (81%)	73 (92%)	6 (8%)	0	100	100
37	l	154/186 (83%)	136 (88%)	18 (12%)	0	100	100
38	m	126/129 (98%)	116 (92%)	10 (8%)	0	100	100
39	n	169/179 (94%)	156 (92%)	12 (7%)	1 (1%)	21	54
40	o	118/137 (86%)	111 (94%)	7 (6%)	0	100	100
41	p	171/176 (97%)	165 (96%)	6 (4%)	0	100	100
42	q	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
43	r	92/113 (81%)	84 (91%)	8 (9%)	0	100	100
44	s	43/109 (39%)	39 (91%)	4 (9%)	0	100	100
All	All	7901/9213 (86%)	7371 (93%)	525 (7%)	5 (0%)	49	79

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	72	GLN
11	K	2	SER
34	i	37	GLN
22	W	95	VAL
39	n	31	ILE

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%)	88 (96%)	4 (4%)	26	50
2	B	134/175 (77%)	129 (96%)	5 (4%)	30	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	190/228 (83%)	186 (98%)	4 (2%)	47	64
4	D	334/392 (85%)	326 (98%)	8 (2%)	43	62
5	E	183/205 (89%)	176 (96%)	7 (4%)	29	53
6	F	345/368 (94%)	337 (98%)	8 (2%)	44	63
7	G	578/608 (95%)	563 (97%)	15 (3%)	40	60
8	H	274/274 (100%)	268 (98%)	6 (2%)	45	63
9	I	151/175 (86%)	146 (97%)	5 (3%)	33	56
10	J	127/141 (90%)	122 (96%)	5 (4%)	28	52
11	K	73/85 (86%)	72 (99%)	1 (1%)	59	70
12	L	479/533 (90%)	471 (98%)	8 (2%)	53	67
13	M	412/412 (100%)	405 (98%)	7 (2%)	53	67
14	N	315/315 (100%)	311 (99%)	4 (1%)	61	71
15	O	283/303 (93%)	276 (98%)	7 (2%)	42	61
16	P	276/327 (84%)	272 (99%)	4 (1%)	59	70
17	Q	112/153 (73%)	110 (98%)	2 (2%)	51	67
18	R	79/97 (81%)	76 (96%)	3 (4%)	29	53
19	S	77/82 (94%)	76 (99%)	1 (1%)	61	71
20	T	78/135 (58%)	77 (99%)	1 (1%)	61	71
20	U	81/135 (60%)	77 (95%)	4 (5%)	22	47
21	V	101/102 (99%)	98 (97%)	3 (3%)	36	57
22	W	108/114 (95%)	106 (98%)	2 (2%)	50	66
23	X	154/155 (99%)	149 (97%)	5 (3%)	34	56
24	Y	25/102 (24%)	24 (96%)	1 (4%)	28	52
25	Z	120/121 (99%)	116 (97%)	4 (3%)	33	56
26	a	59/59 (100%)	57 (97%)	2 (3%)	32	55
27	b	71/72 (99%)	70 (99%)	1 (1%)	59	70
28	c	44/68 (65%)	44 (100%)	0	100	100
29	d	105/105 (100%)	102 (97%)	3 (3%)	37	58
30	e	89/96 (93%)	84 (94%)	5 (6%)	19	45
31	f	54/54 (100%)	48 (89%)	6 (11%)	6	24
32	g	81/131 (62%)	80 (99%)	1 (1%)	63	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	h	124/158 (78%)	122 (98%)	2 (2%)	55	68
34	i	120/121 (99%)	114 (95%)	6 (5%)	22	47
35	j	61/84 (73%)	58 (95%)	3 (5%)	22	47
36	k	63/76 (83%)	63 (100%)	0	100	100
37	l	140/159 (88%)	137 (98%)	3 (2%)	47	64
38	m	113/114 (99%)	108 (96%)	5 (4%)	25	49
39	n	156/161 (97%)	154 (99%)	2 (1%)	61	71
40	o	109/120 (91%)	108 (99%)	1 (1%)	70	74
41	p	156/157 (99%)	152 (97%)	4 (3%)	40	60
42	q	130/130 (100%)	128 (98%)	2 (2%)	57	69
43	r	86/97 (89%)	85 (99%)	1 (1%)	63	72
44	s	44/92 (48%)	41 (93%)	3 (7%)	14	40
All	All	6986/7891 (88%)	6812 (98%)	174 (2%)	42	61

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	28	ASN
1	A	84	LEU
1	A	115	GLU
2	B	27	GLU
2	B	54	CYS
2	B	71	ARG
2	B	85	VAL
2	B	93	THR
3	C	109	THR
3	C	111	THR
3	C	112	ASP
3	C	114	LEU
4	D	47	LEU
4	D	71	GLU
4	D	95	THR
4	D	209	ASP
4	D	275	TYR
4	D	376	VAL
4	D	420	THR
4	D	429	ASP

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Mol	Chain	Res	Type
5	E	52	ASP
5	E	74	GLN
5	E	99	HIS
5	E	104	THR
5	E	106	THR
5	E	181	ILE
5	E	204	GLU
6	F	172	ASP
6	F	241	TRP
6	F	257	ASN
6	F	262	VAL
6	F	314	THR
6	F	318	ASP
6	F	359	CYS
6	F	405	CYS
7	G	14	ASP
7	G	110	GLN
7	G	139	ASP
7	G	156	CYS
7	G	209	THR
7	G	229	ASP
7	G	242	THR
7	G	326	GLU
7	G	357	ASP
7	G	366	THR
7	G	595	GLU
7	G	606	ILE
7	G	609	MET
7	G	617	ASP
7	G	634	ASP
8	H	8	MET
8	H	49	ILE
8	H	176	LEU
8	H	194	ASN
8	H	224	PHE
8	H	251	MET
9	I	47	THR
9	I	86	VAL
9	I	111	ILE
9	I	117	ILE
9	I	129	ASP
10	J	31	LEU

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Mol	Chain	Res	Type
10	J	72	THR
10	J	101	PHE
10	J	110	ASP
10	J	160	SER
11	K	46	LEU
12	L	62	ILE
12	L	123	LEU
12	L	149	ILE
12	L	249	SER
12	L	332	HIS
12	L	353	GLU
12	L	409	LEU
12	L	457	LEU
13	M	33	LEU
13	M	83	HIS
13	M	139	GLN
13	M	290	SER
13	M	294	MET
13	M	390	ASN
13	M	413	MET
14	N	49	ASN
14	N	62	THR
14	N	212	THR
14	N	228	LEU
15	O	1	LEU
15	O	85	ASP
15	O	158	VAL
15	O	163	TYR
15	O	252	ASN
15	O	279	LEU
15	O	290	ASP
16	P	87	HIS
16	P	136	ASN
16	P	170	GLU
16	P	278	TRP
17	Q	21	THR
17	Q	44	ASN
18	R	32	GLN
18	R	71	VAL
18	R	80	LYS
19	S	13	LEU
20	T	78	ASP

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Mol	Chain	Res	Type
20	U	39	ASP
20	U	43	ASP
20	U	60	PHE
20	U	65	ILE
21	V	3	LEU
21	V	15	VAL
21	V	95	GLN
22	W	14	THR
22	W	71	HIS
23	X	5	GLU
23	X	13	LYS
23	X	65	CYS
23	X	112	ASP
23	X	130	VAL
24	Y	140	VAL
25	Z	26	ARG
25	Z	42	LEU
25	Z	63	ASP
25	Z	65	GLU
26	a	54	VAL
26	a	68	ASN
27	b	14	LYS
29	d	16	ASP
29	d	28	ASP
29	d	103	GLU
30	e	66	LEU
30	e	85	LEU
30	e	86	ILE
30	e	90	LYS
30	e	96	HIS
31	f	1	MET
31	f	9	ASP
31	f	25	TYR
31	f	42	LEU
31	f	46	ARG
31	f	53	GLU
32	g	57	ASN
33	h	41	THR
33	h	43	ILE
34	i	11	LEU
34	i	24	ASP
34	i	34	LEU

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Mol	Chain	Res	Type
34	i	52	ASP
34	i	69	PHE
34	i	85	LEU
35	j	42	HIS
35	j	43	ASP
35	j	51	PHE
37	l	33	ASP
37	l	35	GLU
37	l	145	ASP
38	m	13	LEU
38	m	39	ARG
38	m	74	ASN
38	m	76	TYR
38	m	128	TYR
39	n	72	HIS
39	n	175	GLU
40	o	54	GLN
41	p	46	LEU
41	p	62	TYR
41	p	92	ARG
41	p	103	ASN
42	q	59	HIS
42	q	76	ASP
43	r	105	LEU
44	s	43	HIS
44	s	72	SER
44	s	75	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
3	C	102	ASN
4	D	231	ASN
5	E	37	ASN
5	E	150	ASN
6	F	361	GLN
6	F	421	HIS
7	G	7	ASN
7	G	179	ASN
7	G	402	ASN
7	G	517	ASN

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Mol	Chain	Res	Type
7	G	549	HIS
7	G	665	GLN
8	H	5	ASN
8	H	292	ASN
12	L	31	ASN
12	L	113	ASN
12	L	296	ASN
12	L	479	GLN
12	L	546	GLN
13	M	48	ASN
15	O	167	HIS
15	O	204	ASN
17	Q	29	HIS
19	S	61	GLN
19	S	79	ASN
20	U	35	HIS
23	X	34	GLN
25	Z	111	HIS
27	b	73	GLN
37	l	155	HIS
39	n	123	GLN
40	o	3	HIS
41	p	58	ASN
41	p	103	ASN
42	q	31	ASN
42	q	112	ASN
43	r	35	GLN
44	s	55	ASN
44	s	75	HIS

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	2 (33%)	6,8,10	1.27	1 (16%)
11	FME	K	1	11	8,9,10	1.55	1 (12%)	8,9,11	1.24	1 (12%)
4	2MR	D	85	4	10,12,13	2.44	2 (20%)	5,13,15	1.40	1 (20%)
38	SAC	m	1	38	7,8,9	1.75	1 (14%)	7,9,11	1.75	2 (28%)
42	AME	q	1	42	9,10,11	1.52	1 (11%)	9,11,13	1.40	1 (11%)
12	FME	L	1	12	8,9,10	1.52	1 (12%)	8,9,11	1.38	1 (12%)
10	FME	J	1	10	8,9,10	1.53	1 (12%)	8,9,11	1.30	0
29	AME	d	1	29	9,10,11	1.59	1 (11%)	9,11,13	1.30	0
34	SAC	i	1	34	7,8,9	1.74	1 (14%)	7,9,11	1.31	1 (14%)
13	FME	M	1	13	8,9,10	1.49	1 (12%)	8,9,11	1.54	2 (25%)
14	FME	N	1	14	8,9,10	1.51	1 (12%)	8,9,11	1.49	1 (12%)
43	AYA	r	1	43	6,7,8	1.88	1 (16%)	6,8,10	1.24	1 (16%)
1	FME	A	1	1	8,9,10	1.52	1 (12%)	8,9,11	1.39	2 (25%)
8	FME	H	1	8	8,9,10	1.52	1 (12%)	8,9,11	1.24	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	2/7/9/11	-
8	FME	H	1	8	-	0/7/9/11	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NH2	5.31	1.44	1.33
4	D	85	2MR	CZ-NE	5.13	1.45	1.34
11	K	1	FME	CN-N	3.91	1.46	1.33
10	J	1	FME	CN-N	3.83	1.45	1.33
8	H	1	FME	CN-N	3.80	1.45	1.33
1	A	1	FME	CN-N	3.79	1.45	1.33
29	d	1	AME	CT1-N	3.78	1.46	1.34
12	L	1	FME	CN-N	3.72	1.45	1.33
14	N	1	FME	CN-N	3.68	1.45	1.33
34	i	1	SAC	C1A-N	3.67	1.46	1.34
27	b	1	AYA	CT-N	3.66	1.46	1.34
38	m	1	SAC	C1A-N	3.60	1.46	1.34
13	M	1	FME	CN-N	3.57	1.45	1.33
42	q	1	AME	CT1-N	3.46	1.45	1.34
43	r	1	AYA	CT-N	3.45	1.45	1.34
27	b	1	AYA	OT-CT	-2.04	1.18	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	m	1	SAC	C2A-C1A-N	3.33	121.64	116.12
42	q	1	AME	CT2-CT1-N	2.50	120.26	116.12
1	A	1	FME	O1-CN-N	-2.41	119.09	125.32
27	b	1	AYA	CM-CT-N	2.35	120.01	116.12
4	D	85	2MR	CD-NE-CZ	-2.34	118.96	123.36
13	M	1	FME	CA-N-CN	-2.33	119.24	122.82
43	r	1	AYA	CM-CT-N	2.23	119.81	116.12
34	i	1	SAC	C2A-C1A-N	2.22	119.81	116.12
14	N	1	FME	O1-CN-N	-2.19	119.66	125.32
13	M	1	FME	O1-CN-N	-2.16	119.74	125.32
38	m	1	SAC	O-C-CA	-2.09	119.41	124.77
1	A	1	FME	CE-SD-CG	2.08	111.08	100.32
12	L	1	FME	O1-CN-N	-2.06	120.00	125.32
11	K	1	FME	O1-CN-N	-2.02	120.11	125.32

There are no chirality outliers.

All (28) torsion outliers are listed below:

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

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	FME	1	0
4	D	85	2MR	1	0
38	m	1	SAC	2	0
12	L	1	FME	1	0
29	d	1	AME	2	0
34	i	1	SAC	1	0
14	N	1	FME	1	0
8	H	1	FME	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
45	3PE	A	201	-	42,42,50	0.94	4 (9%)	45,47,55	1.15	2 (4%)
46	PC1	d	202	-	32,32,53	1.20	4 (12%)	38,40,61	1.10	2 (5%)
45	3PE	h	201	-	31,31,50	1.11	4 (12%)	34,36,55	1.15	2 (5%)
45	3PE	Y	601	-	38,38,50	0.99	4 (10%)	41,43,55	1.12	2 (4%)
57	CHD	i	201	-	32,32,32	3.27	11 (34%)	51,51,51	2.62	17 (33%)
45	3PE	d	201	-	48,48,50	0.89	4 (8%)	51,53,55	1.04	2 (3%)
46	PC1	H	401	-	42,42,53	1.06	4 (9%)	48,50,61	1.12	2 (4%)
46	PC1	A	202	-	49,49,53	0.99	4 (8%)	55,57,61	0.98	2 (3%)
45	3PE	J	201	-	38,38,50	0.99	4 (10%)	41,43,55	1.17	2 (4%)
51	CDL	q	201	-	59,59,99	1.13	7 (11%)	65,71,111	1.14	5 (7%)
47	SF4	G	803	7	0,12,12	-	-	-	-	-
49	FMN	F	502	-	33,33,33	2.73	10 (30%)	48,50,50	1.75	12 (25%)
45	3PE	M	501	-	37,37,50	1.00	4 (10%)	40,42,55	1.12	2 (5%)
46	PC1	H	402	-	36,36,53	1.15	4 (11%)	42,44,61	1.06	2 (4%)
45	3PE	D	501	-	50,50,50	0.88	3 (6%)	53,55,55	1.09	2 (3%)
47	SF4	B	201	2	0,12,12	-	-	-	-	-
45	3PE	Z	201	-	48,48,50	0.88	4 (8%)	51,53,55	1.07	2 (3%)
56	EHZ	U	101	20	31,36,37	1.58	5 (16%)	36,44,47	1.42	2 (5%)
48	FES	G	802	7	0,4,4	-	-	-	-	-
48	FES	E	301	5	0,4,4	-	-	-	-	-
47	SF4	F	501	6	0,12,12	-	-	-	-	-
45	3PE	I	203	-	32,32,50	1.08	3 (9%)	35,37,55	1.17	3 (8%)
51	CDL	N	402	-	72,72,99	1.03	8 (11%)	78,84,111	1.12	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	SF4	I	201	9	0,12,12	-	-	-		
52	DGT	O	401	53	32,33,33	3.38	14 (43%)	48,52,52	1.91	14 (29%)
47	SF4	I	202	9	0,12,12	-	-	-		
58	MYR	o	201	40	13,14,15	0.42	0	12,13,15	0.80	0
54	NDP	P	501	-	51,52,52	4.03	28 (54%)	71,80,80	1.99	14 (19%)
45	3PE	N	401	-	34,34,50	1.05	4 (11%)	37,39,55	1.13	2 (5%)
51	CDL	d	203	-	64,64,99	1.09	8 (12%)	70,76,111	1.08	4 (5%)
56	EHZ	T	101	20	31,36,37	1.61	5 (16%)	36,44,47	1.83	11 (30%)
46	PC1	B	202	-	50,50,53	0.99	4 (8%)	56,58,61	1.07	2 (3%)
51	CDL	X	201	-	78,78,99	0.99	8 (10%)	84,90,111	1.13	4 (4%)
47	SF4	G	804	7	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	A	201	-	-	15/46/46/54	-
46	PC1	d	202	-	-	10/36/36/57	-
45	3PE	h	201	-	-	15/35/35/54	-
45	3PE	Y	601	-	-	18/42/42/54	-
57	CHD	i	201	-	-	8/9/74/74	1/4/4/4
45	3PE	d	201	-	-	16/52/52/54	-
46	PC1	H	401	-	-	15/46/46/57	-
46	PC1	A	202	-	-	22/53/53/57	-
45	3PE	J	201	-	-	14/42/42/54	-
51	CDL	q	201	-	-	33/70/70/110	-
47	SF4	G	803	7	-	-	0/6/5/5
49	FMN	F	502	-	-	8/18/18/18	0/3/3/3
45	3PE	M	501	-	-	21/41/41/54	-
46	PC1	H	402	-	-	19/40/40/57	-
45	3PE	D	501	-	-	16/54/54/54	-
47	SF4	B	201	2	-	-	0/6/5/5
45	3PE	Z	201	-	-	21/52/52/54	-
56	EHZ	U	101	20	-	11/42/44/45	-
48	FES	G	802	7	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	FES	E	301	5	-	-	0/1/1/1
47	SF4	F	501	6	-	-	0/6/5/5
45	3PE	I	203	-	-	11/36/36/54	-
51	CDL	N	402	-	-	32/83/83/110	-
47	SF4	I	201	9	-	-	0/6/5/5
52	DGT	O	401	53	-	4/22/34/34	0/3/3/3
47	SF4	I	202	9	-	-	0/6/5/5
58	MYR	o	201	40	-	6/12/12/13	-
54	NDP	P	501	-	-	4/34/77/77	0/5/5/5
45	3PE	N	401	-	-	14/38/38/54	-
51	CDL	d	203	-	-	35/75/75/110	-
56	EHZ	T	101	20	-	14/42/44/45	-
46	PC1	B	202	-	-	19/54/54/57	-
51	CDL	X	201	-	-	42/89/89/110	-
47	SF4	G	804	7	-	-	0/6/5/5

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	501	NDP	PA-O3	10.31	1.70	1.59
54	P	501	NDP	C2B-C1B	-9.23	1.30	1.53
57	i	201	CHD	C11-C12	8.94	1.67	1.53
52	O	401	DGT	O6-C6	8.88	1.40	1.23
54	P	501	NDP	O4B-C1B	8.36	1.61	1.42
54	P	501	NDP	O4D-C1D	8.14	1.60	1.42
54	P	501	NDP	C7N-N7N	7.70	1.55	1.33
54	P	501	NDP	C2D-C1D	-7.38	1.30	1.53
54	P	501	NDP	C6N-C5N	7.20	1.55	1.33
57	i	201	CHD	C16-C15	7.12	1.73	1.54
54	P	501	NDP	O4D-C4D	-6.80	1.29	1.45
52	O	401	DGT	C5-N7	6.77	1.52	1.39
49	F	502	FMN	C10-N1	6.63	1.46	1.33
49	F	502	FMN	C4A-N5	6.42	1.44	1.30
57	i	201	CHD	C20-C17	-6.11	1.43	1.54
57	i	201	CHD	C13-C17	5.75	1.65	1.55
52	O	401	DGT	PA-O3A	5.66	1.65	1.59
54	P	501	NDP	P2B-O2B	5.58	1.69	1.59
52	O	401	DGT	PB-O3A	5.52	1.65	1.59
57	i	201	CHD	C8-C9	5.52	1.64	1.53
54	P	501	NDP	C6A-N6A	5.47	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	F	502	FMN	C5A-N5	5.46	1.49	1.39
52	O	401	DGT	PB-O3B	5.44	1.65	1.59
56	T	101	EHZ	C15-N2	5.40	1.46	1.33
57	i	201	CHD	O12-C12	-5.34	1.34	1.43
54	P	501	NDP	O4B-C4B	-5.22	1.33	1.45
49	F	502	FMN	C2-N1	5.11	1.48	1.36
56	U	101	EHZ	C12-N1	5.10	1.45	1.33
56	U	101	EHZ	C15-N2	5.05	1.45	1.33
56	T	101	EHZ	C12-N1	5.04	1.45	1.33
54	P	501	NDP	PN-O3	4.95	1.64	1.59
52	O	401	DGT	C2-N2	4.88	1.45	1.34
52	O	401	DGT	C2-N1	4.83	1.49	1.37
57	i	201	CHD	C6-C5	4.71	1.61	1.53
54	P	501	NDP	C2N-C3N	4.57	1.47	1.35
49	F	502	FMN	C9A-N10	4.50	1.49	1.41
49	F	502	FMN	C2-N3	4.47	1.48	1.39
54	P	501	NDP	C5A-C4A	-4.41	1.31	1.39
52	O	401	DGT	C2-N3	4.41	1.43	1.33
52	O	401	DGT	C8-N9	-4.09	1.28	1.37
54	P	501	NDP	O7N-C7N	-4.05	1.15	1.24
57	i	201	CHD	C15-C14	4.03	1.62	1.54
54	P	501	NDP	C8A-N9A	-3.82	1.31	1.37
54	P	501	NDP	O2D-C2D	3.77	1.52	1.43
52	O	401	DGT	C4-N9	-3.75	1.28	1.38
49	F	502	FMN	C4-N3	3.65	1.45	1.38
49	F	502	FMN	C10-N10	3.65	1.45	1.37
57	i	201	CHD	C6-C7	3.28	1.58	1.52
54	P	501	NDP	C4N-C3N	3.25	1.56	1.50
51	q	201	CDL	OB6-CB4	-3.02	1.39	1.46
51	q	201	CDL	OA6-CA4	-2.92	1.39	1.46
45	D	501	3PE	O21-C2	-2.90	1.39	1.46
54	P	501	NDP	C4N-C5N	2.88	1.56	1.49
45	I	203	3PE	O21-C2	-2.87	1.39	1.46
49	F	502	FMN	O2-C2	-2.84	1.18	1.24
49	F	502	FMN	O4-C4	-2.83	1.18	1.23
57	i	201	CHD	C13-C12	-2.81	1.50	1.54
51	N	402	CDL	OB6-CB4	-2.81	1.40	1.46
54	P	501	NDP	C5A-N7A	-2.77	1.34	1.39
51	N	402	CDL	OA6-CA4	-2.77	1.40	1.46
45	N	401	3PE	O21-C2	-2.76	1.40	1.46
46	A	202	PC1	O21-C2	-2.74	1.40	1.46
46	H	402	PC1	O21-C2	-2.71	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	d	202	PC1	O21-C2	-2.71	1.40	1.46
45	Y	601	3PE	O21-C2	-2.70	1.40	1.46
46	B	202	PC1	O21-C2	-2.70	1.40	1.46
51	X	201	CDL	OA6-CA4	-2.68	1.40	1.46
51	d	203	CDL	OA6-CA4	-2.66	1.40	1.46
45	h	201	3PE	O21-C2	-2.64	1.40	1.46
45	M	501	3PE	O21-C2	-2.64	1.40	1.46
51	X	201	CDL	OB6-CB4	-2.60	1.40	1.46
45	h	201	3PE	O31-C31	2.60	1.40	1.33
45	d	201	3PE	O21-C2	-2.60	1.40	1.46
46	H	401	PC1	O21-C2	-2.59	1.40	1.46
45	J	201	3PE	O21-C2	-2.56	1.40	1.46
45	A	201	3PE	O21-C2	-2.55	1.40	1.46
46	d	202	PC1	O31-C31	2.51	1.40	1.33
51	q	201	CDL	OB8-CB7	2.51	1.40	1.33
51	N	402	CDL	OB8-CB7	2.51	1.40	1.33
51	d	203	CDL	OB8-CB7	2.50	1.40	1.33
52	O	401	DGT	C1'-N9	-2.49	1.41	1.48
54	P	501	NDP	O3B-C3B	-2.49	1.36	1.43
51	d	203	CDL	OB6-CB4	-2.47	1.40	1.46
51	X	201	CDL	OB8-CB7	2.46	1.40	1.33
54	P	501	NDP	O3D-C3D	-2.46	1.36	1.43
54	P	501	NDP	C6N-N1N	2.43	1.43	1.37
54	P	501	NDP	PA-O5B	2.43	1.68	1.59
45	D	501	3PE	O31-C3	-2.42	1.39	1.45
45	Z	201	3PE	O21-C2	-2.42	1.40	1.46
45	I	203	3PE	O31-C31	2.41	1.40	1.33
56	T	101	EHZ	O3-C12	-2.41	1.18	1.23
56	U	101	EHZ	C9-S1	2.41	1.81	1.76
45	d	201	3PE	O31-C31	2.40	1.40	1.33
45	N	401	3PE	O31-C31	2.39	1.40	1.33
45	Z	201	3PE	O31-C31	2.39	1.40	1.33
46	H	402	PC1	O31-C31	2.37	1.40	1.33
56	U	101	EHZ	O4-C15	-2.37	1.18	1.23
51	N	402	CDL	OA8-CA7	2.36	1.40	1.33
45	A	201	3PE	O31-C31	2.36	1.40	1.33
54	P	501	NDP	C7N-C3N	2.36	1.53	1.48
46	B	202	PC1	O31-C31	2.35	1.40	1.33
56	T	101	EHZ	O4-C15	-2.35	1.18	1.23
51	d	203	CDL	OA8-CA7	2.34	1.40	1.33
46	B	202	PC1	O31-C3	-2.34	1.39	1.45
46	H	401	PC1	O31-C31	2.33	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	U	101	EHZ	O3-C12	-2.33	1.18	1.23
51	X	201	CDL	OA8-CA7	2.32	1.40	1.33
56	T	101	EHZ	C9-S1	2.31	1.81	1.76
51	q	201	CDL	OA8-CA7	2.30	1.40	1.33
46	A	202	PC1	O31-C31	2.30	1.40	1.33
51	d	203	CDL	OB6-CB5	2.30	1.40	1.34
45	M	501	3PE	O31-C31	2.29	1.40	1.33
45	D	501	3PE	O31-C31	2.29	1.40	1.33
54	P	501	NDP	P2B-O1X	2.28	1.57	1.50
51	N	402	CDL	OA8-CA6	-2.28	1.40	1.45
45	J	201	3PE	O31-C31	2.27	1.40	1.33
51	X	201	CDL	OA8-CA6	-2.26	1.40	1.45
52	O	401	DGT	PG-O1G	-2.25	1.46	1.54
51	q	201	CDL	OA8-CA6	-2.24	1.40	1.45
52	O	401	DGT	C4-N3	2.24	1.39	1.34
46	H	401	PC1	O31-C3	-2.24	1.40	1.45
45	Y	601	3PE	O31-C3	-2.23	1.40	1.45
46	B	202	PC1	O21-C21	2.23	1.40	1.34
54	P	501	NDP	C5B-C4B	2.23	1.58	1.51
46	A	202	PC1	O31-C3	-2.22	1.40	1.45
51	d	203	CDL	OA8-CA6	-2.22	1.40	1.45
52	O	401	DGT	PG-O2G	-2.22	1.46	1.54
45	J	201	3PE	O31-C3	-2.21	1.40	1.45
45	J	201	3PE	O21-C21	2.21	1.40	1.34
51	d	203	CDL	OB8-CB6	-2.21	1.40	1.45
45	Y	601	3PE	O31-C31	2.21	1.39	1.33
45	M	501	3PE	O31-C3	-2.20	1.40	1.45
45	d	201	3PE	O21-C21	2.20	1.40	1.34
51	X	201	CDL	OB6-CB5	2.19	1.40	1.34
45	A	201	3PE	O31-C3	-2.18	1.40	1.45
45	A	201	3PE	O21-C21	2.15	1.40	1.34
46	H	401	PC1	O21-C21	2.15	1.40	1.34
46	H	402	PC1	O21-C21	2.15	1.40	1.34
45	h	201	3PE	O21-C21	2.14	1.40	1.34
45	N	401	3PE	O31-C3	-2.14	1.40	1.45
45	I	203	3PE	O31-C3	-2.14	1.40	1.45
51	q	201	CDL	OB8-CB6	-2.13	1.40	1.45
46	H	402	PC1	O31-C3	-2.13	1.40	1.45
45	M	501	3PE	O21-C21	2.13	1.40	1.34
45	Z	201	3PE	O31-C3	-2.13	1.40	1.45
51	d	203	CDL	OA6-CA5	2.10	1.40	1.34
51	N	402	CDL	OB8-CB6	-2.10	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	d	202	PC1	O31-C3	-2.10	1.40	1.45
45	d	201	3PE	O31-C3	-2.09	1.40	1.45
45	h	201	3PE	O31-C3	-2.08	1.40	1.45
51	X	201	CDL	OA6-CA5	2.08	1.40	1.34
46	d	202	PC1	O21-C21	2.08	1.40	1.34
57	i	201	CHD	O7-C7	-2.08	1.39	1.43
51	X	201	CDL	OB8-CB6	-2.08	1.40	1.45
45	Z	201	3PE	O21-C21	2.08	1.40	1.34
45	Y	601	3PE	O21-C21	2.06	1.40	1.34
51	q	201	CDL	OA6-CA5	2.05	1.40	1.34
51	N	402	CDL	OA6-CA5	2.04	1.40	1.34
45	N	401	3PE	O21-C21	2.03	1.40	1.34
46	A	202	PC1	O21-C21	2.01	1.39	1.34
51	N	402	CDL	OB6-CB5	2.01	1.39	1.34
54	P	501	NDP	C5D-C4D	2.00	1.57	1.51

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	i	201	CHD	C17-C13-C14	8.37	108.51	100.11
57	i	201	CHD	C13-C17-C20	-8.07	109.71	119.48
52	O	401	DGT	C8-N9-C4	7.28	119.67	106.03
54	P	501	NDP	C4A-N9A-C1B	-5.77	113.13	126.63
54	P	501	NDP	N3A-C2A-N1A	-5.70	119.96	128.58
54	P	501	NDP	N6A-C6A-N1A	-5.60	105.91	118.38
56	T	101	EHZ	C8-C9-S1	5.32	120.27	113.56
54	P	501	NDP	C1B-N9A-C8A	5.25	138.75	127.09
57	i	201	CHD	C17-C13-C12	4.94	122.11	117.67
54	P	501	NDP	C5A-C4A-N3A	-4.82	120.08	126.72
49	F	502	FMN	C7M-C7-C6	4.71	127.87	119.57
49	F	502	FMN	C9-C8-C7	4.47	126.26	119.69
57	i	201	CHD	C16-C17-C13	4.42	107.83	103.54
45	M	501	3PE	O21-C21-C22	4.32	120.83	111.48
45	J	201	3PE	O21-C21-C22	4.26	120.69	111.48
56	U	101	EHZ	C8-C9-S1	4.25	118.92	113.56
51	X	201	CDL	OB6-CB5-C51	4.24	120.65	111.48
46	H	401	PC1	O21-C21-C22	4.21	120.58	111.48
57	i	201	CHD	C18-C13-C12	-4.17	104.88	109.06
57	i	201	CHD	C18-C13-C14	-4.17	104.67	111.20
45	D	501	3PE	O21-C21-C22	4.15	120.45	111.48
54	P	501	NDP	N9A-C8A-N7A	-4.13	108.07	113.94
45	Z	201	3PE	O21-C21-C22	4.13	120.42	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	X	201	CDL	OA6-CA5-C11	4.10	120.36	111.48
46	H	402	PC1	O21-C21-C22	4.10	120.34	111.48
54	P	501	NDP	C5A-C6A-N6A	4.08	133.39	123.29
45	Y	601	3PE	O21-C21-C22	4.08	120.31	111.48
46	B	202	PC1	O21-C21-C22	4.05	120.25	111.48
45	A	201	3PE	O21-C21-C22	4.05	120.24	111.48
51	N	402	CDL	OA6-CA5-C11	4.02	120.18	111.48
56	T	101	EHZ	C16-C15-N2	3.92	123.93	116.48
57	i	201	CHD	C18-C13-C17	-3.89	105.10	111.20
45	h	201	3PE	O21-C21-C22	3.89	119.89	111.48
46	A	202	PC1	O21-C21-C22	3.86	119.84	111.48
51	q	201	CDL	OA6-CA5-C11	3.86	119.83	111.48
46	d	202	PC1	O21-C21-C22	3.82	119.75	111.48
45	I	203	3PE	O21-C21-C22	3.79	119.69	111.48
45	d	201	3PE	O21-C21-C22	3.75	119.60	111.48
51	N	402	CDL	OB6-CB5-C51	3.74	119.58	111.48
45	N	401	3PE	O21-C21-C22	3.70	119.49	111.48
51	d	203	CDL	OA6-CA5-C11	3.69	119.46	111.48
57	i	201	CHD	C1-C10-C5	3.55	112.84	107.75
49	F	502	FMN	C4-N3-C2	-3.53	119.36	125.64
51	q	201	CDL	OB6-CB5-C51	3.48	119.01	111.48
54	P	501	NDP	C2A-N3A-C4A	3.45	120.26	111.83
52	O	401	DGT	C1'-N9-C8	-3.43	120.22	127.91
57	i	201	CHD	C5-C6-C7	-3.35	110.42	114.40
56	U	101	EHZ	C10-S1-C9	3.25	111.46	101.84
49	F	502	FMN	C8M-C8-C7	-3.23	114.16	120.76
56	T	101	EHZ	C14-C13-C12	-3.12	107.19	112.39
52	O	401	DGT	C2-N1-C6	-3.11	119.47	125.11
45	h	201	3PE	O31-C31-C32	3.06	121.17	111.83
57	i	201	CHD	C14-C8-C9	3.02	113.96	109.75
46	d	202	PC1	O31-C31-C32	2.99	120.94	111.83
45	A	201	3PE	O31-C31-C32	2.98	120.92	111.83
45	Y	601	3PE	O31-C31-C32	2.98	120.91	111.83
46	H	401	PC1	O31-C31-C32	2.97	120.90	111.83
52	O	401	DGT	C2'-C3'-C4'	2.97	108.83	102.80
52	O	401	DGT	O2G-PG-O3B	2.96	114.57	104.64
54	P	501	NDP	N3A-C4A-N9A	2.94	132.17	127.17
46	B	202	PC1	O31-C31-C32	2.90	120.67	111.83
57	i	201	CHD	C14-C13-C12	2.90	110.06	107.42
45	N	401	3PE	O31-C31-C32	2.88	120.61	111.83
56	T	101	EHZ	O2-C9-C8	-2.87	119.23	123.74
56	T	101	EHZ	C13-C12-N1	2.84	121.52	116.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	d	203	CDL	OB8-CB7-C71	2.83	120.48	111.83
51	X	201	CDL	OA8-CA7-C31	2.81	120.39	111.83
51	X	201	CDL	OB8-CB7-C71	2.80	120.39	111.83
45	J	201	3PE	O31-C31-C32	2.78	120.32	111.83
45	I	203	3PE	O31-C31-C32	2.74	120.18	111.83
54	P	501	NDP	C5A-N7A-C8A	2.74	107.75	103.45
51	q	201	CDL	OB8-CB7-C71	2.72	120.14	111.83
45	d	201	3PE	O31-C31-C32	2.72	120.13	111.83
49	F	502	FMN	C4A-C4-N3	2.69	120.10	113.25
54	P	501	NDP	C3N-C2N-N1N	-2.68	119.27	123.20
45	Z	201	3PE	O31-C31-C32	2.66	119.95	111.83
57	i	201	CHD	C23-C22-C20	-2.66	109.49	114.46
52	O	401	DGT	O1G-PG-O3B	2.66	113.55	104.64
49	F	502	FMN	O4-C4-C4A	-2.65	119.55	126.53
51	d	203	CDL	OA8-CA7-C31	2.64	119.88	111.83
51	N	402	CDL	OB8-CB7-C71	2.64	119.87	111.83
46	H	402	PC1	O31-C31-C32	2.63	119.86	111.83
49	F	502	FMN	C5A-C9A-N10	2.59	120.31	117.97
45	D	501	3PE	O31-C31-C32	2.56	119.64	111.83
52	O	401	DGT	O1B-PB-O2B	-2.56	100.55	112.44
51	N	402	CDL	OA8-CA7-C31	2.55	119.60	111.83
51	q	201	CDL	OA8-CA7-C31	2.54	119.57	111.83
57	i	201	CHD	C15-C14-C8	2.50	121.78	118.36
45	M	501	3PE	O31-C31-C32	2.50	119.45	111.83
57	i	201	CHD	C13-C14-C8	-2.50	111.55	114.72
49	F	502	FMN	C4A-C10-N10	2.49	120.05	116.48
52	O	401	DGT	O1A-PA-O2A	-2.48	100.91	112.44
46	A	202	PC1	O31-C31-C32	2.47	119.38	111.83
52	O	401	DGT	C5-C6-N1	2.47	119.54	113.25
49	F	502	FMN	C9A-C5A-N5	-2.46	119.84	122.45
51	d	203	CDL	OB6-CB5-C51	2.46	119.96	110.93
49	F	502	FMN	C6-C7-C8	-2.44	116.10	119.69
54	P	501	NDP	P2B-O2B-C2B	-2.44	116.92	123.43
57	i	201	CHD	C11-C9-C8	2.40	114.44	110.89
56	T	101	EHZ	O4-C15-N2	-2.38	117.95	122.98
56	T	101	EHZ	C19-C17-C16	2.35	112.78	108.77
52	O	401	DGT	O6-C6-C5	-2.33	120.38	126.53
49	F	502	FMN	C7M-C7-C8	-2.32	116.03	120.76
54	P	501	NDP	C3D-C2D-C1D	2.29	105.80	101.46
56	T	101	EHZ	C10-S1-C9	2.29	108.60	101.84
57	i	201	CHD	C11-C9-C10	-2.27	111.40	113.70
54	P	501	NDP	C4A-N9A-C8A	2.27	108.12	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	I	203	3PE	C2-O21-C21	-2.22	112.47	117.80
49	F	502	FMN	C10-C4A-N5	-2.16	120.40	124.81
57	i	201	CHD	C1-C10-C9	-2.15	108.00	111.34
52	O	401	DGT	N9-C4-N3	2.12	130.19	125.95
52	O	401	DGT	C5-C4-N9	-2.11	101.87	105.66
56	T	101	EHZ	O3-C12-N1	-2.10	118.90	123.03
51	q	201	CDL	CA4-OA6-CA5	-2.03	112.95	117.80
52	O	401	DGT	C6-C5-N7	2.03	133.98	130.29
56	T	101	EHZ	C11-N1-C12	-2.01	119.08	122.82
56	T	101	EHZ	C7-C8-C9	-2.01	109.38	113.86
52	O	401	DGT	C1'-N9-C4	-2.00	120.10	125.50

There are no chirality outliers.

All (443) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	D	501	3PE	C1-O11-P-O12
45	D	501	3PE	C1-O11-P-O13
45	D	501	3PE	C11-O13-P-O11
45	D	501	3PE	C11-O13-P-O12
45	D	501	3PE	C11-O13-P-O14
45	D	501	3PE	O11-C1-C2-O21
45	I	203	3PE	O11-C1-C2-O21
45	I	203	3PE	O32-C31-O31-C3
45	I	203	3PE	C22-C21-O21-C2
45	J	201	3PE	C1-O11-P-O13
45	J	201	3PE	C11-O13-P-O11
45	J	201	3PE	C11-O13-P-O14
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	C1-O11-P-O14
45	M	501	3PE	C11-O13-P-O11
45	M	501	3PE	C11-O13-P-O14
45	M	501	3PE	C22-C21-O21-C2
45	N	401	3PE	C11-O13-P-O11
45	N	401	3PE	C11-O13-P-O14
45	N	401	3PE	O22-C21-O21-C2
45	Y	601	3PE	C1-O11-P-O12
45	Y	601	3PE	C1-O11-P-O13
45	Y	601	3PE	C11-O13-P-O11
45	Z	201	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
45	Z	201	3PE	C22-C21-O21-C2
45	d	201	3PE	C11-O13-P-O11
45	d	201	3PE	C11-O13-P-O12
45	d	201	3PE	C11-O13-P-O14
45	d	201	3PE	C12-C11-O13-P
46	A	202	PC1	C11-O13-P-O12
46	A	202	PC1	C11-O13-P-O11
46	A	202	PC1	C1-O11-P-O12
46	A	202	PC1	C1-O11-P-O14
46	A	202	PC1	C1-O11-P-O13
46	A	202	PC1	O13-C11-C12-N
46	A	202	PC1	O21-C2-C3-O31
46	B	202	PC1	C11-O13-P-O14
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C22-C21-O21-C2
46	H	401	PC1	C1-O11-P-O12
46	H	401	PC1	C1-O11-P-O14
46	H	401	PC1	C22-C21-O21-C2
46	H	402	PC1	C1-O11-P-O14
46	d	202	PC1	C1-O11-P-O12
46	d	202	PC1	C1-O11-P-O14
46	d	202	PC1	C1-O11-P-O13
49	F	502	FMN	N10-C1'-C2'-O2'
49	F	502	FMN	N10-C1'-C2'-C3'
51	N	402	CDL	CA3-OA5-PA1-OA4
51	N	402	CDL	CB2-OB2-PB2-OB5
51	N	402	CDL	CB3-OB5-PB2-OB2
51	X	201	CDL	CA2-OA2-PA1-OA3
51	X	201	CDL	CA2-OA2-PA1-OA5
51	X	201	CDL	CB3-OB5-PB2-OB2
51	X	201	CDL	CB3-OB5-PB2-OB4
51	X	201	CDL	C51-CB5-OB6-CB4
51	d	203	CDL	CA2-OA2-PA1-OA4
51	d	203	CDL	CA2-OA2-PA1-OA5
51	d	203	CDL	CA3-OA5-PA1-OA2
51	d	203	CDL	CA3-OA5-PA1-OA3
51	d	203	CDL	C11-CA5-OA6-CA4
51	d	203	CDL	CB2-OB2-PB2-OB4
51	d	203	CDL	C51-CB5-OB6-CB4
51	q	201	CDL	O1-C1-CA2-OA2
51	q	201	CDL	C11-CA5-OA6-CA4
51	q	201	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
51	q	201	CDL	CB2-OB2-PB2-OB5
51	q	201	CDL	CB3-OB5-PB2-OB2
51	q	201	CDL	CB3-OB5-PB2-OB3
51	q	201	CDL	OB5-CB3-CB4-OB6
54	P	501	NDP	O4D-C1D-N1N-C6N
54	P	501	NDP	C2N-C3N-C7N-N7N
56	T	101	EHZ	C5-C6-C7-O1
56	T	101	EHZ	C5-C6-C7-C8
56	T	101	EHZ	C12-C13-C14-N2
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	T	101	EHZ	O2-C9-S1-C10
56	T	101	EHZ	C8-C9-S1-C10
56	U	101	EHZ	C6-C7-C8-C9
56	U	101	EHZ	S1-C10-C11-N1
56	U	101	EHZ	C11-C10-S1-C9
56	U	101	EHZ	O2-C9-S1-C10
56	U	101	EHZ	C8-C9-S1-C10
57	i	201	CHD	C13-C17-C20-C21
57	i	201	CHD	C13-C17-C20-C22
57	i	201	CHD	C16-C17-C20-C22
58	o	201	MYR	C1-C2-C3-C4
45	h	201	3PE	O32-C31-O31-C3
46	H	402	PC1	O32-C31-O31-C3
46	d	202	PC1	O32-C31-O31-C3
45	h	201	3PE	C32-C31-O31-C3
46	d	202	PC1	C32-C31-O31-C3
46	H	401	PC1	O32-C31-O31-C3
57	i	201	CHD	C16-C17-C20-C21
45	J	201	3PE	O32-C31-O31-C3
45	I	203	3PE	O22-C21-O21-C2
45	J	201	3PE	O22-C21-O21-C2
45	Z	201	3PE	O22-C21-O21-C2
46	B	202	PC1	O22-C21-O21-C2
46	H	401	PC1	O22-C21-O21-C2
46	H	402	PC1	O22-C21-O21-C2
51	X	201	CDL	OB7-CB5-OB6-CB4
51	d	203	CDL	OA7-CA5-OA6-CA4
51	d	203	CDL	OB7-CB5-OB6-CB4
51	q	201	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
45	I	203	3PE	C32-C31-O31-C3
46	B	202	PC1	C32-C31-O31-C3
46	H	401	PC1	C32-C31-O31-C3
46	H	402	PC1	C32-C31-O31-C3
45	N	401	3PE	C22-C21-O21-C2
46	H	402	PC1	C22-C21-O21-C2
45	J	201	3PE	C32-C31-O31-C3
45	N	401	3PE	O32-C31-O31-C3
45	M	501	3PE	O22-C21-O21-C2
51	q	201	CDL	O1-C1-CB2-OB2
45	N	401	3PE	C32-C31-O31-C3
45	d	201	3PE	C32-C31-O31-C3
51	N	402	CDL	C31-CA7-OA8-CA6
46	B	202	PC1	O32-C31-O31-C3
56	T	101	EHZ	O4-C15-N2-C14
51	d	203	CDL	C71-CB7-OB8-CB6
45	d	201	3PE	O32-C31-O31-C3
51	N	402	CDL	OA9-CA7-OA8-CA6
57	i	201	CHD	C17-C20-C22-C23
51	d	203	CDL	OB9-CB7-OB8-CB6
51	q	201	CDL	C51-CB5-OB6-CB4
57	i	201	CHD	C21-C20-C22-C23
51	q	201	CDL	CB2-C1-CA2-OA2
51	X	201	CDL	C31-CA7-OA8-CA6
51	X	201	CDL	C71-CB7-OB8-CB6
51	q	201	CDL	C71-CB7-OB8-CB6
51	X	201	CDL	OA9-CA7-OA8-CA6
51	X	201	CDL	OB9-CB7-OB8-CB6
45	Y	601	3PE	O21-C2-C3-O31
51	q	201	CDL	OB6-CB4-CB6-OB8
51	N	402	CDL	C71-CB7-OB8-CB6
51	d	203	CDL	CA5-C11-C12-C13
51	q	201	CDL	CB5-C51-C52-C53
49	F	502	FMN	O3'-C3'-C4'-C5'
49	F	502	FMN	C2'-C3'-C4'-C5'
51	d	203	CDL	CB7-C71-C72-C73
46	H	402	PC1	C21-C22-C23-C24
51	X	201	CDL	CB5-C51-C52-C53
51	X	201	CDL	CB7-C71-C72-C73
51	q	201	CDL	OB9-CB7-OB8-CB6
51	q	201	CDL	OB7-CB5-OB6-CB4
45	D	501	3PE	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
45	A	201	3PE	C32-C31-O31-C3
51	d	203	CDL	CB4-CB3-OB5-PB2
45	Z	201	3PE	C1-C2-O21-C21
51	N	402	CDL	OB9-CB7-OB8-CB6
49	F	502	FMN	C2'-C3'-C4'-O4'
45	M	501	3PE	C32-C31-O31-C3
45	M	501	3PE	C23-C24-C25-C26
45	d	201	3PE	C2E-C2F-C2G-C2H
45	h	201	3PE	C26-C27-C28-C29
45	D	501	3PE	C33-C34-C35-C36
45	d	201	3PE	C2B-C2C-C2D-C2E
51	N	402	CDL	C20-C21-C22-C23
58	o	201	MYR	C4-C5-C6-C7
45	D	501	3PE	C24-C25-C26-C27
45	D	501	3PE	O32-C31-O31-C3
45	Z	201	3PE	C29-C2A-C2B-C2C
51	X	201	CDL	C20-C21-C22-C23
51	d	203	CDL	C76-C77-C78-C79
45	N	401	3PE	C21-C22-C23-C24
45	A	201	3PE	C32-C33-C34-C35
46	A	202	PC1	C24-C25-C26-C27
51	N	402	CDL	C34-C35-C36-C37
51	X	201	CDL	C61-C62-C63-C64
45	J	201	3PE	C35-C36-C37-C38
45	N	401	3PE	C25-C26-C27-C28
45	A	201	3PE	O32-C31-O31-C3
51	X	201	CDL	C72-C73-C74-C75
46	H	402	PC1	C35-C36-C37-C38
45	J	201	3PE	C27-C28-C29-C2A
51	q	201	CDL	CB7-C71-C72-C73
51	X	201	CDL	C60-C61-C62-C63
51	N	402	CDL	CA7-C31-C32-C33
46	A	202	PC1	C3A-C3B-C3C-C3D
45	M	501	3PE	O32-C31-O31-C3
51	N	402	CDL	C54-C55-C56-C57
51	N	402	CDL	C38-C39-C40-C41
51	X	201	CDL	C59-C60-C61-C62
45	Y	601	3PE	C22-C21-O21-C2
45	d	201	3PE	C22-C21-O21-C2
51	N	402	CDL	C51-CB5-OB6-CB4
51	X	201	CDL	C11-CA5-OA6-CA4
51	q	201	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
45	Y	601	3PE	O22-C21-O21-C2
51	N	402	CDL	OB7-CB5-OB6-CB4
46	H	401	PC1	C26-C27-C28-C29
56	T	101	EHZ	C1-C2-C3-C4
51	d	203	CDL	C71-C72-C73-C74
45	Y	601	3PE	C32-C33-C34-C35
45	h	201	3PE	C23-C24-C25-C26
46	B	202	PC1	C36-C37-C38-C39
45	d	201	3PE	O22-C21-O21-C2
46	B	202	PC1	O11-C1-C2-O21
45	Z	201	3PE	C34-C35-C36-C37
51	X	201	CDL	CA7-C31-C32-C33
45	A	201	3PE	C23-C24-C25-C26
45	M	501	3PE	C2-C1-O11-P
51	X	201	CDL	OA7-CA5-OA6-CA4
51	q	201	CDL	CA2-C1-CB2-OB2
45	Z	201	3PE	C23-C24-C25-C26
51	d	203	CDL	C42-C43-C44-C45
45	Y	601	3PE	O11-C1-C2-C3
45	h	201	3PE	O11-C1-C2-C3
46	A	202	PC1	O11-C1-C2-C3
46	B	202	PC1	O11-C1-C2-C3
51	d	203	CDL	OB5-CB3-CB4-CB6
49	F	502	FMN	O3'-C3'-C4'-O4'
46	d	202	PC1	C31-C32-C33-C34
52	O	401	DGT	O4'-C4'-C5'-O5'
45	M	501	3PE	C31-C32-C33-C34
46	H	401	PC1	C23-C24-C25-C26
51	X	201	CDL	C75-C76-C77-C78
51	q	201	CDL	CA3-CA4-CA6-OA8
45	J	201	3PE	C24-C25-C26-C27
51	X	201	CDL	C12-C13-C14-C15
45	Y	601	3PE	C26-C27-C28-C29
51	q	201	CDL	C16-C17-C18-C19
51	X	201	CDL	CB6-CB4-OB6-CB5
46	H	401	PC1	C29-C2A-C2B-C2C
51	N	402	CDL	C71-C72-C73-C74
51	d	203	CDL	C44-C45-C46-C47
45	D	501	3PE	C3A-C3B-C3C-C3D
45	M	501	3PE	C36-C37-C38-C39
45	Z	201	3PE	C3B-C3C-C3D-C3E
58	o	201	MYR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
45	d	201	3PE	C33-C34-C35-C36
46	A	202	PC1	C37-C38-C39-C3A
56	U	101	EHZ	C3-C4-C5-C6
49	F	502	FMN	C4'-C5'-O5'-P
51	d	203	CDL	C1-CB2-OB2-PB2
45	M	501	3PE	O11-C1-C2-C3
51	N	402	CDL	C11-CA5-OA6-CA4
46	A	202	PC1	C39-C3A-C3B-C3C
45	Y	601	3PE	C1-C2-C3-O31
46	d	202	PC1	C1-C2-C3-O31
51	N	402	CDL	CB3-CB4-CB6-OB8
51	q	201	CDL	CB3-CB4-CB6-OB8
45	A	201	3PE	C35-C36-C37-C38
45	D	501	3PE	C29-C2A-C2B-C2C
45	A	201	3PE	O11-C1-C2-O21
45	M	501	3PE	O11-C1-C2-O21
45	Y	601	3PE	O11-C1-C2-O21
46	H	402	PC1	O11-C1-C2-O21
51	N	402	CDL	C1-CA2-OA2-PA1
51	X	201	CDL	C1-CA2-OA2-PA1
45	I	203	3PE	C24-C25-C26-C27
56	U	101	EHZ	O1-C7-C8-C9
45	J	201	3PE	C23-C24-C25-C26
51	q	201	CDL	OA6-CA4-CA6-OA8
45	D	501	3PE	C23-C24-C25-C26
46	B	202	PC1	C29-C2A-C2B-C2C
46	H	402	PC1	C23-C24-C25-C26
46	H	401	PC1	C33-C34-C35-C36
45	M	501	3PE	C29-C2A-C2B-C2C
56	T	101	EHZ	C3-C4-C5-C6
45	A	201	3PE	O11-C1-C2-C3
45	D	501	3PE	O11-C1-C2-C3
45	I	203	3PE	O11-C1-C2-C3
51	X	201	CDL	OA5-CA3-CA4-CA6
51	q	201	CDL	OB5-CB3-CB4-CB6
51	d	203	CDL	C33-C34-C35-C36
45	M	501	3PE	C2B-C2C-C2D-C2E
45	M	501	3PE	C3-C2-O21-C21
51	N	402	CDL	OA7-CA5-OA6-CA4
45	N	401	3PE	O11-C1-C2-O21
46	A	202	PC1	O11-C1-C2-O21
51	X	201	CDL	OA5-CA3-CA4-OA6

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Mol	Chain	Res	Type	Atoms
45	Z	201	3PE	C1-C2-C3-O31
46	A	202	PC1	C1-C2-C3-O31
45	A	201	3PE	C12-C11-O13-P
45	Z	201	3PE	C12-C11-O13-P
56	U	101	EHZ	C2-C1-C21-C22
46	H	402	PC1	O21-C2-C3-O31
46	d	202	PC1	O21-C2-C3-O31
51	N	402	CDL	OB6-CB4-CB6-OB8
51	N	402	CDL	C56-C57-C58-C59
46	B	202	PC1	C39-C3A-C3B-C3C
51	q	201	CDL	C72-C73-C74-C75
45	h	201	3PE	C27-C28-C29-C2A
46	B	202	PC1	C32-C33-C34-C35
52	O	401	DGT	C3'-C4'-C5'-O5'
46	A	202	PC1	C32-C31-O31-C3
45	d	201	3PE	C27-C28-C29-C2A
46	H	402	PC1	O13-C11-C12-N
54	P	501	NDP	PN-O3-PA-O2A
56	U	101	EHZ	C2-C3-C4-C5
51	X	201	CDL	C74-C75-C76-C77
45	D	501	3PE	C37-C38-C39-C3A
45	Y	601	3PE	C25-C26-C27-C28
45	Z	201	3PE	C26-C27-C28-C29
51	q	201	CDL	C31-C32-C33-C34
46	A	202	PC1	O32-C31-O31-C3
56	T	101	EHZ	C11-C10-S1-C9
45	h	201	3PE	O11-C1-C2-O21
51	d	203	CDL	OB5-CB3-CB4-OB6
51	d	203	CDL	C74-C75-C76-C77
54	P	501	NDP	C2N-C3N-C7N-O7N
51	d	203	CDL	C36-C37-C38-C39
45	h	201	3PE	O21-C2-C3-O31
51	d	203	CDL	OA6-CA4-CA6-OA8
46	H	402	PC1	C1-C2-C3-O31
51	d	203	CDL	CA3-CA4-CA6-OA8
51	N	402	CDL	C31-C32-C33-C34
45	J	201	3PE	C32-C33-C34-C35
45	A	201	3PE	C1-O11-P-O12
45	A	201	3PE	C1-O11-P-O13
45	A	201	3PE	C1-O11-P-O14
45	I	203	3PE	O13-C11-C12-N
45	J	201	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
45	N	401	3PE	C11-O13-P-O12
45	Y	601	3PE	C11-O13-P-O12
45	Z	201	3PE	C11-O13-P-O11
46	H	401	PC1	C1-O11-P-O13
51	N	402	CDL	CA3-OA5-PA1-OA2
51	N	402	CDL	CA3-OA5-PA1-OA3
51	N	402	CDL	CB2-OB2-PB2-OB3
51	X	201	CDL	CA2-OA2-PA1-OA4
51	X	201	CDL	CA3-OA5-PA1-OA2
51	X	201	CDL	CA3-OA5-PA1-OA3
51	X	201	CDL	CA3-OA5-PA1-OA4
51	d	203	CDL	CB2-OB2-PB2-OB5
51	d	203	CDL	CB3-OB5-PB2-OB2
51	d	203	CDL	CB3-OB5-PB2-OB3
52	O	401	DGT	C5'-O5'-PA-O2A
45	N	401	3PE	C32-C33-C34-C35
45	D	501	3PE	C2C-C2D-C2E-C2F
51	d	203	CDL	CA4-CA3-OA5-PA1
46	H	401	PC1	C2B-C2C-C2D-C2E
58	o	201	MYR	C11-C10-C9-C8
51	d	203	CDL	CB6-CB4-OB6-CB5
46	H	402	PC1	O11-C1-C2-C3
46	B	202	PC1	C27-C28-C29-C2A
46	A	202	PC1	C33-C34-C35-C36
45	A	201	3PE	C28-C29-C2A-C2B
51	q	201	CDL	CA5-C11-C12-C13
52	O	401	DGT	PB-O3A-PA-O2A
51	N	402	CDL	C52-C51-CB5-OB6
45	M	501	3PE	C33-C34-C35-C36
51	d	203	CDL	C52-C51-CB5-OB6
46	B	202	PC1	C3E-C3F-C3G-C3H
45	N	401	3PE	O11-C1-C2-C3
45	d	201	3PE	C29-C2A-C2B-C2C
46	A	202	PC1	C3E-C3F-C3G-C3H
51	X	201	CDL	O1-C1-CA2-OA2
51	N	402	CDL	C13-C14-C15-C16
45	Z	201	3PE	C2C-C2D-C2E-C2F
51	d	203	CDL	C34-C35-C36-C37
45	M	501	3PE	C26-C27-C28-C29
45	Z	201	3PE	C22-C23-C24-C25
45	d	201	3PE	C24-C25-C26-C27
56	T	101	EHZ	C1-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
56	U	101	EHZ	C21-C22-C23-C24
45	Z	201	3PE	C35-C36-C37-C38
46	H	402	PC1	C24-C25-C26-C27
51	d	203	CDL	C41-C42-C43-C44
45	h	201	3PE	C28-C29-C2A-C2B
45	Y	601	3PE	C24-C25-C26-C27
51	X	201	CDL	C13-C14-C15-C16
45	Y	601	3PE	C2-C1-O11-P
51	q	201	CDL	C18-C19-C20-C21
45	Y	601	3PE	O21-C21-C22-C23
45	I	203	3PE	C23-C24-C25-C26
51	N	402	CDL	CA2-C1-CB2-OB2
51	q	201	CDL	C32-C31-CA7-OA8
45	I	203	3PE	C32-C33-C34-C35
51	X	201	CDL	C54-C55-C56-C57
45	N	401	3PE	C2A-C2B-C2C-C2D
45	h	201	3PE	C1-C2-C3-O31
46	H	402	PC1	C22-C23-C24-C25
58	o	201	MYR	C6-C7-C8-C9
46	B	202	PC1	C28-C29-C2A-C2B
45	A	201	3PE	C27-C28-C29-C2A
45	Z	201	3PE	C2E-C2F-C2G-C2H
51	X	201	CDL	CB2-C1-CA2-OA2
46	H	402	PC1	C26-C27-C28-C29
51	X	201	CDL	C31-C32-C33-C34
45	I	203	3PE	C25-C26-C27-C28
46	A	202	PC1	C38-C39-C3A-C3B
51	q	201	CDL	C19-C20-C21-C22
45	d	201	3PE	O31-C31-C32-C33
51	d	203	CDL	C52-C51-CB5-OB7
49	F	502	FMN	C5'-O5'-P-O2P
45	A	201	3PE	O21-C21-C22-C23
51	N	402	CDL	CA5-C11-C12-C13
57	i	201	CHD	C22-C23-C24-O26
57	i	201	CHD	C22-C23-C24-O25
45	Z	201	3PE	C39-C3A-C3B-C3C
56	U	101	EHZ	C10-C11-N1-C12
51	X	201	CDL	C57-C58-C59-C60
45	M	501	3PE	C12-C11-O13-P
45	h	201	3PE	C12-C11-O13-P
46	H	401	PC1	C2E-C2F-C2G-C2H
51	X	201	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
51	X	201	CDL	C12-C11-CA5-OA6
46	d	202	PC1	C35-C36-C37-C38
45	A	201	3PE	C33-C34-C35-C36
45	d	201	3PE	C3B-C3C-C3D-C3E
46	H	401	PC1	O21-C21-C22-C23
45	J	201	3PE	C25-C26-C27-C28
46	H	402	PC1	O21-C21-C22-C23
46	B	202	PC1	O31-C31-C32-C33
51	N	402	CDL	C32-C31-CA7-OA8
45	h	201	3PE	O21-C21-C22-C23
46	A	202	PC1	O21-C21-C22-C23
46	A	202	PC1	C29-C2A-C2B-C2C
51	N	402	CDL	O1-C1-CB2-OB2
51	X	201	CDL	C52-C51-CB5-OB6
51	q	201	CDL	C72-C71-CB7-OB8
45	N	401	3PE	C2-C1-O11-P
51	X	201	CDL	C12-C11-CA5-OA7
45	h	201	3PE	O31-C31-C32-C33
46	H	402	PC1	O22-C21-C22-C23
51	N	402	CDL	C32-C31-CA7-OA9
46	H	402	PC1	C37-C38-C39-C3A
46	B	202	PC1	O32-C31-C32-C33
45	Y	601	3PE	C33-C34-C35-C36
45	Y	601	3PE	C2D-C2E-C2F-C2G
45	Z	201	3PE	O21-C2-C3-O31
51	X	201	CDL	C32-C33-C34-C35
45	Z	201	3PE	C2D-C2E-C2F-C2G
46	B	202	PC1	C21-C22-C23-C24
45	h	201	3PE	O22-C21-C22-C23
46	d	202	PC1	C36-C37-C38-C39
46	A	202	PC1	O31-C31-C32-C33
46	H	401	PC1	O22-C21-C22-C23
45	h	201	3PE	O32-C31-C32-C33
51	q	201	CDL	C72-C71-CB7-OB9
46	B	202	PC1	O21-C21-C22-C23
45	Z	201	3PE	C3A-C3B-C3C-C3D
58	o	201	MYR	C2-C3-C4-C5
51	q	201	CDL	C12-C13-C14-C15
45	Z	201	3PE	C32-C33-C34-C35

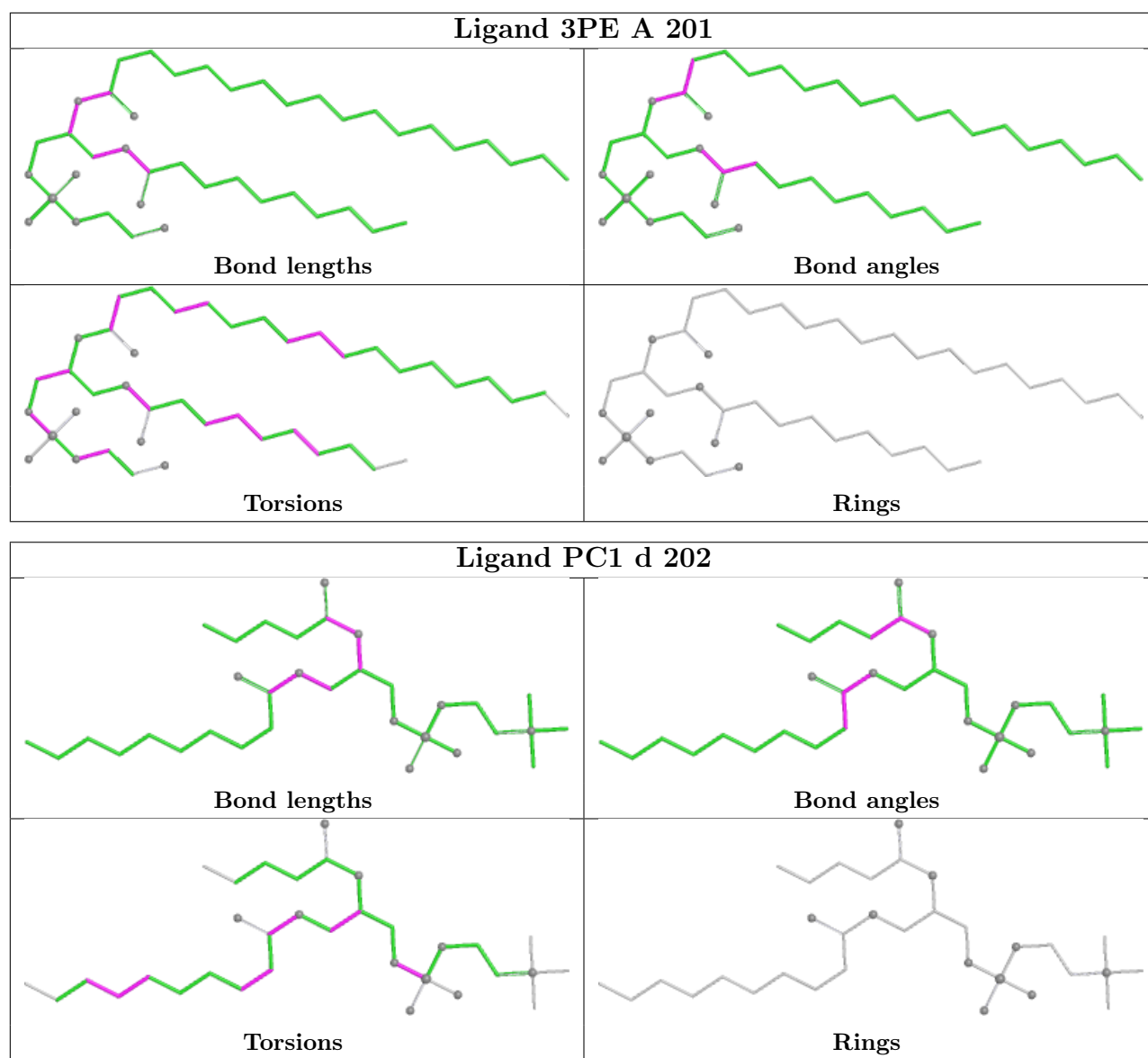
All (1) ring outliers are listed below:

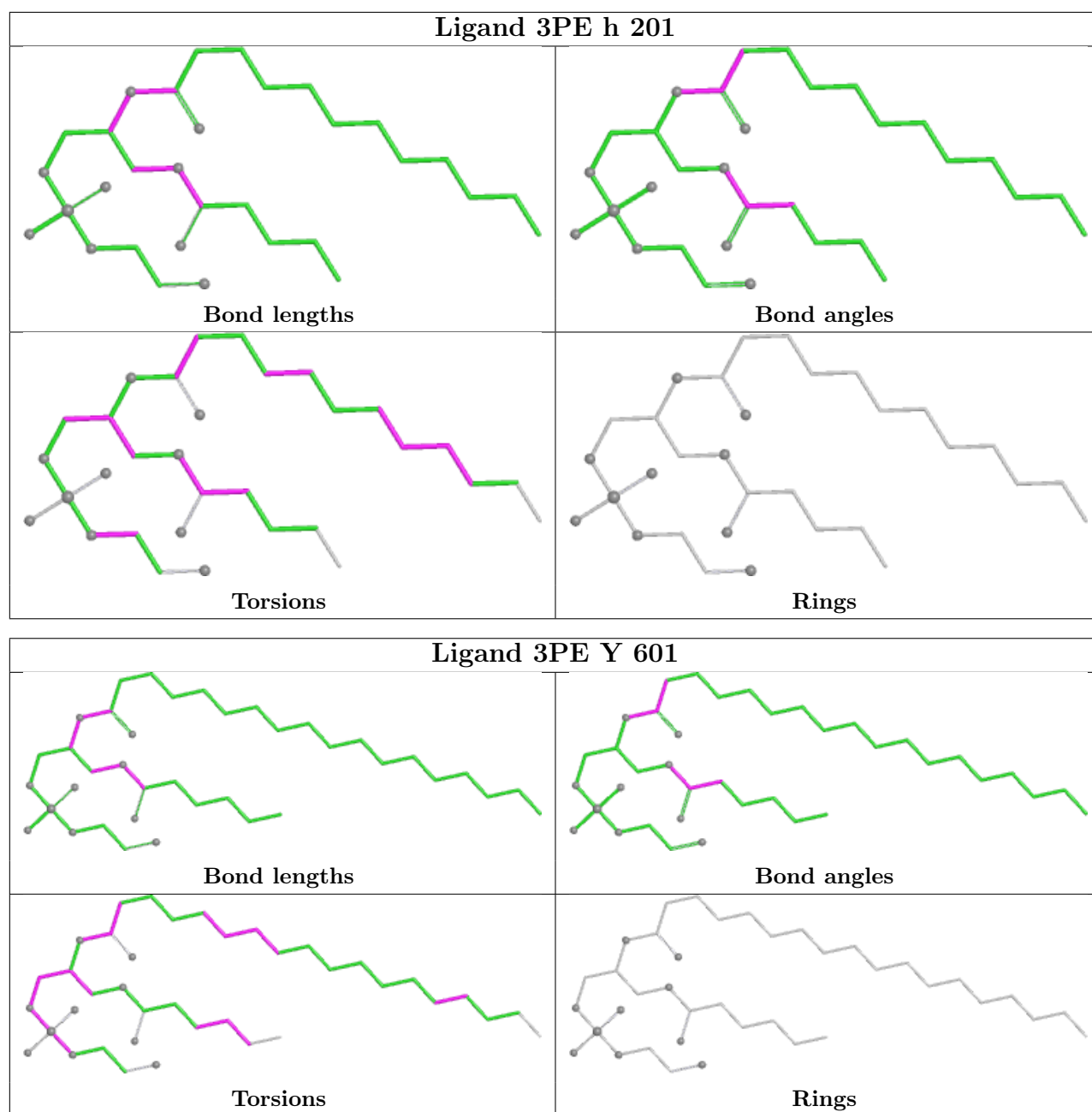
Mol	Chain	Res	Type	Atoms
57	i	201	CHD	C10-C5-C6-C7-C8-C9

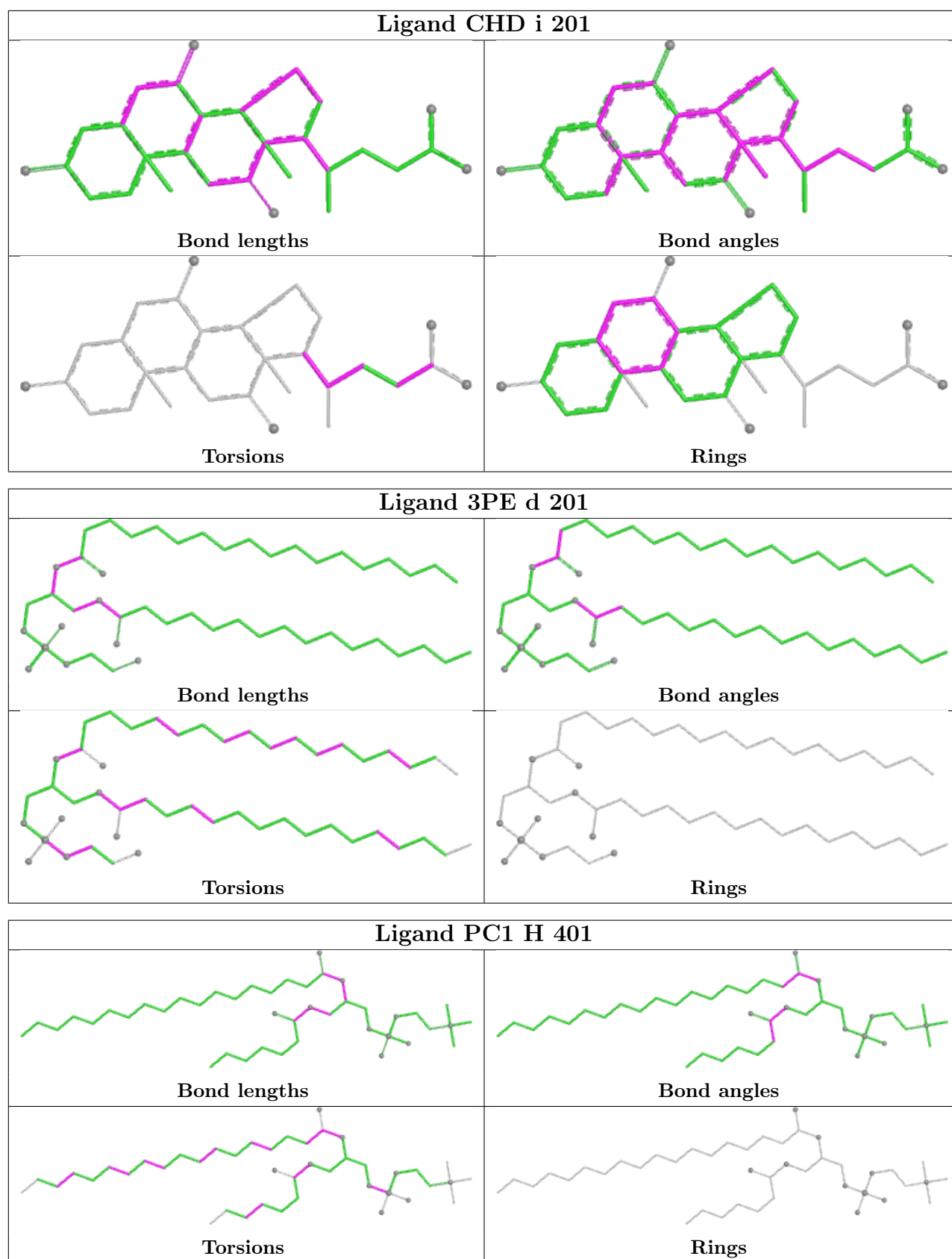
21 monomers are involved in 37 short contacts:

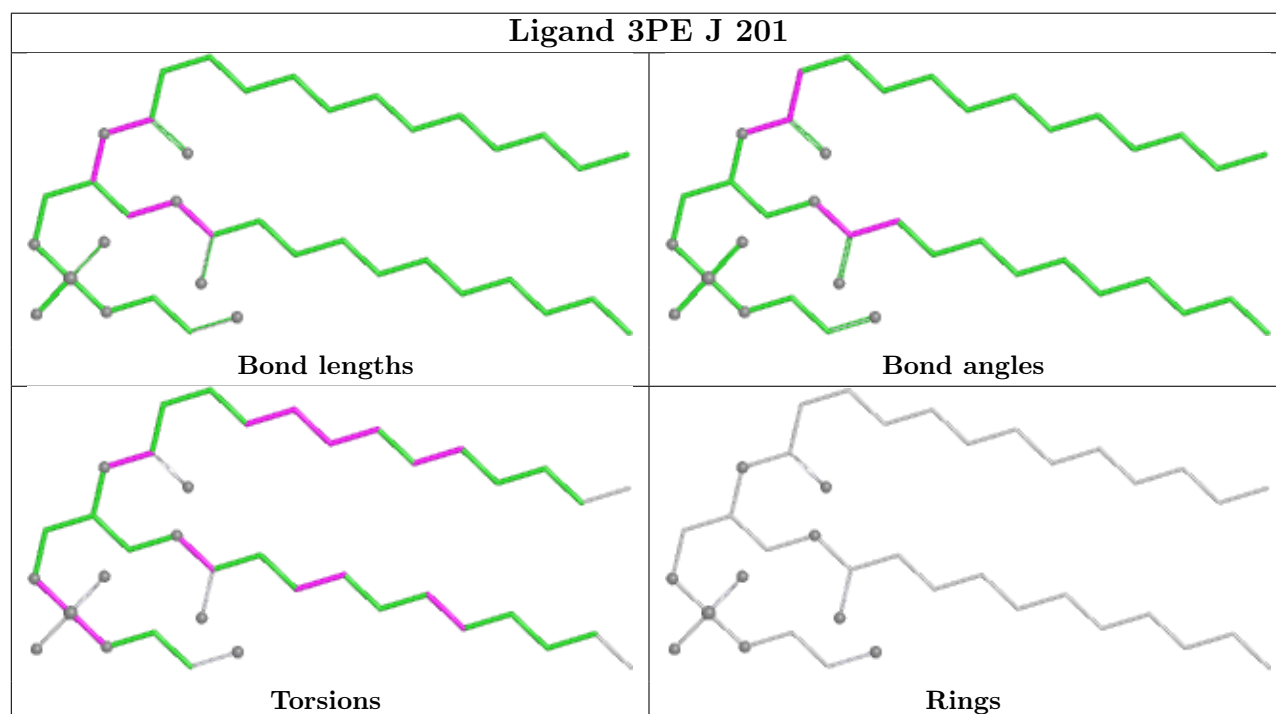
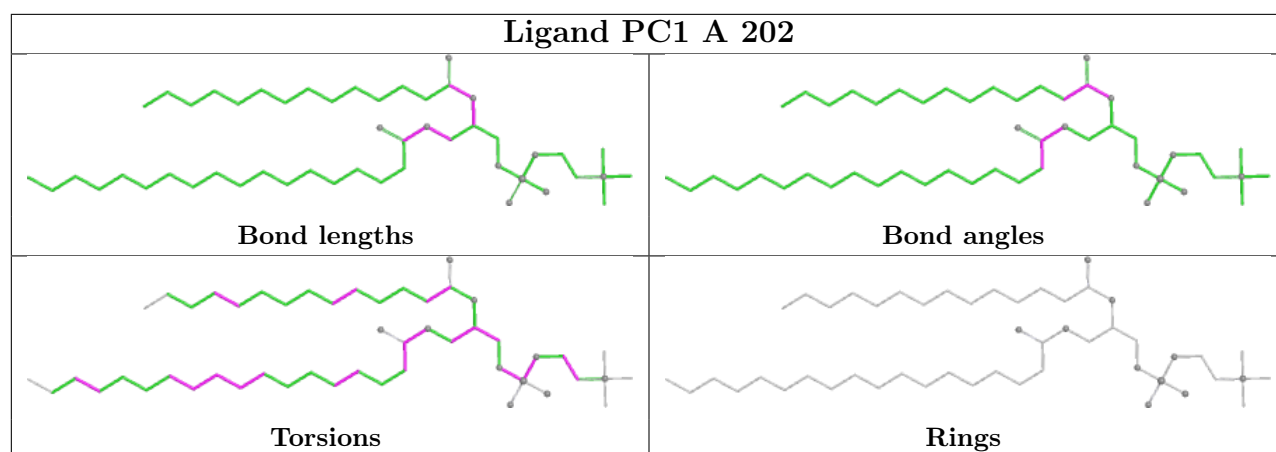
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	A	201	3PE	1	0
46	d	202	PC1	1	0
57	i	201	CHD	5	0
46	H	401	PC1	4	0
51	q	201	CDL	2	0
47	G	803	SF4	1	0
49	F	502	FMN	3	0
45	M	501	3PE	1	0
45	D	501	3PE	1	0
47	B	201	SF4	1	0
56	U	101	EHZ	3	0
48	E	301	FES	1	0
47	F	501	SF4	1	0
45	I	203	3PE	1	0
47	I	201	SF4	1	0
52	O	401	DGT	3	0
54	P	501	NDP	1	0
45	N	401	3PE	1	0
56	T	101	EHZ	2	0
46	B	202	PC1	2	0
47	G	804	SF4	1	0

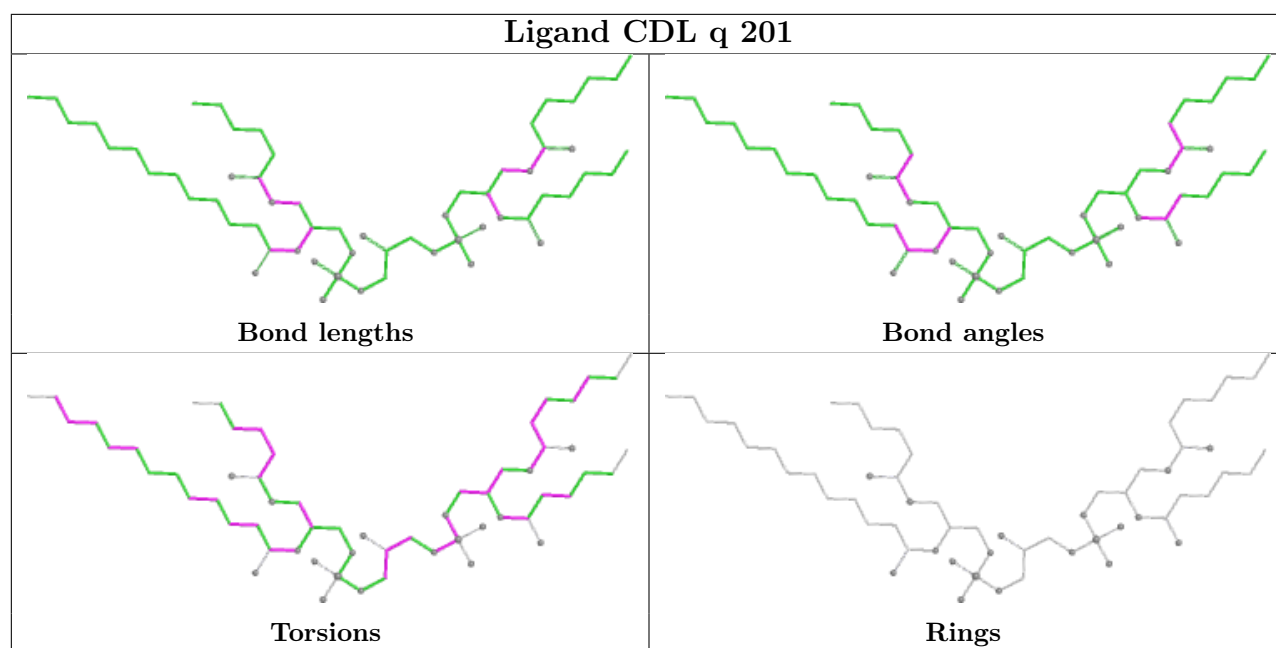
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

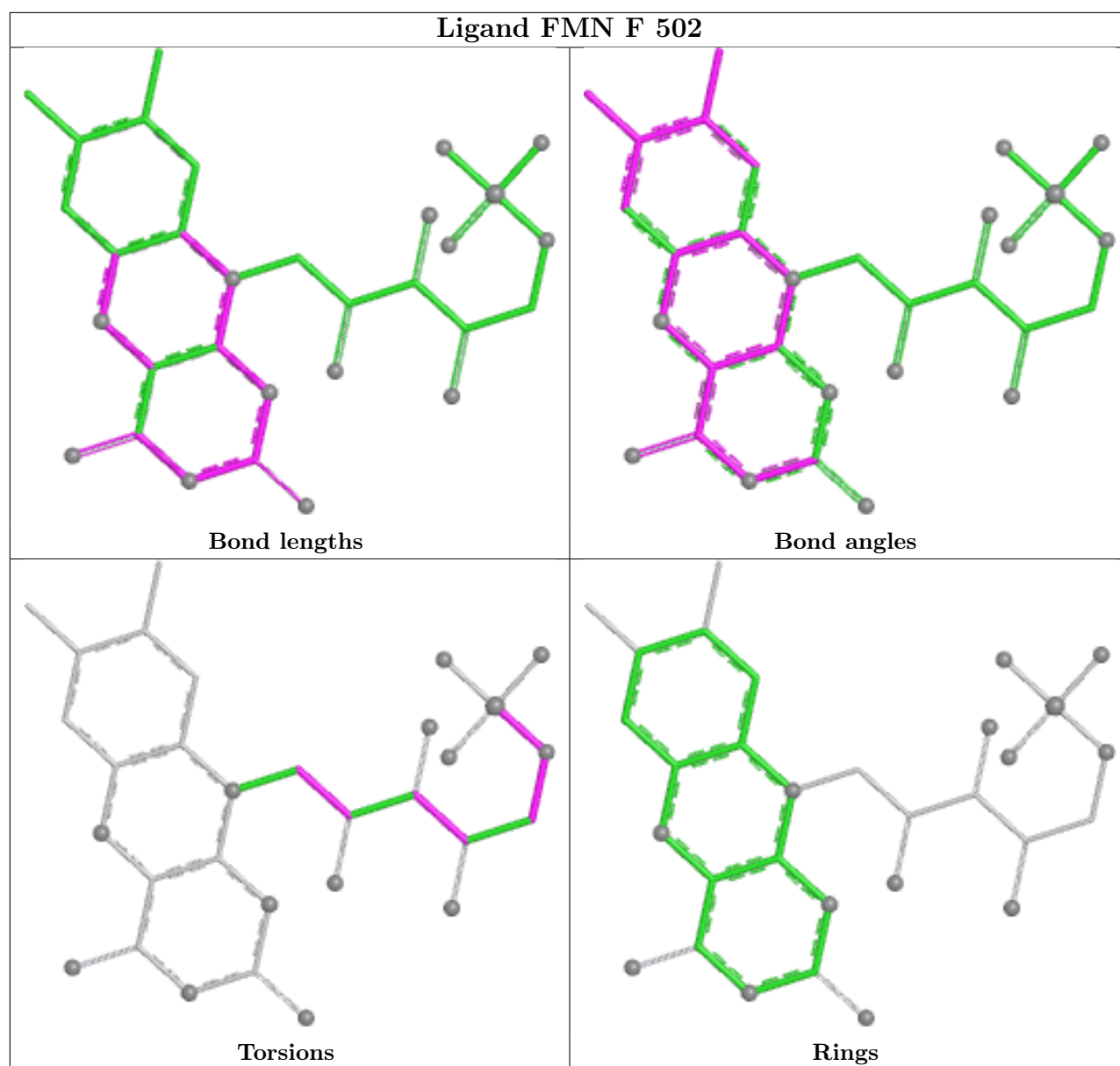


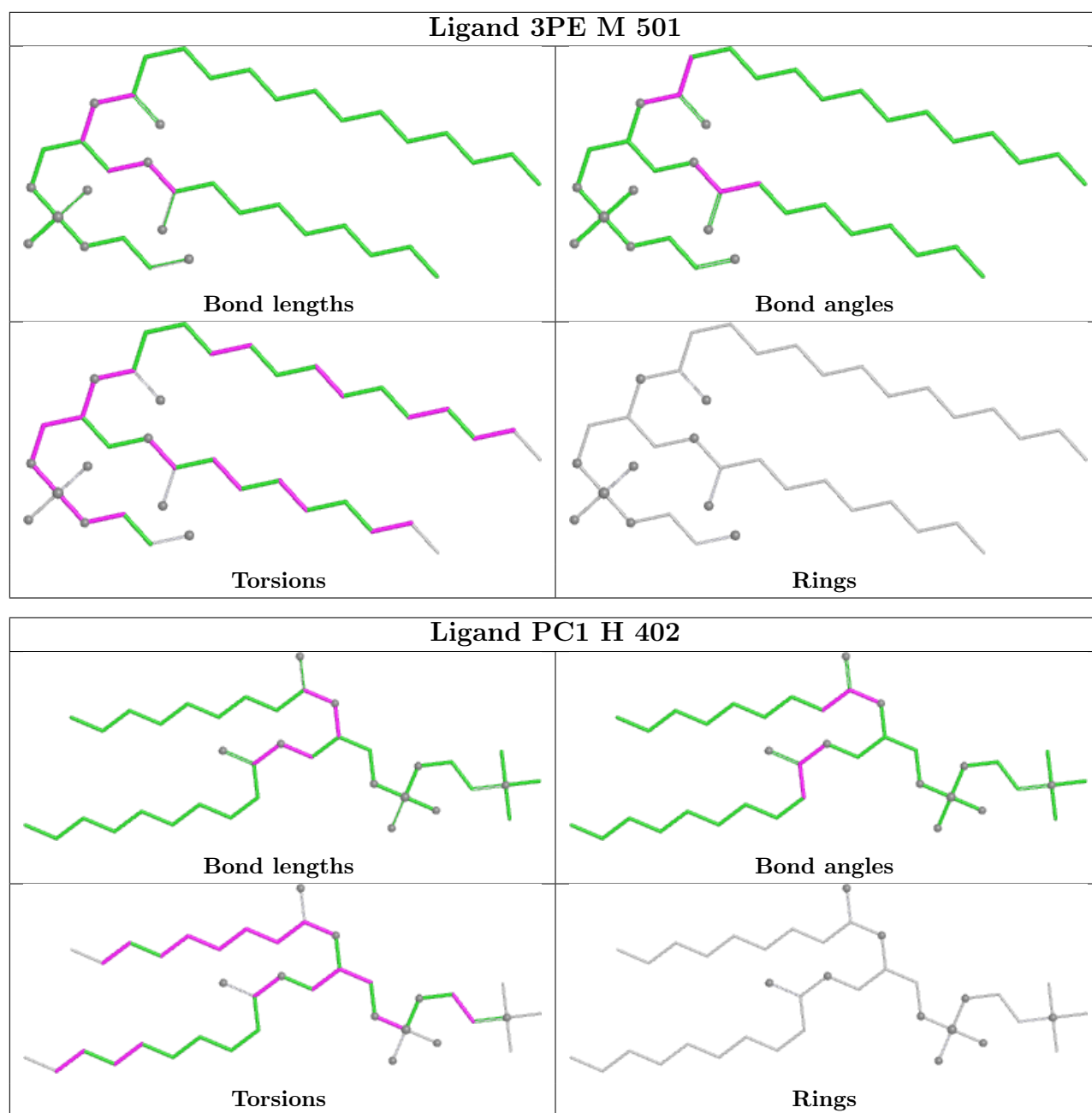


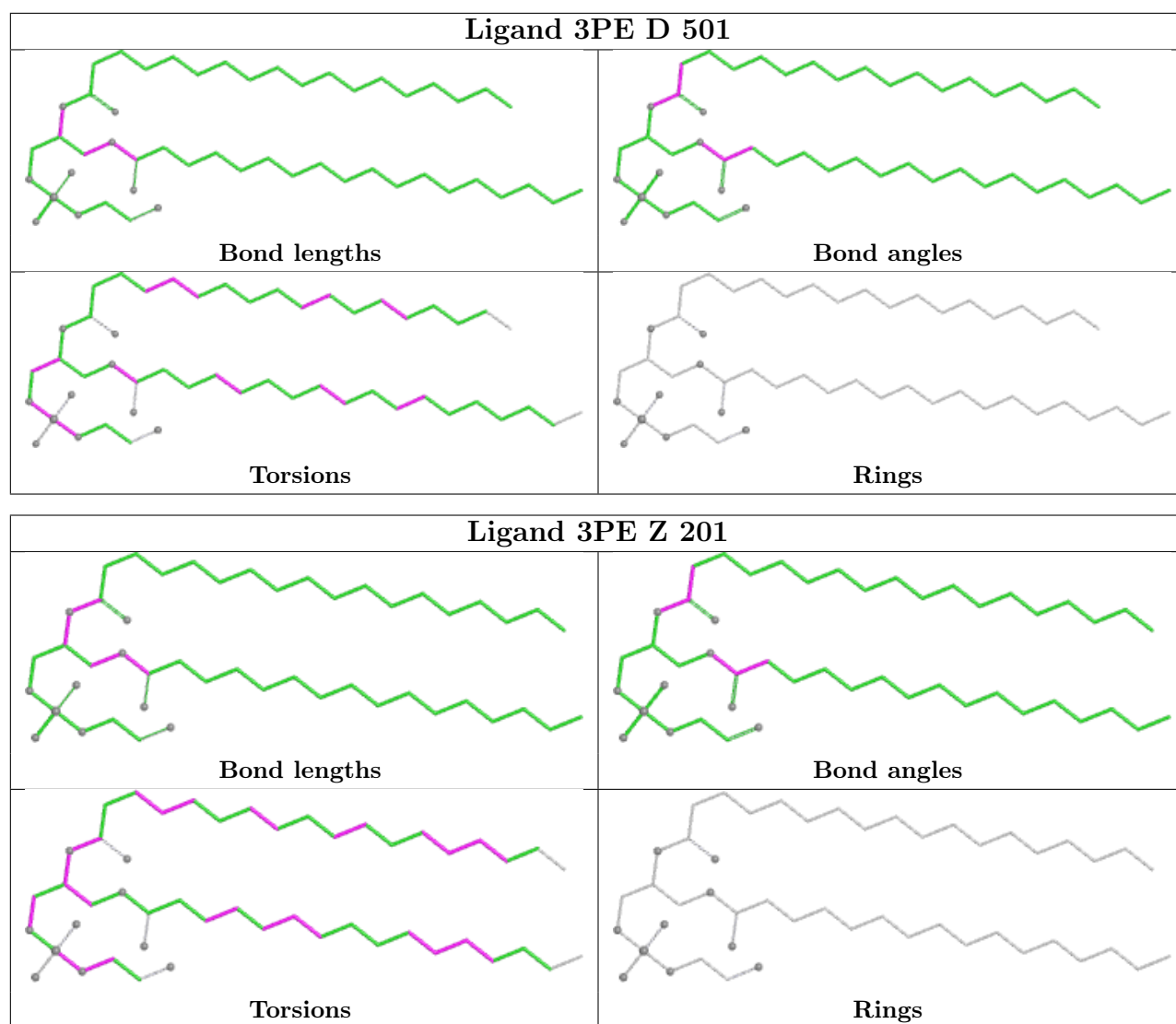


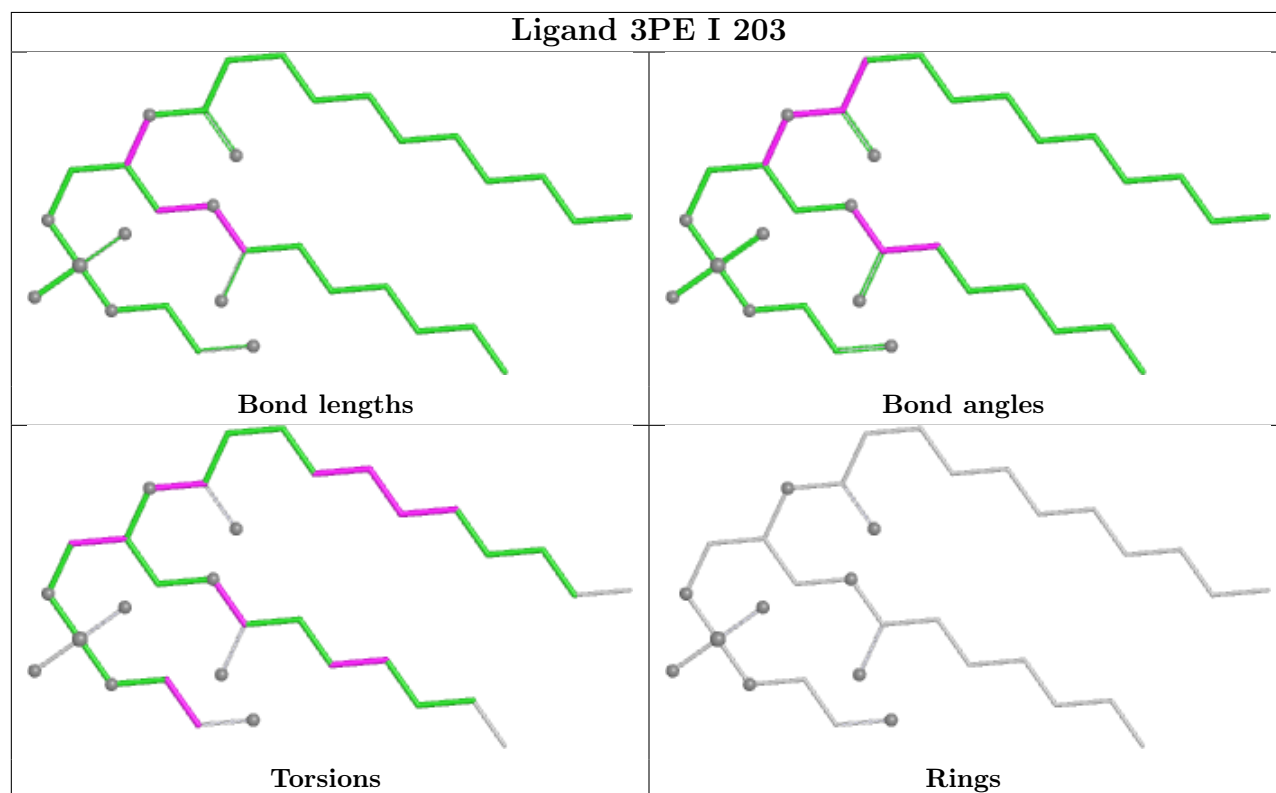
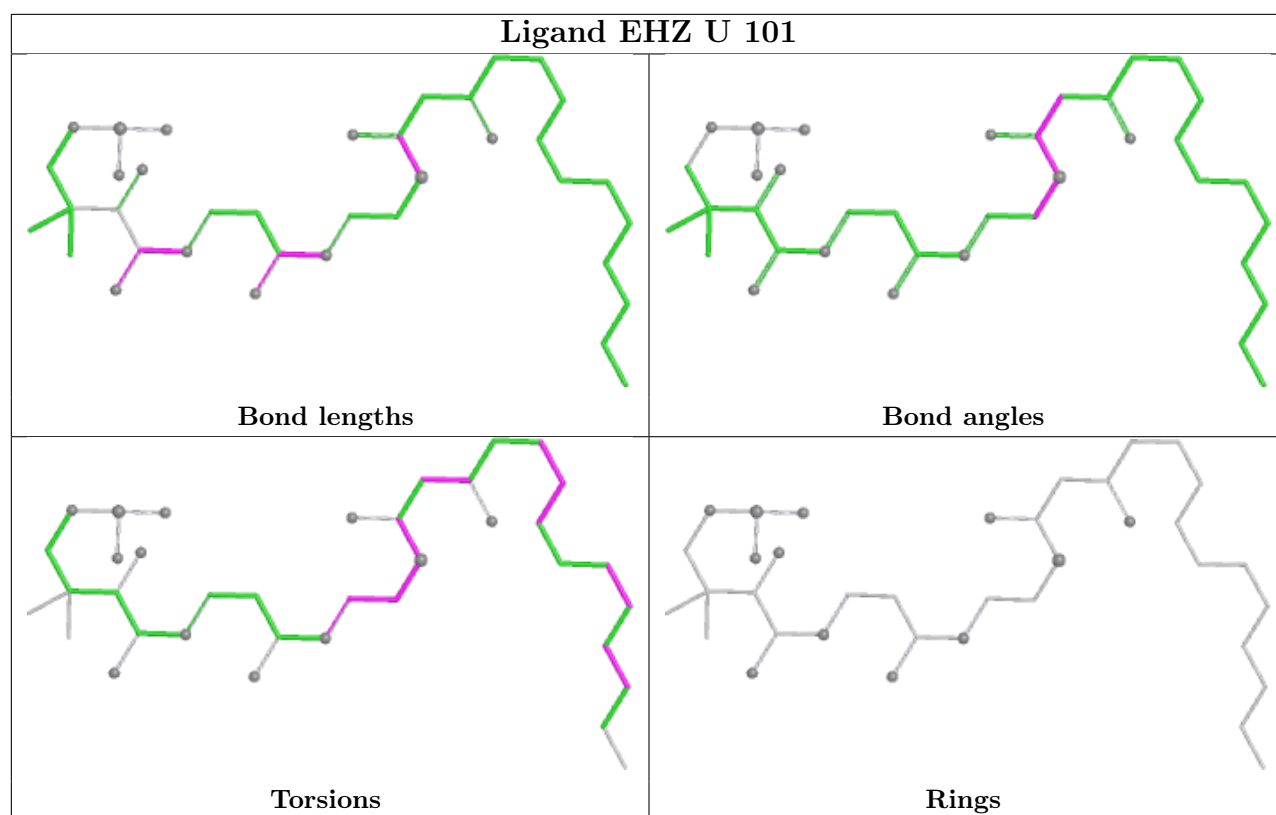


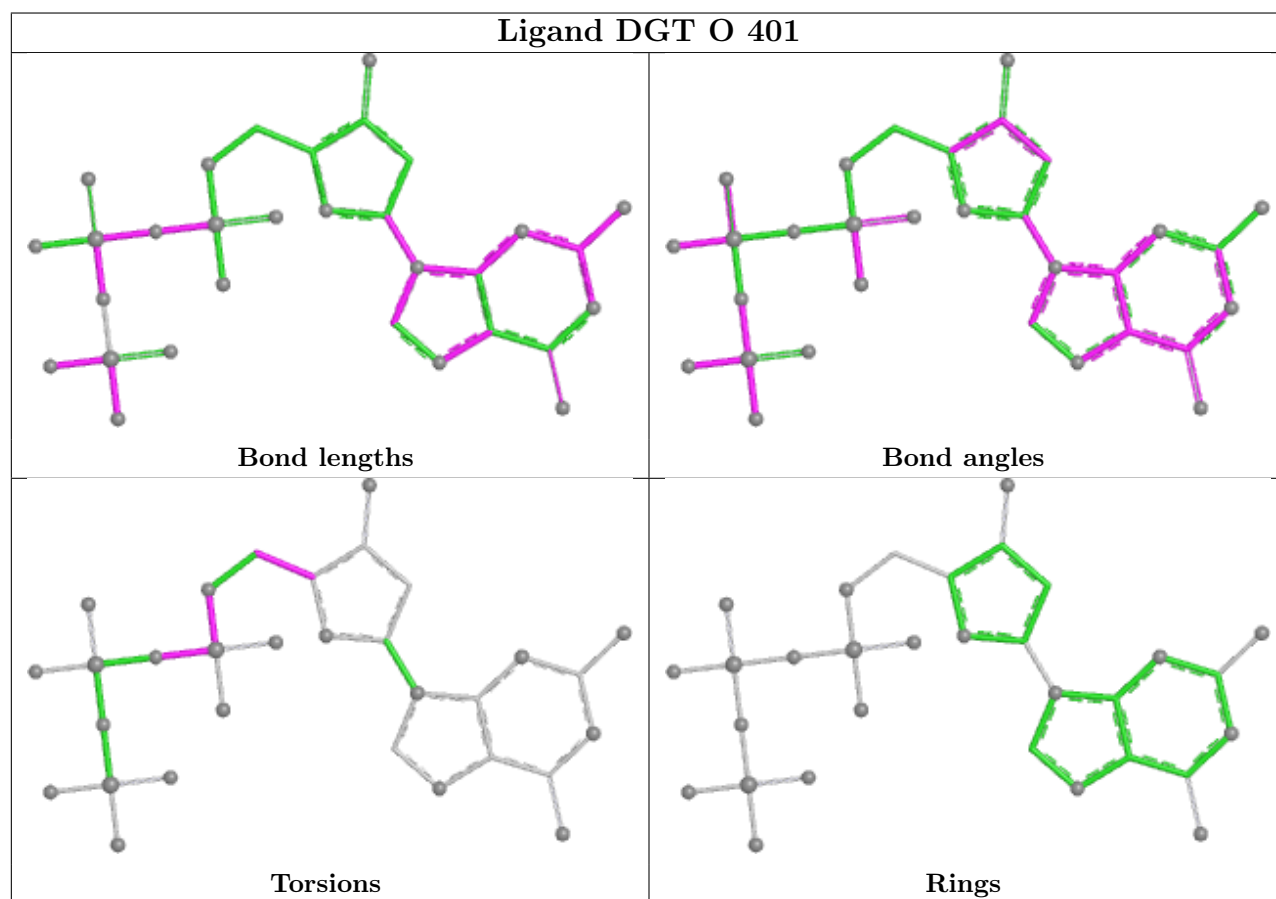
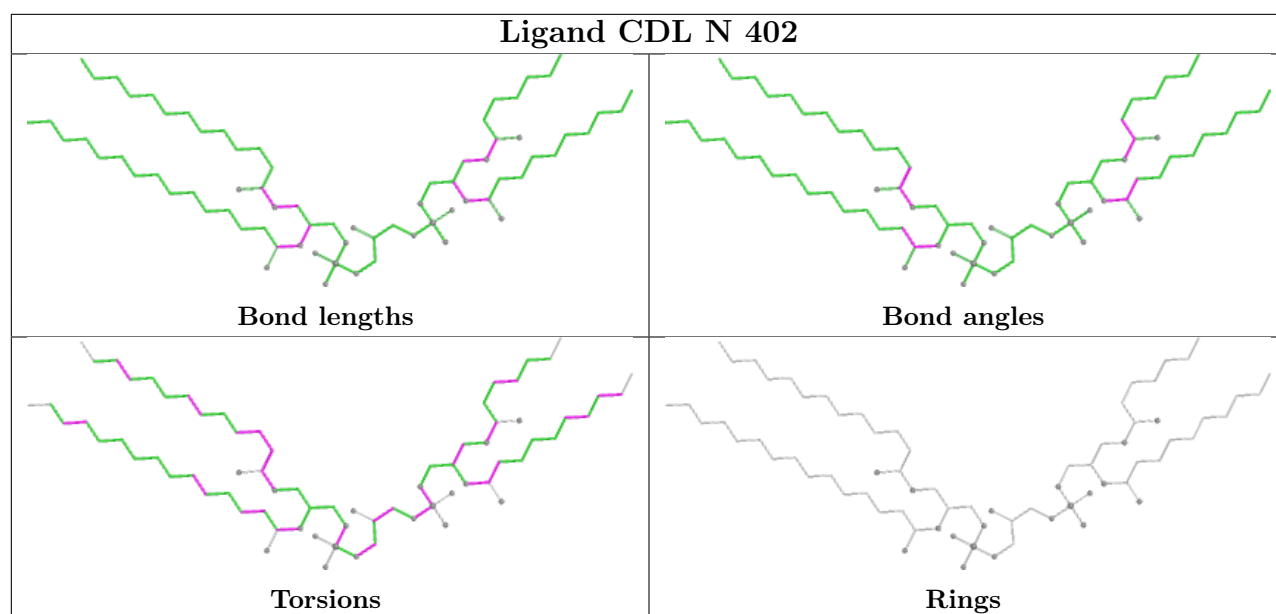


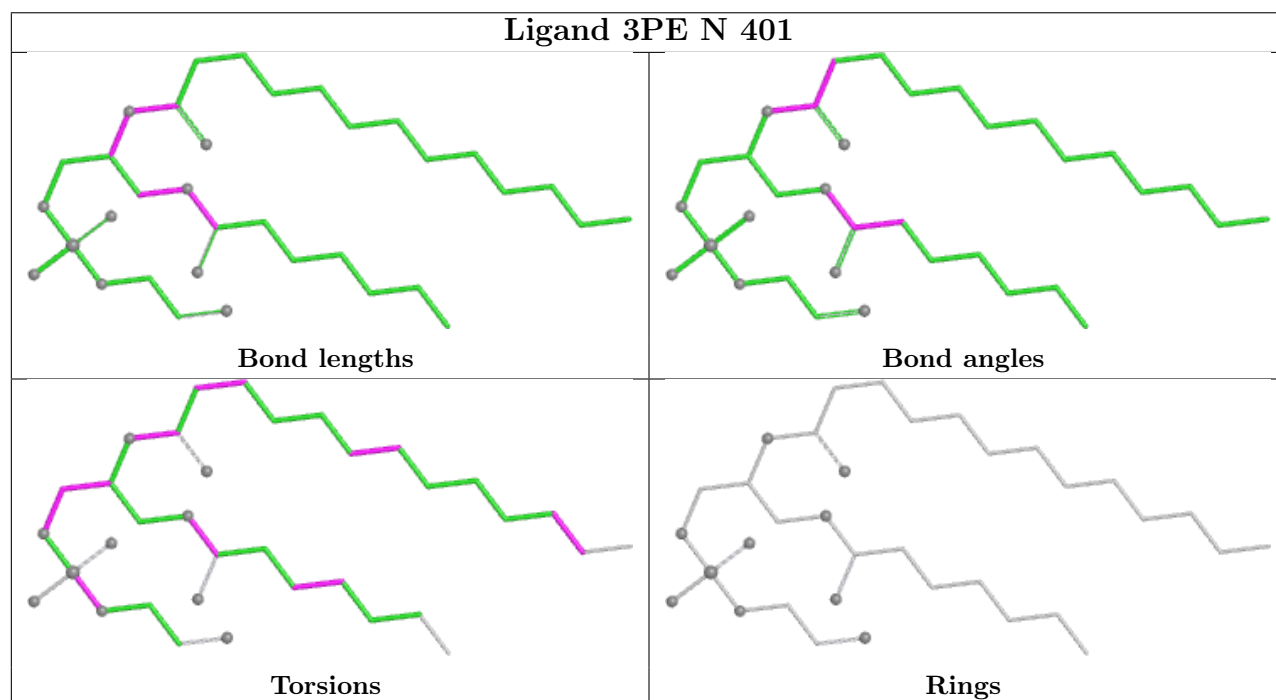
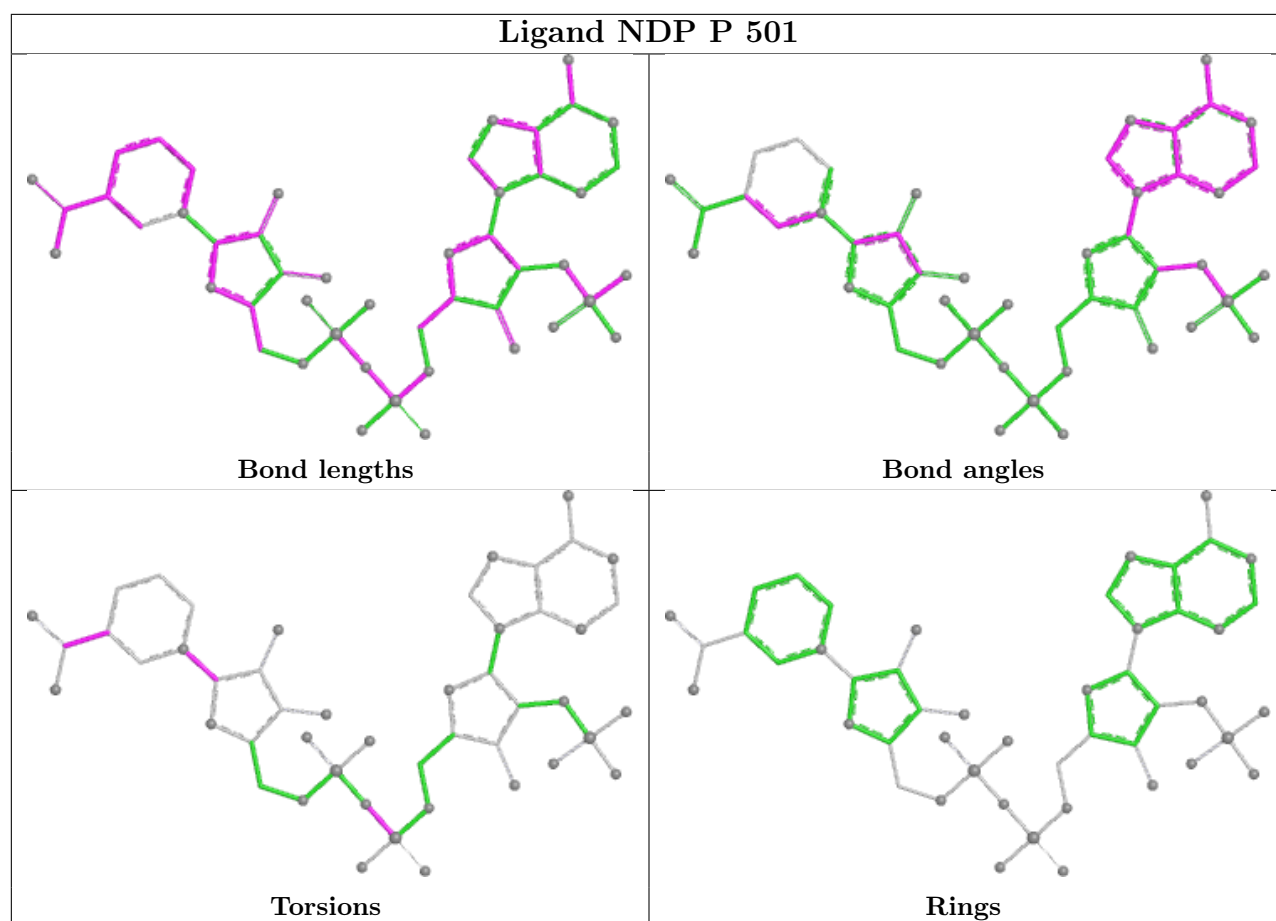


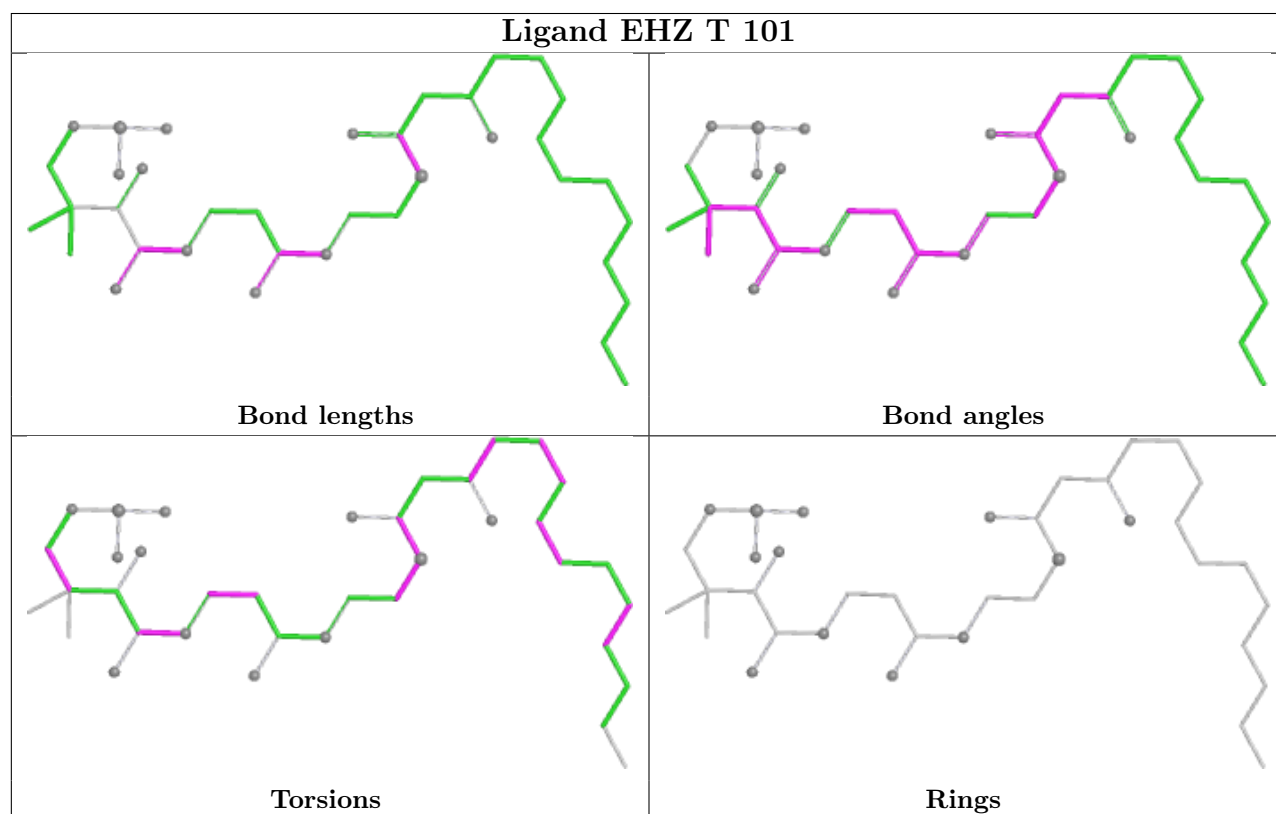
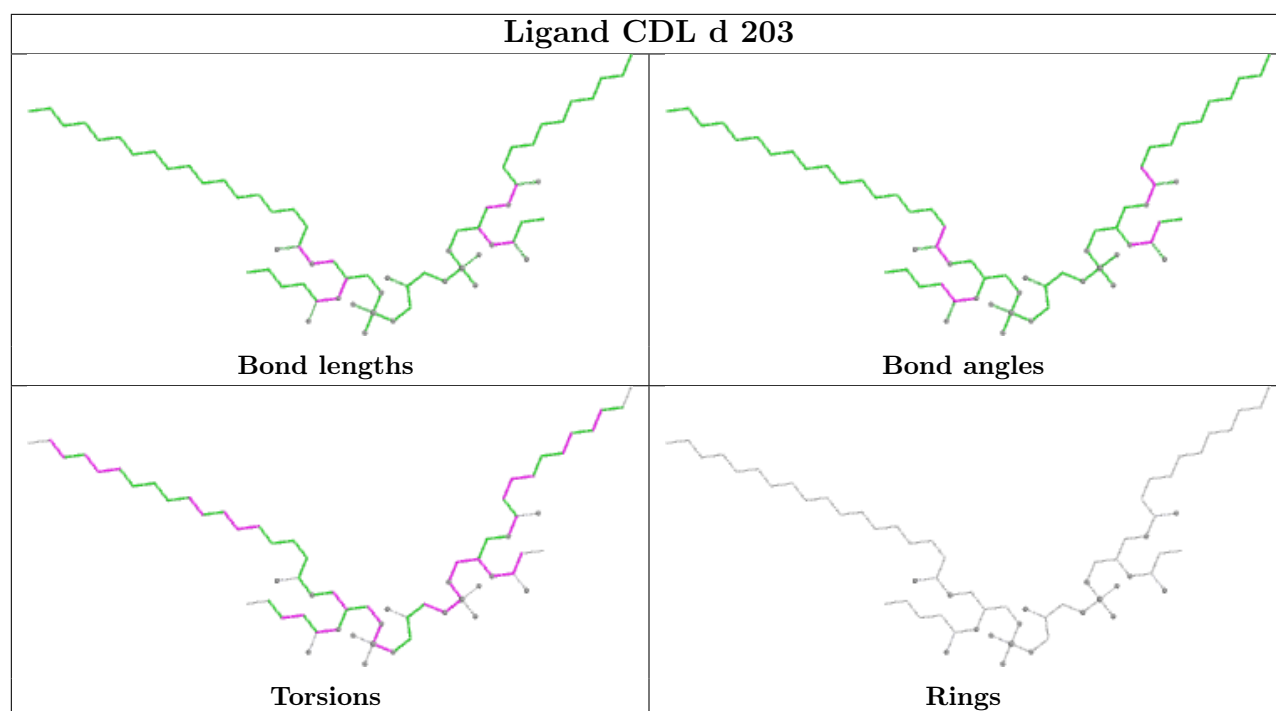


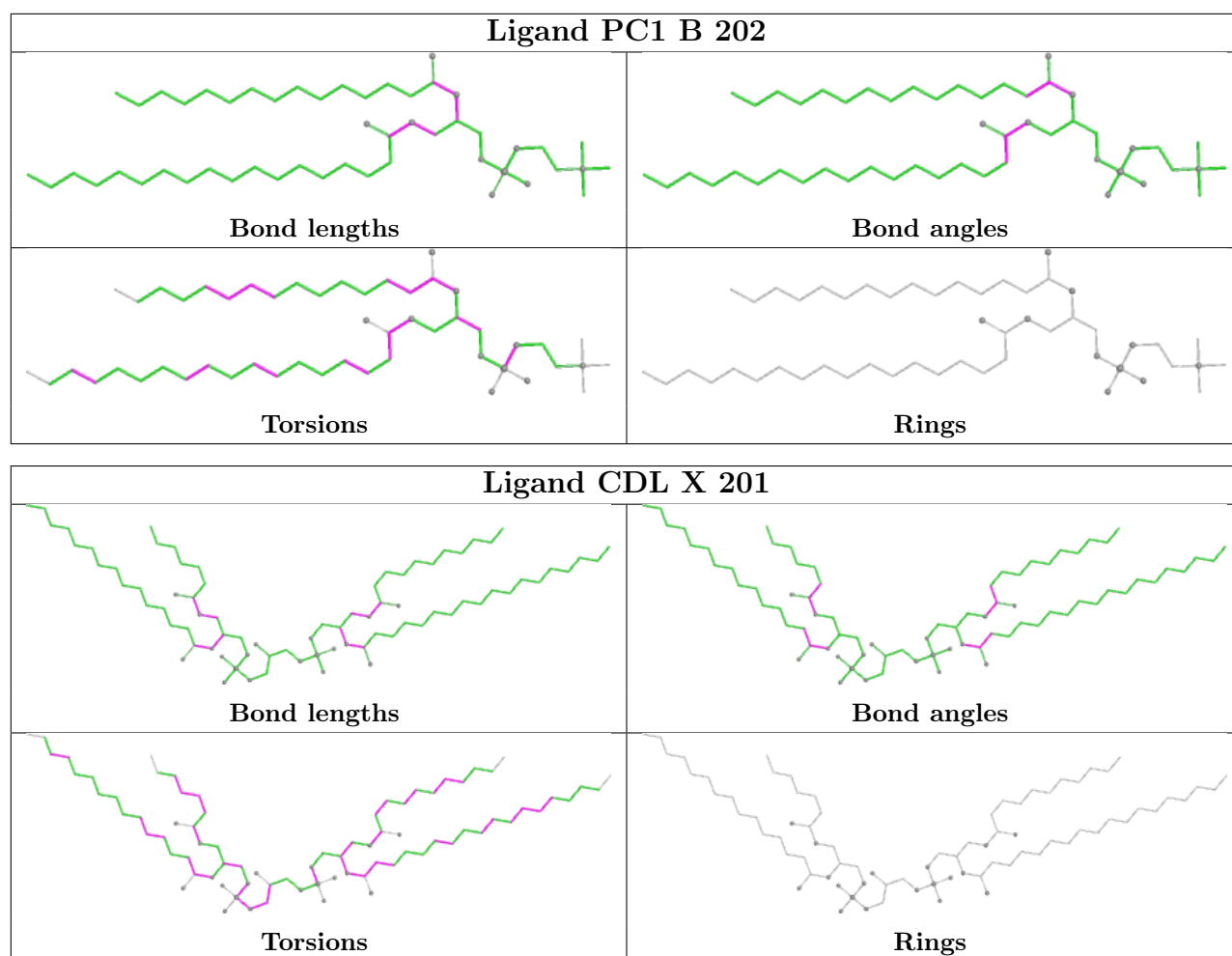












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

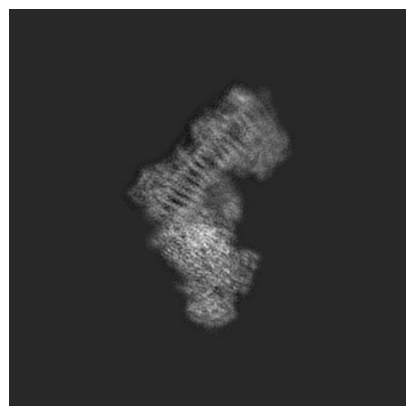
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18054. These allow visual inspection of the internal detail of the map and identification of artifacts.

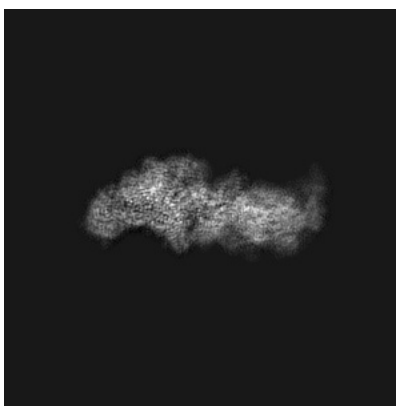
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

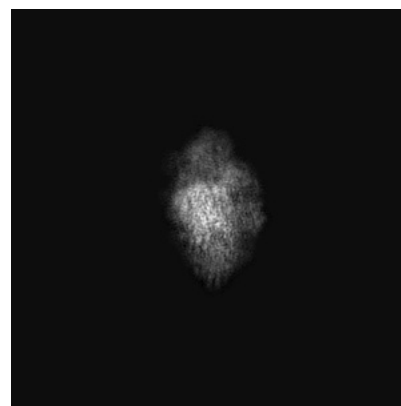
6.1.1 Primary map



X

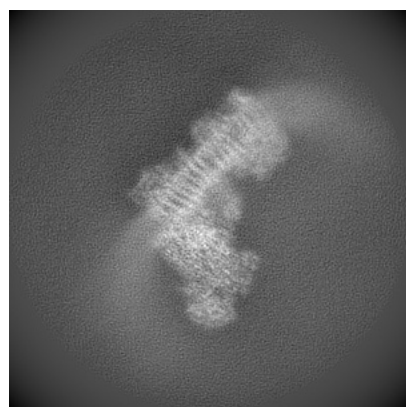


Y

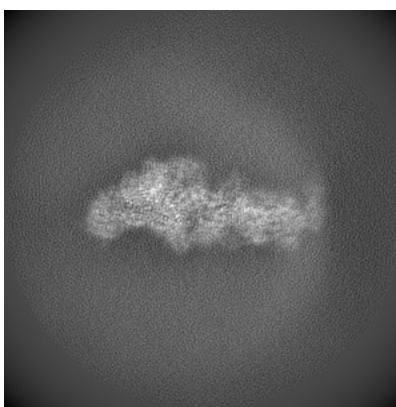


Z

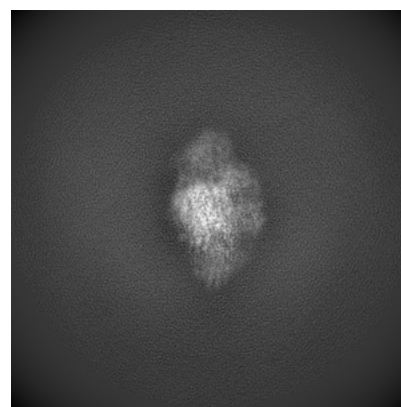
6.1.2 Raw map



X



Y

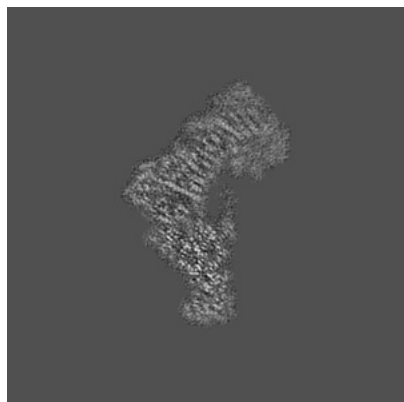


Z

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

6.2 Central slices [i](#)

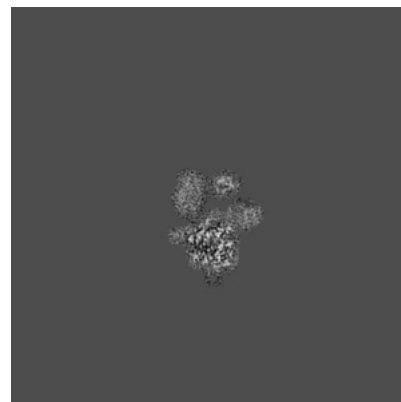
6.2.1 Primary map



X Index: 180

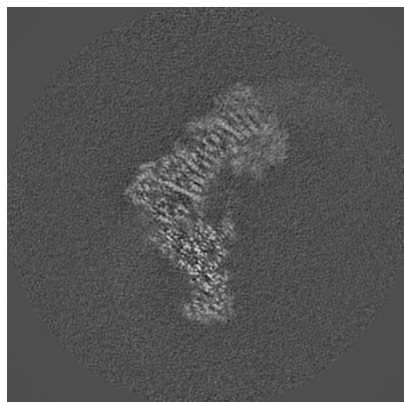


Y Index: 180

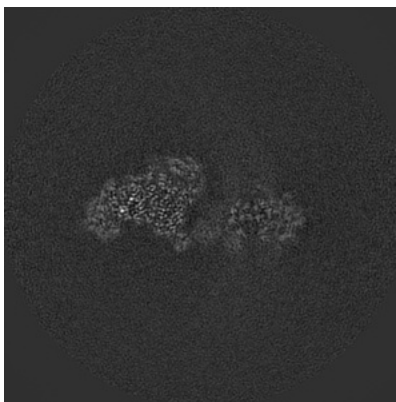


Z Index: 180

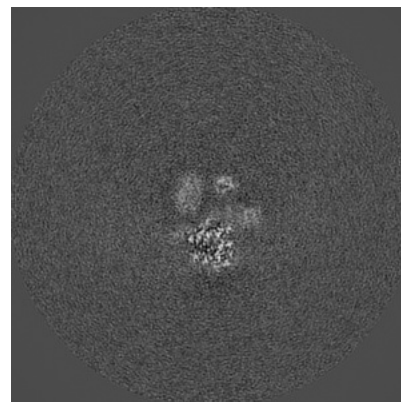
6.2.2 Raw map



X Index: 180



Y Index: 180



Z Index: 180

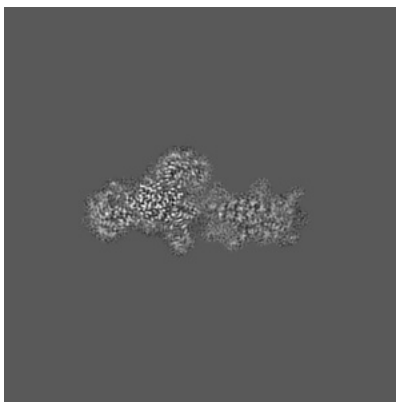
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

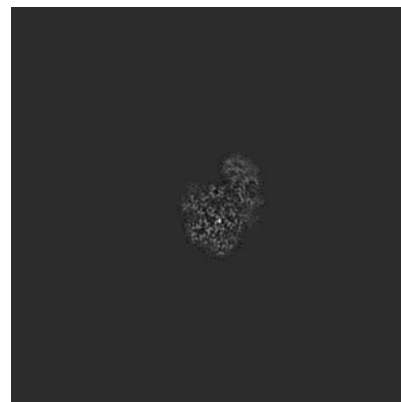
6.3.1 Primary map



X Index: 187

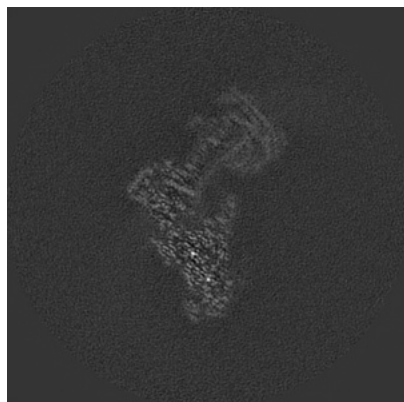


Y Index: 172

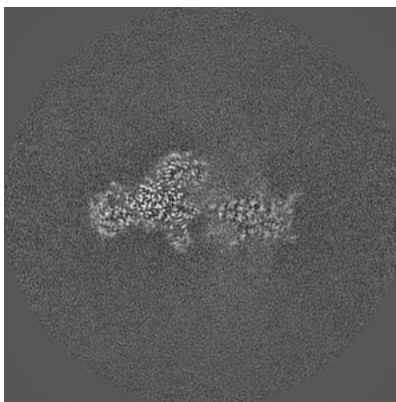


Z Index: 138

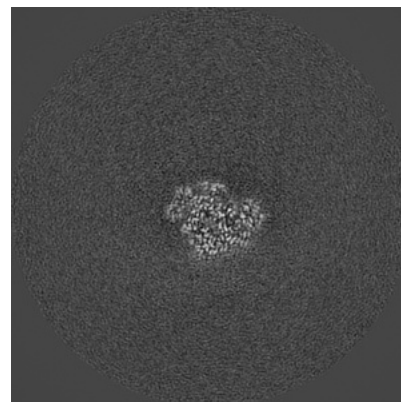
6.3.2 Raw map



X Index: 187



Y Index: 172

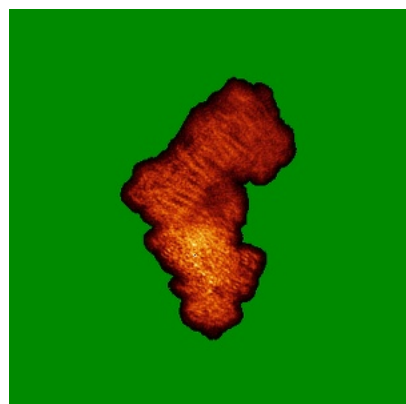


Z Index: 157

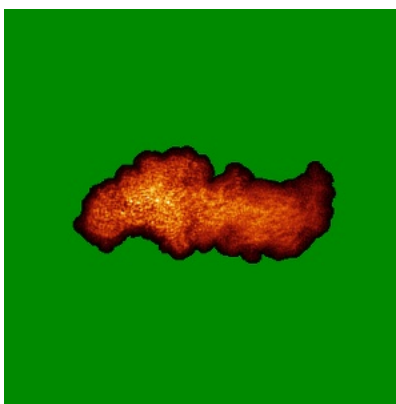
The images above show the largest variance slices of the map in three orthogonal directions.

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

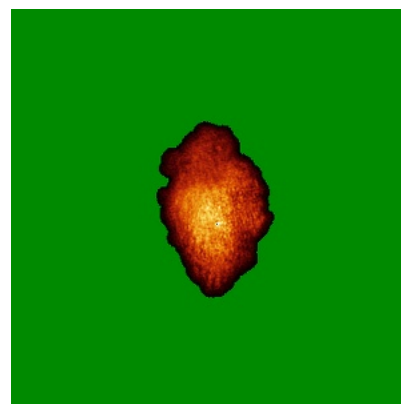
6.4.1 Primary map



X

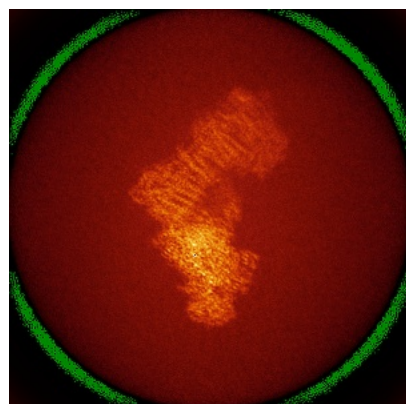


Y

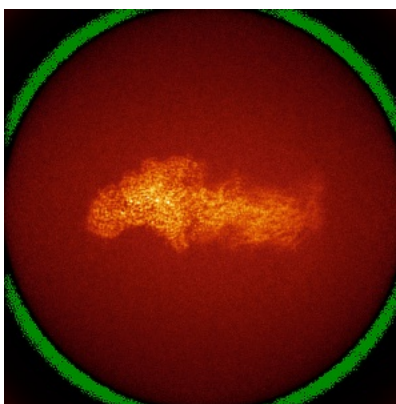


Z

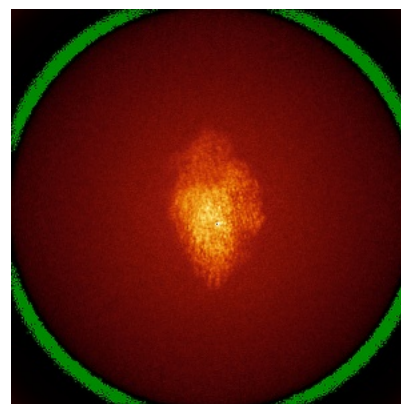
6.4.2 Raw map



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](#)

This section was not generated.

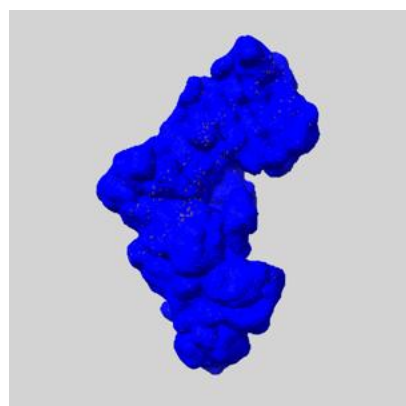
6.6 Mask visualisation [i](#)

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

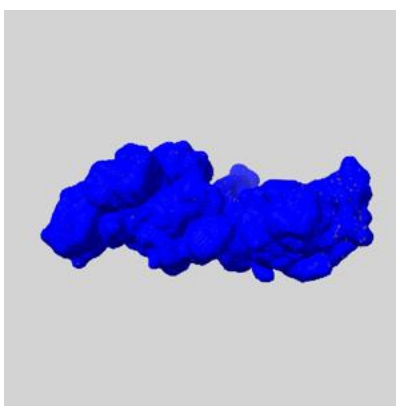
A mask typically either:

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

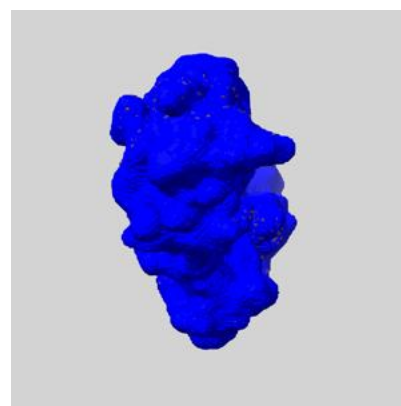
6.6.1 emd_18054_msk_1.map [i](#)



X



Y

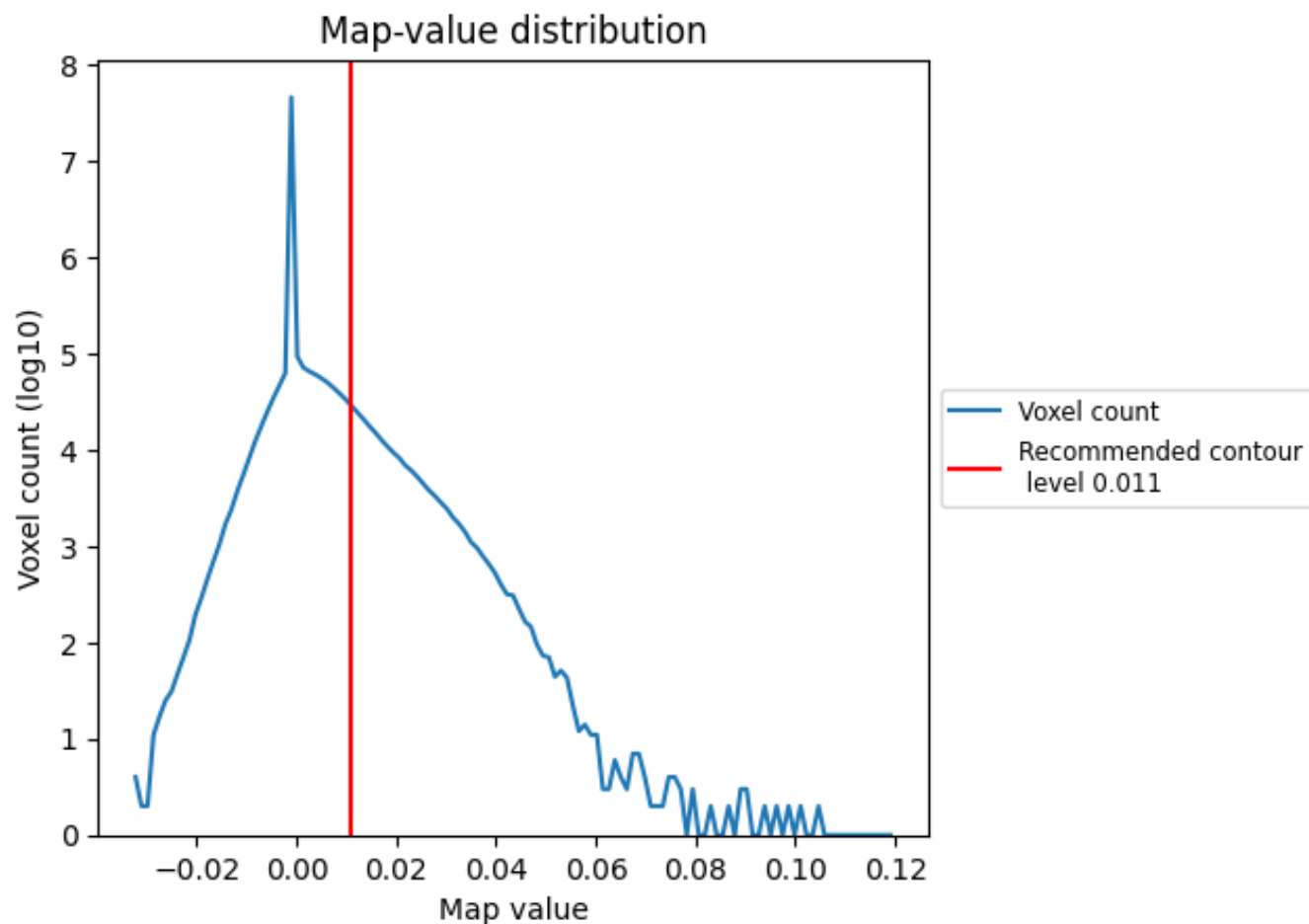


Z

7 Map analysis [i](#)

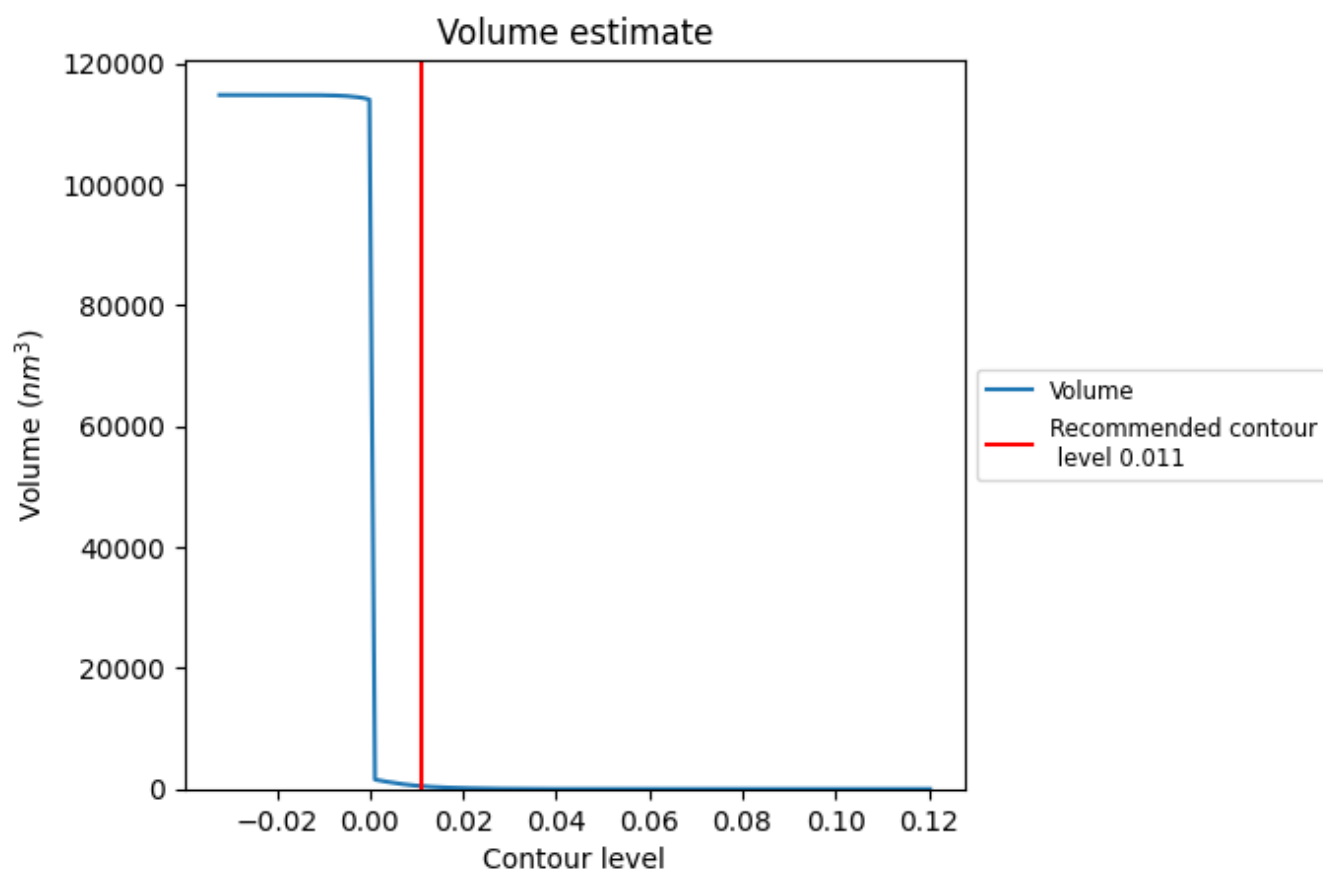
This section contains the results of statistical analysis of the map.

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.

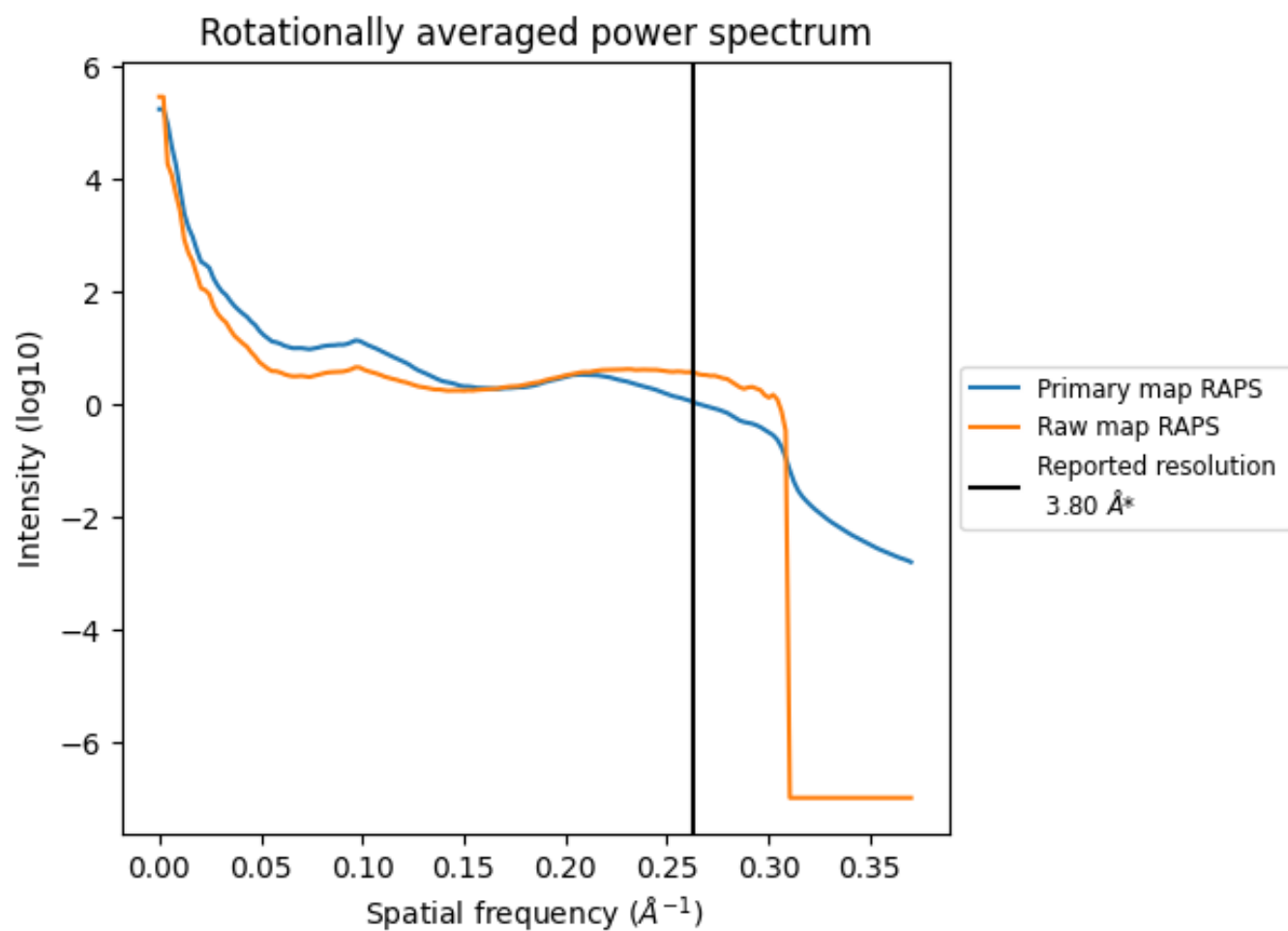
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 480 nm^3 ; this corresponds to an approximate mass of 434 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

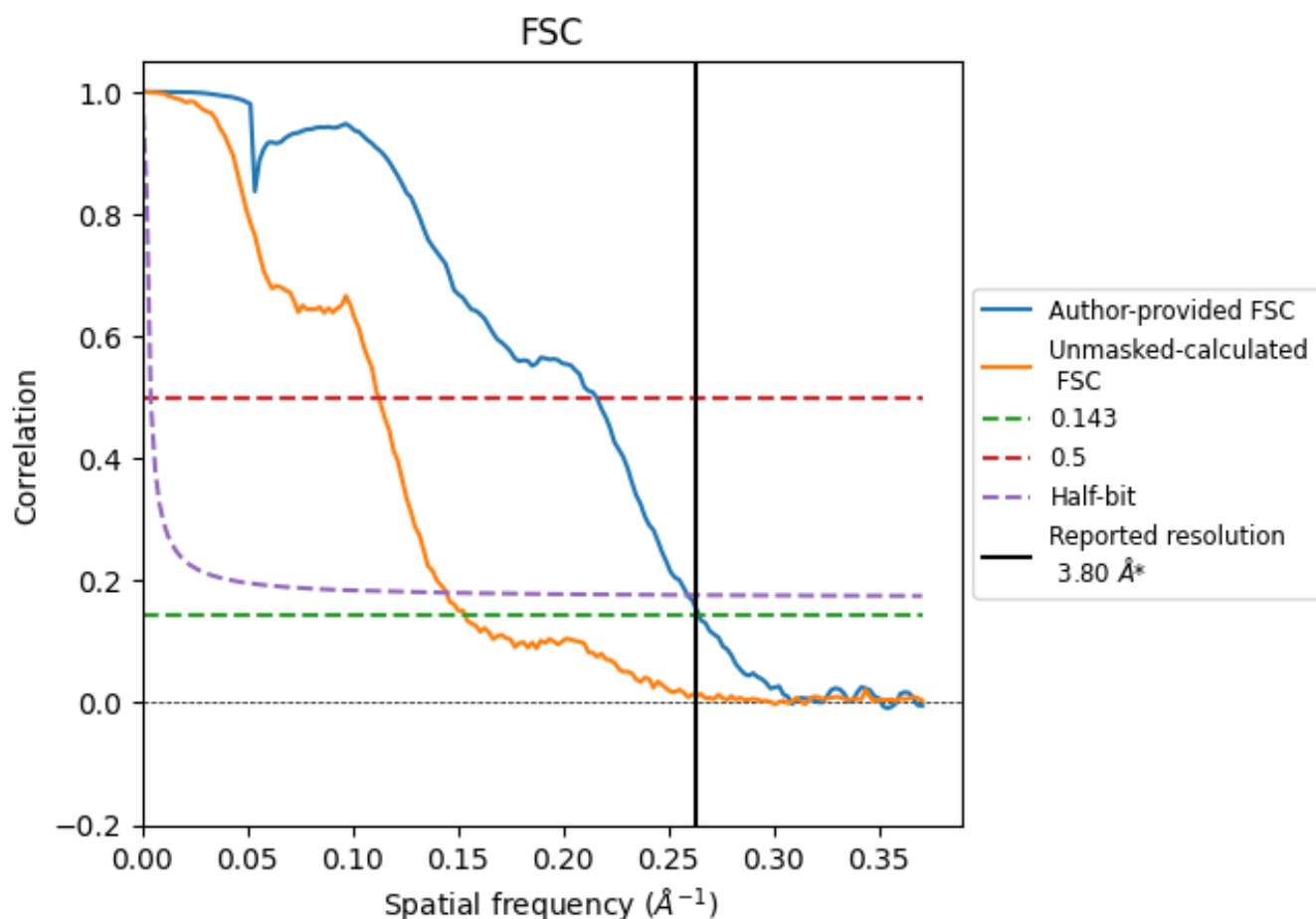


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.78	4.63	3.86
Unmasked-calculated*	6.52	8.91	6.92

*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 6.52 differs from the reported value 3.8 by more than 10 %

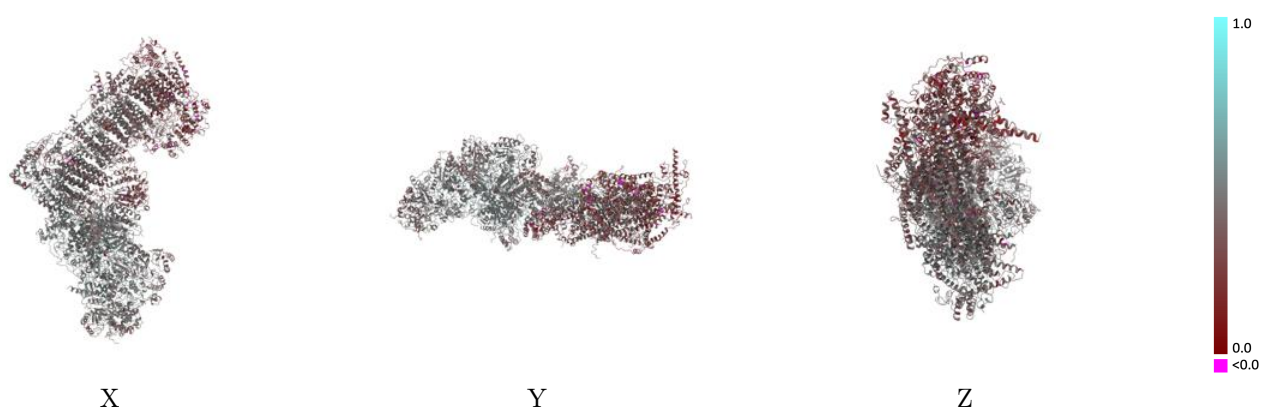
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18054 and PDB model 8Q0J. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)

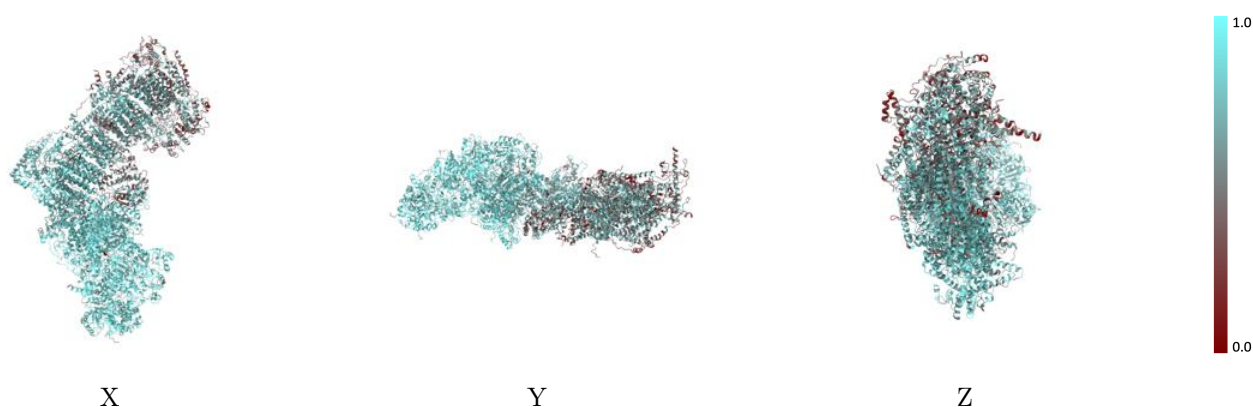
This section was not generated.

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



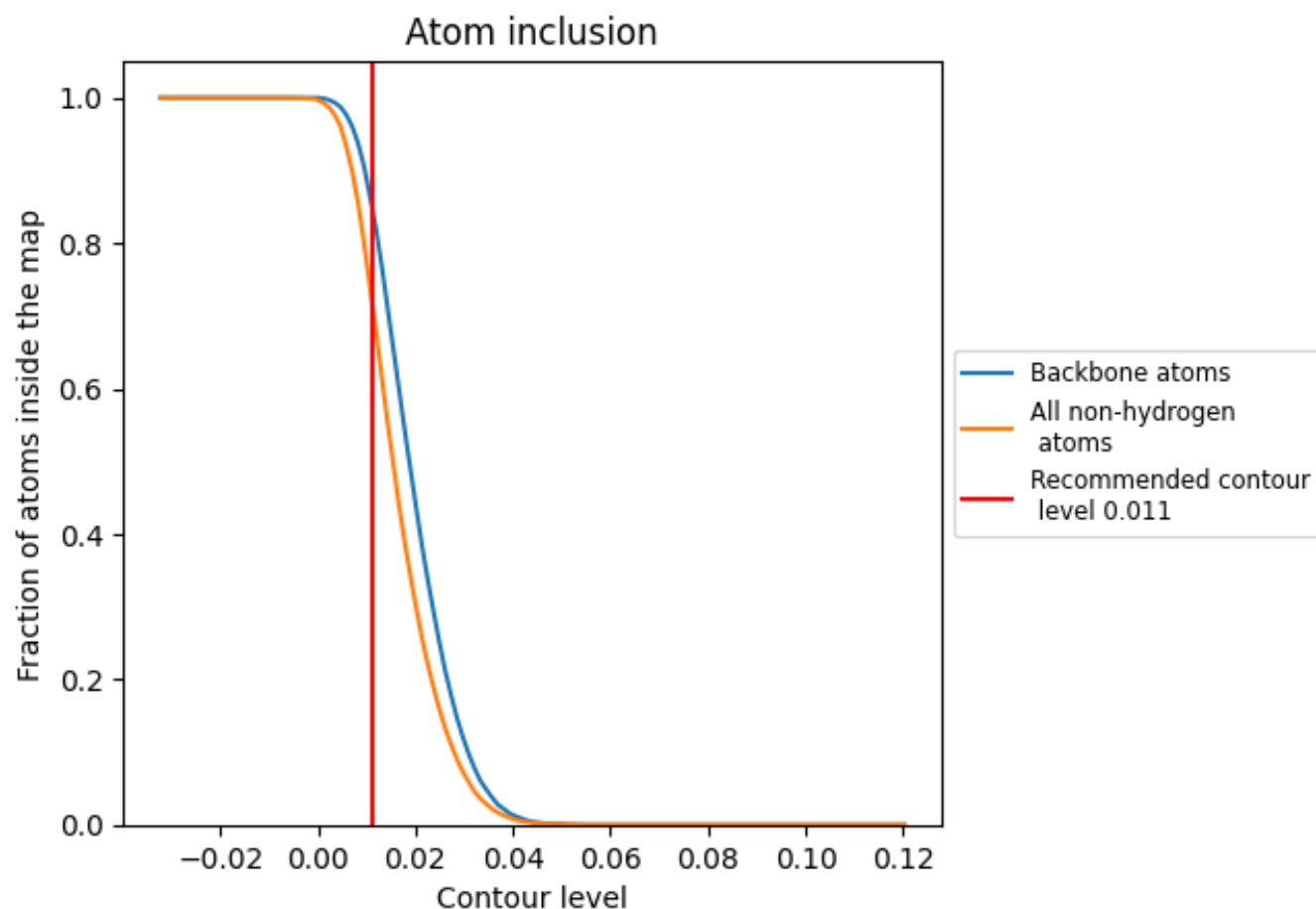
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 85% of all backbone atoms, 72% 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	 0.7240	 0.4190
A	 0.7320	 0.4460
B	 0.8630	 0.5010
C	 0.8870	 0.5150
D	 0.8690	 0.5110
E	 0.8320	 0.4380
F	 0.8640	 0.4480
G	 0.8660	 0.4850
H	 0.8360	 0.4790
I	 0.9080	 0.5190
J	 0.6920	 0.4060
K	 0.7660	 0.4290
L	 0.5900	 0.3320
M	 0.7120	 0.4170
N	 0.7400	 0.4270
O	 0.4620	 0.2980
P	 0.8080	 0.4470
Q	 0.8460	 0.5120
R	 0.7860	 0.4740
S	 0.8130	 0.4230
T	 0.7220	 0.3720
U	 0.4540	 0.2830
V	 0.8560	 0.4620
W	 0.8220	 0.4600
X	 0.7320	 0.4400
Y	 0.3240	 0.3690
Z	 0.7700	 0.4420
a	 0.8340	 0.4790
b	 0.7670	 0.4550
c	 0.5680	 0.3530
d	 0.6580	 0.4070
e	 0.7640	 0.4520
f	 0.5620	 0.4020
g	 0.5980	 0.3610
h	 0.6870	 0.3920



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Chain	Atom inclusion	Q-score
i	 0.4280	 0.2830
j	 0.4850	 0.2990
k	 0.4000	 0.2790
l	 0.4840	 0.3210
m	 0.4880	 0.3120
n	 0.5210	 0.3000
o	 0.4330	 0.2730
p	 0.5660	 0.3630
q	 0.8760	 0.5020
r	 0.8670	 0.4940
s	 0.7250	 0.3910