



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 12:59 PM UTC

PDB ID : 7W35 / pdb_00007w35
EMDB ID : EMD-32271
Title : Deactive state CI from DQ-NADH dataset, Subclass 3
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-25
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

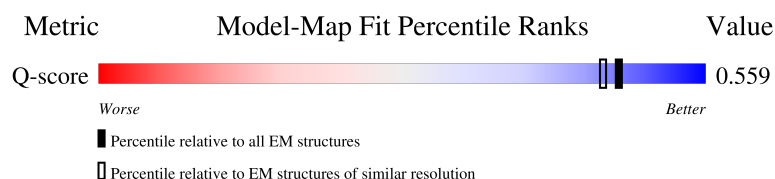
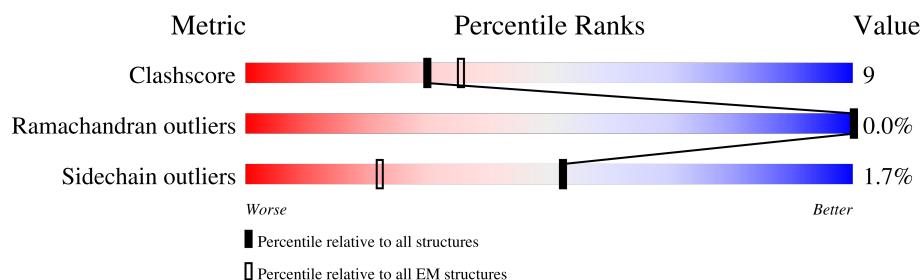
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	433	 8% 77% 23%
2	B	176	 8% 80% 20%
3	C	156	 8% 78% 20%
4	E	115	 8% 82% 18%

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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	122	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66632 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3318	2095	591	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			695	448	103	139	5		

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	331	Total	C	N	O	S	0	0
			2615	1694	459	454	8		

- Molecule 10 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5296	3320	923	1014	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1668	1064	281	313	10		

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1738	1124	298	314	2		

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3377	2162	578	613	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			558	356	104	94	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1018	648	174	190	6		

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1167	752	200	206	9		

- Molecule 22 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			600	393	98	108	1		

- Molecule 23 is a protein called Complex I-B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	84	Total	C	N	O	S	0	0
			674	437	116	120	1		

- Molecule 24 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1165	762	199	201	3		

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			879	573	158	147	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1315	853	213	241	8		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1461	916	265	272	8		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			342	225	58	59		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			999	650	173	170	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	105	Total	C	N	O	S	0	0
			867	550	161	150	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	347	Total	C	N	O	S	0	0
			2710	1782	420	462	46		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	98	Total	C	N	O	S	0	0
			748	493	113	128	14		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4720	3118	739	814	49		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			919	614	137	160	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	56	Total	C	N	O	S	0	0
			479	311	88	79	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1062	691	182	189			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1530	980	279	263	8		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3631	2412	572	609	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			998	625	183	181	9		

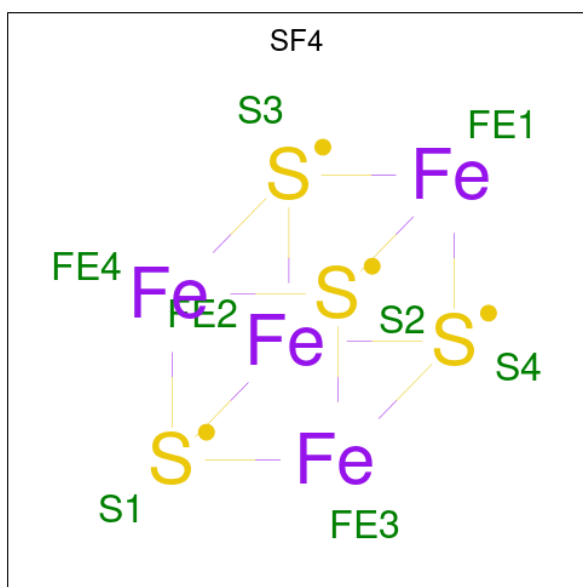
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

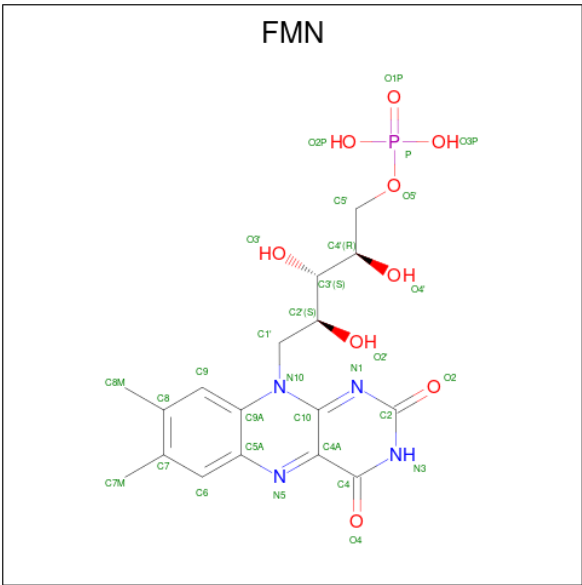
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

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



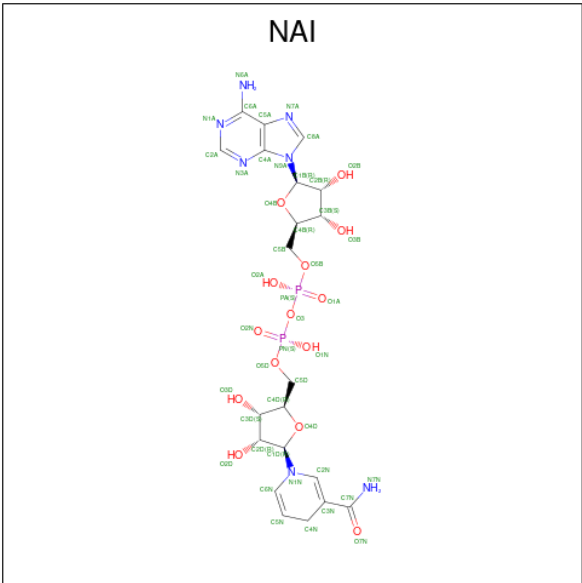
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



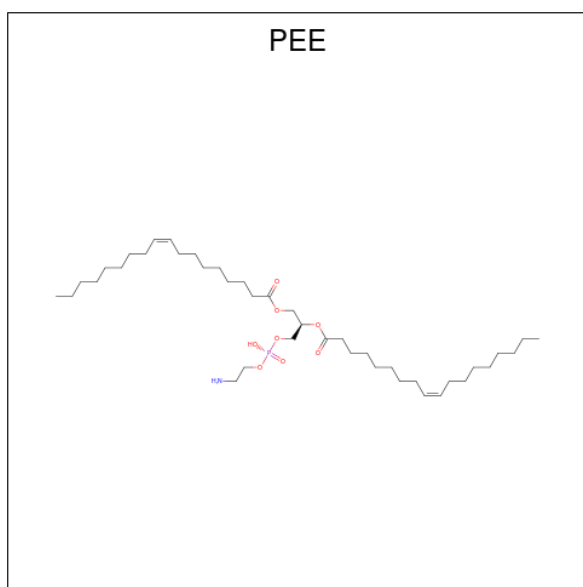
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



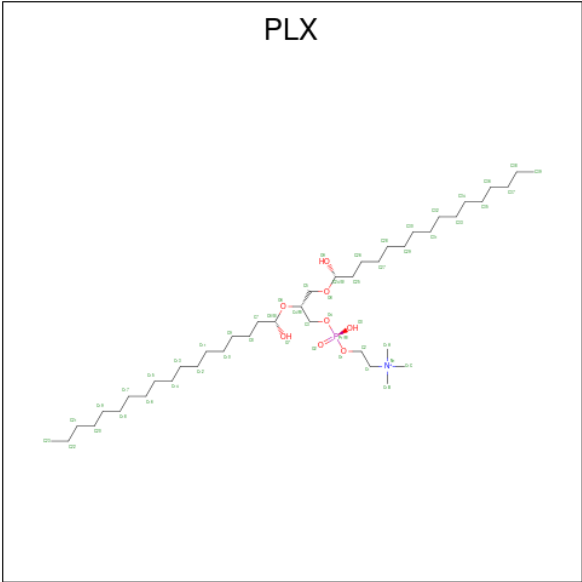
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



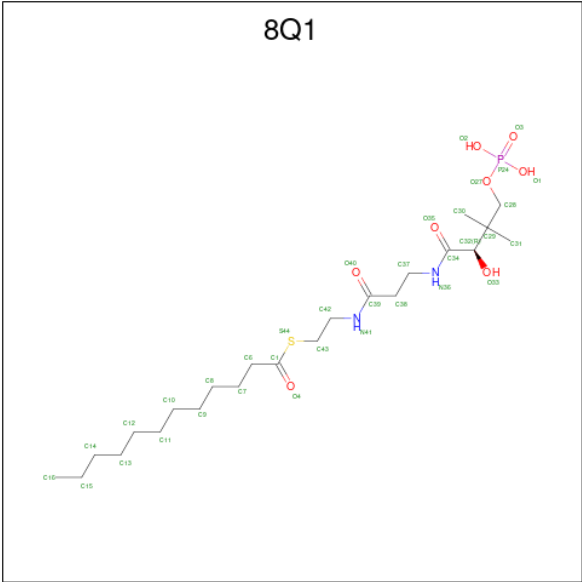
Mol	Chain	Residues	Atoms					AltConf
48	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
48	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
48	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
48	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
48	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 49 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



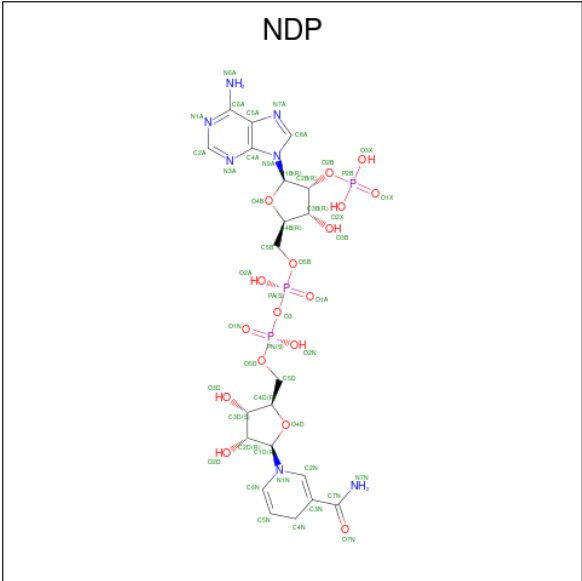
Mol	Chain	Residues	Atoms					AltConf
49	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
49	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



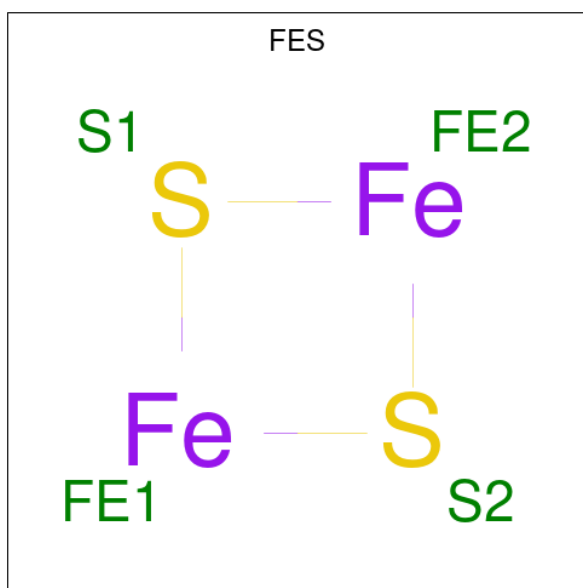
Mol	Chain	Residues	Atoms						AltConf
50	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
50	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



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

- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	Fe	S	0
			4	2	2	
52	O	1	Total	Fe	S	0
			4	2	2	

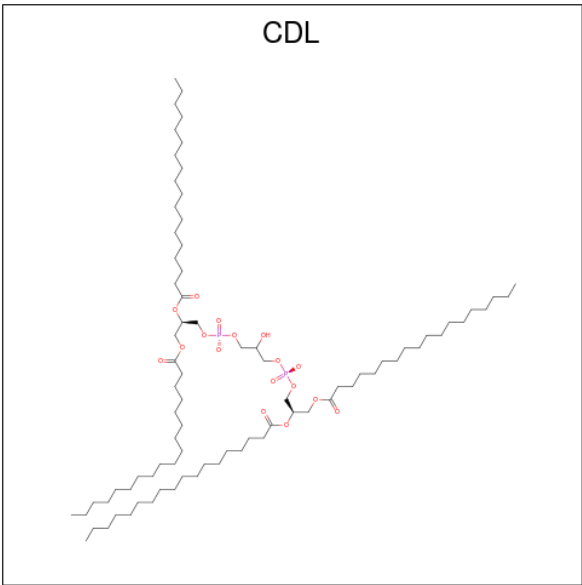
- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

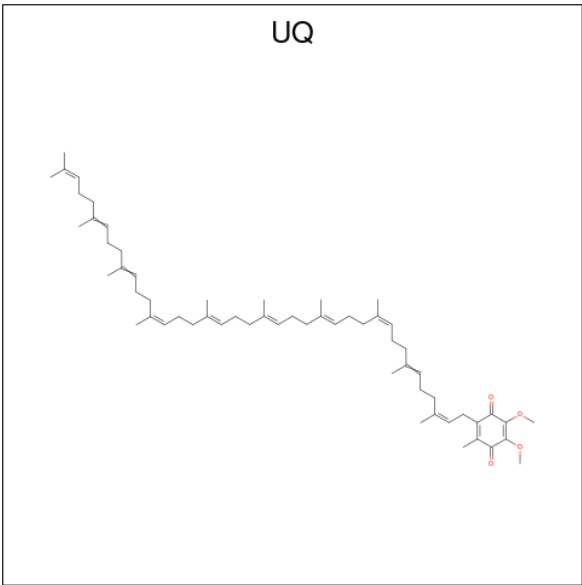
Mol	Chain	Residues	Atoms		AltConf
54	T	1	Total	Zn	0
			1	1	

- Molecule 55 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).



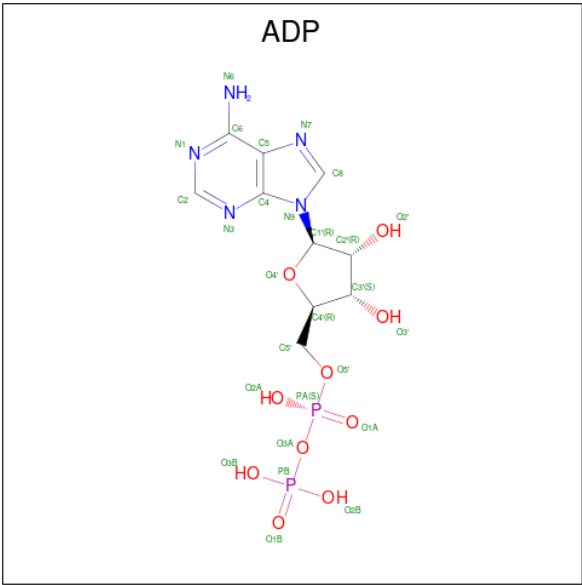
Mol	Chain	Residues	Atoms				AltConf
55	a	1	Total	C	O	P	0
			91	72	17	2	
55	i	1	Total	C	O	P	0
			66	47	17	2	
55	l	1	Total	C	O	P	0
			100	81	17	2	
55	r	1	Total	C	O	P	0
			99	80	17	2	
55	r	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
56	s	1	28	24	4	0

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

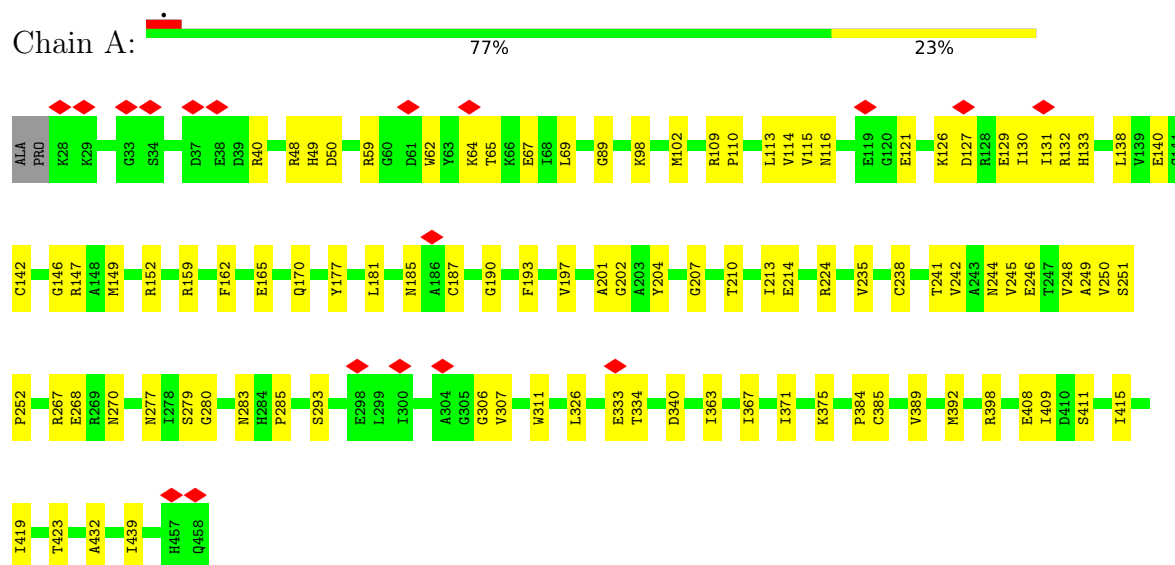


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

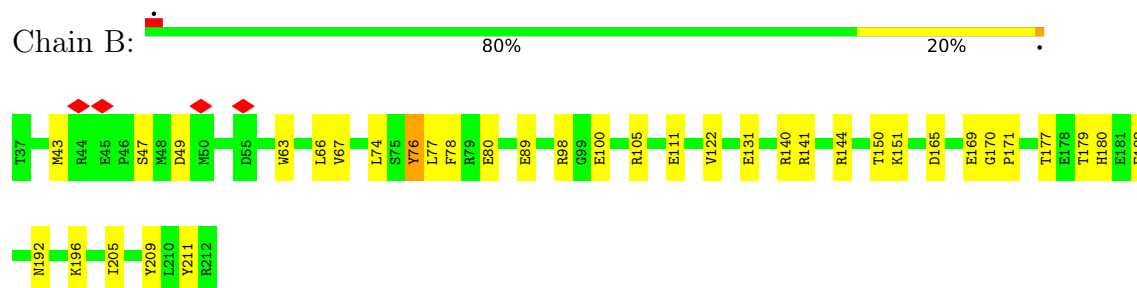
3 Residue-property plots

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

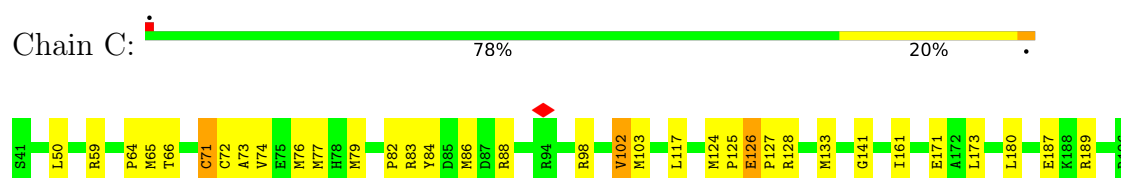
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



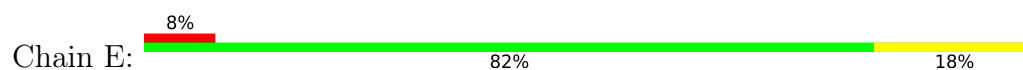
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



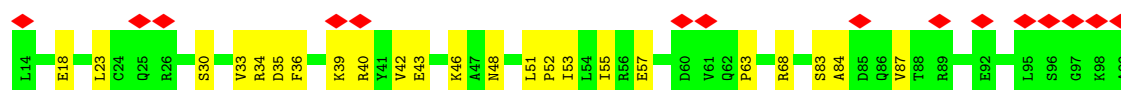
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



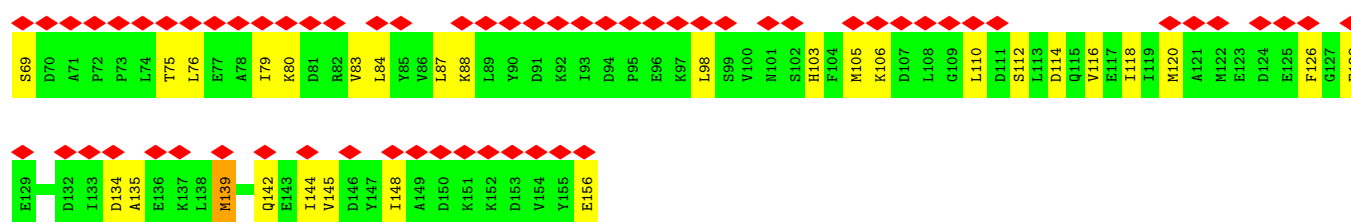
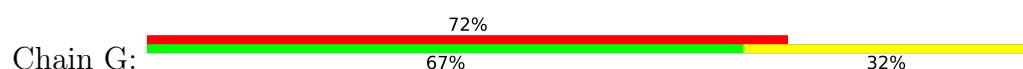
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



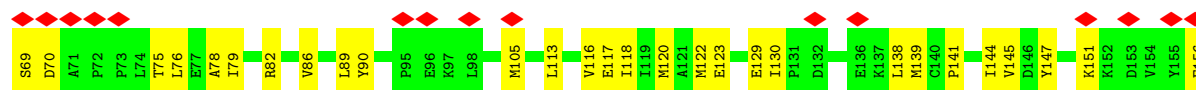
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



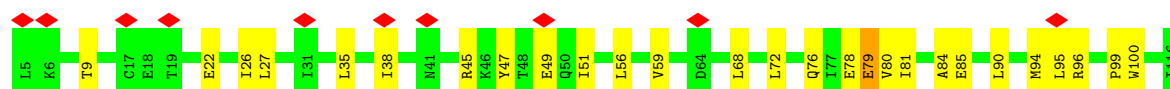
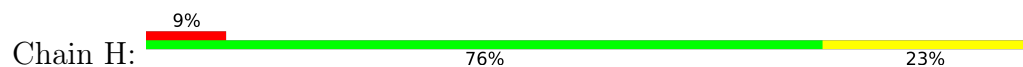
- Molecule 6: Acyl carrier protein



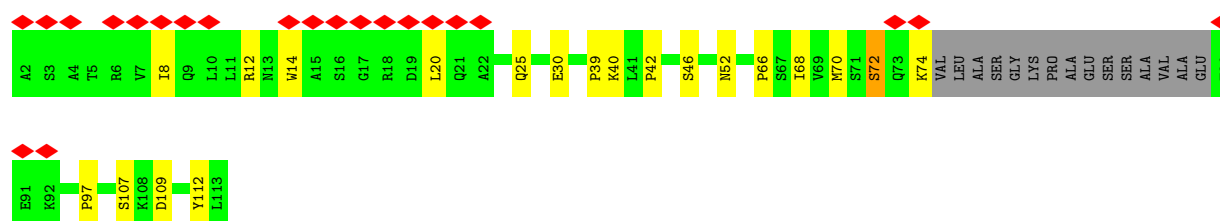
- Molecule 6: Acyl carrier protein



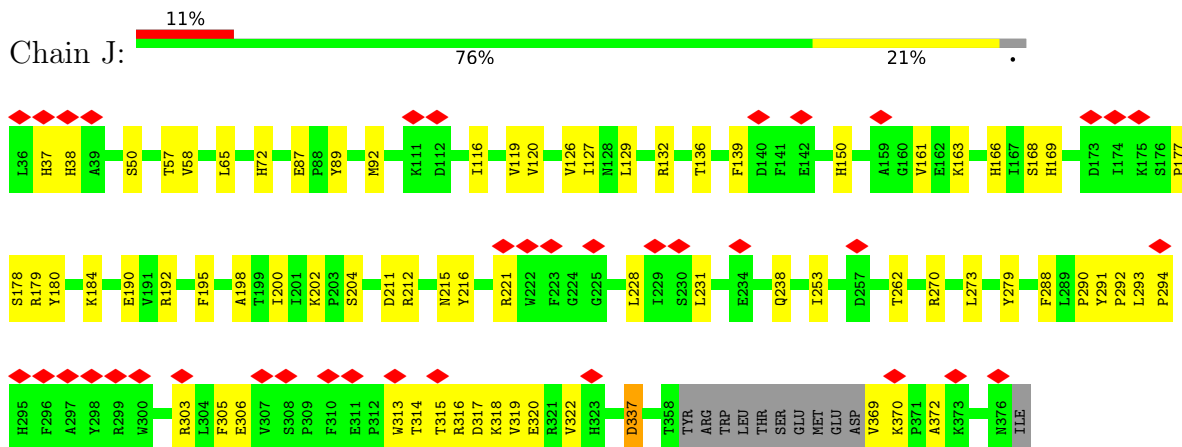
- Molecule 7: Complex I subunit B13



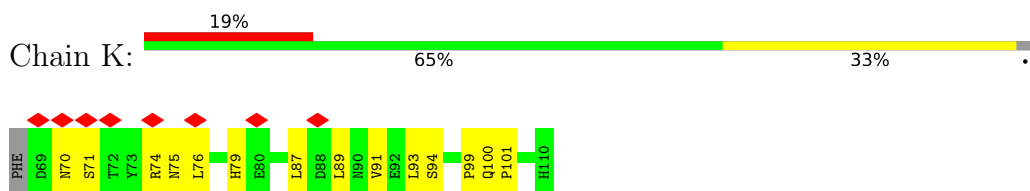
- Molecule 8: Complex I-B14.5a



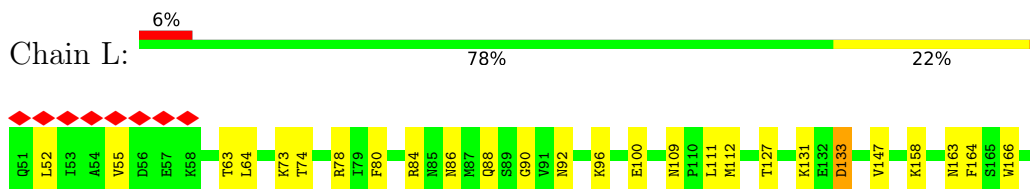
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



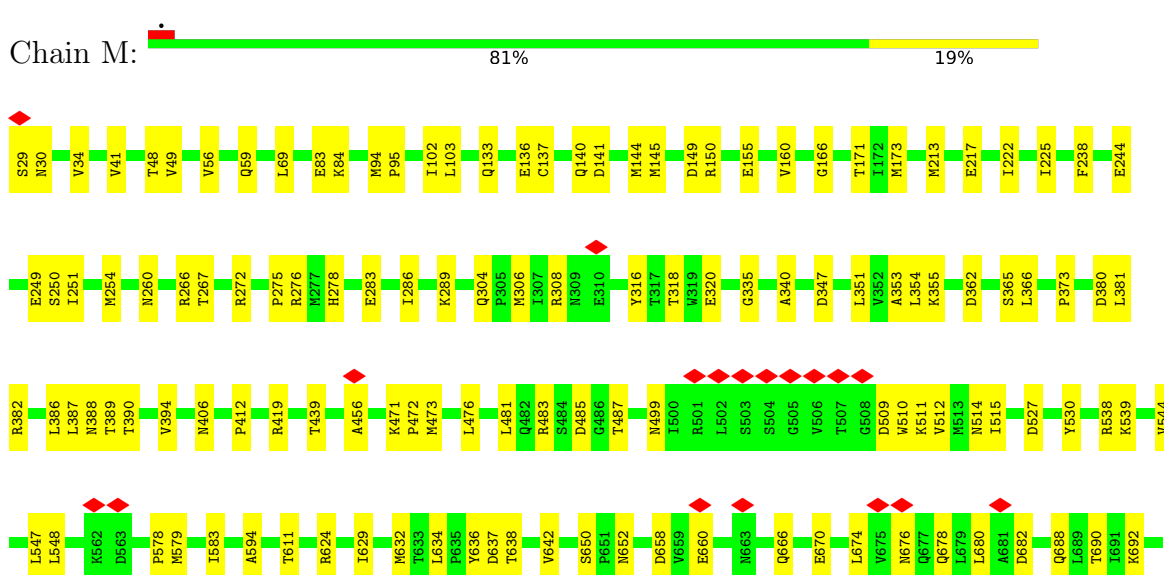
- Molecule 10: Complex I-9kD

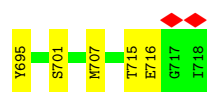


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

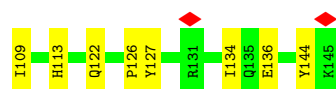
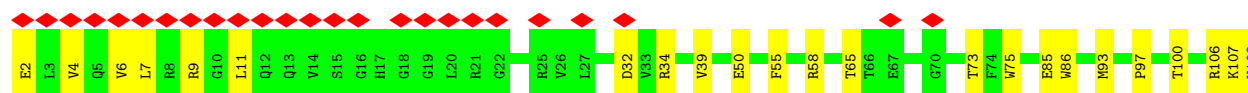
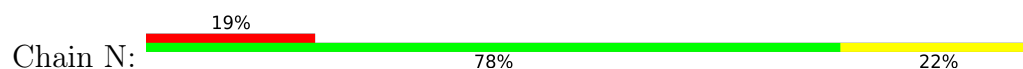


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

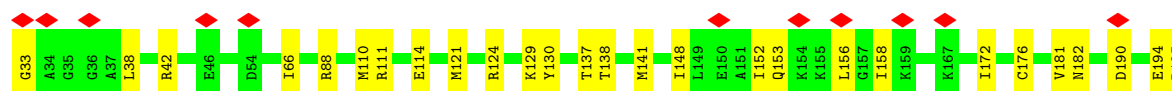
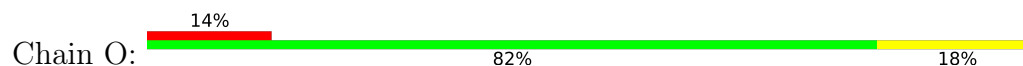




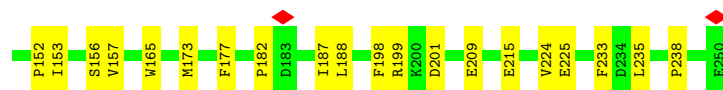
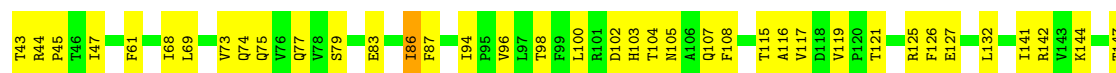
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



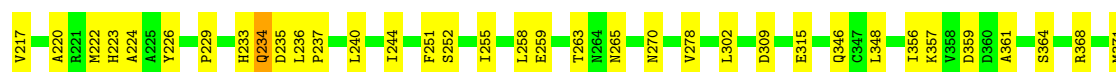
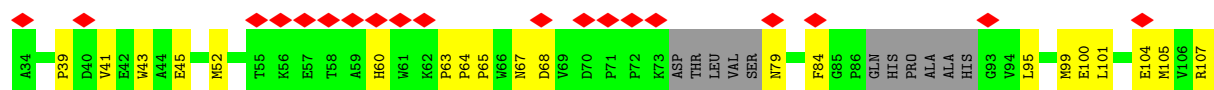
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: Complex I-30kD

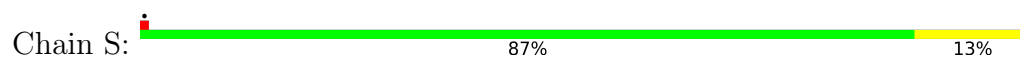


- Molecule 16: Complex I-49kD

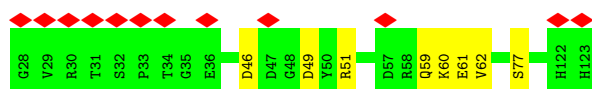




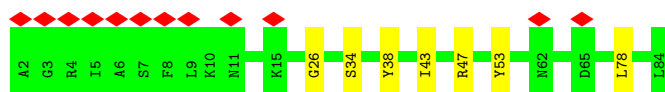
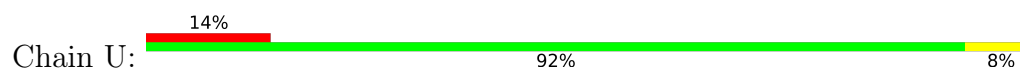
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



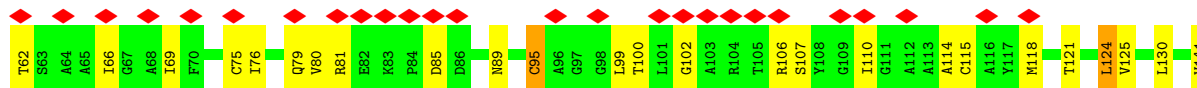
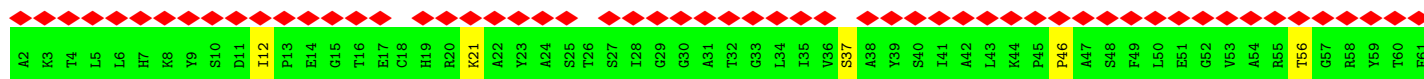
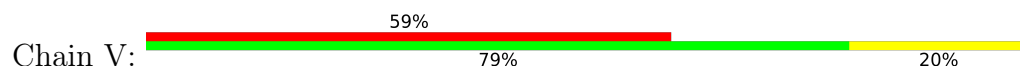
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



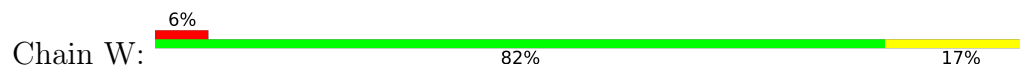
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

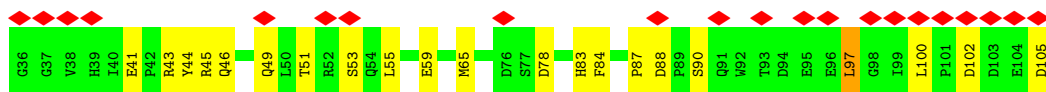


- Molecule 21: Complex I-B16.6

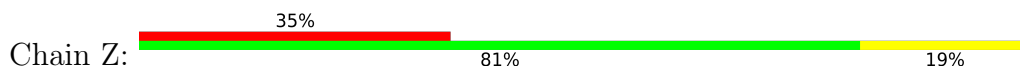


- Molecule 22: Complex I-AGGG

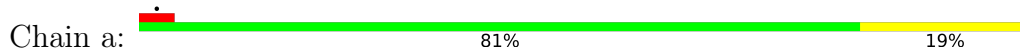




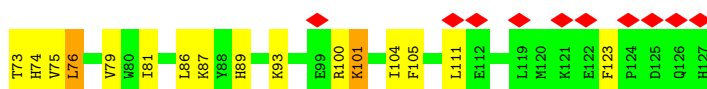
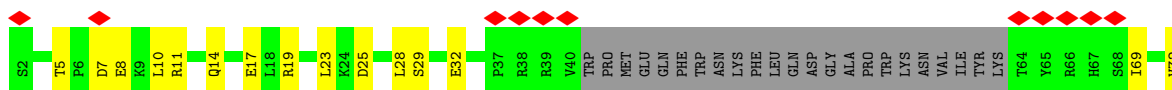
• Molecule 23: Complex I-B12



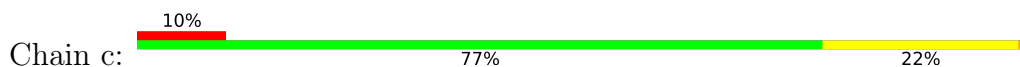
• Molecule 24: Complex I-SGDH



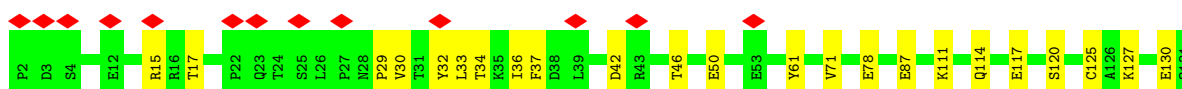
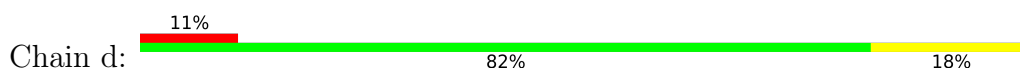
• Molecule 25: Complex I-B17

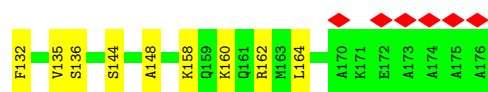


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

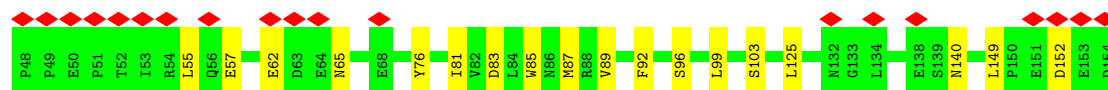
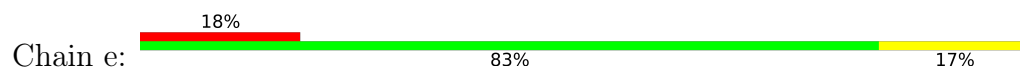


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10





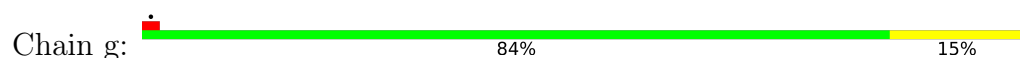
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



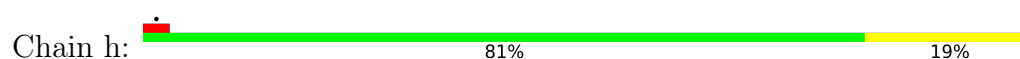
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



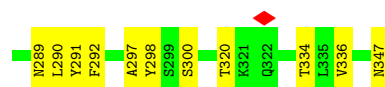
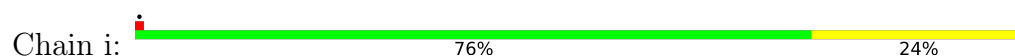
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



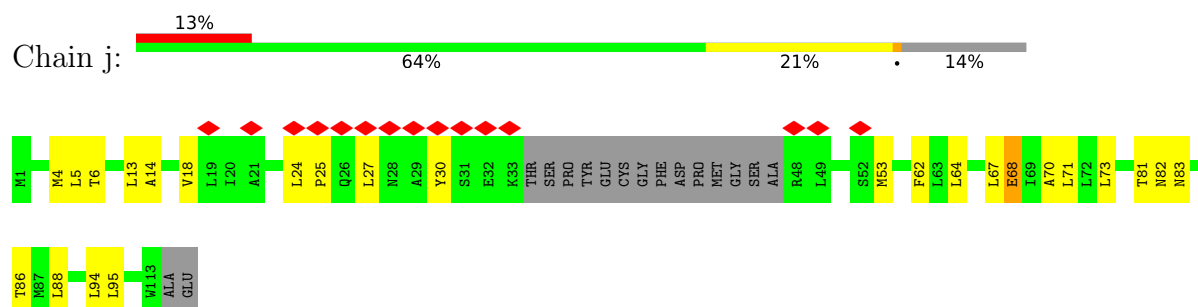
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



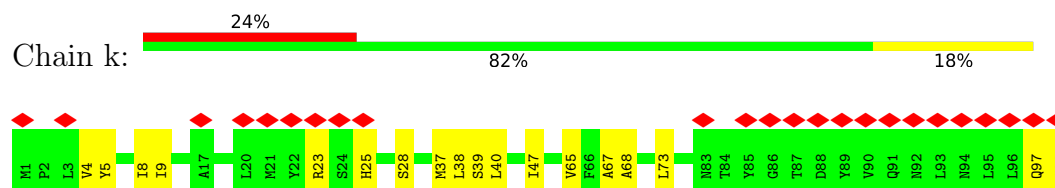
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



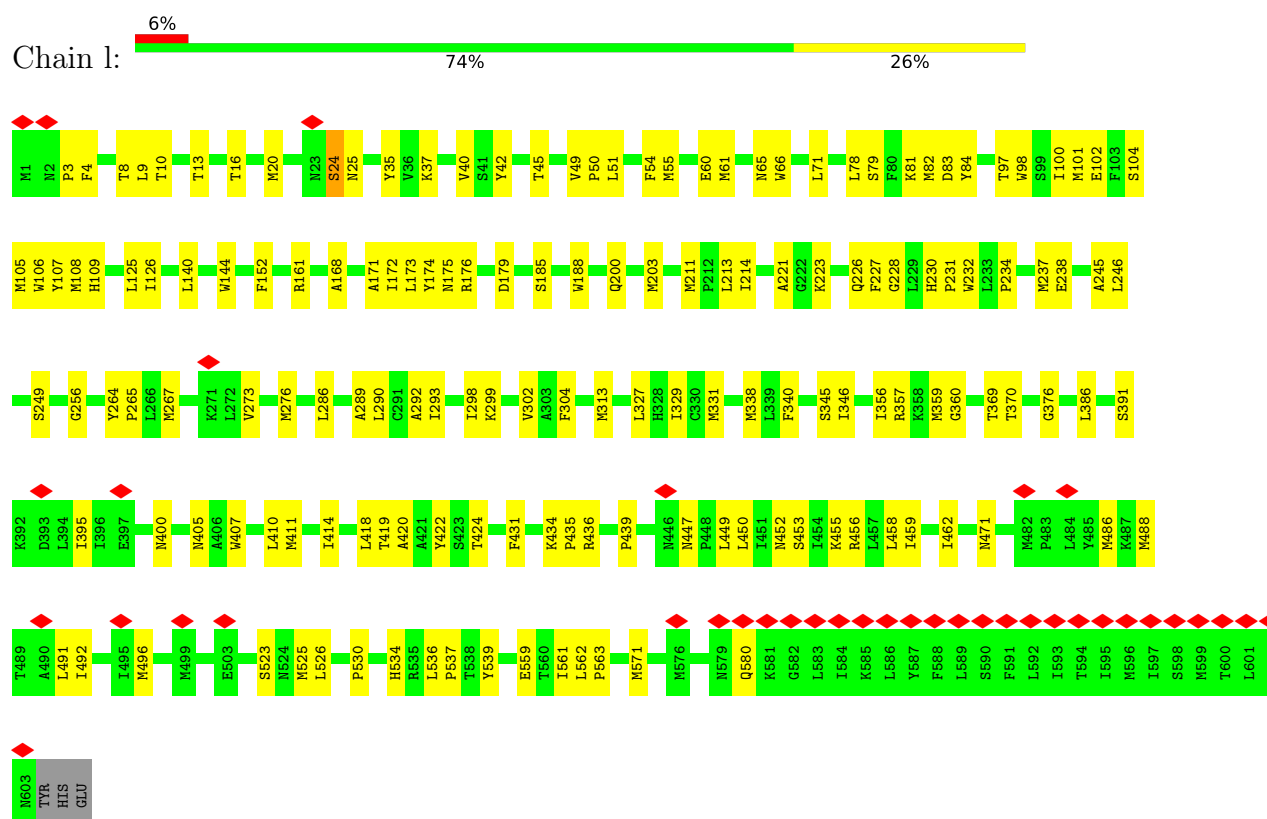
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



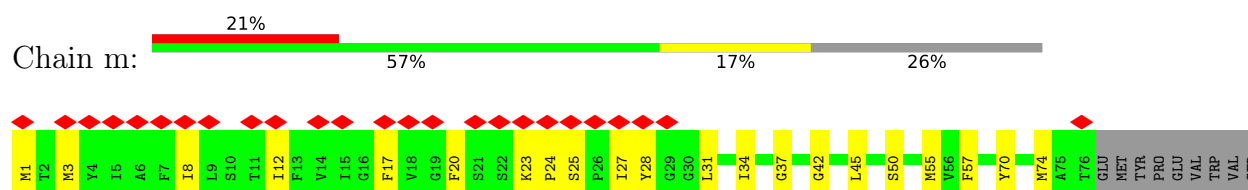
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

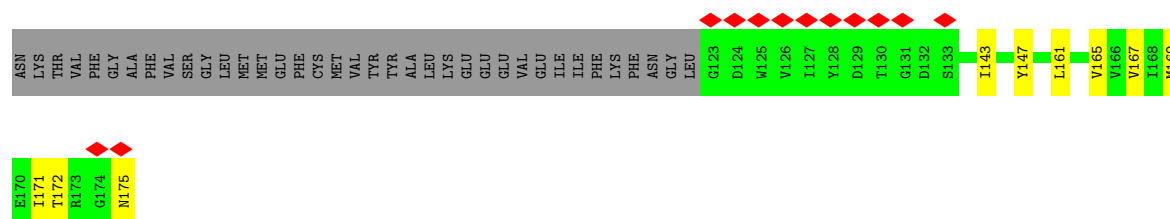


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

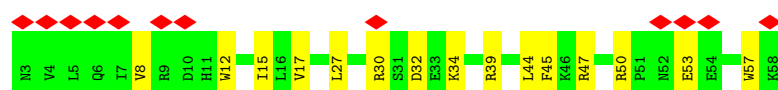
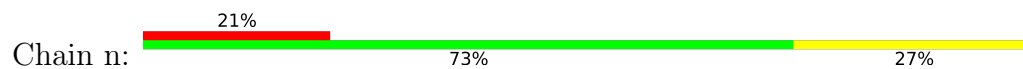


- Molecule 36: NADH-ubiquinone oxidoreductase chain 6

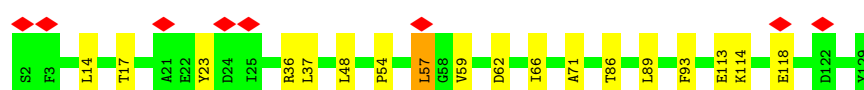
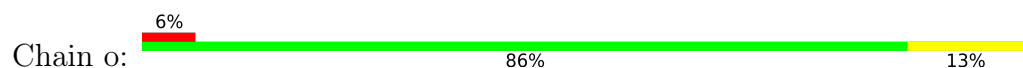




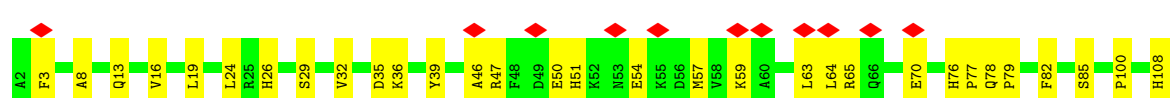
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



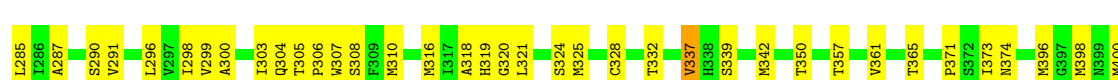
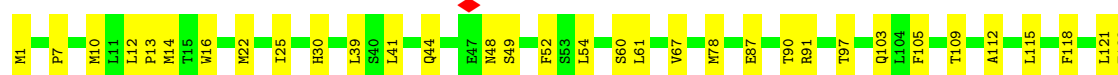
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



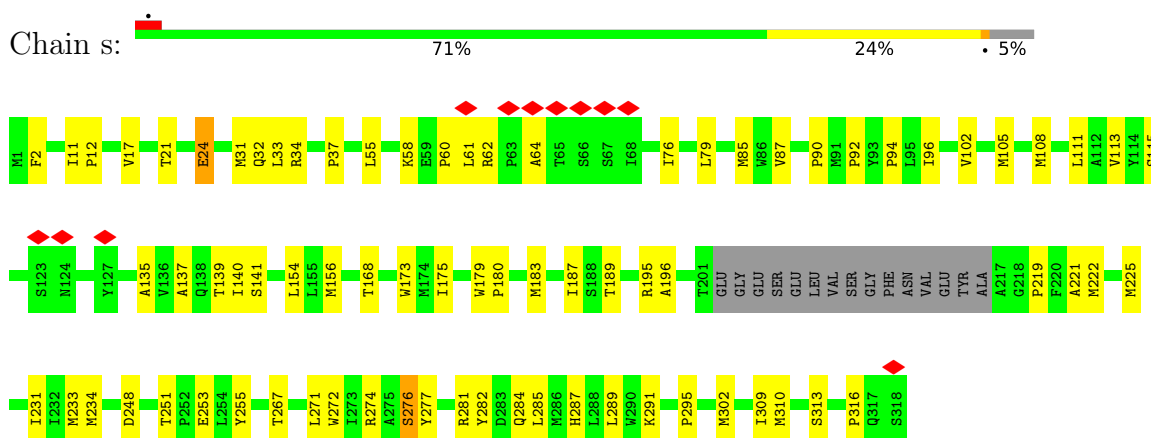
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



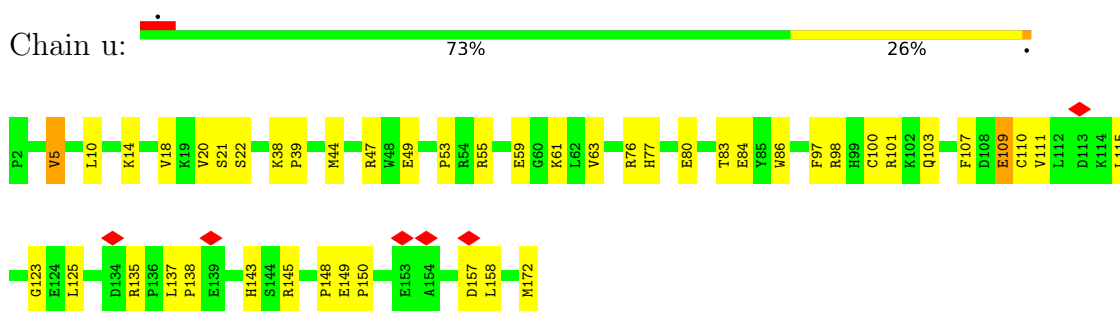
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4



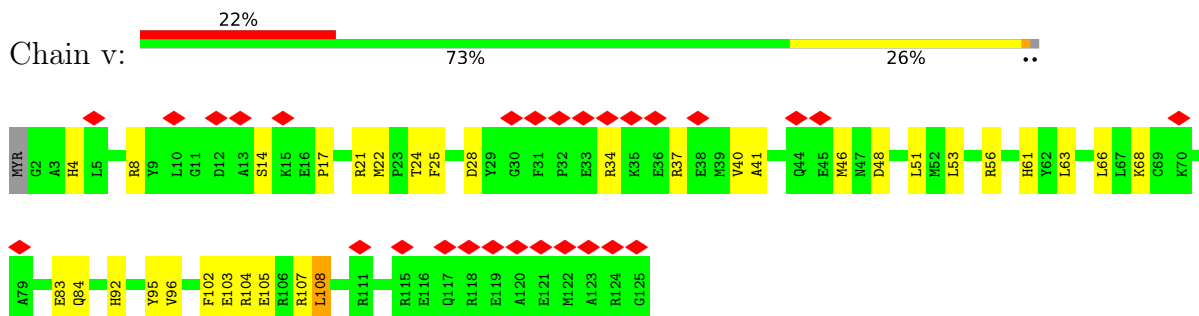
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1



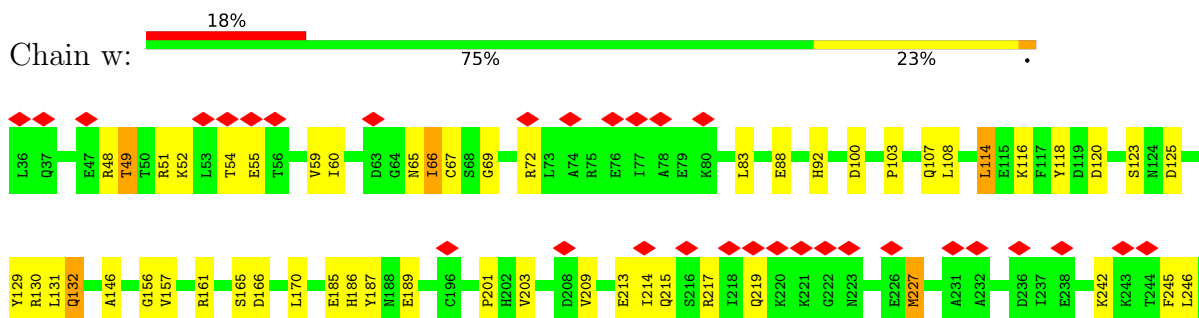
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	124144	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.191	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, PEE, 2MR, PLX, FES, ADP, SF4, NAI, MG, FMN, NDP, UQ, ZN, 8Q1

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	0.14	0/3393	0.35	0/4584
2	B	0.11	0/1443	0.28	0/1952
3	C	0.23	0/1279	0.39	0/1730
4	E	0.14	0/995	0.33	0/1340
5	F	0.13	0/702	0.35	0/945
6	G	0.17	0/705	0.41	0/956
6	X	0.12	0/707	0.32	0/958
7	H	0.15	0/929	0.39	0/1258
8	I	0.13	0/798	0.37	0/1079
9	J	0.12	0/2684	0.33	0/3638
10	K	0.12	0/365	0.37	0/493
11	L	0.12	0/1039	0.30	0/1403
12	M	0.12	0/5384	0.33	1/7295 (0.0%)
13	N	0.11	0/1245	0.30	0/1694
14	O	0.13	0/1708	0.35	0/2324
15	P	0.12	0/1789	0.35	0/2436
16	Q	0.14	0/3451	0.39	2/4672 (0.0%)
17	S	0.21	0/572	0.53	1/771 (0.1%)
18	T	0.08	0/755	0.24	0/1018
19	U	0.12	0/664	0.30	0/912
20	V	0.14	0/1039	0.37	0/1407
21	W	0.12	0/1198	0.28	0/1617
22	Y	0.17	0/626	0.38	0/857
23	Z	0.13	0/695	0.36	0/939
24	a	0.13	0/1199	0.42	2/1623 (0.1%)
25	b	0.14	0/906	0.37	0/1232
26	c	0.14	0/1371	0.35	0/1875
27	d	0.12	0/1494	0.31	0/2015
28	e	0.11	0/916	0.30	0/1246
29	f	0.10	0/350	0.21	0/473
30	g	0.11	0/1030	0.26	0/1393
31	h	0.12	0/889	0.34	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.14	0/2773	0.34	0/3768
33	j	0.16	0/819	0.37	0/1117
34	k	0.14	0/759	0.31	0/1029
35	l	0.13	0/4845	0.33	0/6595
36	m	0.13	0/938	0.35	0/1271
37	n	0.11	0/491	0.31	0/663
38	o	0.11	0/1092	0.33	0/1481
39	p	0.15	0/1586	0.40	1/2150 (0.0%)
40	r	0.14	0/3723	0.34	0/5078
41	s	0.15	0/2464	0.37	0/3369
42	u	0.11	0/1436	0.31	0/1938
43	v	0.14	0/1022	0.37	0/1377
44	w	0.12	0/2642	0.32	0/3580
All	All	0.13	0/66910	0.34	7/90741 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	233	HIS	N-CA-C	9.19	120.91	111.07
16	Q	234	GLN	N-CA-C	8.15	122.63	111.71
24	a	128	GLY	CA-C-N	6.87	126.67	119.05
24	a	128	GLY	C-N-CA	6.87	126.67	119.05
12	M	695	TYR	N-CA-C	6.43	118.29	111.28
17	S	18	ILE	CB-CA-C	-6.31	107.66	114.35
39	p	133	TRP	N-CA-C	5.60	117.39	111.28

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	3318	0	3280	71	0
2	B	1412	0	1363	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1248	0	1254	32	0
4	E	971	0	975	13	0
5	F	691	0	704	15	0
6	G	693	0	671	23	0
6	X	695	0	669	19	0
7	H	910	0	950	20	0
8	I	780	0	808	19	0
9	J	2615	0	2635	55	0
10	K	355	0	329	11	0
11	L	1016	0	1016	24	0
12	M	5296	0	5326	81	0
13	N	1204	0	1162	22	0
14	O	1668	0	1671	27	0
15	P	1738	0	1693	41	0
16	Q	3377	0	3320	76	0
17	S	558	0	551	7	0
18	T	741	0	702	7	0
19	U	643	0	642	6	0
20	V	1018	0	1018	27	0
21	W	1167	0	1155	24	0
22	Y	600	0	539	20	0
23	Z	674	0	643	14	0
24	a	1165	0	1174	22	0
25	b	879	0	899	30	0
26	c	1315	0	1208	31	0
27	d	1461	0	1429	22	0
28	e	890	0	837	14	0
29	f	342	0	341	6	0
30	g	999	0	991	15	0
31	h	867	0	871	17	0
32	i	2710	0	2874	62	0
33	j	800	0	855	25	0
34	k	748	0	799	17	0
35	l	4720	0	4797	99	0
36	m	919	0	920	31	0
37	n	479	0	486	10	0
38	o	1062	0	1072	15	0
39	p	1530	0	1466	42	0
40	r	3631	0	3839	79	0
41	s	2394	0	2508	70	0
42	u	1398	0	1378	33	0
43	v	998	0	919	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	w	2582	0	2531	50	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	6	0
47	A	44	0	27	6	0
48	B	51	0	82	5	0
48	b	46	0	69	7	0
48	i	47	0	71	2	0
48	j	51	0	82	4	0
48	l	46	0	69	3	0
48	m	41	0	59	4	0
48	r	51	0	82	6	0
49	C	52	0	88	5	0
49	g	52	0	88	4	0
49	j	52	0	88	4	0
49	r	104	0	176	8	0
50	G	35	0	0	2	0
50	X	35	0	0	3	0
51	J	48	0	25	2	0
52	M	4	0	0	0	0
52	O	4	0	0	0	0
53	M	1	0	0	0	0
54	T	1	0	0	0	0
55	a	91	0	132	6	0
55	i	66	0	76	3	0
55	l	100	0	156	9	0
55	r	199	0	307	19	0
56	s	28	0	31	4	0
57	w	27	0	11	2	0
All	All	66632	0	67008	1212	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 (1212) 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)
20:V:69:ILE:HD13	20:V:100:THR:CG2	1.55	1.34
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.69	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.12
20:V:69:ILE:HD13	20:V:100:THR:CB	1.88	1.02
20:V:69:ILE:CD1	20:V:100:THR:HG21	1.90	1.02
20:V:62:THR:O	20:V:66:ILE:HG13	1.57	1.01
45:C:301:SF4:S4	16:Q:223:HIS:CD2	2.54	1.00
20:V:69:ILE:CD1	20:V:100:THR:CB	2.39	0.98
26:c:184:TYR:HA	43:v:34:ARG:HH12	1.28	0.97
20:V:69:ILE:HD13	20:V:100:THR:HG21	0.95	0.94
9:J:231:LEU:CD1	9:J:292:PRO:HD3	2.01	0.90
9:J:231:LEU:HD13	9:J:292:PRO:HD3	1.51	0.90
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.56	0.88
20:V:69:ILE:CD1	20:V:100:THR:HB	2.04	0.87
20:V:69:ILE:CD1	20:V:100:THR:CG2	2.49	0.86
9:J:212:ARG:O	9:J:216:TYR:HB3	1.77	0.85
4:E:37:ARG:HG2	6:G:120:MET:HE2	1.56	0.84
3:C:98:ARG:HH21	41:s:61:LEU:HD13	1.42	0.81
22:Y:97:LEU:HD21	43:v:104:ARG:HA	1.63	0.80
44:w:350:LYS:HD3	44:w:351:TRP:H	1.48	0.78
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.64	0.77
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.66	0.77
1:A:127:ASP:O	1:A:131:ILE:HG13	1.86	0.76
7:H:72:LEU:HD13	7:H:80:VAL:HG11	1.69	0.75
35:l:286:LEU:HD22	35:l:411:MET:HE3	1.68	0.75
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.68	0.75
42:u:76:ARG:HG2	42:u:77:HIS:HD2	1.51	0.75
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.20	0.74
16:Q:100:GLU:HG2	16:Q:108:LYS:HB3	1.68	0.74
32:i:87:THR:HG22	32:i:88:LYS:H	1.52	0.73
32:i:91:ASN:ND2	32:i:92:PRO:HD2	2.02	0.73
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.21	0.73
5:F:40:ARG:HH12	5:F:84:ALA:HB1	1.54	0.72
33:j:18:VAL:HG21	41:s:76:ILE:HG12	1.71	0.71
1:A:210:THR:HB	1:A:224:ARG:H	1.56	0.70
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.71	0.70
40:r:324:SER:HG	40:r:440:HIS:HE2	1.37	0.70
24:a:141:GLN:NE2	24:a:145:GLU:OE1	2.24	0.70
2:B:111:GLU:O	2:B:141:ARG:NH1	2.24	0.70
44:w:242:LYS:HA	44:w:246:LEU:HD23	1.74	0.69
16:Q:184:ILE:HG12	16:Q:203:MET:HE3	1.73	0.69
27:d:114:GLN:HG3	35:l:203:MET:HG2	1.73	0.69
35:l:357:ARG:HG3	39:p:32:VAL:HG13	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:69:ILE:HD12	20:V:100:THR:CB	2.22	0.69
32:i:177:LYS:NZ	34:k:97:GLN:O	2.25	0.69
20:V:69:ILE:HG21	20:V:100:THR:HG21	1.75	0.69
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.75	0.68
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.73	0.68
9:J:293:LEU:HG	9:J:294:PRO:HD2	1.76	0.68
3:C:66:THR:HG21	3:C:76:MET:HG2	1.75	0.68
55:r:504:CDL:H612	55:r:504:CDL:H451	1.75	0.68
9:J:212:ARG:O	9:J:216:TYR:CB	2.41	0.68
26:c:46:GLU:OE1	26:c:46:GLU:N	2.22	0.68
1:A:409:ILE:HG23	1:A:439:ILE:HD12	1.75	0.67
21:W:66:GLU:HG3	42:u:125:LEU:HB2	1.74	0.67
26:c:116:ARG:HG2	48:l:702:PEE:H49	1.76	0.67
19:U:26:GLY:HA3	48:j:201:PEE:H37	1.77	0.67
1:A:159:ARG:NH2	14:O:176:CYS:O	2.27	0.67
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.27	0.67
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.22	0.67
16:Q:52:MET:O	32:i:171:ASN:ND2	2.26	0.67
6:G:105:MET:SD	6:G:139:MET:HE2	2.35	0.67
36:m:55:MET:HA	36:m:55:MET:HE2	1.77	0.67
32:i:239:VAL:HG23	55:r:505:CDL:H311	1.78	0.66
55:r:504:CDL:H312	55:r:504:CDL:H742	1.78	0.66
1:A:50:ASP:O	1:A:59:ARG:NH2	2.28	0.66
35:l:400:ASN:HB3	35:l:486:MET:HE3	1.76	0.66
5:F:46:LYS:HE3	12:M:674:LEU:HD11	1.78	0.66
24:a:70:LEU:HD13	28:e:87:MET:HE3	1.76	0.66
1:A:49:HIS:HA	10:K:74:ARG:HH11	1.60	0.66
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.34	0.66
11:L:109:ASN:ND2	11:L:111:LEU:O	2.28	0.66
28:e:81:ILE:HD12	28:e:81:ILE:H	1.60	0.66
6:G:144:ILE:O	6:G:148:ILE:HD12	1.94	0.66
9:J:211:ASP:OD1	9:J:215:ASN:ND2	2.29	0.66
27:d:164:LEU:HD12	28:e:149:LEU:HD23	1.78	0.66
8:I:42:PRO:HB3	21:W:6:VAL:HG11	1.76	0.66
39:p:57:MET:HE2	39:p:57:MET:HA	1.78	0.66
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.29	0.65
16:Q:178:THR:HG1	16:Q:214:TYR:HH	1.42	0.65
24:a:131:LYS:NZ	37:n:32:ASP:OD2	2.27	0.65
27:d:30:VAL:O	27:d:34:THR:HG23	1.97	0.65
1:A:152:ARG:NH2	10:K:99:PRO:O	2.29	0.65
25:b:28:LEU:HG	25:b:32:GLU:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:20:MET:HG2	55:r:504:CDL:H832	1.79	0.65
41:s:281:ARG:HB2	41:s:284:GLN:HG3	1.79	0.65
20:V:107:SER:HB3	20:V:110:ILE:HB	1.77	0.65
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.78	0.65
43:v:83:GLU:OE1	43:v:83:GLU:N	2.21	0.65
1:A:140:GLU:OE2	1:A:252:PRO:HB3	1.97	0.64
1:A:392:MET:HE1	1:A:432:ALA:HA	1.79	0.64
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.78	0.64
40:r:269:MET:HE1	40:r:296:LEU:HD13	1.78	0.64
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.31	0.64
22:Y:41:GLU:OE2	22:Y:41:GLU:N	2.30	0.64
43:v:51:LEU:HD13	43:v:63:LEU:HD23	1.80	0.64
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.80	0.64
25:b:101:LYS:HG3	25:b:101:LYS:O	1.97	0.64
29:f:62:HIS:O	29:f:66:VAL:HG23	1.98	0.64
44:w:114:LEU:HD12	44:w:131:LEU:HD21	1.78	0.64
27:d:144:SER:OG	27:d:158:LYS:NZ	2.25	0.64
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.80	0.64
20:V:69:ILE:HD12	20:V:100:THR:OG1	1.98	0.64
40:r:285:LEU:HD22	40:r:410:MET:HE2	1.80	0.64
41:s:55:LEU:HD13	41:s:221:ALA:HB2	1.80	0.64
12:M:676:ASN:O	12:M:678:GLN:NE2	2.31	0.63
23:Z:24:ILE:HG22	23:Z:30:GLU:HG2	1.81	0.63
36:m:1:MET:HE3	36:m:3:MET:HA	1.81	0.63
36:m:8:ILE:O	36:m:12:ILE:HG13	1.98	0.63
1:A:185:ASN:OD1	1:A:190:GLY:N	2.31	0.63
2:B:76:TYR:HE1	41:s:33:LEU:HD13	1.63	0.63
2:B:177:THR:HG22	2:B:179:THR:H	1.62	0.63
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.81	0.63
29:f:65:ASP:OD2	30:g:79:LYS:NZ	2.31	0.63
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.32	0.63
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.80	0.63
40:r:210:TYR:O	40:r:213:HIS:ND1	2.32	0.63
15:P:43:THR:HA	15:P:47:ILE:HD12	1.80	0.63
23:Z:68:LEU:HB3	23:Z:71:PHE:HB2	1.80	0.62
7:H:22:GLU:O	7:H:26:ILE:HD12	1.99	0.62
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.32	0.62
13:N:39:VAL:HG23	13:N:50:GLU:HG2	1.80	0.62
12:M:690:THR:HG22	12:M:692:LYS:H	1.63	0.62
6:X:141:PRO:O	6:X:145:VAL:HG23	1.99	0.62
27:d:111:LYS:NZ	35:l:200:GLN:OE1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:182:ASN:OD1	16:Q:404:LYS:NZ	2.33	0.62
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.81	0.62
40:r:14:MET:SD	40:r:30:HIS:ND1	2.69	0.62
7:H:47:TYR:O	7:H:51:ILE:HG13	2.00	0.62
37:n:47:ARG:NH2	37:n:53:GLU:OE1	2.33	0.62
40:r:191:SER:HB3	48:r:501:PEE:H3	1.82	0.62
43:v:22:MET:HE1	43:v:102:PHE:HA	1.80	0.62
26:c:160:GLN:OE1	43:v:37:ARG:NH1	2.33	0.62
49:g:201:PLX:H301	32:i:347:ASN:HB3	1.81	0.62
35:l:40:VAL:HG21	35:l:101:MET:HE3	1.81	0.62
21:W:50:MET:HE1	41:s:168:THR:HG22	1.82	0.61
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.82	0.61
16:Q:198:THR:HG23	41:s:32:GLN:HG2	1.82	0.61
25:b:7:ASP:OD1	25:b:8:GLU:N	2.34	0.61
50:X:201:8Q1:N36	50:X:201:8Q1:O40	2.33	0.61
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.83	0.61
10:K:100:GLN:HG3	10:K:101:PRO:HD2	1.82	0.61
16:Q:196:ALA:O	16:Q:197:MET:HG3	2.01	0.61
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.81	0.61
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.82	0.61
34:k:25:HIS:O	34:k:28:SER:N	2.32	0.61
35:l:227:PHE:O	35:l:230:HIS:ND1	2.32	0.61
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.81	0.61
12:M:136:GLU:OE2	12:M:272:ARG:NH2	2.34	0.60
15:P:117:VAL:HB	15:P:127:GLU:HG2	1.83	0.60
25:b:79:VAL:HG22	35:l:10:THR:HG21	1.82	0.60
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.33	0.60
44:w:249:MET:HE3	44:w:252:LYS:HE3	1.81	0.60
3:C:77:MET:HE1	16:Q:185:MET:HE1	1.83	0.60
3:C:125:PRO:HG3	41:s:61:LEU:CD1	2.31	0.60
9:J:192:ARG:NH1	9:J:198:ALA:O	2.35	0.60
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.81	0.60
9:J:50:SER:OG	15:P:225:GLU:OE2	2.20	0.60
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.82	0.60
32:i:283:ALA:HB1	40:r:158:LEU:HD13	1.83	0.60
44:w:88:GLU:OE1	44:w:161:ARG:NH1	2.35	0.60
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.83	0.60
12:M:171:THR:HG23	12:M:173:MET:HE3	1.84	0.60
12:M:306:MET:HB2	12:M:583:ILE:HB	1.83	0.60
14:O:38:LEU:O	14:O:124:ARG:NH2	2.35	0.60
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:201:MET:HE2	48:r:501:PEE:H78	1.84	0.60
3:C:125:PRO:HG3	41:s:61:LEU:HD12	1.84	0.60
39:p:13:GLN:OE1	39:p:13:GLN:N	2.34	0.60
26:c:165:ASP:OD2	26:c:170:ARG:NH2	2.35	0.60
44:w:92:HIS:HD2	44:w:103:PRO:HB2	1.66	0.60
1:A:129:GLU:OE2	1:A:132:ARG:HD3	2.01	0.59
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.84	0.59
48:B:303:PEE:H59	41:s:277:TYR:HE2	1.67	0.59
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	1.84	0.59
55:a:201:CDL:H191	55:a:201:CDL:H732	1.84	0.59
26:c:155:PRO:HG3	43:v:4:HIS:CD2	2.37	0.59
32:i:133:TRP:HE3	55:i:401:CDL:H391	1.66	0.59
44:w:289:ARG:HH21	44:w:293:ARG:HH12	1.50	0.59
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.33	0.59
32:i:236:LYS:HG2	32:i:237:MET:HG3	1.84	0.59
55:r:505:CDL:H742	55:r:505:CDL:H271	1.84	0.59
1:A:102:MET:HE3	1:A:149:MET:HB3	1.84	0.59
12:M:254:MET:HE2	12:M:289:LYS:HG2	1.82	0.59
27:d:71:VAL:HG11	27:d:87:GLU:HB3	1.85	0.59
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.84	0.59
32:i:334:THR:HG21	55:r:505:CDL:H391	1.84	0.59
40:r:403:THR:HA	40:r:406:TYR:CE2	2.38	0.59
20:V:69:ILE:HG21	20:V:100:THR:CG2	2.33	0.59
13:N:7:LEU:O	13:N:11:LEU:HD12	2.03	0.59
32:i:278:MET:HG2	32:i:282:MET:HE2	1.84	0.59
33:j:73:LEU:HD13	36:m:55:MET:HE1	1.85	0.59
40:r:325:MET:HG3	40:r:440:HIS:HB3	1.85	0.59
3:C:73:ALA:O	3:C:76:MET:HB3	2.03	0.59
50:G:201:8Q1:O40	50:G:201:8Q1:N36	2.35	0.59
39:p:35:ASP:OD1	39:p:36:LYS:N	2.36	0.59
7:H:96:ARG:O	7:H:96:ARG:NE	2.36	0.58
10:K:89:LEU:O	10:K:93:LEU:HD12	2.02	0.58
35:l:24:SER:OG	35:l:25:ASN:N	2.34	0.58
7:H:9:THR:O	7:H:76:GLN:NE2	2.35	0.58
17:S:51:ASP:OD2	42:u:22:SER:OG	2.21	0.58
26:c:126:TRP:HA	26:c:129:MET:HE2	1.84	0.58
36:m:25:SER:O	36:m:28:TYR:N	2.34	0.58
44:w:59:VAL:HG13	44:w:201:PRO:HA	1.86	0.58
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.32	0.58
5:F:18:GLU:HB3	5:F:52:PRO:HG2	1.85	0.58
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LYS:NZ	14:O:33:GLY:O	2.36	0.58
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.86	0.58
48:B:303:PEE:H72	41:s:183:MET:HG2	1.86	0.58
28:e:85:TRP:O	28:e:89:VAL:HG13	2.04	0.58
1:A:214:GLU:OE2	1:A:224:ARG:NH2	2.32	0.58
7:H:38:ILE:HG13	7:H:95:LEU:HD23	1.86	0.58
9:J:204:SER:OG	9:J:238:GLN:O	2.20	0.58
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.86	0.58
48:m:201:PEE:H53	48:m:201:PEE:H25	1.86	0.58
6:X:69:SER:OG	6:X:70:ASP:N	2.37	0.57
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.36	0.57
35:l:338:MET:HE1	35:l:376:GLY:HA3	1.86	0.57
39:p:176:GLU:HG3	39:p:177:ARG:HG2	1.85	0.57
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.87	0.57
35:l:419:THR:HA	35:l:422:TYR:CE2	2.39	0.57
12:M:166:GLY:HA2	12:M:213:MET:HE2	1.85	0.57
26:c:84:GLN:O	26:c:98:ARG:NH1	2.37	0.57
9:J:132:ARG:NH2	51:J:401:NDP:O2X	2.37	0.57
6:X:120:MET:HE1	39:p:24:LEU:HB2	1.86	0.57
25:b:75:VAL:O	25:b:79:VAL:HG23	2.04	0.57
9:J:313:TRP:H	9:J:313:TRP:CD1	2.22	0.57
13:N:122:GLN:HA	18:T:59:GLN:HG2	1.87	0.57
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.23	0.57
6:X:86:VAL:HA	6:X:89:LEU:HD12	1.86	0.57
44:w:120:ASP:OD1	44:w:120:ASP:N	2.38	0.57
2:B:78:PHE:O	8:I:12:ARG:NH2	2.38	0.57
3:C:79:MET:HE3	3:C:86:MET:HE3	1.85	0.57
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.86	0.57
41:s:32:GLN:OE1	41:s:34:ARG:NH2	2.37	0.57
3:C:133:MET:HE3	3:C:173:LEU:HD22	1.87	0.57
6:G:110:LEU:HD23	6:G:114:ASP:HB3	1.87	0.57
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.87	0.57
1:A:98:LYS:NZ	47:A:503:NAI:O3B	2.37	0.56
2:B:47:SER:OG	2:B:49:ASP:OD1	2.23	0.56
32:i:149:ILE:HD11	32:i:195:PRO:HG3	1.87	0.56
35:l:4:PHE:HD2	35:l:61:MET:HE2	1.70	0.56
40:r:282:LEU:HG	40:r:342:MET:HG2	1.86	0.56
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.88	0.56
27:d:46:THR:O	27:d:50:GLU:HG2	2.05	0.56
42:u:83:THR:HA	42:u:86:TRP:CD1	2.41	0.56
26:c:69:GLY:HA3	38:o:86:THR:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.87	0.56
35:l:264:TYR:HA	35:l:267:MET:HB2	1.86	0.56
35:l:391:SER:O	35:l:395:ILE:HG12	2.05	0.56
43:v:66:LEU:HD11	43:v:84:GLN:HG2	1.87	0.56
44:w:246:LEU:HD12	44:w:255:VAL:HG11	1.87	0.56
1:A:185:ASN:ND2	1:A:187:CYS:O	2.38	0.56
1:A:138:LEU:HD13	1:A:245:VAL:HG13	1.86	0.56
9:J:136:THR:HG23	9:J:139:PHE:H	1.70	0.56
35:l:105:MET:HB3	35:l:449:LEU:HD13	1.88	0.56
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.87	0.56
12:M:456:ALA:O	12:M:499:ASN:ND2	2.39	0.56
15:P:209:GLU:HG2	15:P:224:VAL:HA	1.87	0.56
20:V:124:LEU:HD21	48:r:501:PEE:H64	1.88	0.56
28:e:57:GLU:HG2	44:w:320:GLY:HA3	1.88	0.56
6:G:84:LEU:O	6:G:88:LYS:HG2	2.05	0.56
24:a:94:GLY:HA2	24:a:116:PRO:HG3	1.88	0.56
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.88	0.56
33:j:18:VAL:HG22	41:s:222:MET:HE1	1.88	0.56
34:k:5:TYR:O	34:k:9:ILE:HG13	2.06	0.56
12:M:34:VAL:HG23	12:M:41:VAL:HG13	1.87	0.56
31:h:18:MET:HG2	32:i:25:HIS:HE2	1.70	0.56
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.88	0.56
41:s:141:SER:HB3	41:s:289:LEU:HD22	1.88	0.56
6:G:103:HIS:CE1	6:G:105:MET:HG2	2.41	0.55
32:i:159:MET:HE3	32:i:163:LEU:HG	1.87	0.55
33:j:67:LEU:HD22	34:k:65:VAL:HA	1.88	0.55
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.70	0.55
3:C:59:ARG:NH1	49:C:302:PLX:O3	2.39	0.55
6:G:75:THR:OG1	6:G:156:GLU:OE1	2.23	0.55
3:C:50:LEU:HD21	49:C:302:PLX:H371	1.88	0.55
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.42	0.55
11:L:163:ASN:O	11:L:171:ARG:HA	2.06	0.55
56:s:401:UQ:H152	56:s:401:UQ:H101	1.86	0.55
43:v:25:PHE:HD2	43:v:108:LEU:HD23	1.71	0.55
1:A:116:ASN:ND2	1:A:207:GLY:O	2.39	0.55
12:M:472:PRO:O	12:M:510:TRP:NE1	2.32	0.55
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	1.88	0.55
36:m:31:LEU:HA	36:m:34:ILE:HD12	1.87	0.55
55:r:504:CDL:HA62	55:r:504:CDL:H511	1.88	0.55
9:J:305:PHE:HD2	9:J:314:THR:HG22	1.71	0.55
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:37:LYS:HE3	35:l:105:MET:HE1	1.89	0.55
41:s:287:HIS:CD2	41:s:291:LYS:HD2	2.42	0.55
1:A:64:LYS:HG3	1:A:67:GLU:HB2	1.88	0.55
14:O:148:ILE:O	14:O:152:ILE:HG13	2.07	0.55
28:e:92:PHE:O	28:e:96:SER:HB2	2.07	0.55
32:i:20:VAL:HG13	32:i:29:ILE:HG23	1.88	0.55
35:l:228:GLY:HA3	48:l:702:PEE:H38	1.88	0.55
12:M:419:ARG:NH1	12:M:439:THR:O	2.40	0.55
21:W:85:GLN:O	21:W:89:GLU:HG3	2.07	0.55
29:f:55:TRP:NE1	30:g:68:THR:OG1	2.40	0.55
42:u:149:GLU:OE1	42:u:150:PRO:HD2	2.06	0.55
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.88	0.55
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.30	0.54
40:r:112:ALA:HB1	40:r:118:PHE:HB2	1.89	0.54
4:E:15:THR:OG1	11:L:55:VAL:O	2.24	0.54
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.89	0.54
6:G:83:VAL:O	6:G:87:LEU:HD23	2.06	0.54
23:Z:64:VAL:O	23:Z:68:LEU:HD12	2.07	0.54
35:l:559:GLU:O	35:l:563:PRO:HD2	2.08	0.54
12:M:373:PRO:HB3	12:M:487:THR:HG22	1.90	0.54
35:l:356:ILE:HA	35:l:359:MET:SD	2.48	0.54
44:w:49:THR:HA	44:w:52:LYS:HE2	1.90	0.54
14:O:207:GLU:HG3	14:O:212:LYS:HZ3	1.73	0.54
44:w:209:VAL:HG22	44:w:260:ALA:HB2	1.90	0.54
20:V:121:THR:O	20:V:125:VAL:HG23	2.07	0.54
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.90	0.54
42:u:100:CYS:HB2	42:u:103:GLN:OE1	2.08	0.54
16:Q:259:GLU:O	16:Q:263:THR:HG22	2.08	0.54
19:U:47:ARG:HA	33:j:82:ASN:ND2	2.23	0.54
33:j:14:ALA:O	33:j:18:VAL:HG23	2.08	0.54
44:w:250:SER:O	44:w:280:LYS:NZ	2.33	0.54
1:A:270:ASN:ND2	1:A:340:ASP:OD2	2.36	0.54
3:C:126:GLU:HG2	33:j:30:TYR:CD1	2.43	0.54
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.89	0.54
44:w:132:GLN:HE21	44:w:170:LEU:HB2	1.73	0.54
50:X:201:8Q1:S44	39:p:63:LEU:HB3	2.48	0.53
14:O:152:ILE:HG23	14:O:205:ILE:HD11	1.90	0.53
20:V:69:ILE:CD1	20:V:100:THR:OG1	2.55	0.53
44:w:215:GLN:O	44:w:219:GLN:HG2	2.08	0.53
6:G:112:SER:O	6:G:116:VAL:HG23	2.09	0.53
10:K:91:VAL:O	10:K:94:SER:OG	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:131:LYS:HD2	11:L:147:VAL:HG11	1.89	0.53
12:M:547:LEU:HD11	12:M:579:MET:HE3	1.89	0.53
13:N:2:GLU:HG3	13:N:4:VAL:HG22	1.91	0.53
42:u:107:PHE:O	42:u:111:VAL:HG13	2.09	0.53
2:B:77:LEU:HD12	41:s:31:MET:HG3	1.90	0.53
22:Y:84:PHE:CD1	43:v:92:HIS:HD2	2.26	0.53
35:l:231:PRO:HA	35:l:234:PRO:HG2	1.90	0.53
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.91	0.53
10:K:76:LEU:O	10:K:79:HIS:HB2	2.08	0.53
21:W:80:ASP:HB3	42:u:53:PRO:HB3	1.90	0.53
6:G:126:PHE:HB3	6:G:128:PHE:HE1	1.74	0.53
20:V:76:ILE:O	20:V:80:VAL:HG13	2.09	0.53
22:Y:51:THR:HG22	22:Y:53:SER:H	1.74	0.53
39:p:136:GLU:OE2	39:p:167:TRP:NE1	2.42	0.53
44:w:65:ASN:OD1	44:w:66:ILE:N	2.38	0.53
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.35	0.53
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	1.90	0.53
36:m:57:PHE:HE1	41:s:111:LEU:HD22	1.74	0.53
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.91	0.53
15:P:87:PHE:CE2	15:P:144:LYS:HD2	2.44	0.53
13:N:39:VAL:CG2	13:N:50:GLU:HG2	2.38	0.53
26:c:42:PRO:HD3	26:c:74:ASP:HB3	1.89	0.53
44:w:54:THR:O	44:w:55:GLU:HG3	2.09	0.53
25:b:14:GLN:O	25:b:17:GLU:HG3	2.09	0.52
44:w:350:LYS:CD	44:w:351:TRP:H	2.21	0.52
22:Y:87:PRO:HG3	43:v:96:VAL:HG22	1.90	0.52
31:h:59:GLU:OE2	42:u:145:ARG:NH1	2.42	0.52
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.92	0.52
36:m:165:VAL:O	36:m:169:MET:HG2	2.08	0.52
16:Q:105:MET:HE2	16:Q:105:MET:N	2.25	0.52
20:V:81:ARG:NH1	20:V:89:ASN:OD1	2.39	0.52
23:Z:25:GLU:HA	23:Z:30:GLU:OE1	2.08	0.52
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.42	0.52
1:A:277:ASN:HD21	14:O:181:VAL:HB	1.74	0.52
24:a:144:ALA:O	24:a:148:GLU:HG2	2.10	0.52
1:A:126:LYS:O	1:A:130:ILE:HG23	2.09	0.52
24:a:140:LEU:HD21	40:r:177:LEU:HB3	1.92	0.52
36:m:45:LEU:HD23	36:m:50:SER:HA	1.91	0.52
44:w:129:TYR:OH	44:w:186:HIS:ND1	2.28	0.52
25:b:11:ARG:HB2	39:p:156:PRO:HB3	1.92	0.52
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:25:PHE:CD2	43:v:108:LEU:HD23	2.45	0.52
7:H:27:LEU:HD13	7:H:84:ALA:HB3	1.91	0.52
8:I:12:ARG:HD3	8:I:20:LEU:HD22	1.92	0.52
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.45	0.52
5:F:33:VAL:O	5:F:36:PHE:HB3	2.09	0.52
22:Y:78:ASP:OD2	22:Y:83:HIS:ND1	2.25	0.52
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.45	0.51
12:M:539:LYS:HE3	12:M:539:LYS:HA	1.91	0.51
21:W:114:THR:OG1	42:u:143:HIS:ND1	2.40	0.51
50:X:201:8Q1:O27	50:X:201:8Q1:O33	2.25	0.51
35:l:51:LEU:O	35:l:55:MET:HG3	2.09	0.51
44:w:125:ASP:O	44:w:130:ARG:NH2	2.43	0.51
8:I:66:PRO:HB3	15:P:79:SER:HA	1.92	0.51
40:r:115:LEU:HD12	40:r:174:LEU:HD22	1.92	0.51
1:A:214:GLU:OE1	11:L:175:LYS:NZ	2.44	0.51
13:N:127:TYR:OH	18:T:61:GLU:O	2.23	0.51
15:P:156:SER:O	15:P:156:SER:OG	2.27	0.51
35:l:293:ILE:HD13	35:l:418:LEU:HD22	1.91	0.51
40:r:216:LEU:HD23	40:r:287:ALA:HB1	1.93	0.51
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.92	0.51
24:a:67:PHE:CE2	40:r:434:ASN:HB3	2.46	0.51
31:h:18:MET:HG2	32:i:25:HIS:NE2	2.25	0.51
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.93	0.51
35:l:106:TRP:CD1	35:l:447:ASN:HD22	2.29	0.51
3:C:84:TYR:CE1	3:C:171:GLU:HG3	2.46	0.51
5:F:18:GLU:OE2	5:F:68:ARG:NH1	2.43	0.51
22:Y:43:ARG:HG3	22:Y:46:GLN:HB2	1.93	0.51
35:l:144:TRP:HH2	35:l:256:GLY:HA2	1.74	0.51
40:r:41:LEU:O	40:r:44:GLN:NE2	2.41	0.51
1:A:244:ASN:N	46:A:502:FMN:O1P	2.35	0.51
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.92	0.51
20:V:37:SER:HB3	20:V:56:THR:HG22	1.93	0.51
30:g:101:GLU:OE1	30:g:101:GLU:N	2.29	0.51
41:s:21:THR:HB	56:s:401:UQ:HM23	1.93	0.51
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.29	0.51
30:g:31:PRO:HD2	42:u:172:MET:HE1	1.92	0.51
55:r:504:CDL:H421	55:r:504:CDL:H602	1.93	0.51
43:v:103:GLU:O	43:v:107:ARG:HG2	2.10	0.51
16:Q:41:VAL:O	16:Q:45:GLU:HG2	2.10	0.51
9:J:168:SER:O	9:J:202:LYS:HA	2.11	0.51
13:N:65:THR:O	13:N:73:THR:OG1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.44	0.51
30:g:4:MET:O	30:g:10:ARG:NH1	2.42	0.51
38:o:57:LEU:HD13	38:o:57:LEU:O	2.11	0.51
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.92	0.50
9:J:178:SER:HB3	9:J:320:GLU:HG2	1.93	0.50
15:P:44:ARG:HE	15:P:45:PRO:HD3	1.75	0.50
25:b:101:LYS:NZ	27:d:117:GLU:OE2	2.35	0.50
41:s:135:ALA:O	41:s:139:THR:OG1	2.26	0.50
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.41	0.50
23:Z:33:GLN:OE1	23:Z:33:GLN:HA	2.11	0.50
38:o:89:LEU:HD22	38:o:93:PHE:HE2	1.76	0.50
40:r:10:MET:C	40:r:13:PRO:HD2	2.37	0.50
40:r:324:SER:OG	40:r:440:HIS:NE2	2.31	0.50
48:r:501:PEE:H69	49:r:502:PLX:H381	1.92	0.50
12:M:308:ARG:NH2	12:M:578:PRO:O	2.44	0.50
20:V:114:ALA:O	20:V:118:MET:HG2	2.11	0.50
25:b:72:VAL:HA	25:b:76:LEU:HB2	1.91	0.50
25:b:93:LYS:HD2	25:b:93:LYS:H	1.75	0.50
35:l:161:ARG:NH1	35:l:238:GLU:OE1	2.43	0.50
40:r:97:THR:HG21	55:r:505:CDL:H242	1.93	0.50
6:G:79:ILE:HG22	6:G:145:VAL:HG23	1.94	0.50
8:I:68:ILE:HG12	15:P:77:GLN:HE21	1.77	0.50
12:M:49:VAL:HG13	12:M:102:ILE:HD13	1.94	0.50
39:p:13:GLN:H	39:p:13:GLN:CD	2.17	0.50
1:A:244:ASN:O	1:A:248:VAL:HG23	2.11	0.50
3:C:126:GLU:HG3	3:C:127:PRO:HA	1.94	0.50
6:G:148:ILE:HD12	6:G:148:ILE:H	1.76	0.50
9:J:72:HIS:NE2	15:P:215:GLU:OE1	2.45	0.50
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.47	0.50
12:M:538:ARG:HG3	12:M:538:ARG:HH11	1.77	0.50
13:N:97:PRO:HG2	13:N:100:THR:HG23	1.94	0.50
22:Y:84:PHE:HB3	43:v:92:HIS:CD2	2.46	0.50
35:l:144:TRP:CE2	35:l:223:LYS:HD2	2.47	0.50
40:r:303:ILE:HG22	40:r:305:THR:HG23	1.93	0.50
40:r:337:VAL:HG12	40:r:339:SER:H	1.76	0.50
4:E:25:MET:HE1	4:E:79:VAL:HG21	1.93	0.50
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.94	0.50
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.77	0.50
40:r:67:VAL:HG12	49:r:503:PLX:H382	1.92	0.50
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.32	0.50
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:347:ASN:N	32:i:347:ASN:OD1	2.45	0.50
36:m:57:PHE:CE1	41:s:111:LEU:HD22	2.47	0.50
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.93	0.49
15:P:73:VAL:HG13	15:P:86:ILE:HG23	1.94	0.49
32:i:291:TYR:HA	40:r:151:PHE:HZ	1.76	0.49
38:o:17:THR:O	38:o:23:TYR:OH	2.25	0.49
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.47	0.49
30:g:12:PRO:HG3	31:h:8:LYS:HD2	1.93	0.49
31:h:38:LYS:HE2	31:h:42:GLU:OE1	2.12	0.49
41:s:85:MET:SD	41:s:108:MET:HB2	2.52	0.49
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.92	0.49
35:l:293:ILE:HD12	55:l:701:CDL:H521	1.94	0.49
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.94	0.49
41:s:62:ARG:HD3	41:s:64:ALA:H	1.77	0.49
41:s:85:MET:HE3	41:s:105:MET:HE3	1.94	0.49
9:J:293:LEU:HG	9:J:294:PRO:CD	2.42	0.49
11:L:90:GLY:HA2	12:M:59:GLN:HE22	1.78	0.49
12:M:389:THR:O	12:M:390:THR:OG1	2.25	0.49
21:W:76:GLN:NE2	21:W:80:ASP:OD1	2.45	0.49
44:w:213:GLU:O	44:w:217:ARG:HG3	2.12	0.49
2:B:171:PRO:HB3	13:N:93:MET:HE1	1.94	0.49
3:C:64:PRO:HB3	3:C:102:VAL:HG13	1.94	0.49
4:E:23:ARG:HH22	11:L:52:LEU:N	2.10	0.49
16:Q:196:ALA:C	16:Q:197:MET:HG3	2.38	0.49
19:U:78:LEU:HD12	42:u:123:GLY:HA3	1.93	0.49
27:d:160:LYS:NZ	30:g:114:ILE:O	2.44	0.49
38:o:62:ASP:O	38:o:66:ILE:HD12	2.12	0.49
12:M:483:ARG:HH22	12:M:682:ASP:HB3	1.76	0.49
16:Q:158:LEU:HD12	16:Q:411:LEU:HD23	1.95	0.49
38:o:37:LEU:HD13	39:p:8:ALA:HA	1.95	0.49
40:r:48:ASN:N	40:r:48:ASN:OD1	2.43	0.49
41:s:225:MET:SD	56:s:401:UQ:H153	2.52	0.49
35:l:106:TRP:O	35:l:109:HIS:ND1	2.35	0.49
40:r:122:PHE:CZ	40:r:206:LYS:HD2	2.48	0.49
42:u:18:VAL:HG12	42:u:20:VAL:HG22	1.94	0.49
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.95	0.49
36:m:42:GLY:HA2	48:m:201:PEE:H23	1.94	0.49
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.47	0.49
40:r:207:MET:HG2	40:r:298:ILE:HG13	1.94	0.49
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.48	0.49
1:A:204:TYR:OH	47:A:503:NAI:H5N	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:VAL:O	1:A:251:SER:OG	2.30	0.49
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.95	0.49
15:P:100:LEU:O	15:P:108:PHE:N	2.39	0.49
31:h:37:GLU:HG3	31:h:63:PHE:CZ	2.48	0.49
41:s:251:THR:HG23	41:s:251:THR:O	2.13	0.49
41:s:251:THR:OG1	41:s:253:GLU:OE1	2.29	0.49
8:I:107:SER:O	8:I:107:SER:OG	2.31	0.48
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.42	0.48
3:C:82:PRO:HA	41:s:34:ARG:HB3	1.95	0.48
8:I:40:LYS:HB3	21:W:7:LYS:H	1.78	0.48
25:b:111:LEU:HD23	27:d:17:THR:HG23	1.95	0.48
39:p:47:ARG:NH2	39:p:70:GLU:OE2	2.47	0.48
4:E:16:SER:HB3	11:L:52:LEU:HG	1.95	0.48
12:M:275:PRO:HB3	12:M:286:ILE:HG23	1.95	0.48
41:s:189:THR:HG22	41:s:234:MET:HE3	1.94	0.48
21:W:144:THR:HB	41:s:96:ILE:HG23	1.94	0.48
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.48	0.48
1:A:170:GLN:HE21	1:A:197:VAL:HB	1.79	0.48
8:I:40:LYS:HB3	21:W:6:VAL:HA	1.95	0.48
14:O:88:ARG:NH2	14:O:190:ASP:OD2	2.47	0.48
16:Q:237:PRO:HD2	16:Q:240:LEU:HD22	1.95	0.48
19:U:43:ILE:O	19:U:47:ARG:HG3	2.13	0.48
20:V:85:ASP:HB3	20:V:130:LEU:HD21	1.96	0.48
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.77	0.48
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.94	0.48
44:w:67:CYS:N	57:w:401:ADP:O2A	2.38	0.48
5:F:23:LEU:O	5:F:57:GLU:HA	2.12	0.48
9:J:293:LEU:CG	9:J:294:PRO:HD2	2.41	0.48
33:j:83:ASN:OD1	33:j:86:THR:HG22	2.13	0.48
44:w:83:LEU:HD22	44:w:156:GLY:HA3	1.95	0.48
1:A:246:GLU:O	1:A:250:VAL:HG13	2.14	0.48
2:B:151:LYS:HA	3:C:141:GLY:HA2	1.95	0.48
8:I:14:TRP:O	21:W:28:ARG:NH2	2.47	0.48
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.47	0.48
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.96	0.48
16:Q:84:PHE:CE2	16:Q:99:MET:HG3	2.48	0.48
16:Q:84:PHE:HE2	16:Q:99:MET:HG3	1.79	0.48
23:Z:57:PHE:O	35:l:434:LYS:NZ	2.37	0.48
35:l:102:GLU:HG2	35:l:453:SER:HB3	1.95	0.48
42:u:83:THR:HA	42:u:86:TRP:NE1	2.29	0.48
42:u:157:ASP:OD1	42:u:157:ASP:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:353:TRP:H	44:w:353:TRP:CD1	2.31	0.48
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.96	0.48
12:M:638:THR:O	12:M:642:VAL:HG23	2.14	0.48
32:i:246:VAL:HG21	55:r:505:CDL:H362	1.96	0.48
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.95	0.48
9:J:293:LEU:CD1	9:J:294:PRO:HD2	2.44	0.48
14:O:129:LYS:HD3	14:O:130:TYR:CE1	2.49	0.48
26:c:175:THR:O	26:c:175:THR:OG1	2.29	0.48
30:g:73:PHE:HE2	49:g:201:PLX:H392	1.79	0.48
32:i:258:SER:OG	32:i:336:VAL:HG22	2.14	0.48
39:p:19:LEU:HD22	39:p:64:LEU:HD12	1.94	0.48
44:w:116:LYS:NZ	44:w:123:SER:OG	2.47	0.48
2:B:196:LYS:HE3	13:N:113:HIS:CE1	2.49	0.47
9:J:132:ARG:HA	9:J:132:ARG:HD3	1.67	0.47
33:j:68:GLU:HG3	36:m:161:LEU:HD13	1.96	0.47
35:l:172:ILE:HG21	40:r:408:LEU:HD12	1.95	0.47
36:m:74:MET:HE2	36:m:74:MET:HB3	1.82	0.47
37:n:8:VAL:O	37:n:12:TRP:HB3	2.14	0.47
38:o:114:LYS:O	38:o:118:GLU:HG3	2.14	0.47
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.96	0.47
5:F:83:SER:O	5:F:87:VAL:HG23	2.13	0.47
23:Z:57:PHE:CG	35:l:435:PRO:HG3	2.49	0.47
55:a:201:CDL:H212	55:a:201:CDL:H761	1.96	0.47
26:c:170:ARG:HG2	43:v:53:LEU:HD21	1.96	0.47
35:l:290:LEU:O	35:l:523:SER:OG	2.31	0.47
40:r:218:LYS:O	40:r:222:GLU:HG2	2.14	0.47
21:W:60:LEU:HD13	42:u:98:ARG:HD2	1.96	0.47
6:X:151:LYS:HA	6:X:151:LYS:HD2	1.66	0.47
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.48	0.47
56:s:401:UQ:H71	56:s:401:UQ:H111	1.60	0.47
2:B:100:GLU:O	2:B:170:GLY:N	2.41	0.47
3:C:127:PRO:HB3	3:C:189:ARG:HH22	1.79	0.47
9:J:57:THR:HG21	9:J:120:VAL:HG12	1.95	0.47
15:P:69:LEU:HD22	15:P:96:VAL:HG22	1.97	0.47
19:U:38:TYR:HB2	41:s:310:MET:O	2.14	0.47
21:W:88:ARG:O	21:W:92:GLU:HG2	2.14	0.47
24:a:136:THR:HG21	40:r:48:ASN:ND2	2.29	0.47
25:b:19:ARG:HA	39:p:171:VAL:HG13	1.96	0.47
32:i:65:THR:O	32:i:69:MET:HG3	2.15	0.47
35:l:455:LYS:O	35:l:459:ILE:HG13	2.14	0.47
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:111:LEU:HD22	25:b:111:LEU:H	1.79	0.47
32:i:278:MET:O	32:i:282:MET:HG3	2.14	0.47
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.97	0.47
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.79	0.47
32:i:68:MET:HE2	34:k:37:MET:HA	1.97	0.47
32:i:320:THR:OG1	44:w:300:ASN:HB2	2.14	0.47
48:j:201:PEE:H59	48:j:201:PEE:H64	1.67	0.47
36:m:25:SER:O	36:m:27:ILE:N	2.47	0.47
49:r:502:PLX:H301	49:r:502:PLX:H331	1.49	0.47
2:B:98:ARG:HB3	2:B:169:GLU:CD	2.40	0.47
9:J:65:LEU:HG	9:J:129:LEU:HD21	1.97	0.47
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.96	0.47
14:O:153:GLN:HG3	14:O:158:ILE:O	2.15	0.47
14:O:198:PRO:O	14:O:201:ILE:HG22	2.14	0.47
6:X:75:THR:O	6:X:79:ILE:HG13	2.15	0.47
22:Y:45:ARG:HG2	35:l:439:PRO:HB3	1.97	0.47
24:a:157:ARG:HD2	30:g:2:THR:N	2.30	0.47
32:i:91:ASN:CG	32:i:92:PRO:HD2	2.40	0.47
35:l:13:THR:O	35:l:16:THR:OG1	2.30	0.47
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.96	0.47
35:l:345:SER:HB2	35:l:450:LEU:HD11	1.97	0.47
35:l:346:ILE:HG13	35:l:369:THR:HG21	1.96	0.47
35:l:407:TRP:O	35:l:411:MET:HG2	2.14	0.47
41:s:156:MET:HE2	41:s:156:MET:HB2	1.78	0.47
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.37	0.47
49:C:302:PLX:H31	13:N:75:TRP:CD2	2.50	0.47
15:P:94:ILE:O	15:P:98:THR:OG1	2.24	0.47
20:V:118:MET:HE2	20:V:118:MET:HB3	1.74	0.47
22:Y:55:LEU:O	22:Y:59:GLU:HG2	2.15	0.47
23:Z:24:ILE:HD11	23:Z:46:GLY:C	2.40	0.47
24:a:115:HIS:O	24:a:119:ARG:HG3	2.14	0.47
32:i:41:ILE:HG13	34:k:73:LEU:HD21	1.97	0.47
32:i:96:THR:O	32:i:100:MET:HG3	2.15	0.47
32:i:291:TYR:CE2	48:i:402:PEE:H49	2.50	0.47
55:l:701:CDL:H572	55:l:701:CDL:H541	1.70	0.47
1:A:224:ARG:HD3	11:L:164:PHE:CE2	2.50	0.47
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.44	0.47
16:Q:235:ASP:N	16:Q:356:ILE:HD13	2.29	0.47
33:j:70:ALA:HA	33:j:73:LEU:HD12	1.96	0.47
48:j:201:PEE:H35	48:j:201:PEE:H30	1.79	0.47
41:s:233:MET:HE3	41:s:233:MET:HB3	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:60:ILE:HG12	44:w:203:VAL:HB	1.96	0.47
3:C:88:ARG:HA	41:s:37:PRO:HA	1.97	0.47
3:C:128:ARG:N	9:J:89:TYR:OH	2.39	0.47
9:J:319:VAL:HA	9:J:322:VAL:HG12	1.97	0.47
12:M:29:SER:HG	12:M:30:ASN:H	1.61	0.47
13:N:6:VAL:HG12	13:N:9:ARG:NH2	2.30	0.47
14:O:110:MET:O	14:O:114:GLU:HG3	2.15	0.47
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.50	0.47
16:Q:270:ASN:HB3	41:s:284:GLN:HE22	1.80	0.47
55:l:701:CDL:H391	55:l:701:CDL:H421	1.80	0.47
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.50	0.46
15:P:104:THR:O	15:P:107:GLN:NE2	2.47	0.46
22:Y:84:PHE:CG	43:v:92:HIS:HD2	2.33	0.46
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.31	0.46
2:B:80:GLU:HG3	17:S:1:MET:SD	2.55	0.46
48:B:303:PEE:H21	48:B:303:PEE:H16	1.63	0.46
3:C:71:CYS:HB3	16:Q:141:TYR:HB2	1.97	0.46
4:E:89:GLU:OE1	4:E:98:LYS:NZ	2.44	0.46
12:M:382:ARG:HE	12:M:527:ASP:CG	2.23	0.46
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.97	0.46
12:M:485:ASP:OD1	12:M:485:ASP:N	2.48	0.46
21:W:51:MET:HA	41:s:313:SER:HB2	1.97	0.46
25:b:100:ARG:HH11	35:l:60:GLU:HG3	1.80	0.46
29:f:55:TRP:O	29:f:59:ILE:HG13	2.15	0.46
40:r:396:MET:O	40:r:400:MET:HG3	2.15	0.46
11:L:133:ASP:OD1	11:L:133:ASP:N	2.47	0.46
16:Q:100:GLU:HG3	16:Q:107:ARG:HB2	1.97	0.46
16:Q:446:ASP:OD1	41:s:281:ARG:NH1	2.48	0.46
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.50	0.46
32:i:40:MET:HE1	32:i:129:LEU:HD23	1.98	0.46
7:H:76:GLN:O	7:H:78:GLU:N	2.48	0.46
9:J:238:GLN:HG2	9:J:270:ARG:HG2	1.97	0.46
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.79	0.46
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.98	0.46
27:d:132:PHE:HA	27:d:135:VAL:HG12	1.97	0.46
40:r:22:MET:HE3	40:r:22:MET:HB3	1.75	0.46
1:A:89:GLY:O	47:A:503:NAI:H2N	2.14	0.46
8:I:46:SER:O	8:I:52:ASN:ND2	2.47	0.46
21:W:10:MET:SD	21:W:11:PRO:HD2	2.56	0.46
32:i:170:LEU:HD23	32:i:292:PHE:HB3	1.97	0.46
35:l:419:THR:HA	35:l:422:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:14:LYS:O	42:u:61:LYS:NZ	2.49	0.46
21:W:50:MET:HE3	41:s:156:MET:HG2	1.96	0.46
6:X:105:MET:HE3	6:X:139:MET:HE1	1.97	0.46
40:r:87:GLU:OE2	40:r:91:ARG:HB2	2.15	0.46
40:r:105:PHE:O	40:r:109:THR:OG1	2.25	0.46
9:J:337:ASP:OD1	9:J:337:ASP:N	2.49	0.46
12:M:335:GLY:HA2	12:M:362:ASP:O	2.16	0.46
21:W:128:ARG:NH1	31:h:102:GLU:OE2	2.37	0.46
24:a:141:GLN:O	24:a:145:GLU:HG3	2.15	0.46
27:d:127:LYS:NZ	27:d:130:GLU:OE1	2.49	0.46
31:h:88:LYS:HB2	31:h:88:LYS:HE2	1.69	0.46
44:w:248:GLU:HG3	44:w:249:MET:HG2	1.97	0.46
44:w:351:TRP:HA	44:w:351:TRP:CE3	2.51	0.46
8:I:74:LYS:HD2	8:I:74:LYS:HA	1.78	0.46
18:T:49:ASP:OD2	18:T:51:ARG:HB2	2.15	0.46
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.98	0.46
26:c:38:PRO:HG2	38:o:71:ALA:HB2	1.97	0.46
32:i:267:ILE:HG12	32:i:279:PRO:HB3	1.97	0.46
34:k:4:VAL:O	34:k:8:ILE:HD13	2.15	0.46
35:l:107:TYR:HD2	35:l:108:MET:HE2	1.81	0.46
39:p:176:GLU:HG3	39:p:177:ARG:N	2.30	0.46
40:r:445:LEU:HD22	55:r:504:CDL:H401	1.97	0.46
42:u:80:GLU:O	42:u:84:GLU:HG2	2.16	0.46
16:Q:188:THR:HB	16:Q:200:PHE:HA	1.98	0.46
16:Q:251:PHE:O	16:Q:255:ILE:HG13	2.16	0.46
26:c:127:ASN:O	26:c:131:LYS:HG3	2.16	0.46
55:i:401:CDL:H142	55:i:401:CDL:H171	1.81	0.46
7:H:94:MET:SD	7:H:99:PRO:HG3	2.56	0.46
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.97	0.46
18:T:46:ASP:OD1	18:T:49:ASP:HB2	2.15	0.46
27:d:32:TYR:O	27:d:36:ILE:HG23	2.15	0.46
35:l:561:ILE:HG22	35:l:562:LEU:N	2.31	0.46
39:p:108:HIS:CD2	39:p:109:PRO:HD2	2.51	0.46
41:s:90:PRO:HB3	41:s:94:PRO:HD3	1.97	0.46
3:C:124:MET:HE2	3:C:128:ARG:HB2	1.98	0.45
7:H:35:LEU:HD13	7:H:49:GLU:HG2	1.98	0.45
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.97	0.45
35:l:370:THR:HA	35:l:431:PHE:CE2	2.51	0.45
41:s:173:TRP:HB3	41:s:175:ILE:HG22	1.98	0.45
1:A:69:LEU:HD13	1:A:147:ARG:HG2	1.97	0.45
48:j:201:PEE:H26	41:s:295:PRO:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:171:ALA:O	35:l:175:ASN:ND2	2.31	0.45
40:r:135:ARG:HH21	55:r:505:CDL:H122	1.82	0.45
40:r:307:TRP:HA	40:r:310:MET:HE2	1.97	0.45
1:A:133:HIS:CE1	10:K:75:ASN:HD22	2.34	0.45
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.24	0.45
33:j:5:LEU:HD23	41:s:2:PHE:HD2	1.82	0.45
44:w:166:ASP:OD1	44:w:187:TYR:OH	2.33	0.45
9:J:231:LEU:CD1	9:J:292:PRO:CD	2.84	0.45
24:a:96:ALA:HB2	27:d:61:TYR:CZ	2.52	0.45
26:c:113:ILE:HD11	26:c:116:ARG:HD2	1.99	0.45
32:i:102:LEU:HD13	32:i:142:LEU:HG	1.97	0.45
37:n:34:LYS:HB3	37:n:34:LYS:HE3	1.57	0.45
1:A:213:ILE:HG23	1:A:235:VAL:HA	1.98	0.45
12:M:260:ASN:HD21	12:M:278:HIS:HD2	1.65	0.45
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.51	0.45
26:c:163:TYR:OH	43:v:41:ALA:O	2.29	0.45
30:g:110:THR:O	30:g:113:GLU:HG2	2.17	0.45
33:j:95:LEU:HD13	41:s:302:MET:HG3	1.98	0.45
40:r:121:LEU:O	40:r:125:THR:HG23	2.17	0.45
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.51	0.45
3:C:73:ALA:O	3:C:76:MET:CB	2.64	0.45
11:L:158:LYS:NZ	12:M:69:LEU:O	2.46	0.45
12:M:485:ASP:OD2	12:M:680:LEU:HG	2.17	0.45
14:O:156:LEU:HB3	14:O:158:ILE:HG12	1.97	0.45
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.97	0.45
25:b:29:SER:OG	25:b:32:GLU:OE1	2.30	0.45
27:d:37:PHE:CE2	35:l:3:PRO:HB3	2.52	0.45
28:e:62:GLU:OE1	28:e:62:GLU:N	2.47	0.45
35:l:359:MET:O	35:l:436:ARG:NH2	2.50	0.45
36:m:169:MET:HE3	36:m:169:MET:HB3	1.79	0.45
39:p:127:ARG:HG2	39:p:131:GLU:OE2	2.16	0.45
4:E:115:PRO:HB2	4:E:120:SER:OG	2.16	0.45
32:i:247:THR:O	32:i:251:MET:HG3	2.16	0.45
35:l:42:TYR:HA	35:l:45:THR:HG22	1.99	0.45
35:l:313:MET:HE2	35:l:329:ILE:HA	1.99	0.45
55:r:505:CDL:H612	55:r:505:CDL:H662	1.98	0.45
44:w:69:GLY:HA3	44:w:72:ARG:HE	1.82	0.45
9:J:288:PHE:CZ	9:J:290:PRO:HB3	2.51	0.45
12:M:634:LEU:HD13	12:M:636:TYR:OH	2.17	0.45
16:Q:184:ILE:HD12	16:Q:210:MET:HE1	1.98	0.45
16:Q:220:ALA:HB3	16:Q:224:ALA:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:78:ALA:O	6:X:82:ARG:HG3	2.17	0.45
22:Y:97:LEU:HD13	43:v:107:ARG:HD2	1.99	0.45
25:b:81:ILE:HG23	48:b:201:PEE:H58	1.97	0.45
32:i:276:ILE:HG21	48:r:501:PEE:H14	1.99	0.45
35:l:289:ALA:O	35:l:293:ILE:HG23	2.17	0.45
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.52	0.45
40:r:78:MET:HE1	40:r:439:LEU:HD12	1.99	0.45
7:H:81:ILE:HG22	7:H:85:GLU:OE1	2.17	0.45
9:J:291:TYR:O	9:J:291:TYR:CD1	2.70	0.45
11:L:73:LYS:H	11:L:73:LYS:HG2	1.56	0.45
11:L:112:MET:SD	13:N:126:PRO:HB2	2.56	0.45
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.99	0.45
12:M:476:LEU:HD21	12:M:481:LEU:HD21	1.99	0.45
24:a:130:GLU:H	24:a:130:GLU:CD	2.25	0.45
7:H:56:LEU:HA	7:H:59:VAL:HG12	1.98	0.44
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.99	0.44
15:P:152:PRO:HB3	15:P:177:PHE:HD2	1.83	0.44
21:W:109:SER:HB2	42:u:5:VAL:HG22	1.99	0.44
35:l:65:ASN:HD21	35:l:78:LEU:HD23	1.82	0.44
1:A:185:ASN:C	1:A:187:CYS:H	2.25	0.44
12:M:650:SER:OG	12:M:652:ASN:OD1	2.32	0.44
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.53	0.44
27:d:15:ARG:HG3	27:d:15:ARG:O	2.16	0.44
32:i:89:MET:HG3	32:i:95:MET:SD	2.57	0.44
33:j:53:MET:HE2	36:m:172:THR:HB	1.99	0.44
49:j:202:PLX:H151	49:j:202:PLX:H341	1.99	0.44
35:l:298:ILE:O	35:l:302:VAL:HG23	2.17	0.44
39:p:82:PHE:HB2	39:p:85:SER:OG	2.17	0.44
40:r:10:MET:O	40:r:13:PRO:HD2	2.17	0.44
44:w:185:GLU:O	44:w:189:GLU:HG3	2.16	0.44
6:G:116:VAL:HG12	6:G:120:MET:HE3	1.98	0.44
12:M:632:MET:HE3	12:M:632:MET:HB2	1.82	0.44
20:V:62:THR:HG22	20:V:66:ILE:HD11	1.98	0.44
21:W:88:ARG:HG2	42:u:10:LEU:HG	1.99	0.44
6:G:79:ILE:HG23	6:G:126:PHE:CZ	2.53	0.44
6:G:142:GLN:O	6:G:145:VAL:HG12	2.18	0.44
7:H:38:ILE:O	7:H:45:ARG:NH1	2.48	0.44
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.49	0.44
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.51	0.44
23:Z:22:TRP:HB3	23:Z:50:ALA:HB3	1.98	0.44
23:Z:32:VAL:HG13	39:p:39:TYR:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.99	0.44
41:s:282:TYR:O	41:s:285:LEU:HG	2.17	0.44
1:A:177:TYR:CD2	10:K:93:LEU:HD23	2.52	0.44
11:L:84:ARG:NH1	11:L:88:GLN:O	2.50	0.44
14:O:137:THR:HG22	14:O:138:THR:H	1.83	0.44
23:Z:41:LEU:HD21	39:p:46:ALA:HB2	1.99	0.44
24:a:188:ASP:N	24:a:188:ASP:OD1	2.51	0.44
30:g:122:ARG:NH2	38:o:113:GLU:OE2	2.48	0.44
32:i:222:SER:O	32:i:224:ALA:N	2.50	0.44
33:j:67:LEU:HD21	34:k:68:ALA:HB3	1.99	0.44
35:l:488:MET:HE3	35:l:488:MET:HB3	1.91	0.44
39:p:63:LEU:O	39:p:64:LEU:HB3	2.17	0.44
1:A:185:ASN:O	1:A:187:CYS:N	2.50	0.44
2:B:205:ILE:O	2:B:209:TYR:HB3	2.18	0.44
12:M:382:ARG:HG2	12:M:386:LEU:HD11	1.99	0.44
16:Q:236:LEU:HD22	16:Q:240:LEU:HD23	1.99	0.44
35:l:237:MET:HB3	35:l:299:LYS:HE2	2.00	0.44
42:u:158:LEU:HD23	42:u:158:LEU:HA	1.84	0.44
3:C:74:VAL:HB	16:Q:222:MET:HE1	2.00	0.44
4:E:39:TRP:O	4:E:43:VAL:HG23	2.18	0.44
9:J:204:SER:OG	9:J:204:SER:O	2.35	0.44
12:M:406:ASN:ND2	12:M:688:GLN:O	2.41	0.44
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	1.99	0.44
30:g:32:ARG:HB2	30:g:78:LEU:HD11	1.99	0.44
35:l:536:LEU:HB3	35:l:537:PRO:HD3	2.00	0.44
36:m:45:LEU:HD13	48:m:201:PEE:H51	2.00	0.44
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.81	0.44
25:b:10:LEU:O	25:b:14:GLN:HG3	2.17	0.44
26:c:149:ILE:HD13	26:c:149:ILE:HA	1.86	0.44
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.53	0.44
38:o:59:VAL:HG12	40:r:423:ILE:HG23	1.99	0.44
41:s:92:PRO:HB3	41:s:255:TYR:CD1	2.53	0.44
7:H:38:ILE:HG12	7:H:100:TRP:CH2	2.53	0.44
9:J:180:TYR:HB2	9:J:317:ASP:OD2	2.18	0.44
16:Q:368:ARG:HA	16:Q:371:MET:HE3	2.00	0.44
27:d:29:PRO:O	27:d:33:LEU:HB2	2.17	0.44
29:f:63:LYS:HB2	29:f:63:LYS:HE2	1.69	0.44
35:l:327:LEU:O	35:l:331:MET:HG2	2.18	0.44
49:r:503:PLX:H121	49:r:503:PLX:H152	1.45	0.44
2:B:105:ARG:HD2	13:N:108:TYR:CG	2.53	0.43
3:C:161:ILE:HG13	3:C:180:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:206:GLU:OE2	16:Q:209:LYS:NZ	2.51	0.43
6:X:113:LEU:O	6:X:116:VAL:HG12	2.18	0.43
6:X:138:LEU:HD13	6:X:144:ILE:HG12	1.99	0.43
31:h:47:ILE:HG12	42:u:148:PRO:HG2	2.00	0.43
40:r:260:PRO:HG3	49:r:502:PLX:H132	2.00	0.43
41:s:196:ALA:HB3	41:s:274:ARG:HA	1.99	0.43
12:M:351:LEU:O	12:M:530:TYR:OH	2.32	0.43
35:l:496:MET:HE1	55:l:701:CDL:H582	2.00	0.43
39:p:46:ALA:O	39:p:50:GLU:HG2	2.17	0.43
44:w:107:GLN:NE2	44:w:330:LYS:HE2	2.33	0.43
1:A:102:MET:HG3	1:A:241:THR:OG1	2.17	0.43
1:A:415:ILE:O	1:A:419:ILE:HG13	2.18	0.43
16:Q:155:VAL:HB	16:Q:229:PRO:HB3	2.00	0.43
22:Y:105:ASP:OD1	22:Y:105:ASP:N	2.49	0.43
25:b:123:PHE:HB3	43:v:40:VAL:HG21	2.00	0.43
48:b:201:PEE:H28	55:r:504:CDL:H271	1.99	0.43
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.53	0.43
27:d:162:ARG:NH2	28:e:140:ASN:OD1	2.36	0.43
32:i:46:LYS:HB3	32:i:46:LYS:HE2	1.78	0.43
33:j:88:LEU:HD13	41:s:309:ILE:HD12	2.00	0.43
35:l:51:LEU:HG	35:l:55:MET:HE2	2.00	0.43
44:w:66:ILE:O	44:w:214:ILE:HD12	2.18	0.43
44:w:314:LEU:O	44:w:318:THR:HG22	2.18	0.43
1:A:367:ILE:O	1:A:371:ILE:HG12	2.18	0.43
3:C:127:PRO:HA	9:J:89:TYR:OH	2.17	0.43
9:J:163:LYS:NZ	9:J:253:ILE:O	2.44	0.43
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.53	0.43
25:b:5:THR:OG1	25:b:7:ASP:OD1	2.26	0.43
32:i:13:VAL:HG13	32:i:36:ASN:ND2	2.34	0.43
40:r:371:PRO:HD2	55:r:504:CDL:H391	2.00	0.43
7:H:76:GLN:O	7:H:79:GLU:HG2	2.19	0.43
7:H:90:LEU:HB2	15:P:102:ASP:HB3	2.01	0.43
9:J:38:HIS:ND1	13:N:136:GLU:OE2	2.52	0.43
35:l:458:LEU:O	35:l:462:ILE:HG13	2.18	0.43
36:m:175:ASN:OD1	44:w:289:ARG:NH2	2.50	0.43
37:n:27:LEU:HA	37:n:30:ARG:HB2	2.00	0.43
40:r:398:MET:O	40:r:402:ILE:HG13	2.17	0.43
41:s:179:TRP:CG	41:s:180:PRO:HD3	2.54	0.43
41:s:267:THR:O	41:s:271:LEU:HG	2.18	0.43
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.59	0.43
4:E:71:ALA:HA	50:G:201:8Q1:O40	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.54	0.43
10:K:87:LEU:HD22	14:O:66:ILE:HD11	2.00	0.43
12:M:144:MET:HE3	12:M:144:MET:HB3	1.74	0.43
33:j:71:LEU:O	36:m:147:TYR:OH	2.36	0.43
55:l:701:CDL:H382	55:l:701:CDL:H351	1.78	0.43
38:o:48:LEU:HB3	39:p:166:LEU:HD13	2.00	0.43
44:w:295:ARG:HA	44:w:298:VAL:HG22	2.00	0.43
1:A:114:VAL:O	1:A:242:VAL:HA	2.19	0.43
9:J:58:VAL:HG22	9:J:127:ILE:HD12	2.01	0.43
20:V:12:ILE:HB	20:V:21:LYS:HD3	2.01	0.43
22:Y:88:ASP:OD1	22:Y:90:SER:OG	2.34	0.43
36:m:17:PHE:HA	36:m:20:PHE:CD1	2.54	0.43
40:r:290:SER:HA	40:r:319:HIS:HE2	1.83	0.43
1:A:48:ARG:HD2	10:K:70:ASN:O	2.19	0.43
3:C:65:MET:HE3	3:C:65:MET:HB2	1.90	0.43
14:O:213:ILE:HD12	14:O:214:PRO:HD2	2.00	0.43
6:X:76:LEU:HD12	6:X:156:GLU:O	2.19	0.43
6:X:129:GLU:HB3	39:p:82:PHE:CD2	2.53	0.43
35:l:188:TRP:CD1	35:l:211:MET:HE3	2.53	0.43
39:p:117:ASP:O	39:p:121:LYS:HG3	2.19	0.43
40:r:1:MET:HB2	40:r:52:PHE:CD2	2.53	0.43
44:w:165:SER:HB3	44:w:245:PHE:CE2	2.54	0.43
1:A:279:SER:OG	1:A:280:GLY:N	2.50	0.43
5:F:48:ASN:HB3	5:F:51:LEU:HB3	2.00	0.43
5:F:53:ILE:N	12:M:380:ASP:OD2	2.51	0.43
6:G:126:PHE:HB3	6:G:128:PHE:CE1	2.54	0.43
7:H:76:GLN:HB3	7:H:79:GLU:CD	2.43	0.43
9:J:313:TRP:H	9:J:313:TRP:HD1	1.65	0.43
12:M:658:ASP:OD1	12:M:660:GLU:HG2	2.19	0.43
6:X:130:ILE:HG12	6:X:147:TYR:CE2	2.54	0.43
24:a:120:TRP:O	24:a:124:THR:HG22	2.18	0.43
25:b:105:PHE:HB2	43:v:68:LYS:HD3	2.01	0.43
26:c:87:ASP:OD2	26:c:90:TYR:N	2.52	0.43
31:h:51:ARG:HA	31:h:54:LYS:HG2	2.00	0.43
48:i:402:PEE:H34	40:r:155:ALA:HB2	2.01	0.43
49:j:202:PLX:H322	49:j:202:PLX:H351	1.78	0.43
55:l:701:CDL:H711	55:l:701:CDL:H742	1.64	0.43
40:r:16:TRP:CZ2	55:r:505:CDL:H261	2.54	0.43
40:r:39:LEU:HD12	40:r:39:LEU:HA	1.89	0.43
40:r:300:ALA:O	40:r:308:SER:HB3	2.19	0.43
55:r:504:CDL:H652	55:r:504:CDL:H622	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:195:ARG:HD3	41:s:231:ILE:HD11	2.00	0.43
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.54	0.43
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.54	0.43
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	2.00	0.43
20:V:95:CYS:HA	20:V:115:CYS:HA	2.00	0.43
25:b:69:ILE:O	25:b:73:THR:HG22	2.18	0.43
25:b:74:HIS:NE2	35:l:35:TYR:OH	2.34	0.43
26:c:36:MET:HE2	26:c:36:MET:HB2	1.90	0.43
55:l:701:CDL:H581	55:l:701:CDL:H352	2.01	0.43
48:l:702:PEE:H22	48:l:702:PEE:H64	2.01	0.43
39:p:100:PRO:HG3	40:r:419:TYR:CZ	2.53	0.43
48:r:501:PEE:H33	48:r:501:PEE:H74	2.00	0.43
14:O:172:ILE:HD13	14:O:172:ILE:HA	1.86	0.42
16:Q:144:MET:HE2	16:Q:144:MET:HB2	1.89	0.42
17:S:54:ILE:HD11	42:u:21:SER:HA	1.99	0.42
20:V:75:CYS:O	20:V:79:GLN:HG3	2.19	0.42
32:i:174:GLN:HB2	32:i:177:LYS:HG3	2.00	0.42
35:l:245:ALA:O	35:l:249:SER:OG	2.36	0.42
37:n:39:ARG:HG3	37:n:57:TRP:CE2	2.54	0.42
39:p:170:ILE:O	39:p:173:ARG:HD3	2.19	0.42
40:r:457:PRO:HG2	40:r:458:LEU:HD12	2.01	0.42
42:u:76:ARG:HG2	42:u:77:HIS:CD2	2.41	0.42
43:v:28:ASP:OD1	43:v:28:ASP:N	2.46	0.42
9:J:303:ARG:HB2	9:J:316:ARG:HD3	2.01	0.42
11:L:96:LYS:HA	11:L:96:LYS:HD3	1.83	0.42
12:M:29:SER:OG	12:M:30:ASN:N	2.52	0.42
12:M:222:ILE:HA	12:M:225:ILE:HG12	2.01	0.42
16:Q:234:GLN:O	16:Q:234:GLN:HG2	2.19	0.42
39:p:126:LYS:O	39:p:130:ARG:HG3	2.19	0.42
40:r:233:ALA:HA	40:r:320:GLY:HA2	2.01	0.42
40:r:287:ALA:O	40:r:291:VAL:HG23	2.19	0.42
5:F:55:ILE:HD13	12:M:381:LEU:HD23	2.01	0.42
9:J:195:PHE:HB3	9:J:198:ALA:HB2	2.02	0.42
10:K:79:HIS:CE1	14:O:215:LYS:HB2	2.54	0.42
20:V:102:GLY:O	20:V:106:ARG:N	2.51	0.42
26:c:117:VAL:HG21	35:l:539:TYR:HB2	2.01	0.42
35:l:530:PRO:HA	35:l:534:HIS:HD2	1.84	0.42
40:r:318:ALA:HB1	40:r:374:ASN:CG	2.44	0.42
1:A:110:PRO:O	1:A:238:CYS:HB3	2.19	0.42
5:F:18:GLU:CB	5:F:52:PRO:HG2	2.50	0.42
12:M:84:LYS:HE2	12:M:84:LYS:HB2	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:118:ILE:O	6:X:122:MET:HG2	2.20	0.42
22:Y:65:MET:HB2	35:l:462:ILE:HD13	2.02	0.42
22:Y:100:LEU:O	22:Y:102:ASP:N	2.47	0.42
48:b:201:PEE:H32	35:l:66:TRP:CZ3	2.55	0.42
32:i:68:MET:HE3	34:k:40:LEU:HD12	2.02	0.42
33:j:81:THR:C	33:j:83:ASN:H	2.26	0.42
49:j:202:PLX:H312	49:j:202:PLX:H282	1.66	0.42
35:l:488:MET:O	35:l:492:ILE:HG23	2.19	0.42
40:r:61:LEU:HB2	40:r:457:PRO:HD3	2.01	0.42
55:r:505:CDL:H132	55:r:505:CDL:H161	1.89	0.42
1:A:285:PRO:O	14:O:222:ARG:NH2	2.51	0.42
8:I:25:GLN:H	8:I:25:GLN:HG2	1.71	0.42
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.52	0.42
39:p:120:ALA:O	39:p:124:GLN:HG2	2.19	0.42
1:A:201:ALA:HB1	14:O:121:MET:HB2	2.00	0.42
1:A:283:ASN:ND2	1:A:306:GLY:O	2.53	0.42
7:H:59:VAL:HG23	7:H:68:LEU:HD21	2.00	0.42
12:M:94:MET:HE2	12:M:94:MET:HB2	1.94	0.42
15:P:165:TRP:CZ2	16:Q:111:PRO:HG2	2.55	0.42
16:Q:270:ASN:HB3	41:s:284:GLN:NE2	2.34	0.42
21:W:105:LYS:HE2	21:W:105:LYS:HB3	1.79	0.42
6:X:151:LYS:HD3	39:p:3:PHE:HE2	1.84	0.42
22:Y:43:ARG:CG	22:Y:46:GLN:HB2	2.50	0.42
22:Y:43:ARG:NH2	22:Y:49:GLN:HB2	2.34	0.42
49:g:201:PLX:H1C2	31:h:2:PRO:HD2	2.01	0.42
31:h:19:THR:HA	32:i:84:TRP:HB2	2.01	0.42
31:h:89:GLU:OE1	31:h:91:LYS:N	2.52	0.42
35:l:81:LYS:HE2	35:l:83:ASP:OD2	2.20	0.42
41:s:248:ASP:OD2	41:s:251:THR:HG22	2.19	0.42
44:w:351:TRP:HA	44:w:351:TRP:HE3	1.84	0.42
7:H:51:ILE:HG13	7:H:51:ILE:H	1.66	0.42
9:J:231:LEU:HD13	9:J:292:PRO:CD	2.36	0.42
12:M:707:MET:HE2	12:M:707:MET:HA	2.00	0.42
31:h:2:PRO:HA	32:i:140:SER:HB2	2.02	0.42
35:l:176:ARG:HA	35:l:179:ASP:HB2	2.02	0.42
37:n:44:LEU:HD23	37:n:45:PHE:CE2	2.54	0.42
43:v:83:GLU:H	43:v:83:GLU:CD	2.20	0.42
1:A:130:ILE:HD11	1:A:245:VAL:HG12	2.01	0.42
2:B:105:ARG:HB3	2:B:111:GLU:HA	2.01	0.42
3:C:103:MET:HE1	3:C:117:LEU:HG	2.02	0.42
49:C:302:PLX:H1C3	49:C:302:PLX:H21	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:134:ASP:OD1	6:G:135:ALA:N	2.53	0.42
12:M:249:GLU:HB3	12:M:276:ARG:CZ	2.50	0.42
12:M:353:ALA:HA	12:M:636:TYR:OH	2.19	0.42
12:M:715:THR:HG22	12:M:716:GLU:OE1	2.19	0.42
16:Q:203:MET:HE2	16:Q:258:LEU:HD22	2.02	0.42
27:d:117:GLU:HG3	27:d:125:CYS:SG	2.60	0.42
28:e:55:LEU:HB2	44:w:318:THR:HG23	2.00	0.42
39:p:76:HIS:O	39:p:78:GLN:N	2.52	0.42
49:r:502:PLX:H22	49:r:502:PLX:H1C3	1.78	0.42
44:w:305:LEU:O	44:w:308:THR:OG1	2.36	0.42
5:F:30:SER:OG	5:F:63:PRO:HG3	2.20	0.42
5:F:43:GLU:OE2	5:F:43:GLU:HA	2.19	0.42
12:M:304:GLN:HB2	12:M:316:TYR:CD1	2.55	0.42
12:M:306:MET:HE2	12:M:316:TYR:CE1	2.54	0.42
13:N:85:GLU:HG2	13:N:86:TRP:N	2.35	0.42
15:P:115:THR:OG1	15:P:116:ALA:N	2.52	0.42
16:Q:127:LYS:HB3	16:Q:131:GLN:HB3	2.02	0.42
16:Q:315:GLU:O	16:Q:346:GLN:NE2	2.35	0.42
21:W:130:ASN:HB3	36:m:1:MET:N	2.34	0.42
6:X:82:ARG:HD2	22:Y:44:TYR:CE1	2.54	0.42
6:X:113:LEU:O	6:X:117:GLU:HG3	2.20	0.42
6:X:123:GLU:HG2	6:X:129:GLU:HA	2.02	0.42
24:a:184:LYS:HB3	31:h:30:PRO:HB3	2.01	0.42
26:c:184:TYR:HA	43:v:34:ARG:NH1	2.12	0.42
32:i:243:LEU:HD23	55:r:505:CDL:H361	2.02	0.42
35:l:410:LEU:O	35:l:414:ILE:HG13	2.19	0.42
36:m:17:PHE:HA	36:m:20:PHE:CE1	2.54	0.42
39:p:50:GLU:HB2	39:p:51:HIS:HD2	1.84	0.42
41:s:11:ILE:HB	41:s:12:PRO:HD3	2.01	0.42
41:s:17:VAL:O	41:s:21:THR:HG23	2.20	0.42
1:A:40:ARG:NE	14:O:233:SER:OG	2.53	0.42
11:L:175:LYS:HZ3	11:L:175:LYS:HG2	1.51	0.42
12:M:48:THR:HA	12:M:95:PRO:HA	2.01	0.42
12:M:355:LYS:HG3	12:M:366:LEU:HD13	2.02	0.42
26:c:113:ILE:C	26:c:115:ASN:H	2.28	0.42
33:j:24:LEU:HD12	33:j:27:LEU:HD21	2.01	0.42
33:j:94:LEU:HD12	36:m:147:TYR:HE1	1.85	0.42
35:l:8:THR:OG1	35:l:82:MET:SD	2.62	0.42
7:H:90:LEU:O	7:H:94:MET:HB2	2.19	0.41
9:J:273:LEU:HD11	9:J:322:VAL:HG22	2.02	0.41
15:P:173:MET:HB3	15:P:198:PHE:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:167:TYR:CG	26:c:178:PRO:HG3	2.55	0.41
32:i:278:MET:HB3	32:i:279:PRO:HD3	2.02	0.41
35:l:55:MET:SD	35:l:471:ASN:HB3	2.60	0.41
39:p:63:LEU:C	39:p:65:ARG:H	2.28	0.41
40:r:257:MET:HE3	40:r:257:MET:HB3	1.96	0.41
49:r:502:PLX:H51	49:r:502:PLX:H6	1.39	0.41
43:v:21:ARG:HB3	43:v:21:ARG:NH1	2.34	0.41
44:w:108:LEU:HD21	44:w:330:LYS:HE3	2.02	0.41
1:A:326:LEU:HD22	1:A:363:ILE:HD11	2.02	0.41
4:E:81:LEU:HD23	11:L:64:LEU:HD13	2.02	0.41
9:J:150:HIS:ND1	9:J:190:GLU:HG2	2.35	0.41
9:J:313:TRP:CD1	9:J:313:TRP:N	2.87	0.41
12:M:347:ASP:OD1	12:M:347:ASP:N	2.51	0.41
12:M:509:ASP:OD1	12:M:509:ASP:N	2.44	0.41
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.55	0.41
27:d:148:ALA:HB3	40:r:304:GLN:HG3	2.02	0.41
34:k:38:LEU:HD21	36:m:37:GLY:HA2	2.02	0.41
4:E:56:VAL:HG12	4:E:60:ARG:HD2	2.02	0.41
9:J:169:HIS:HB2	9:J:184:LYS:HE3	2.01	0.41
16:Q:244:ILE:HG22	16:Q:348:LEU:HD11	2.02	0.41
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.76	0.41
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.84	0.41
26:c:148:GLU:OE1	35:l:405:ASN:ND2	2.49	0.41
49:g:201:PLX:H72	49:g:201:PLX:H101	1.78	0.41
32:i:298:TYR:CE2	40:r:143:LEU:HB3	2.54	0.41
34:k:37:MET:HG3	34:k:67:ALA:CB	2.50	0.41
36:m:167:VAL:O	36:m:171:ILE:HG12	2.21	0.41
44:w:51:ARG:HE	44:w:51:ARG:HB3	1.75	0.41
1:A:249:ALA:O	1:A:252:PRO:HD2	2.19	0.41
8:I:70:MET:O	8:I:70:MET:SD	2.78	0.41
9:J:279:TYR:HB2	9:J:372:ALA:HB2	2.02	0.41
12:M:388:ASN:HB3	12:M:511:LYS:HE2	2.02	0.41
15:P:68:ILE:HG22	15:P:69:LEU:HG	2.02	0.41
25:b:89:HIS:CE1	48:b:201:PEE:H50	2.55	0.41
32:i:7:THR:HG23	55:i:401:CDL:H531	2.02	0.41
2:B:144:ARG:NH1	11:L:112:MET:O	2.44	0.41
49:C:302:PLX:H311	49:C:302:PLX:H281	1.61	0.41
9:J:177:PRO:HG2	9:J:320:GLU:OE2	2.20	0.41
15:P:173:MET:HE3	15:P:188:LEU:HB2	2.01	0.41
16:Q:278:VAL:HG13	16:Q:438:MET:HE3	2.03	0.41
48:b:201:PEE:H60	48:b:201:PEE:H55	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:67:LEU:HD11	34:k:68:ALA:HB3	2.02	0.41
49:j:202:PLX:H372	49:j:202:PLX:H342	1.81	0.41
34:k:23:ARG:HG2	36:m:23:LYS:NZ	2.35	0.41
35:l:100:ILE:HG21	35:l:246:LEU:HB2	2.02	0.41
40:r:44:GLN:HG3	40:r:60:SER:HB3	2.03	0.41
43:v:103:GLU:OE2	43:v:103:GLU:HA	2.21	0.41
44:w:100:ASP:OD1	44:w:100:ASP:N	2.53	0.41
12:M:666:GLN:NE2	12:M:670:GLU:OE1	2.52	0.41
14:O:138:THR:HA	14:O:141:MET:HB3	2.02	0.41
15:P:235:LEU:HD12	16:Q:418:ARG:HE	1.85	0.41
16:Q:136:PHE:HA	16:Q:139:LEU:HG	2.03	0.41
17:S:16:LEU:HD23	17:S:16:LEU:HA	1.91	0.41
55:a:201:CDL:H541	48:b:201:PEE:H16	2.02	0.41
25:b:10:LEU:HG	25:b:14:GLN:HE21	1.85	0.41
32:i:89:MET:HE2	32:i:94:ALA:O	2.20	0.41
39:p:13:GLN:HA	39:p:16:VAL:HG22	2.03	0.41
39:p:54:GLU:OE1	39:p:59:LYS:HB3	2.21	0.41
40:r:127:VAL:HB	40:r:128:PRO:HD3	2.01	0.41
40:r:357:THR:O	40:r:361:VAL:HG23	2.20	0.41
44:w:48:ARG:HD2	44:w:288:ASP:OD2	2.20	0.41
2:B:63:TRP:O	2:B:67:VAL:HG23	2.21	0.41
6:G:76:LEU:HB3	6:G:80:LYS:NZ	2.35	0.41
8:I:107:SER:C	8:I:109:ASP:H	2.28	0.41
9:J:179:ARG:H	9:J:179:ARG:HG2	1.64	0.41
16:Q:199:PRO:HA	16:Q:202:TRP:HB2	2.03	0.41
55:a:201:CDL:H752	28:e:103:SER:HB3	2.03	0.41
30:g:87:LEU:HD23	30:g:87:LEU:HA	1.92	0.41
32:i:87:THR:HG22	32:i:88:LYS:N	2.28	0.41
33:j:4:MET:SD	48:m:201:PEE:H21	2.61	0.41
35:l:54:PHE:CZ	35:l:84:TYR:HB2	2.56	0.41
35:l:420:ALA:O	35:l:424:THR:HG22	2.21	0.41
40:r:299:VAL:O	40:r:303:ILE:HG12	2.21	0.41
1:A:109:ARG:HG2	11:L:166:TRP:CD1	2.56	0.41
1:A:385:CYS:O	1:A:389:VAL:HB	2.21	0.41
46:A:502:FMN:N5	47:A:503:NAI:H4N	2.36	0.41
48:B:303:PEE:H59	41:s:277:TYR:CE2	2.52	0.41
6:G:88:LYS:NZ	6:G:98:LEU:HD11	2.35	0.41
6:G:114:ASP:O	6:G:118:ILE:HG13	2.21	0.41
9:J:126:VAL:HG23	9:J:161:VAL:HG11	2.02	0.41
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.51	0.41
15:P:147:THR:HB	15:P:153:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:147:ALA:HB2	40:r:173:SER:HB2	2.02	0.41
31:h:101:LYS:HD3	31:h:101:LYS:N	2.35	0.41
32:i:238:PRO:O	32:i:241:THR:OG1	2.33	0.41
55:l:701:CDL:H591	55:l:701:CDL:H622	1.48	0.41
42:u:47:ARG:NH2	42:u:53:PRO:HG3	2.36	0.41
42:u:97:PHE:HB3	42:u:101:ARG:NH1	2.36	0.41
48:B:303:PEE:H56	41:s:187:ILE:HD12	2.03	0.41
3:C:187:GLU:HB2	9:J:87:GLU:OE2	2.21	0.41
4:E:42:GLU:OE2	4:E:45:ASN:HB3	2.21	0.41
12:M:83:GLU:HG3	12:M:103:LEU:HD11	2.03	0.41
12:M:250:SER:OG	12:M:251:ILE:N	2.49	0.41
12:M:512:VAL:O	12:M:514:ASN:ND2	2.54	0.41
14:O:195:ASP:OD2	14:O:222:ARG:HD3	2.20	0.41
16:Q:104:GLU:HG2	16:Q:443:MET:SD	2.61	0.41
17:S:37:ARG:HG2	17:S:48:MET:HE2	2.03	0.41
28:e:65:ASN:ND2	40:r:427:LYS:HE2	2.36	0.41
28:e:152:ASP:OD1	28:e:152:ASP:N	2.54	0.41
32:i:14:MET:HE3	32:i:14:MET:HB3	1.84	0.41
37:n:17:VAL:HG13	40:r:7:PRO:HB3	2.03	0.41
41:s:219:PRO:HA	41:s:222:MET:HE3	2.01	0.41
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.01	0.41
42:u:59:GLU:O	42:u:63:VAL:HG13	2.20	0.41
43:v:46:MET:HE3	43:v:56:ARG:HB3	2.03	0.41
44:w:146:ALA:HB1	44:w:157:VAL:HG21	2.03	0.41
44:w:219:GLN:HA	44:w:227:MET:HE3	2.02	0.41
1:A:207:GLY:HA3	46:A:502:FMN:N5	2.36	0.41
3:C:72:CYS:HB3	3:C:133:MET:SD	2.61	0.41
3:C:125:PRO:HB2	41:s:58:LYS:HE3	2.03	0.41
24:a:154:LEU:HD23	24:a:154:LEU:HA	1.87	0.41
55:a:201:CDL:H372	55:a:201:CDL:H341	1.75	0.41
55:a:201:CDL:H531	48:b:201:PEE:H56	2.03	0.41
26:c:58:ARG:HD2	38:o:36:ARG:HG3	2.03	0.41
35:l:571:MET:HE2	35:l:571:MET:HB2	1.93	0.41
36:m:70:TYR:O	36:m:74:MET:HG3	2.21	0.41
41:s:272:TRP:O	41:s:276:SER:OG	2.26	0.41
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.55	0.40
13:N:144:TYR:H	13:N:144:TYR:HD1	1.68	0.40
14:O:130:TYR:CE2	14:O:208:LEU:HD22	2.55	0.40
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.56	0.40
15:P:157:VAL:HG21	15:P:182:PRO:HD3	2.02	0.40
16:Q:79:ASN:HA	16:Q:101:LEU:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:393:PRO:HA	16:Q:413:SER:O	2.21	0.40
26:c:155:PRO:HG3	43:v:4:HIS:HD2	1.86	0.40
36:m:23:LYS:N	36:m:24:PRO:HD3	2.36	0.40
40:r:306:PRO:HA	40:r:458:LEU:HD22	2.03	0.40
41:s:79:LEU:HA	41:s:79:LEU:HD23	1.88	0.40
43:v:17:PRO:HB3	43:v:105:GLU:CD	2.46	0.40
1:A:251:SER:OG	1:A:252:PRO:HD3	2.21	0.40
6:G:106:LYS:H	6:G:106:LYS:HG2	1.69	0.40
9:J:116:ILE:O	9:J:120:VAL:HG22	2.21	0.40
15:P:126:PHE:HZ	15:P:199:ARG:HE	1.68	0.40
16:Q:145:MET:HE2	16:Q:226:TYR:HB3	2.02	0.40
19:U:53:TYR:CZ	42:u:44:MET:HG3	2.56	0.40
32:i:115:VAL:HB	32:i:116:PRO:HD3	2.02	0.40
32:i:252:GLY:HA3	32:i:290:LEU:HD13	2.02	0.40
37:n:30:ARG:HA	37:n:30:ARG:HD2	1.63	0.40
38:o:54:PRO:HG3	39:p:129:ARG:NE	2.36	0.40
40:r:325:MET:HG3	40:r:440:HIS:CB	2.51	0.40
49:r:502:PLX:H92	49:r:502:PLX:H121	1.90	0.40
42:u:149:GLU:OE1	42:u:149:GLU:HA	2.21	0.40
44:w:301:LYS:H	44:w:301:LYS:HG2	1.73	0.40
1:A:202:GLY:N	14:O:121:MET:HG3	2.36	0.40
1:A:267:ARG:HG3	1:A:293:SER:OG	2.21	0.40
9:J:315:THR:H	9:J:318:LYS:HB3	1.85	0.40
12:M:133:GLN:O	12:M:137:CYS:HB2	2.22	0.40
12:M:141:ASP:O	12:M:145:MET:HG2	2.21	0.40
16:Q:65:PRO:HB2	16:Q:67:ASN:O	2.22	0.40
22:Y:78:ASP:OD1	22:Y:78:ASP:N	2.54	0.40
24:a:152:LYS:HD3	30:g:96:VAL:HG21	2.02	0.40
25:b:87:LYS:NZ	27:d:42:ASP:OD1	2.54	0.40
26:c:81:ARG:NH2	38:o:14:LEU:O	2.48	0.40
32:i:245:MET:HG3	32:i:297:ALA:HB1	2.04	0.40
32:i:265:MET:HE2	32:i:265:MET:HA	2.02	0.40
34:k:40:LEU:HD23	34:k:40:LEU:HA	1.81	0.40
35:l:16:THR:HG22	35:l:126:ILE:HD13	2.02	0.40
35:l:214:ILE:HG12	35:l:276:MET:HE1	2.03	0.40
35:l:525:MET:SD	39:p:77:PRO:HB2	2.62	0.40
55:l:701:CDL:H181	55:l:701:CDL:H212	1.85	0.40
1:A:411:SER:O	1:A:415:ILE:HG12	2.21	0.40
2:B:43:MET:HG2	8:I:112:TYR:HE1	1.86	0.40
5:F:35:ASP:O	5:F:39:LYS:N	2.52	0.40
8:I:8:ILE:HD13	8:I:8:ILE:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:72:SER:HB3	15:P:74:GLN:O	2.21	0.40
12:M:471:LYS:HB3	12:M:510:TRP:CZ2	2.56	0.40
17:S:50:ARG:O	17:S:54:ILE:HG23	2.21	0.40
18:T:60:LYS:HG2	18:T:62:VAL:HG23	2.02	0.40
21:W:57:ARG:HB3	41:s:316:PRO:HG3	2.03	0.40
33:j:62:PHE:CD1	41:s:140:ILE:HB	2.57	0.40
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.55	0.40
40:r:321:LEU:HD13	40:r:444:LEU:HG	2.02	0.40
40:r:328:CYS:O	40:r:332:THR:HG23	2.22	0.40
41:s:85:MET:HE3	41:s:85:MET:HB3	2.00	0.40
42:u:109:GLU:HG3	42:u:110:CYS:N	2.36	0.40
1:A:146:GLY:HA3	1:A:193:PHE:CE1	2.57	0.40
6:G:69:SER:HA	16:Q:60:HIS:CE1	2.56	0.40
16:Q:63:PRO:HA	16:Q:64:PRO:HD3	1.94	0.40
16:Q:107:ARG:O	16:Q:440:LYS:NZ	2.39	0.40
26:c:164:ASN:OD1	26:c:180:PRO:HA	2.21	0.40
32:i:141:VAL:O	32:i:145:ILE:HG12	2.21	0.40
35:l:213:LEU:HB3	35:l:273:VAL:HG11	2.03	0.40
38:o:89:LEU:HD22	38:o:93:PHE:CE2	2.55	0.40
41:s:62:ARG:HH11	41:s:64:ALA:HA	1.86	0.40
41:s:137:ALA:HB3	41:s:282:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/433 (99%)	413 (96%)	16 (4%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	111 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	101 (92%)	9 (8%)	0	100	100
8	I	93/112 (83%)	84 (90%)	9 (10%)	0	100	100
9	J	327/342 (96%)	316 (97%)	11 (3%)	0	100	100
10	K	40/43 (93%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	671 (98%)	16 (2%)	1 (0%)	48	80
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	412/430 (96%)	397 (96%)	15 (4%)	0	100	100
17	S	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
18	T	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	53
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	93 (94%)	6 (6%)	0	100	100
26	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
27	d	173/175 (99%)	173 (100%)	0	0	100	100
28	e	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
29	f	40/49 (82%)	40 (100%)	0	0	100	100
30	g	119/122 (98%)	116 (98%)	3 (2%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	332 (96%)	12 (4%)	1 (0%)	36	70
33	j	95/115 (83%)	88 (93%)	7 (7%)	0	100	100
34	k	96/98 (98%)	93 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	l	601/606 (99%)	575 (96%)	26 (4%)	0	100	100
36	m	125/175 (71%)	114 (91%)	11 (9%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
39	p	176/178 (99%)	167 (95%)	9 (5%)	0	100	100
40	r	457/459 (100%)	444 (97%)	13 (3%)	0	100	100
41	s	299/318 (94%)	287 (96%)	12 (4%)	0	100	100
42	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
43	v	122/125 (98%)	114 (93%)	8 (7%)	0	100	100
44	w	318/320 (99%)	304 (96%)	14 (4%)	0	100	100
All	All	8067/8326 (97%)	7772 (96%)	292 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	M	283	GLU
32	i	90	PHE
20	V	46	PRO

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	345/346 (100%)	341 (99%)	4 (1%)	63	82
2	B	151/151 (100%)	150 (99%)	1 (1%)	76	86
3	C	132/132 (100%)	129 (98%)	3 (2%)	44	74
4	E	107/107 (100%)	105 (98%)	2 (2%)	50	76
5	F	76/76 (100%)	75 (99%)	1 (1%)	61	81
6	G	76/81 (94%)	75 (99%)	1 (1%)	61	81
6	X	75/81 (93%)	75 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	H	99/99 (100%)	98 (99%)	1 (1%)	68	84
8	I	87/97 (90%)	85 (98%)	2 (2%)	44	74
9	J	278/296 (94%)	273 (98%)	5 (2%)	51	77
10	K	41/42 (98%)	40 (98%)	1 (2%)	43	73
11	L	113/113 (100%)	108 (96%)	5 (4%)	25	60
12	M	580/580 (100%)	570 (98%)	10 (2%)	53	78
13	N	130/130 (100%)	128 (98%)	2 (2%)	57	80
14	O	182/183 (100%)	180 (99%)	2 (1%)	65	83
15	P	190/190 (100%)	189 (100%)	1 (0%)	81	89
16	Q	361/370 (98%)	358 (99%)	3 (1%)	73	86
17	S	56/58 (97%)	56 (100%)	0	100	100
18	T	79/79 (100%)	78 (99%)	1 (1%)	61	81
19	U	69/69 (100%)	68 (99%)	1 (1%)	59	80
20	V	100/101 (99%)	96 (96%)	4 (4%)	28	62
21	W	122/123 (99%)	118 (97%)	4 (3%)	33	67
22	Y	63/63 (100%)	62 (98%)	1 (2%)	55	79
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	120 (98%)	2 (2%)	55	79
25	b	98/119 (82%)	95 (97%)	3 (3%)	35	68
26	c	141/141 (100%)	139 (99%)	2 (1%)	59	80
27	d	155/155 (100%)	152 (98%)	3 (2%)	50	76
28	e	99/99 (100%)	97 (98%)	2 (2%)	48	76
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	107/109 (98%)	107 (100%)	0	100	100
31	h	93/93 (100%)	92 (99%)	1 (1%)	65	83
32	i	311/311 (100%)	308 (99%)	3 (1%)	68	84
33	j	88/100 (88%)	86 (98%)	2 (2%)	44	74
34	k	85/85 (100%)	84 (99%)	1 (1%)	63	82
35	l	518/540 (96%)	509 (98%)	9 (2%)	53	78
36	m	91/141 (64%)	90 (99%)	1 (1%)	65	83
37	n	53/53 (100%)	52 (98%)	1 (2%)	50	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	o	113/113 (100%)	112 (99%)	1 (1%)	70	85
39	p	158/159 (99%)	156 (99%)	2 (1%)	61	81
40	r	410/410 (100%)	399 (97%)	11 (3%)	39	71
41	s	263/275 (96%)	259 (98%)	4 (2%)	57	80
42	u	153/153 (100%)	149 (97%)	4 (3%)	40	72
43	v	98/111 (88%)	94 (96%)	4 (4%)	27	61
44	w	281/283 (99%)	272 (97%)	9 (3%)	34	67
All	All	7049/7249 (97%)	6929 (98%)	120 (2%)	52	78

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	THR
1	A	268	GLU
1	A	307	VAL
1	A	334	THR
2	B	76	TYR
3	C	71	CYS
3	C	102	VAL
3	C	126	GLU
4	E	58	GLN
4	E	99	GLN
5	F	42	VAL
6	G	139	MET
7	H	79	GLU
8	I	30	GLU
8	I	72	SER
9	J	92	MET
9	J	119	VAL
9	J	221	ARG
9	J	228	LEU
9	J	337	ASP
10	K	71	SER
11	L	63	THR
11	L	74	THR
11	L	86	ASN
11	L	127	THR
11	L	133	ASP
12	M	56	VAL
12	M	160	VAL

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Mol	Chain	Res	Type
12	M	244	GLU
12	M	318	THR
12	M	365	SER
12	M	515	ILE
12	M	544	VAL
12	M	611	THR
12	M	629	ILE
12	M	701	SER
13	N	107	LYS
13	N	134	ILE
14	O	42	ARG
14	O	196	LEU
15	P	86	ILE
16	Q	217	VAL
16	Q	252	SER
16	Q	265	ASN
18	T	77	SER
19	U	34	SER
20	V	95	CYS
20	V	99	LEU
20	V	124	LEU
20	V	141	VAL
21	W	66	GLU
21	W	83	VAL
21	W	114	THR
21	W	134	LEU
22	Y	97	LEU
24	a	93	ILE
24	a	97	GLU
25	b	23	LEU
25	b	76	LEU
25	b	101	LYS
26	c	96	ASP
26	c	117	VAL
27	d	78	GLU
27	d	120	SER
27	d	136	SER
28	e	99	LEU
28	e	125	LEU
31	h	82	GLN
32	i	37	LEU
32	i	97	MET

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Mol	Chain	Res	Type
32	i	300	SER
33	j	13	LEU
33	j	68	GLU
34	k	39	SER
35	l	24	SER
35	l	71	LEU
35	l	79	SER
35	l	104	SER
35	l	140	LEU
35	l	185	SER
35	l	340	PHE
35	l	386	LEU
35	l	491	LEU
36	m	143	ILE
37	n	15	ILE
38	o	57	LEU
39	p	110	SER
39	p	176	GLU
40	r	49	SER
40	r	90	THR
40	r	103	GLN
40	r	179	ILE
40	r	218	LYS
40	r	248	THR
40	r	274	SER
40	r	337	VAL
40	r	350	THR
40	r	365	THR
40	r	452	LYS
41	s	24	GLU
41	s	113	VAL
41	s	115	SER
41	s	276	SER
42	u	5	VAL
42	u	55	ARG
42	u	109	GLU
42	u	115	LEU
43	v	14	SER
43	v	24	THR
43	v	61	HIS
43	v	108	LEU
44	w	49	THR

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Mol	Chain	Res	Type
44	w	66	ILE
44	w	114	LEU
44	w	132	GLN
44	w	227	MET
44	w	297	LEU
44	w	306	ASN
44	w	312	VAL
44	w	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	244	ASN
1	A	270	ASN
1	A	277	ASN
1	A	284	HIS
4	E	51	GLN
4	E	126	HIS
5	F	86	GLN
9	J	122	HIS
10	K	75	ASN
11	L	71	HIS
12	M	278	HIS
12	M	388	ASN
12	M	464	GLN
12	M	498	GLN
12	M	604	GLN
12	M	669	ASN
12	M	688	GLN
13	N	12	GLN
14	O	41	HIS
14	O	191	ASN
15	P	77	GLN
15	P	180	ASN
15	P	196	HIS
15	P	247	GLN
16	Q	160	ASN
16	Q	233	HIS
18	T	120	GLN
19	U	74	GLN
24	a	170	GLN

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Mol	Chain	Res	Type
25	b	126	GLN
26	c	94	HIS
27	d	59	ASN
29	f	73	ASN
30	g	90	HIS
32	i	63	GLN
32	i	91	ASN
32	i	120	GLN
35	l	67	HIS
35	l	165	ASN
35	l	192	HIS
35	l	320	ASN
38	o	126	ASN
39	p	51	HIS
40	r	144	ASN
40	r	175	ASN
40	r	184	HIS
40	r	188	ASN
41	s	97	ASN
41	s	235	ASN
41	s	317	GLN
42	u	30	HIS
42	u	35	GLN
42	u	77	HIS
43	v	4	HIS
43	v	92	HIS
44	w	155	GLN
44	w	176	GLN
44	w	306	ASN
44	w	323	GLN
44	w	329	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	2.02	1 (10%)	5,13,15	5.94	3 (60%)

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
16	2MR	Q	118	16	-	2/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.81	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.12	130.59	119.48
16	Q	118	2MR	CD-NE-CZ	4.24	131.33	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.29	130.71	123.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 34 ligands modelled in this entry, 2 are monoatomic - leaving 32 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$
48	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)
55	CDL	i	401	-	65,65,99	1.31	9 (13%)	71,77,111	1.03	4 (5%)
48	PEE	i	402	-	46,46,50	1.23	6 (13%)	49,51,55	0.99	2 (4%)
55	CDL	r	504	-	98,98,99	1.12	8 (8%)	104,110,111	0.90	4 (3%)
49	PLX	r	503	-	51,51,51	1.22	5 (9%)	53,59,59	0.59	1 (1%)
48	PEE	b	201	-	45,45,50	1.25	6 (13%)	48,50,55	1.00	2 (4%)
45	SF4	A	501	1	0,12,12	-	-	-		
45	SF4	M	802	12	0,12,12	-	-	-		
55	CDL	a	201	-	90,90,99	1.16	9 (10%)	96,102,111	0.93	4 (4%)
51	NDP	J	401	-	51,52,52	4.31	25 (49%)	71,80,80	2.20	14 (19%)
48	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	1.02	2 (3%)
56	UQ	s	401	-	28,28,63	3.36	8 (28%)	36,37,79	2.81	13 (36%)
45	SF4	C	301	3,16	0,12,12	-	-	-		
45	SF4	M	801	12	0,12,12	-	-	-		
49	PLX	j	202	-	51,51,51	1.22	4 (7%)	53,59,59	0.59	1 (1%)
50	8Q1	X	201	-	32,34,34	1.64	6 (18%)	39,43,43	1.53	6 (15%)
48	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
50	8Q1	G	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.55	6 (15%)
45	SF4	B	301	2	0,12,12	-	-	-		
55	CDL	r	505	-	99,99,99	1.12	9 (9%)	105,111,111	0.86	4 (3%)
47	NAI	A	503	-	47,48,48	4.02	22 (46%)	64,73,73	1.68	11 (17%)
57	ADP	w	401	-	28,29,29	3.18	9 (32%)	43,45,45	1.90	9 (20%)
52	FES	O	301	14	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	B	302	2	0,12,12	-	-	-		
46	FMN	A	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.24	8 (16%)
55	CDL	l	701	-	99,99,99	1.12	9 (9%)	105,111,111	0.84	4 (3%)
48	PEE	l	702	-	45,45,50	1.25	6 (13%)	48,50,55	1.02	2 (4%)
49	PLX	r	502	-	51,51,51	1.21	5 (9%)	53,59,59	0.63	1 (1%)
48	PEE	m	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.01	2 (4%)
52	FES	M	803	12	0,4,4	-	-	-		
49	PLX	C	302	-	51,51,51	1.22	4 (7%)	53,59,59	0.62	1 (1%)
49	PLX	g	201	-	51,51,51	1.22	5 (9%)	53,59,59	0.60	1 (1%)

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
48	PEE	r	501	-	-	27/54/54/54	-
55	CDL	i	401	-	-	41/76/76/110	-
48	PEE	i	402	-	-	27/50/50/54	-
55	CDL	r	504	-	-	53/109/109/110	-
49	PLX	r	503	-	-	31/55/55/55	-
48	PEE	b	201	-	-	24/49/49/54	-
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	M	802	12	-	-	0/6/5/5
55	CDL	a	201	-	-	51/101/101/110	-
51	NDP	J	401	-	-	7/34/77/77	0/5/5/5
48	PEE	B	303	-	-	21/54/54/54	-
56	UQ	s	401	-	-	10/21/45/87	0/1/1/1
45	SF4	C	301	3,16	-	-	0/6/5/5
49	PLX	j	202	-	-	31/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
50	8Q1	X	201	-	-	13/41/41/41	-
48	PEE	j	201	-	-	23/54/54/54	-
50	8Q1	G	201	-	-	19/41/41/41	-
55	CDL	r	505	-	-	59/110/110/110	-
45	SF4	B	301	2	-	-	0/6/5/5
47	NAI	A	503	-	-	9/29/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
52	FES	O	301	14	-	-	0/1/1/1
45	SF4	B	302	2	-	-	0/6/5/5
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
55	CDL	l	701	-	-	62/110/110/110	-
48	PEE	l	702	-	-	22/49/49/54	-
49	PLX	r	502	-	-	27/55/55/55	-
48	PEE	m	201	-	-	16/44/44/54	-
52	FES	M	803	12	-	-	0/1/1/1
49	PLX	C	302	-	-	23/55/55/55	-
49	PLX	g	201	-	-	21/55/55/55	-

All (186) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-13.09	1.24	1.53
51	J	401	NDP	O4D-C4D	10.85	1.69	1.45
47	A	503	NAI	C3D-C4D	-10.24	1.27	1.53
51	J	401	NDP	C3D-C4D	-9.87	1.28	1.53
56	s	401	UQ	C13-C14	9.68	1.55	1.33
47	A	503	NAI	O4B-C1B	9.38	1.63	1.42
56	s	401	UQ	C8-C9	9.29	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.97	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.17	1.26	1.45
56	s	401	UQ	C18-C19	7.98	1.56	1.32
51	J	401	NDP	O4B-C4B	-7.88	1.27	1.45
57	w	401	ADP	O4'-C4'	7.78	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.66	1.29	1.53
51	J	401	NDP	C2N-C3N	7.50	1.55	1.35
47	A	503	NAI	C2B-C1B	-7.31	1.30	1.53
51	J	401	NDP	C6N-C5N	7.30	1.55	1.33
47	A	503	NAI	O4D-C4D	7.08	1.60	1.45
51	J	401	NDP	PN-O3	6.99	1.67	1.59
47	A	503	NAI	PA-O3	6.49	1.66	1.59
57	w	401	ADP	PA-O3A	6.48	1.66	1.59
51	J	401	NDP	P2B-O2B	6.13	1.70	1.59
47	A	503	NAI	C2D-C3D	6.00	1.69	1.53
51	J	401	NDP	PA-O3	5.90	1.65	1.59
51	J	401	NDP	C6A-N6A	5.76	1.48	1.34
47	A	503	NAI	PN-O3	5.73	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	A	503	NAI	O4D-C1D	5.67	1.55	1.42
51	J	401	NDP	C3B-C4B	5.56	1.67	1.53
57	w	401	ADP	C6-N6	5.49	1.48	1.34
47	A	503	NAI	C7N-N7N	5.32	1.48	1.33
47	A	503	NAI	C4N-C3N	-5.27	1.40	1.50
50	X	201	8Q1	C39-N41	5.20	1.45	1.33
47	A	503	NAI	C6A-N6A	5.13	1.47	1.34
50	G	201	8Q1	C39-N41	5.11	1.45	1.33
50	X	201	8Q1	C34-N36	5.08	1.45	1.33
50	G	201	8Q1	C34-N36	5.06	1.45	1.33
51	J	401	NDP	C6N-N1N	5.06	1.49	1.37
51	J	401	NDP	O4D-C1D	-4.98	1.30	1.42
51	J	401	NDP	O4B-C1B	4.74	1.53	1.42
51	J	401	NDP	C1B-N9A	-4.60	1.33	1.46
57	w	401	ADP	O4'-C1'	-4.56	1.31	1.42
47	A	503	NAI	O2B-C2B	4.37	1.53	1.43
51	J	401	NDP	O2D-C2D	-3.93	1.33	1.43
51	J	401	NDP	C7N-N7N	3.89	1.44	1.33
48	j	201	PEE	C18-C19	3.84	1.53	1.31
48	B	303	PEE	C18-C19	3.83	1.53	1.31
48	l	702	PEE	C18-C19	3.83	1.53	1.31
48	m	201	PEE	C18-C19	3.83	1.53	1.31
48	r	501	PEE	C18-C19	3.83	1.53	1.31
48	b	201	PEE	C18-C19	3.83	1.53	1.31
48	i	402	PEE	C18-C19	3.82	1.53	1.31
48	j	201	PEE	C39-C38	3.75	1.53	1.31
48	i	402	PEE	C39-C38	3.75	1.53	1.31
48	B	303	PEE	C39-C38	3.74	1.53	1.31
48	r	501	PEE	C39-C38	3.74	1.52	1.31
48	l	702	PEE	C39-C38	3.74	1.52	1.31
48	b	201	PEE	C39-C38	3.74	1.52	1.31
47	A	503	NAI	C7N-C3N	3.60	1.56	1.48
55	i	401	CDL	OA8-CA7	3.51	1.43	1.33
55	l	701	CDL	OA8-CA7	3.50	1.43	1.33
55	r	505	CDL	OA8-CA7	3.50	1.43	1.33
46	A	502	FMN	C4A-N5	3.46	1.38	1.30
55	r	504	CDL	OA8-CA7	3.45	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.43	1.40	1.49
55	a	201	CDL	OA8-CA7	3.42	1.43	1.33
57	w	401	ADP	C8-N9	-3.38	1.31	1.37
57	w	401	ADP	O2'-C2'	-3.12	1.35	1.43
51	J	401	NDP	C8A-N9A	-3.12	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	s	401	UQ	C6-C1	3.09	1.55	1.46
55	r	504	CDL	OB6-CB5	3.07	1.42	1.34
55	a	201	CDL	OB6-CB5	3.05	1.42	1.34
55	r	505	CDL	OB6-CB5	3.05	1.42	1.34
55	l	701	CDL	OB8-CB7	3.04	1.42	1.33
55	i	401	CDL	OB6-CB5	3.04	1.42	1.34
55	r	504	CDL	OB8-CB7	3.03	1.42	1.33
55	l	701	CDL	OB6-CB5	3.03	1.42	1.34
51	J	401	NDP	C7N-C3N	3.03	1.55	1.48
55	a	201	CDL	OA6-CA5	3.02	1.42	1.34
55	r	505	CDL	OB8-CB7	3.02	1.42	1.33
55	i	401	CDL	OB8-CB7	3.02	1.42	1.33
55	r	505	CDL	OA6-CA5	3.02	1.42	1.34
55	a	201	CDL	OB8-CB7	3.01	1.42	1.33
55	l	701	CDL	OA6-CA5	3.00	1.42	1.34
55	i	401	CDL	OA6-CA5	2.99	1.42	1.34
57	w	401	ADP	O3'-C3'	2.99	1.50	1.43
51	J	401	NDP	C5A-N7A	-2.98	1.33	1.39
51	J	401	NDP	O3D-C3D	2.97	1.50	1.43
55	r	504	CDL	OA6-CA5	2.94	1.42	1.34
49	C	302	PLX	O6-C4	-2.86	1.40	1.44
49	g	201	PLX	O6-C4	-2.77	1.41	1.44
49	r	503	PLX	O6-C4	-2.73	1.41	1.44
49	j	202	PLX	O6-C4	-2.71	1.41	1.44
51	J	401	NDP	O2B-C2B	2.67	1.53	1.44
47	A	503	NAI	C8A-N9A	-2.67	1.33	1.37
48	B	303	PEE	O2-C2	-2.55	1.40	1.46
48	r	501	PEE	O2-C2	-2.55	1.40	1.46
48	b	201	PEE	O3-C30	2.54	1.40	1.33
55	r	504	CDL	OA6-CA4	-2.54	1.40	1.46
48	b	201	PEE	O2-C2	-2.54	1.40	1.46
48	j	201	PEE	O2-C2	-2.53	1.40	1.46
47	A	503	NAI	PN-O5D	2.53	1.69	1.59
55	a	201	CDL	OA6-CA4	-2.51	1.40	1.46
55	r	505	CDL	OA6-CA4	-2.51	1.40	1.46
48	i	402	PEE	O2-C2	-2.50	1.40	1.46
55	l	701	CDL	OA6-CA4	-2.50	1.40	1.46
55	i	401	CDL	OA6-CA4	-2.49	1.40	1.46
48	i	402	PEE	O3-C30	2.47	1.40	1.33
48	r	501	PEE	O3-C30	2.47	1.40	1.33
48	j	201	PEE	O3-C30	2.47	1.40	1.33
50	X	201	8Q1	C1-S44	2.46	1.82	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	m	201	PEE	O3-C30	2.46	1.40	1.33
46	A	502	FMN	C10-N1	2.46	1.38	1.33
48	l	702	PEE	O3-C30	2.45	1.40	1.33
49	r	502	PLX	C7-C6	2.45	1.55	1.50
48	l	702	PEE	O2-C2	-2.44	1.40	1.46
48	B	303	PEE	O3-C30	2.44	1.40	1.33
49	j	202	PLX	C7-C6	2.44	1.55	1.50
57	w	401	ADP	C5-N7	-2.43	1.34	1.39
48	l	702	PEE	O2-C10	2.42	1.41	1.34
49	r	503	PLX	C7-C6	2.41	1.55	1.50
48	m	201	PEE	O2-C10	2.41	1.41	1.34
49	g	201	PLX	C7-C6	2.41	1.55	1.50
50	X	201	8Q1	C6-C1	2.40	1.53	1.50
48	m	201	PEE	O2-C2	-2.40	1.41	1.46
50	G	201	8Q1	C1-S44	2.40	1.81	1.76
47	A	503	NAI	C6N-C5N	2.39	1.40	1.33
47	A	503	NAI	C5B-C4B	2.38	1.58	1.51
51	J	401	NDP	C2D-C3D	2.38	1.59	1.53
50	G	201	8Q1	O35-C34	-2.35	1.18	1.23
49	C	302	PLX	C7-C6	2.35	1.55	1.50
55	l	701	CDL	OB6-CB4	-2.32	1.41	1.46
47	A	503	NAI	O3B-C3B	-2.32	1.37	1.43
55	i	401	CDL	OB6-CB4	-2.30	1.41	1.46
48	i	402	PEE	O2-C10	2.30	1.40	1.34
55	i	401	CDL	PB2-OB2	2.29	1.68	1.59
48	B	303	PEE	O2-C10	2.29	1.40	1.34
50	X	201	8Q1	O35-C34	-2.28	1.19	1.23
55	r	505	CDL	PB2-OB2	2.28	1.68	1.59
51	J	401	NDP	PA-O5B	2.28	1.68	1.59
49	r	502	PLX	O6-C4	-2.28	1.41	1.44
50	G	201	8Q1	O40-C39	-2.28	1.18	1.23
48	b	201	PEE	O2-C10	2.28	1.40	1.34
50	G	201	8Q1	C6-C1	2.27	1.53	1.50
48	j	201	PEE	O2-C10	2.27	1.40	1.34
55	r	504	CDL	PB2-OB2	2.26	1.68	1.59
48	r	501	PEE	O2-C10	2.25	1.40	1.34
55	i	401	CDL	PB2-OB5	2.25	1.68	1.59
55	a	201	CDL	OB6-CB4	-2.25	1.41	1.46
55	r	504	CDL	PB2-OB5	2.25	1.68	1.59
56	s	401	UQ	C7-C8	2.25	1.54	1.50
55	l	701	CDL	PB2-OB2	2.24	1.68	1.59
55	a	201	CDL	PB2-OB2	2.24	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	r	504	CDL	OB6-CB4	-2.24	1.41	1.46
55	r	505	CDL	PB2-OB5	2.24	1.68	1.59
50	X	201	8Q1	O40-C39	-2.24	1.18	1.23
49	g	201	PLX	P1-O4	2.23	1.68	1.59
55	a	201	CDL	PB2-OB5	2.23	1.68	1.59
55	l	701	CDL	PB2-OB5	2.22	1.68	1.59
49	j	202	PLX	P1-O4	2.21	1.68	1.59
49	r	503	PLX	P1-O4	2.21	1.68	1.59
55	r	505	CDL	OB6-CB4	-2.21	1.41	1.46
49	r	502	PLX	P1-O4	2.20	1.68	1.59
49	C	302	PLX	P1-O4	2.20	1.68	1.59
48	m	201	PEE	O3-C3	-2.17	1.40	1.45
56	s	401	UQ	O3-CM3	-2.16	1.40	1.45
48	l	702	PEE	O3-C3	-2.14	1.40	1.45
56	s	401	UQ	O4-C4	-2.14	1.18	1.23
48	j	201	PEE	O3-C3	-2.13	1.40	1.45
49	j	202	PLX	P1-O1	2.12	1.67	1.59
48	B	303	PEE	O3-C3	-2.12	1.40	1.45
48	r	501	PEE	O3-C3	-2.11	1.40	1.45
48	i	402	PEE	O3-C3	-2.10	1.40	1.45
51	J	401	NDP	O7N-C7N	-2.10	1.19	1.24
47	A	503	NAI	C5A-N7A	-2.09	1.35	1.39
49	C	302	PLX	P1-O1	2.08	1.67	1.59
49	r	503	PLX	P1-O1	2.08	1.67	1.59
49	r	502	PLX	P1-O1	2.08	1.67	1.59
55	a	201	CDL	C11-CA5	2.06	1.56	1.50
49	g	201	PLX	P1-O1	2.06	1.67	1.59
48	b	201	PEE	O3-C3	-2.04	1.40	1.45
49	r	502	PLX	C25-C24	2.04	1.55	1.50
49	r	503	PLX	C1-C2	2.02	1.57	1.51
56	s	401	UQ	O1-C1	-2.01	1.18	1.23
55	r	505	CDL	C11-CA5	2.01	1.56	1.50
55	l	701	CDL	C11-CA5	2.01	1.56	1.50
55	i	401	CDL	C11-CA5	2.01	1.56	1.50
49	g	201	PLX	C1-C2	2.00	1.57	1.51

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C7-C8-C9	-7.97	113.10	126.83
51	J	401	NDP	C3N-C2N-N1N	-7.46	112.25	123.20
51	J	401	NDP	C1D-N1N-C2N	-7.03	109.57	121.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	J	401	NDP	C6N-N1N-C2N	-6.62	112.23	119.32
56	s	401	UQ	C12-C13-C14	-6.23	113.36	127.62
50	X	201	8Q1	C6-C1-S44	5.62	120.10	113.40
51	J	401	NDP	C5A-C4A-N3A	-5.55	119.07	126.72
50	G	201	8Q1	C6-C1-S44	5.54	120.00	113.40
57	w	401	ADP	C5-C4-N3	-5.48	119.17	126.72
56	s	401	UQ	C7-C6-C1	5.38	124.77	118.52
47	A	503	NAI	C5A-C4A-N3A	-5.37	119.32	126.72
51	J	401	NDP	C1D-N1N-C6N	-5.23	109.72	120.77
56	s	401	UQ	C7-C6-C5	-4.93	116.44	124.89
57	w	401	ADP	N3-C2-N1	-4.56	121.67	128.58
56	s	401	UQ	C10-C9-C8	-4.47	112.14	123.63
47	A	503	NAI	N3A-C2A-N1A	-4.41	121.91	128.58
57	w	401	ADP	N3-C4-N9	4.30	134.48	127.17
56	s	401	UQ	C15-C14-C13	-4.27	112.67	123.63
55	a	201	CDL	OA6-CA5-C11	4.16	120.49	111.48
51	J	401	NDP	N3A-C2A-N1A	-4.14	122.31	128.58
55	r	504	CDL	OA6-CA5-C11	4.12	120.40	111.48
48	B	303	PEE	O2-C10-C11	4.10	120.34	111.48
55	i	401	CDL	OA6-CA5-C11	4.06	120.26	111.48
48	r	501	PEE	O2-C10-C11	4.04	120.22	111.48
55	r	504	CDL	OB6-CB5-C51	3.98	120.09	111.48
55	r	505	CDL	OB6-CB5-C51	3.98	120.09	111.48
51	J	401	NDP	N3A-C4A-N9A	3.96	133.91	127.17
48	i	402	PEE	O2-C10-C11	3.96	120.04	111.48
48	l	702	PEE	O2-C10-C11	3.95	120.03	111.48
48	m	201	PEE	O2-C10-C11	3.94	120.01	111.48
48	b	201	PEE	O2-C10-C11	3.94	120.00	111.48
55	a	201	CDL	OB6-CB5-C51	3.93	119.97	111.48
55	i	401	CDL	OB6-CB5-C51	3.92	119.95	111.48
55	r	505	CDL	OA6-CA5-C11	3.91	119.93	111.48
48	j	201	PEE	O2-C10-C11	3.91	119.93	111.48
55	l	701	CDL	OA6-CA5-C11	3.89	119.89	111.48
56	s	401	UQ	C17-C18-C19	-3.86	114.76	127.64
47	A	503	NAI	N3A-C4A-N9A	3.78	133.60	127.17
55	l	701	CDL	OB6-CB5-C51	3.70	119.48	111.48
56	s	401	UQ	C16-C14-C13	-3.66	112.96	121.17
47	A	503	NAI	C2A-N3A-C4A	3.65	120.76	111.83
56	s	401	UQ	C11-C9-C8	-3.65	112.98	121.17
51	J	401	NDP	C2A-N3A-C4A	3.62	120.66	111.83
57	w	401	ADP	C2-N3-C4	3.57	120.56	111.83
57	w	401	ADP	N9-C8-N7	-3.50	108.97	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	A	503	NAI	C4A-C5A-N7A	-3.47	106.61	110.58
47	A	503	NAI	C5A-N7A-C8A	3.42	108.83	103.45
50	G	201	8Q1	O4-C1-C6	-3.39	120.07	123.98
46	A	502	FMN	C4-N3-C2	-3.38	119.63	125.64
50	X	201	8Q1	O4-C1-C6	-3.36	120.10	123.98
47	A	503	NAI	C3D-C2D-C1D	3.35	107.80	101.46
47	A	503	NAI	N9A-C8A-N7A	-3.31	109.24	113.94
51	J	401	NDP	C4A-C5A-N7A	-3.21	106.91	110.58
56	s	401	UQ	C21-C19-C18	-3.20	113.05	122.66
57	w	401	ADP	C5-N7-C8	3.20	108.48	103.45
51	J	401	NDP	N9A-C8A-N7A	-3.15	109.47	113.94
57	w	401	ADP	C4-N9-C8	3.15	109.04	105.74
51	J	401	NDP	C5A-N7A-C8A	3.08	108.29	103.45
50	G	201	8Q1	C37-C38-C39	3.06	117.49	112.39
47	A	503	NAI	C2D-C3D-C4D	2.99	108.39	102.61
57	w	401	ADP	C4-C5-N7	-2.99	107.17	110.58
56	s	401	UQ	CM5-C5-C6	-2.91	119.66	124.45
48	B	303	PEE	O3-C30-C31	2.91	120.70	111.83
48	r	501	PEE	O3-C30-C31	2.81	120.40	111.83
55	i	401	CDL	OA8-CA7-C31	2.81	120.39	111.83
56	s	401	UQ	C20-C19-C18	-2.78	114.31	122.66
55	a	201	CDL	OB8-CB7-C71	2.76	120.25	111.83
55	r	504	CDL	OA8-CA7-C31	2.74	120.20	111.83
48	b	201	PEE	O3-C30-C31	2.73	120.16	111.83
48	j	201	PEE	O3-C30-C31	2.72	120.14	111.83
55	i	401	CDL	OB8-CB7-C71	2.69	120.03	111.83
55	r	505	CDL	OA8-CA7-C31	2.69	120.02	111.83
55	l	701	CDL	OB8-CB7-C71	2.68	120.01	111.83
55	r	504	CDL	OB8-CB7-C71	2.68	120.00	111.83
48	l	702	PEE	O3-C30-C31	2.67	119.99	111.83
48	i	402	PEE	O3-C30-C31	2.67	119.98	111.83
46	A	502	FMN	C4A-C4-N3	2.67	120.05	113.25
55	l	701	CDL	OA8-CA7-C31	2.64	119.88	111.83
55	r	505	CDL	OB8-CB7-C71	2.63	119.86	111.83
55	a	201	CDL	OA8-CA7-C31	2.62	119.82	111.83
48	m	201	PEE	O3-C30-C31	2.59	119.75	111.83
49	r	503	PLX	C1A-N1-C1	2.56	120.10	109.91
50	X	201	8Q1	C37-C38-C39	2.56	116.66	112.39
46	A	502	FMN	O4-C4-C4A	-2.55	119.80	126.53
46	A	502	FMN	C4A-C10-N10	2.54	120.12	116.48
49	r	502	PLX	C1A-N1-C1	2.54	119.99	109.91
49	g	201	PLX	C1A-N1-C1	2.53	119.97	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C6-C5-C4	2.46	121.11	119.17
51	J	401	NDP	C4A-N9A-C8A	2.45	108.31	105.74
50	G	201	8Q1	C43-S44-C1	2.45	109.07	101.84
50	X	201	8Q1	C43-S44-C1	2.40	108.93	101.84
49	j	202	PLX	C1A-N1-C1	2.39	119.40	109.91
51	J	401	NDP	C2B-C3B-C4B	2.39	107.12	101.99
47	A	503	NAI	C4A-N9A-C8A	2.38	108.24	105.74
49	C	302	PLX	C1A-N1-C1	2.31	119.10	109.91
46	A	502	FMN	C5A-C9A-N10	2.30	120.04	117.97
46	A	502	FMN	C10-C4A-N5	-2.28	120.15	124.81
47	A	503	NAI	C4D-O4D-C1D	-2.28	104.43	109.47
50	X	201	8Q1	O4-C1-S44	-2.27	119.80	122.68
50	X	201	8Q1	C38-C39-N41	2.20	120.35	116.34
46	A	502	FMN	C9A-C5A-N5	-2.19	120.13	122.45
50	G	201	8Q1	O4-C1-S44	-2.17	119.93	122.68
50	G	201	8Q1	C38-C39-N41	2.11	120.19	116.34
46	A	502	FMN	C4A-C10-N1	-2.07	119.51	124.59
57	w	401	ADP	C2'-C3'-C4'	2.05	106.58	102.61
51	J	401	NDP	C2B-C1B-N9A	-2.05	110.37	113.75

There are no chirality outliers.

All (627) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C1'-C2'-C3'-O3'
46	A	502	FMN	C1'-C2'-C3'-C4'
47	A	503	NAI	C5B-O5B-PA-O1A
48	b	201	PEE	C1-O3P-P-O1P
48	b	201	PEE	O4P-C4-C5-N
48	i	402	PEE	C11-C10-O2-C2
48	i	402	PEE	C4-O4P-P-O1P
48	j	201	PEE	C11-C10-O2-C2
48	j	201	PEE	O4-C10-O2-C2
48	j	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C1-O3P-P-O4P
48	l	702	PEE	C11-C10-O2-C2
48	l	702	PEE	C4-O4P-P-O3P
48	l	702	PEE	C4-O4P-P-O2P
48	l	702	PEE	C4-O4P-P-O1P

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Mol	Chain	Res	Type	Atoms
48	m	201	PEE	C17-C18-C19-C20
48	m	201	PEE	C11-C10-O2-C2
48	r	501	PEE	C1-O3P-P-O1P
49	C	302	PLX	C3-O4-P1-O1
49	C	302	PLX	C3-O4-P1-O2
49	C	302	PLX	C3-O4-P1-O3
49	C	302	PLX	N1-C1-C2-O1
49	g	201	PLX	O7-C6-O6-C4
49	j	202	PLX	O7-C6-C7-C8
49	j	202	PLX	O7-C6-O6-C4
49	j	202	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	C2-O1-P1-O4
49	r	502	PLX	C2-O1-P1-O2
49	r	502	PLX	O9-C24-C25-C26
49	r	503	PLX	O7-C6-O6-C4
49	r	503	PLX	C2-O1-P1-O4
49	r	503	PLX	C2-O1-P1-O2
49	r	503	PLX	C2-O1-P1-O3
49	r	503	PLX	O9-C24-O8-C5
49	r	503	PLX	O9-C24-C25-C26
50	G	201	8Q1	O4-C1-S44-C43
50	G	201	8Q1	C6-C1-S44-C43
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-O33
50	G	201	8Q1	N36-C37-C38-C39
50	G	201	8Q1	N41-C42-C43-S44
50	G	201	8Q1	C28-O27-P24-O2
50	G	201	8Q1	C28-O27-P24-O1
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C28-O27-P24-O2

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Mol	Chain	Res	Type	Atoms
50	X	201	8Q1	C28-O27-P24-O1
55	a	201	CDL	CA2-C1-CB2-OB2
55	a	201	CDL	CA2-OA2-PA1-OA3
55	a	201	CDL	CA3-OA5-PA1-OA2
55	a	201	CDL	CA3-OA5-PA1-OA4
55	a	201	CDL	OA5-CA3-CA4-OA6
55	a	201	CDL	CB2-OB2-PB2-OB3
55	a	201	CDL	CB3-OB5-PB2-OB2
55	a	201	CDL	CB3-OB5-PB2-OB3
55	a	201	CDL	CB3-OB5-PB2-OB4
55	i	401	CDL	CA2-OA2-PA1-OA3
55	i	401	CDL	CA2-OA2-PA1-OA4
55	i	401	CDL	CA2-OA2-PA1-OA5
55	i	401	CDL	CA3-OA5-PA1-OA2
55	i	401	CDL	CA3-OA5-PA1-OA3
55	i	401	CDL	CA3-OA5-PA1-OA4
55	i	401	CDL	CB2-OB2-PB2-OB4
55	i	401	CDL	CB2-OB2-PB2-OB5
55	i	401	CDL	CB3-OB5-PB2-OB2
55	i	401	CDL	CB3-OB5-PB2-OB3
55	l	701	CDL	CA2-OA2-PA1-OA4
55	l	701	CDL	CA2-OA2-PA1-OA5
55	l	701	CDL	CA3-OA5-PA1-OA2
55	l	701	CDL	CA3-OA5-PA1-OA4
55	l	701	CDL	OA6-CA4-CA6-OA8
55	l	701	CDL	CB2-OB2-PB2-OB3
55	l	701	CDL	CB2-OB2-PB2-OB4
55	l	701	CDL	CB2-OB2-PB2-OB5
55	l	701	CDL	OB6-CB4-CB6-OB8
55	r	504	CDL	O1-C1-CA2-OA2
55	r	504	CDL	O1-C1-CB2-OB2
55	r	504	CDL	CA2-C1-CB2-OB2
55	r	504	CDL	CA2-OA2-PA1-OA3
55	r	504	CDL	CA2-OA2-PA1-OA5
55	r	504	CDL	CB3-OB5-PB2-OB2
55	r	504	CDL	CB3-OB5-PB2-OB3
55	r	504	CDL	CB3-OB5-PB2-OB4
55	r	505	CDL	CA2-OA2-PA1-OA3
55	r	505	CDL	CA2-OA2-PA1-OA4
55	r	505	CDL	CA2-OA2-PA1-OA5
55	r	505	CDL	CA3-OA5-PA1-OA2
55	r	505	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
55	r	505	CDL	OA6-CA4-CA6-OA8
55	r	505	CDL	CB2-OB2-PB2-OB3
55	r	505	CDL	CB2-OB2-PB2-OB4
55	r	505	CDL	CB2-OB2-PB2-OB5
55	r	505	CDL	CB3-OB5-PB2-OB3
55	r	505	CDL	OB7-CB5-OB6-CB4
55	r	505	CDL	C51-CB5-OB6-CB4
56	s	401	UQ	C1-C6-C7-C8
56	s	401	UQ	C5-C6-C7-C8
56	s	401	UQ	C7-C8-C9-C10
56	s	401	UQ	C12-C13-C14-C16
57	w	401	ADP	C5'-O5'-PA-O2A
55	r	504	CDL	OA9-CA7-OA8-CA6
55	i	401	CDL	OA9-CA7-OA8-CA6
48	i	402	PEE	O4-C10-O2-C2
48	l	702	PEE	O4-C10-O2-C2
48	m	201	PEE	O4-C10-O2-C2
55	r	504	CDL	C31-CA7-OA8-CA6
55	r	505	CDL	C71-CB7-OB8-CB6
56	s	401	UQ	C12-C11-C9-C8
48	b	201	PEE	C31-C30-O3-C3
48	l	702	PEE	C31-C30-O3-C3
55	i	401	CDL	C31-CA7-OA8-CA6
48	j	201	PEE	C17-C18-C19-C20
55	r	505	CDL	OB9-CB7-OB8-CB6
55	a	201	CDL	O1-C1-CB2-OB2
55	l	701	CDL	O1-C1-CB2-OB2
55	l	701	CDL	C71-CB7-OB8-CB6
48	l	702	PEE	O5-C30-O3-C3
48	b	201	PEE	C11-C10-O2-C2
55	a	201	CDL	C51-CB5-OB6-CB4
56	s	401	UQ	C17-C18-C19-C21
48	b	201	PEE	O5-C30-O3-C3
49	r	503	PLX	C12-C13-C14-C15
55	l	701	CDL	C11-C12-C13-C14
48	b	201	PEE	C37-C38-C39-C40
48	r	501	PEE	C17-C18-C19-C20
55	l	701	CDL	OB9-CB7-OB8-CB6
49	g	201	PLX	C7-C8-C9-C10
55	l	701	CDL	C59-C60-C61-C62
55	r	504	CDL	C62-C63-C64-C65
49	r	502	PLX	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
55	a	201	CDL	CB2-C1-CA2-OA2
55	r	504	CDL	CB2-C1-CA2-OA2
55	r	505	CDL	CB2-C1-CA2-OA2
48	m	201	PEE	C31-C30-O3-C3
55	a	201	CDL	C71-CB7-OB8-CB6
55	r	504	CDL	C71-CB7-OB8-CB6
49	j	202	PLX	C28-C29-C30-C31
55	r	504	CDL	C32-C33-C34-C35
49	r	502	PLX	C9-C10-C11-C12
49	C	302	PLX	C28-C29-C30-C31
55	r	505	CDL	O1-C1-CA2-OA2
48	m	201	PEE	O5-C30-O3-C3
48	l	702	PEE	O3P-C1-C2-O2
55	l	701	CDL	C35-C36-C37-C38
55	i	401	CDL	CA7-C31-C32-C33
55	r	504	CDL	OB9-CB7-OB8-CB6
55	i	401	CDL	C31-C32-C33-C34
55	a	201	CDL	CA7-C31-C32-C33
55	l	701	CDL	CB7-C71-C72-C73
48	b	201	PEE	O4-C10-O2-C2
48	m	201	PEE	C13-C14-C15-C16
55	a	201	CDL	CB5-C51-C52-C53
55	r	504	CDL	CA7-C31-C32-C33
55	r	504	CDL	CB7-C71-C72-C73
55	r	505	CDL	CB7-C71-C72-C73
48	r	501	PEE	C10-C11-C12-C13
55	i	401	CDL	CB7-C71-C72-C73
48	B	303	PEE	C12-C13-C14-C15
55	a	201	CDL	C31-C32-C33-C34
55	l	701	CDL	C39-C40-C41-C42
55	a	201	CDL	O1-C1-CA2-OA2
55	i	401	CDL	O1-C1-CA2-OA2
55	a	201	CDL	OB9-CB7-OB8-CB6
48	b	201	PEE	C10-C11-C12-C13
55	r	504	CDL	CB5-C51-C52-C53
55	a	201	CDL	OB7-CB5-OB6-CB4
48	B	303	PEE	C37-C38-C39-C40
48	i	402	PEE	C17-C18-C19-C20
48	j	201	PEE	C37-C38-C39-C40
55	r	505	CDL	CA7-C31-C32-C33
51	J	401	NDP	C2D-C1D-N1N-C6N
48	r	501	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
55	i	401	CDL	CB2-C1-CA2-OA2
49	r	503	PLX	C2-C1-N1-C1A
48	B	303	PEE	C17-C18-C19-C20
55	r	504	CDL	C20-C21-C22-C23
55	r	505	CDL	C74-C75-C76-C77
49	j	202	PLX	C15-C16-C17-C18
55	l	701	CDL	C71-C72-C73-C74
48	r	501	PEE	C11-C10-O2-C2
49	r	503	PLX	C2-C1-N1-C1C
48	b	201	PEE	C22-C23-C24-C25
55	a	201	CDL	C37-C38-C39-C40
55	i	401	CDL	C11-C12-C13-C14
55	r	504	CDL	C75-C76-C77-C78
48	j	201	PEE	C43-C44-C45-C46
48	r	501	PEE	C20-C21-C22-C23
49	g	201	PLX	C30-C31-C32-C33
49	g	201	PLX	C33-C34-C35-C36
55	r	504	CDL	C71-C72-C73-C74
55	r	505	CDL	C55-C56-C57-C58
55	r	505	CDL	C73-C74-C75-C76
48	l	702	PEE	C37-C38-C39-C40
49	g	201	PLX	C32-C33-C34-C35
55	r	504	CDL	C73-C74-C75-C76
55	i	401	CDL	C71-CB7-OB8-CB6
49	C	302	PLX	O7-C6-C7-C8
48	l	702	PEE	C21-C22-C23-C24
49	j	202	PLX	C10-C11-C12-C13
49	r	502	PLX	C27-C28-C29-C30
55	l	701	CDL	C37-C38-C39-C40
55	l	701	CDL	C60-C61-C62-C63
49	r	502	PLX	C15-C16-C17-C18
49	j	202	PLX	C25-C26-C27-C28
49	j	202	PLX	C27-C28-C29-C30
55	r	505	CDL	CB5-C51-C52-C53
49	r	503	PLX	C25-C26-C27-C28
55	a	201	CDL	C71-C72-C73-C74
55	r	505	CDL	C75-C76-C77-C78
49	g	201	PLX	C28-C29-C30-C31
55	l	701	CDL	C55-C56-C57-C58
56	s	401	UQ	C13-C14-C16-C17
49	g	201	PLX	C10-C11-C12-C13
49	r	502	PLX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
55	r	504	CDL	C81-C82-C83-C84
55	l	701	CDL	C75-C76-C77-C78
49	r	503	PLX	C16-C17-C18-C19
49	r	503	PLX	C14-C15-C16-C17
49	r	503	PLX	C27-C28-C29-C30
55	l	701	CDL	C73-C74-C75-C76
55	r	504	CDL	C56-C57-C58-C59
55	r	505	CDL	C56-C57-C58-C59
55	l	701	CDL	C56-C57-C58-C59
55	r	504	CDL	C14-C15-C16-C17
49	g	201	PLX	C11-C10-C9-C8
49	r	503	PLX	C33-C34-C35-C36
55	a	201	CDL	C21-C22-C23-C24
55	a	201	CDL	C75-C76-C77-C78
55	i	401	CDL	C35-C36-C37-C38
55	l	701	CDL	C54-C55-C56-C57
55	i	401	CDL	CB5-C51-C52-C53
48	b	201	PEE	C31-C32-C33-C34
49	g	201	PLX	C27-C28-C29-C30
46	A	502	FMN	O2'-C2'-C3'-C4'
48	b	201	PEE	C33-C34-C35-C36
48	b	201	PEE	C14-C15-C16-C17
49	j	202	PLX	C12-C13-C14-C15
55	r	505	CDL	C52-C53-C54-C55
55	i	401	CDL	OB9-CB7-OB8-CB6
49	C	302	PLX	C7-C8-C9-C10
49	r	503	PLX	C13-C14-C15-C16
55	i	401	CDL	C52-C53-C54-C55
48	r	501	PEE	O4-C10-O2-C2
56	s	401	UQ	C12-C11-C9-C10
55	l	701	CDL	C40-C41-C42-C43
49	g	201	PLX	C9-C10-C11-C12
55	l	701	CDL	C63-C64-C65-C66
48	l	702	PEE	C31-C32-C33-C34
49	j	202	PLX	C7-C8-C9-C10
55	r	504	CDL	C35-C36-C37-C38
48	r	501	PEE	C31-C32-C33-C34
49	C	302	PLX	C15-C16-C17-C18
55	r	505	CDL	C71-C72-C73-C74
49	r	502	PLX	C10-C11-C12-C13
49	C	302	PLX	C17-C18-C19-C20
55	l	701	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
49	r	503	PLX	C11-C12-C13-C14
55	r	505	CDL	C43-C44-C45-C46
48	B	303	PEE	C11-C10-O2-C2
48	b	201	PEE	C13-C14-C15-C16
48	B	303	PEE	O4-C10-O2-C2
48	i	402	PEE	C19-C20-C21-C22
55	a	201	CDL	C13-C14-C15-C16
49	r	502	PLX	C33-C34-C35-C36
49	r	503	PLX	C2-C1-N1-C1B
48	i	402	PEE	C11-C12-C13-C14
49	C	302	PLX	O4-C3-C4-O6
49	j	202	PLX	C13-C14-C15-C16
49	g	201	PLX	C25-C26-C27-C28
49	r	502	PLX	C31-C32-C33-C34
49	r	503	PLX	C10-C11-C12-C13
48	B	303	PEE	C15-C16-C17-C18
48	i	402	PEE	C35-C36-C37-C38
48	m	201	PEE	C15-C16-C17-C18
55	r	504	CDL	OB6-CB4-CB6-OB8
48	B	303	PEE	C32-C33-C34-C35
48	B	303	PEE	C33-C34-C35-C36
48	m	201	PEE	C11-C12-C13-C14
55	r	504	CDL	C54-C55-C56-C57
48	j	201	PEE	C36-C37-C38-C39
48	r	501	PEE	C36-C37-C38-C39
49	C	302	PLX	C11-C12-C13-C14
49	r	502	PLX	C12-C13-C14-C15
55	r	505	CDL	C32-C33-C34-C35
55	r	505	CDL	C42-C43-C44-C45
48	B	303	PEE	C31-C30-O3-C3
48	i	402	PEE	C14-C15-C16-C17
49	r	503	PLX	C28-C29-C30-C31
55	i	401	CDL	C71-C72-C73-C74
55	l	701	CDL	C51-CB5-OB6-CB4
48	j	201	PEE	C23-C24-C25-C26
55	i	401	CDL	C32-C33-C34-C35
55	r	504	CDL	C39-C40-C41-C42
49	r	503	PLX	C30-C31-C32-C33
55	r	505	CDL	C41-C42-C43-C44
49	j	202	PLX	C26-C27-C28-C29
55	l	701	CDL	C57-C58-C59-C60
55	a	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C14-C15-C16-C17
48	B	303	PEE	C42-C43-C44-C45
49	r	502	PLX	C16-C17-C18-C19
55	a	201	CDL	C54-C55-C56-C57
48	B	303	PEE	C14-C15-C16-C17
48	m	201	PEE	C33-C34-C35-C36
48	b	201	PEE	C1-C2-C3-O3
48	i	402	PEE	C1-C2-C3-O3
49	r	503	PLX	C3-C4-C5-O8
55	l	701	CDL	CB3-CB4-CB6-OB8
55	r	504	CDL	CB3-CB4-CB6-OB8
49	C	302	PLX	C33-C34-C35-C36
49	j	202	PLX	C9-C10-C11-C12
48	B	303	PEE	C39-C40-C41-C42
48	b	201	PEE	C15-C16-C17-C18
48	j	201	PEE	C19-C20-C21-C22
48	r	501	PEE	C19-C20-C21-C22
48	i	402	PEE	C13-C14-C15-C16
55	r	504	CDL	C74-C75-C76-C77
48	j	201	PEE	C31-C30-O3-C3
48	B	303	PEE	C21-C22-C23-C24
49	C	302	PLX	C9-C10-C11-C12
50	G	201	8Q1	C28-O27-P24-O3
50	X	201	8Q1	C28-O27-P24-O3
55	l	701	CDL	C17-C18-C19-C20
55	r	505	CDL	C62-C63-C64-C65
49	j	202	PLX	C34-C35-C36-C37
49	C	302	PLX	C30-C31-C32-C33
49	C	302	PLX	C31-C32-C33-C34
55	a	201	CDL	C34-C35-C36-C37
55	a	201	CDL	C14-C15-C16-C17
47	A	503	NAI	C3D-C4D-C5D-O5D
48	B	303	PEE	O5-C30-O3-C3
55	i	401	CDL	C14-C15-C16-C17
48	r	501	PEE	C44-C45-C46-C47
49	g	201	PLX	C12-C13-C14-C15
55	l	701	CDL	C58-C59-C60-C61
55	r	504	CDL	C55-C56-C57-C58
48	b	201	PEE	C32-C33-C34-C35
49	r	503	PLX	C9-C10-C11-C12
49	r	503	PLX	C31-C32-C33-C34
55	i	401	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
55	l	701	CDL	C64-C65-C66-C67
48	r	501	PEE	C31-C30-O3-C3
55	i	401	CDL	C33-C34-C35-C36
55	r	505	CDL	C84-C85-C86-C87
49	C	302	PLX	C27-C28-C29-C30
55	l	701	CDL	C77-C78-C79-C80
48	b	201	PEE	C34-C35-C36-C37
49	r	503	PLX	C29-C30-C31-C32
55	a	201	CDL	CA5-C11-C12-C13
55	r	505	CDL	C59-C60-C61-C62
49	j	202	PLX	C11-C12-C13-C14
55	r	504	CDL	C51-C52-C53-C54
48	l	702	PEE	C22-C23-C24-C25
49	j	202	PLX	C30-C31-C32-C33
49	C	302	PLX	C16-C17-C18-C19
55	a	201	CDL	C11-C12-C13-C14
48	l	702	PEE	O3P-C1-C2-C3
49	C	302	PLX	O4-C3-C4-C5
55	a	201	CDL	OA5-CA3-CA4-CA6
48	l	702	PEE	C32-C33-C34-C35
48	j	201	PEE	O5-C30-O3-C3
49	r	503	PLX	C26-C27-C28-C29
55	a	201	CDL	C55-C56-C57-C58
55	r	504	CDL	C11-C12-C13-C14
48	r	501	PEE	C21-C22-C23-C24
55	a	201	CDL	C73-C74-C75-C76
48	i	402	PEE	C23-C24-C25-C26
48	r	501	PEE	C1-C2-C3-O3
49	j	202	PLX	C3-C4-C5-O8
50	X	201	8Q1	O33-C32-C34-N36
55	l	701	CDL	CA3-CA4-CA6-OA8
55	r	505	CDL	CA3-CA4-CA6-OA8
49	r	502	PLX	C13-C14-C15-C16
50	G	201	8Q1	C12-C13-C14-C15
48	B	303	PEE	C20-C21-C22-C23
49	g	201	PLX	C13-C14-C15-C16
49	r	503	PLX	C36-C37-C38-C39
55	r	504	CDL	C36-C37-C38-C39
49	j	202	PLX	O4-C3-C4-O6
55	a	201	CDL	OB5-CB3-CB4-OB6
55	i	401	CDL	C73-C74-C75-C76
49	j	202	PLX	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C31-C32-C33-C34
55	a	201	CDL	C74-C75-C76-C77
48	b	201	PEE	O2-C2-C3-O3
48	l	702	PEE	O2-C2-C3-O3
48	r	501	PEE	O2-C2-C3-O3
49	j	202	PLX	O6-C4-C5-O8
55	i	401	CDL	OB6-CB4-CB6-OB8
55	r	505	CDL	OB6-CB4-CB6-OB8
55	r	505	CDL	C17-C18-C19-C20
48	j	201	PEE	C44-C45-C46-C47
48	B	303	PEE	C36-C37-C38-C39
49	r	502	PLX	C7-C8-C9-C10
49	g	201	PLX	C14-C15-C16-C17
49	r	502	PLX	C29-C30-C31-C32
50	G	201	8Q1	C10-C11-C12-C13
49	C	302	PLX	C13-C14-C15-C16
55	l	701	CDL	CA2-C1-CB2-OB2
55	a	201	CDL	C72-C73-C74-C75
55	r	505	CDL	C80-C81-C82-C83
55	l	701	CDL	C72-C73-C74-C75
48	B	303	PEE	O3P-C1-C2-C3
48	b	201	PEE	O3P-C1-C2-C3
49	j	202	PLX	O4-C3-C4-C5
48	i	402	PEE	C24-C25-C26-C27
48	j	201	PEE	C38-C39-C40-C41
48	l	702	PEE	C30-C31-C32-C33
48	r	501	PEE	O5-C30-O3-C3
55	l	701	CDL	OB7-CB5-OB6-CB4
48	l	702	PEE	C15-C16-C17-C18
55	a	201	CDL	C60-C61-C62-C63
55	r	505	CDL	C51-C52-C53-C54
48	b	201	PEE	O3P-C1-C2-O2
49	r	502	PLX	C26-C27-C28-C29
49	r	502	PLX	C3-C4-C5-O8
55	r	505	CDL	CB3-CB4-CB6-OB8
56	s	401	UQ	C14-C16-C17-C18
48	i	402	PEE	C18-C19-C20-C21
49	r	503	PLX	C7-C8-C9-C10
48	j	201	PEE	C21-C22-C23-C24
55	r	504	CDL	C42-C43-C44-C45
49	r	502	PLX	O6-C4-C5-O8
55	r	505	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
48	r	501	PEE	C22-C23-C24-C25
55	l	701	CDL	C14-C15-C16-C17
49	j	202	PLX	C7-C6-O6-C4
48	r	501	PEE	C12-C13-C14-C15
55	r	505	CDL	C60-C61-C62-C63
55	r	505	CDL	C79-C80-C81-C82
55	r	504	CDL	C11-CA5-OA6-CA4
46	A	502	FMN	O2'-C2'-C3'-O3'
49	j	202	PLX	C32-C33-C34-C35
55	l	701	CDL	C31-C32-C33-C34
55	l	701	CDL	O1-C1-CA2-OA2
48	i	402	PEE	C31-C32-C33-C34
55	i	401	CDL	C37-C38-C39-C40
55	i	401	CDL	C15-C16-C17-C18
48	i	402	PEE	C21-C22-C23-C24
48	b	201	PEE	C11-C12-C13-C14
55	r	505	CDL	C44-C45-C46-C47
49	g	201	PLX	C25-C24-O8-C5
49	j	202	PLX	C25-C24-O8-C5
55	r	504	CDL	C78-C79-C80-C81
55	l	701	CDL	C62-C63-C64-C65
55	r	504	CDL	C33-C34-C35-C36
55	r	505	CDL	C16-C17-C18-C19
48	r	501	PEE	O3P-C1-C2-C3
55	a	201	CDL	C76-C77-C78-C79
55	r	505	CDL	C64-C65-C66-C67
55	a	201	CDL	C52-C53-C54-C55
55	r	505	CDL	CB4-CB3-OB5-PB2
50	G	201	8Q1	C42-C43-S44-C1
49	j	202	PLX	C33-C34-C35-C36
49	j	202	PLX	O6-C6-C7-C8
49	r	502	PLX	O8-C24-C25-C26
49	r	503	PLX	O8-C24-C25-C26
48	B	303	PEE	O3P-C1-C2-O2
48	r	501	PEE	O3P-C1-C2-O2
55	i	401	CDL	OA5-CA3-CA4-OA6
48	i	402	PEE	C10-C11-C12-C13
55	r	505	CDL	C54-C55-C56-C57
55	r	504	CDL	C37-C38-C39-C40
51	J	401	NDP	O4D-C1D-N1N-C6N
49	r	503	PLX	O6-C4-C5-O8
55	l	701	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
48	l	702	PEE	C1-C2-C3-O3
49	C	302	PLX	C25-C26-C27-C28
47	A	503	NAI	C2D-C1D-N1N-C2N
55	a	201	CDL	C31-CA7-OA8-CA6
48	b	201	PEE	C38-C39-C40-C41
48	r	501	PEE	C16-C17-C18-C19
48	m	201	PEE	C24-C25-C26-C27
55	a	201	CDL	OA9-CA7-OA8-CA6
51	J	401	NDP	O4D-C4D-C5D-O5D
55	r	505	CDL	C15-C16-C17-C18
47	A	503	NAI	C5B-O5B-PA-O3
48	i	402	PEE	C4-O4P-P-O3P
48	l	702	PEE	O4P-C4-C5-N
48	m	201	PEE	C4-O4P-P-O3P
48	m	201	PEE	C4-O4P-P-O2P
48	m	201	PEE	C4-O4P-P-O1P
48	r	501	PEE	C4-O4P-P-O1P
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C2-O1-P1-O2
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	C2-O1-P1-O3
49	r	503	PLX	C3-O4-P1-O2
51	J	401	NDP	C5B-O5B-PA-O1A
55	a	201	CDL	CA2-OA2-PA1-OA4
55	a	201	CDL	CA2-OA2-PA1-OA5
55	a	201	CDL	CB2-OB2-PB2-OB4
55	a	201	CDL	CB2-OB2-PB2-OB5
55	i	401	CDL	CB2-OB2-PB2-OB3
55	l	701	CDL	CA2-OA2-PA1-OA3
55	l	701	CDL	CB3-OB5-PB2-OB2
55	l	701	CDL	CB3-OB5-PB2-OB3
55	l	701	CDL	CB3-OB5-PB2-OB4
55	r	504	CDL	CB2-OB2-PB2-OB3
55	r	504	CDL	CB2-OB2-PB2-OB5
55	r	505	CDL	CA3-OA5-PA1-OA3
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O3A
55	r	505	CDL	C12-C13-C14-C15
55	r	505	CDL	C14-C15-C16-C17
48	i	402	PEE	C2-C1-O3P-P
55	r	504	CDL	OA7-CA5-OA6-CA4
56	s	401	UQ	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
48	b	201	PEE	C16-C17-C18-C19
48	r	501	PEE	C13-C14-C15-C16
55	i	401	CDL	OA5-CA3-CA4-CA6
55	l	701	CDL	OA5-CA3-CA4-CA6
49	g	201	PLX	O4-C3-C4-O6
55	l	701	CDL	OA5-CA3-CA4-OA6
55	l	701	CDL	C12-C13-C14-C15
48	b	201	PEE	C18-C19-C20-C21
48	m	201	PEE	C31-C32-C33-C34
55	i	401	CDL	C34-C35-C36-C37
48	i	402	PEE	O2-C2-C3-O3
55	a	201	CDL	C11-CA5-OA6-CA4
48	B	303	PEE	C23-C24-C25-C26
55	l	701	CDL	C44-C45-C46-C47
49	g	201	PLX	O8-C24-C25-C26
55	i	401	CDL	C75-C76-C77-C78
48	B	303	PEE	C24-C25-C26-C27
48	j	201	PEE	C40-C41-C42-C43
55	l	701	CDL	C21-C22-C23-C24
55	l	701	CDL	C18-C19-C20-C21
55	r	504	CDL	C52-C53-C54-C55
48	j	201	PEE	C12-C13-C14-C15
48	i	402	PEE	C22-C23-C24-C25
55	a	201	CDL	OA7-CA5-OA6-CA4
47	A	503	NAI	O4D-C1D-N1N-C2N
48	m	201	PEE	C18-C19-C20-C21
48	r	501	PEE	C30-C31-C32-C33
48	l	702	PEE	C39-C40-C41-C42
55	i	401	CDL	CB3-CB4-CB6-OB8
48	i	402	PEE	C30-C31-C32-C33
49	C	302	PLX	C36-C37-C38-C39
48	m	201	PEE	C3-C2-O2-C10
48	i	402	PEE	C16-C17-C18-C19
47	A	503	NAI	C2D-C1D-N1N-C6N
48	B	303	PEE	C13-C14-C15-C16
55	r	505	CDL	C1-CB2-OB2-PB2
48	i	402	PEE	O3P-C1-C2-C3
49	g	201	PLX	O4-C3-C4-C5
55	r	505	CDL	C20-C21-C22-C23
47	A	503	NAI	C2N-C3N-C7N-N7N
51	J	401	NDP	C2B-O2B-P2B-O1X
49	j	202	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
49	C	302	PLX	C18-C19-C20-C21
50	G	201	8Q1	C9-C10-C11-C12
50	G	201	8Q1	C1-C6-C7-C8
55	r	504	CDL	C44-C45-C46-C47
50	G	201	8Q1	C11-C10-C9-C8
55	r	504	CDL	C23-C24-C25-C26
47	A	503	NAI	O4D-C4D-C5D-O5D
49	g	201	PLX	O9-C24-C25-C26
55	r	504	CDL	C82-C83-C84-C85
55	r	505	CDL	OA9-CA7-OA8-CA6
48	j	201	PEE	C42-C43-C44-C45
48	r	501	PEE	C11-C12-C13-C14
55	r	505	CDL	C76-C77-C78-C79
55	r	505	CDL	C31-C32-C33-C34
55	i	401	CDL	OA6-CA4-CA6-OA8
55	r	505	CDL	C31-CA7-OA8-CA6
49	j	202	PLX	C4-C5-O8-C24
48	j	201	PEE	C30-C31-C32-C33
55	l	701	CDL	C41-C42-C43-C44
55	a	201	CDL	C43-C44-C45-C46
48	i	402	PEE	C36-C37-C38-C39
48	l	702	PEE	C36-C37-C38-C39
55	i	401	CDL	CA3-CA4-CA6-OA8
55	a	201	CDL	C20-C21-C22-C23
48	i	402	PEE	C38-C39-C40-C41
48	i	402	PEE	C32-C33-C34-C35
55	a	201	CDL	C35-C36-C37-C38
47	A	503	NAI	O4D-C1D-N1N-C6N
48	j	201	PEE	C16-C17-C18-C19
48	l	702	PEE	C16-C17-C18-C19
51	J	401	NDP	O4B-C4B-C5B-O5B
57	w	401	ADP	PB-O3A-PA-O2A
55	l	701	CDL	C76-C77-C78-C79
49	j	202	PLX	C18-C19-C20-C21
50	X	201	8Q1	C29-C32-C34-O35
55	r	504	CDL	C72-C71-CB7-OB8
55	l	701	CDL	C12-C11-CA5-OA6
55	l	701	CDL	C43-C44-C45-C46
48	j	201	PEE	O2-C10-C11-C12
49	r	502	PLX	C25-C24-O8-C5
55	r	504	CDL	C61-C62-C63-C64
49	r	503	PLX	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
55	r	504	CDL	C12-C11-CA5-OA6
48	i	402	PEE	C34-C35-C36-C37
50	X	201	8Q1	C29-C32-C34-N36
49	C	302	PLX	C11-C10-C9-C8
55	l	701	CDL	C82-C83-C84-C85
55	l	701	CDL	C32-C31-CA7-OA8
55	r	505	CDL	OB5-CB3-CB4-OB6
55	r	504	CDL	C72-C71-CB7-OB9
49	j	202	PLX	C11-C10-C9-C8
49	r	502	PLX	O9-C24-O8-C5
48	j	201	PEE	O4-C10-C11-C12
55	i	401	CDL	C72-C73-C74-C75
55	r	504	CDL	C83-C84-C85-C86
51	J	401	NDP	C3D-C4D-C5D-O5D
55	a	201	CDL	C58-C59-C60-C61
55	l	701	CDL	C32-C33-C34-C35
48	r	501	PEE	C38-C39-C40-C41
55	l	701	CDL	C12-C11-CA5-OA7
55	r	504	CDL	C12-C11-CA5-OA7
55	r	505	CDL	C39-C40-C41-C42
48	r	501	PEE	C24-C25-C26-C27

There are no ring outliers.

26 monomers are involved in 111 short contacts:

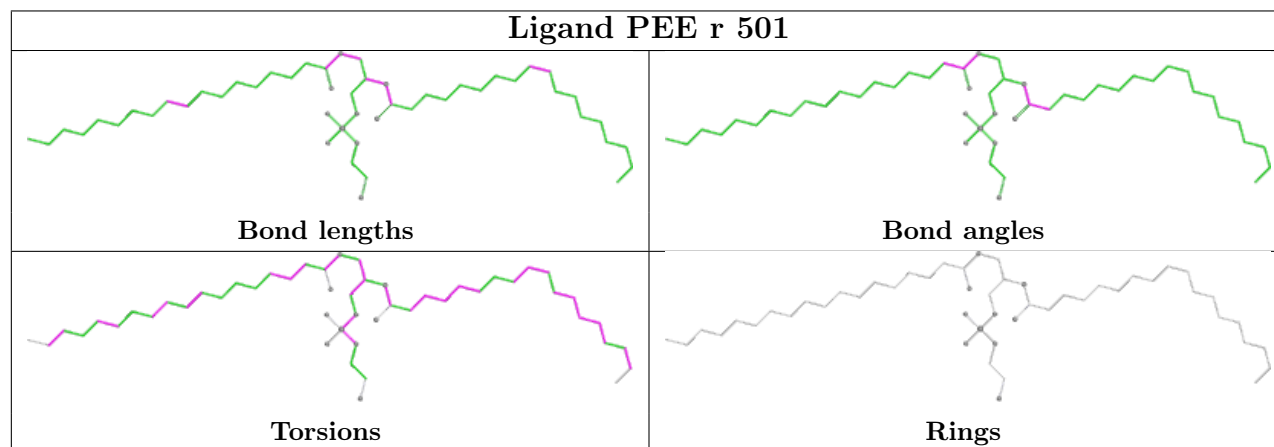
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	r	501	PEE	6	0
55	i	401	CDL	3	0
48	i	402	PEE	2	0
55	r	504	CDL	9	0
49	r	503	PLX	2	0
48	b	201	PEE	7	0
45	A	501	SF4	1	0
55	a	201	CDL	6	0
51	J	401	NDP	2	0
48	B	303	PEE	5	0
56	s	401	UQ	4	0
45	C	301	SF4	1	0
49	j	202	PLX	4	0
50	X	201	8Q1	3	0
48	j	201	PEE	4	0
50	G	201	8Q1	2	0

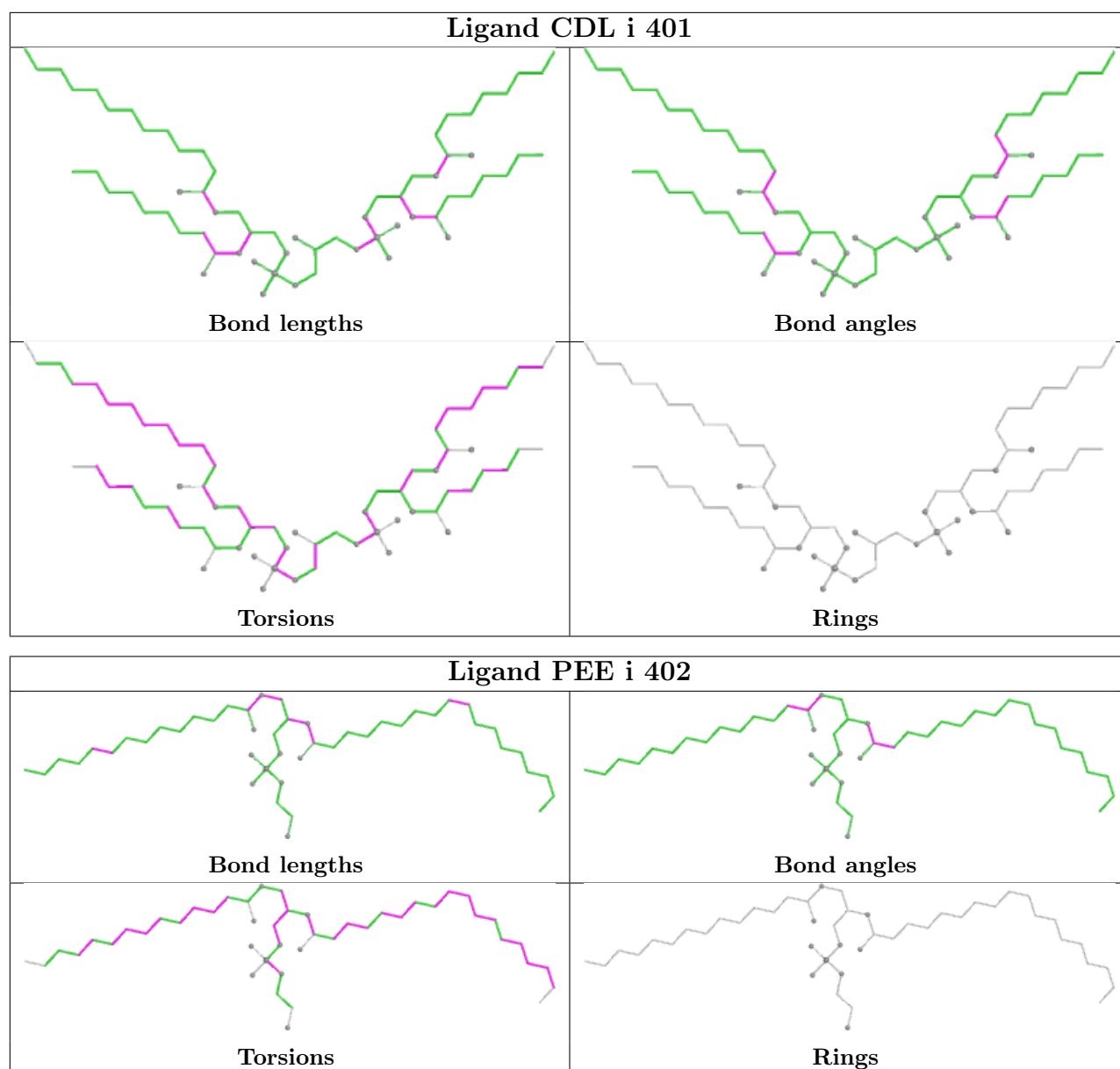
Continued on next page...

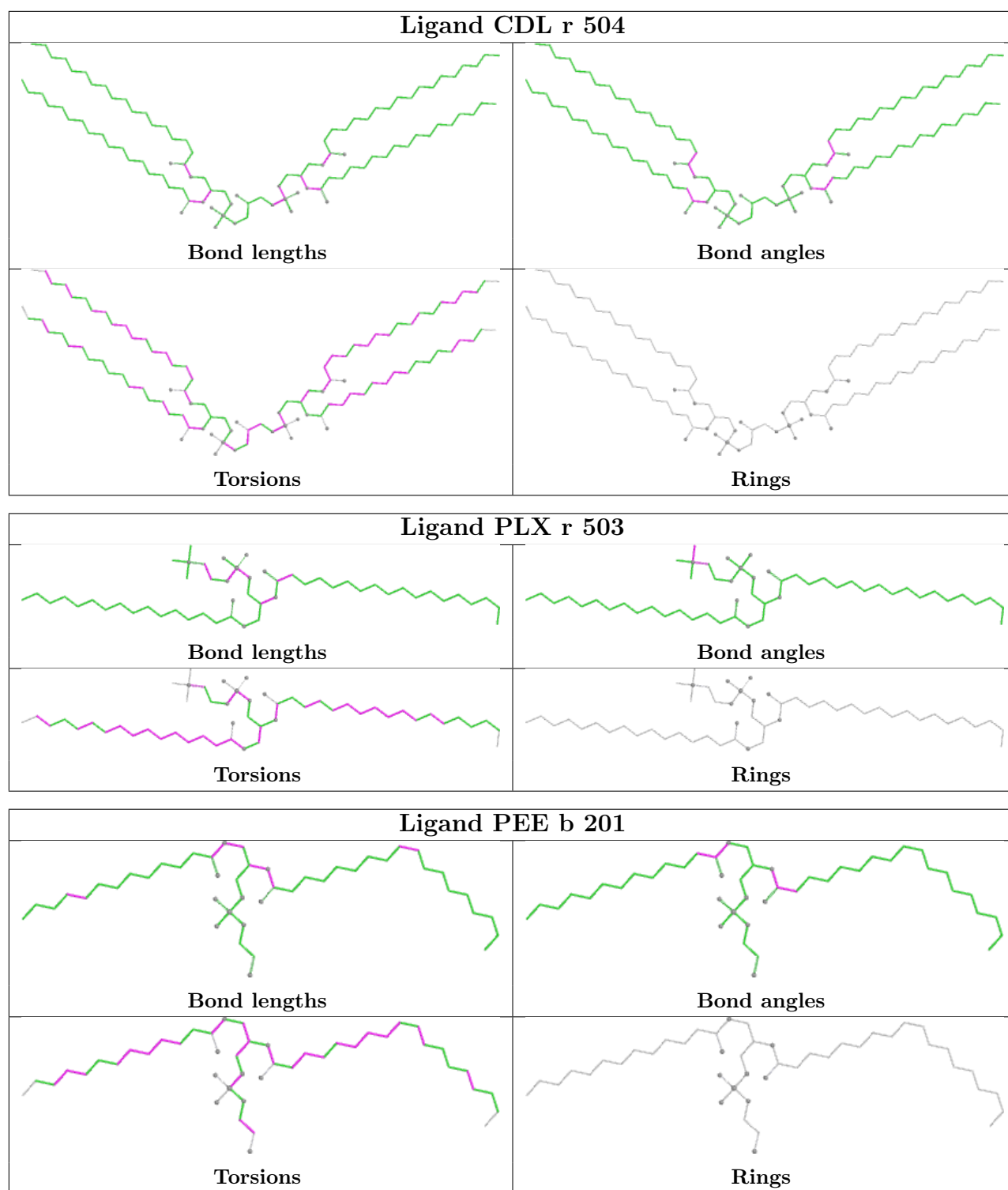
Continued from previous page...

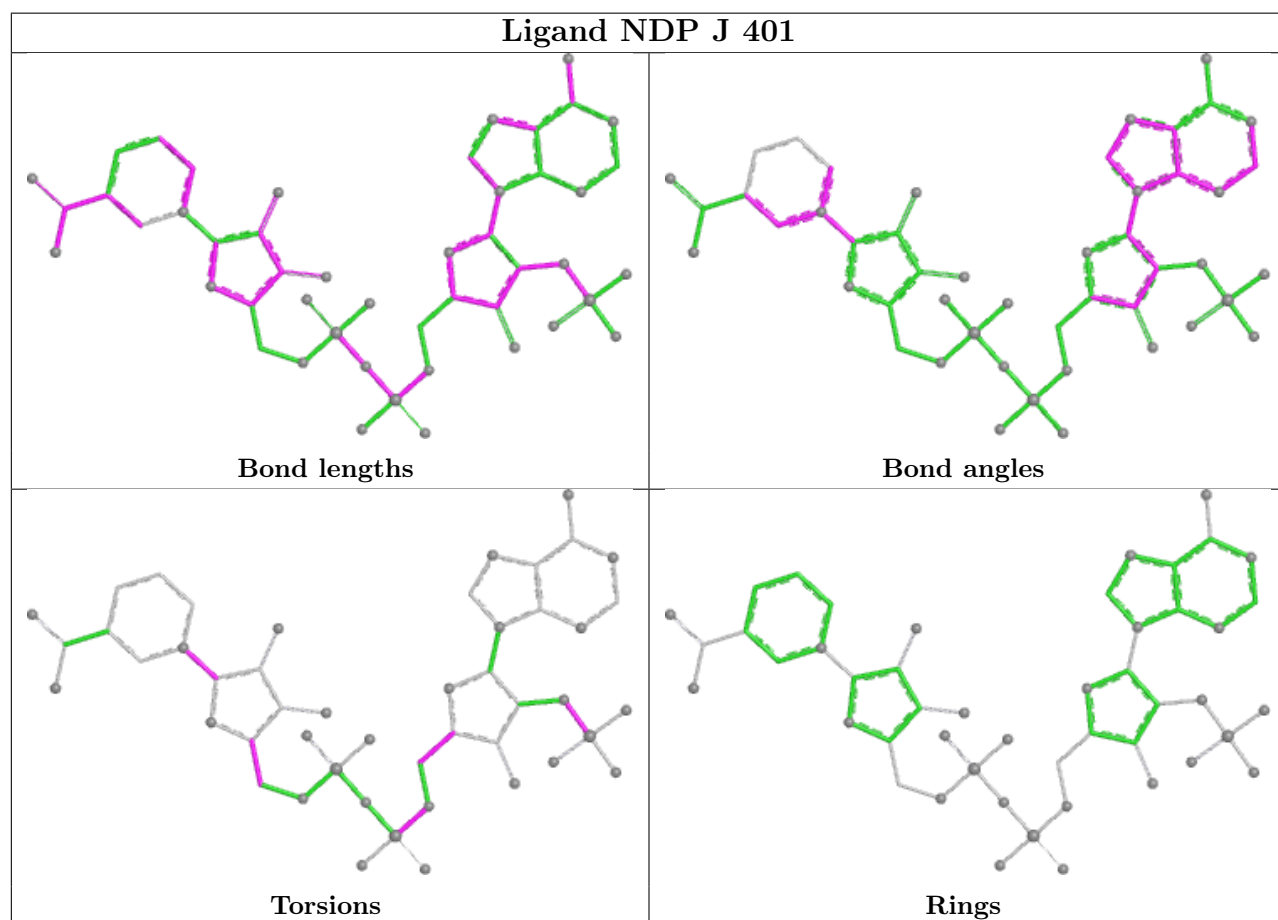
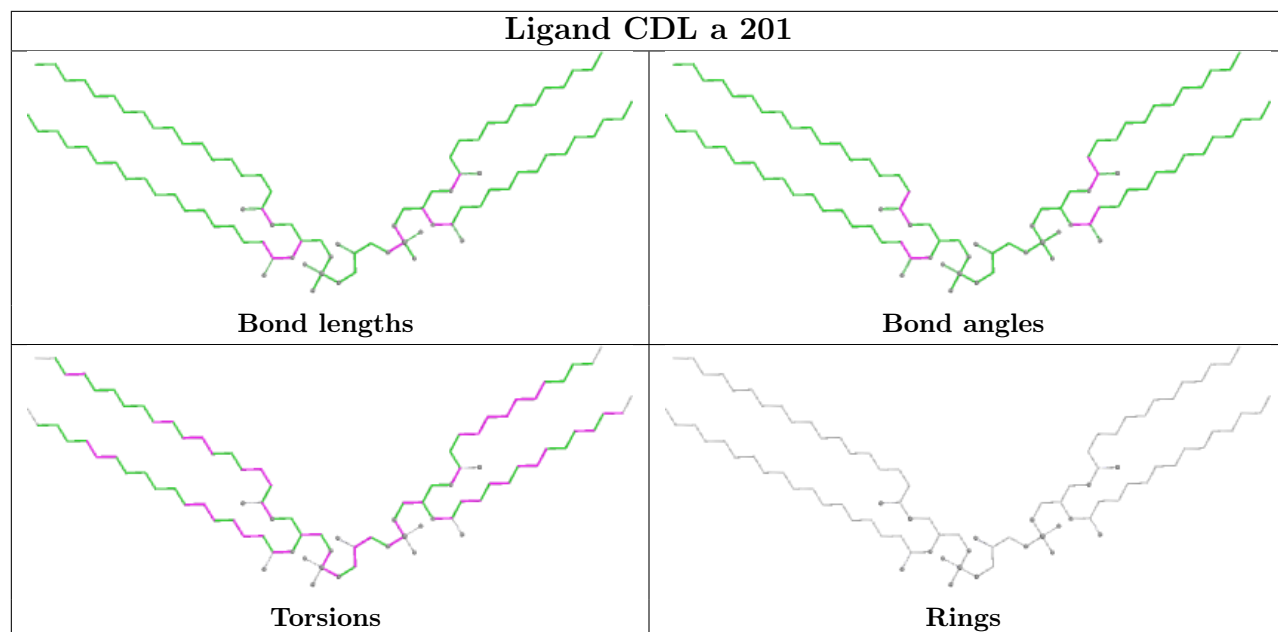
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	r	505	CDL	10	0
47	A	503	NAI	6	0
57	w	401	ADP	2	0
46	A	502	FMN	6	0
55	l	701	CDL	9	0
48	l	702	PEE	3	0
49	r	502	PLX	6	0
48	m	201	PEE	4	0
49	C	302	PLX	5	0
49	g	201	PLX	4	0

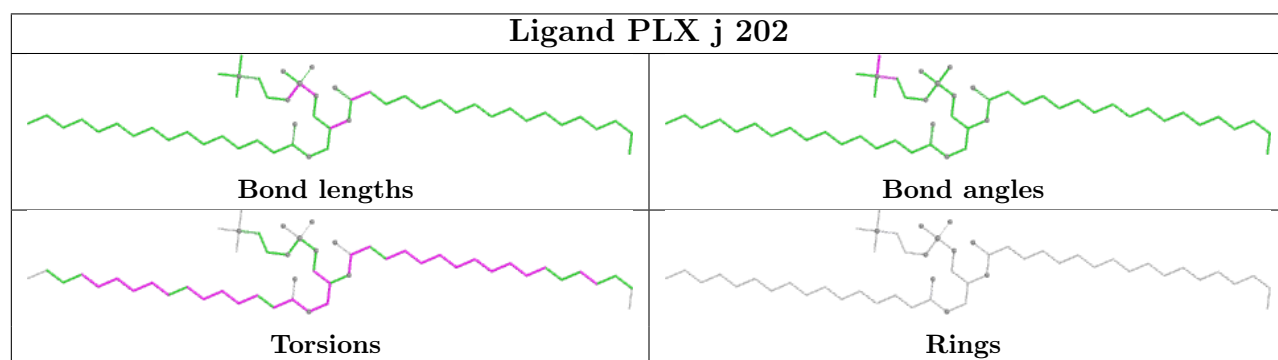
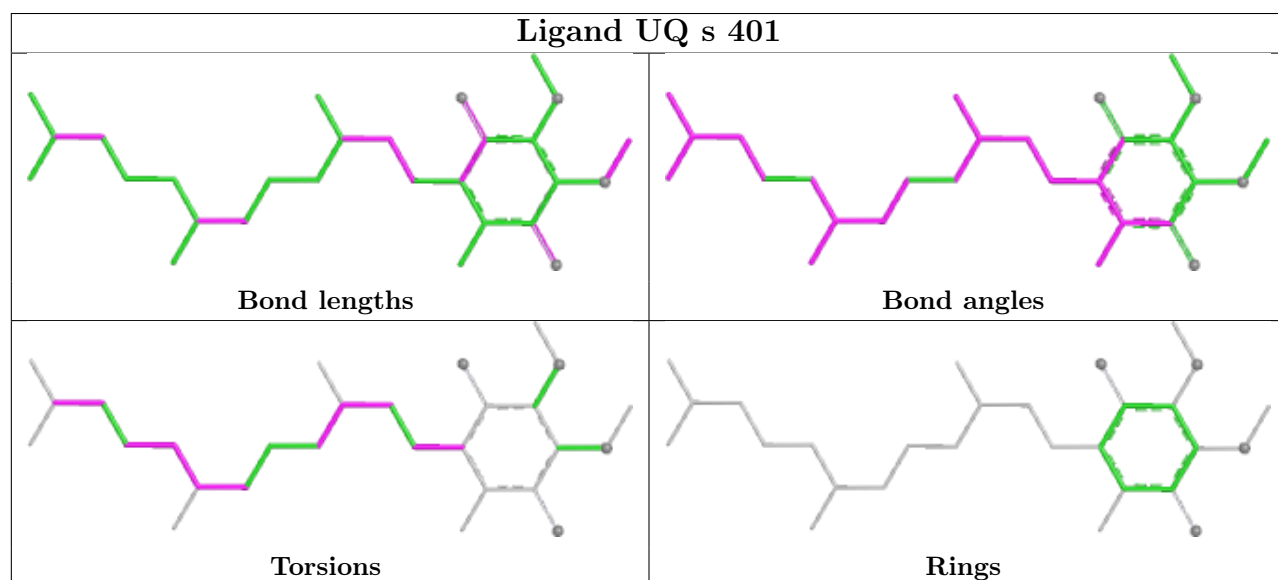
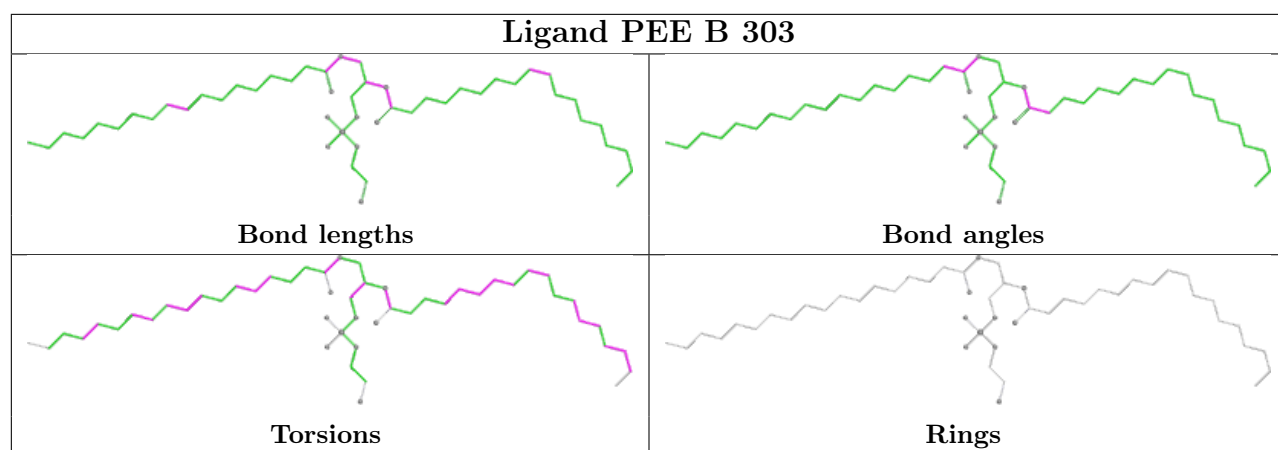
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

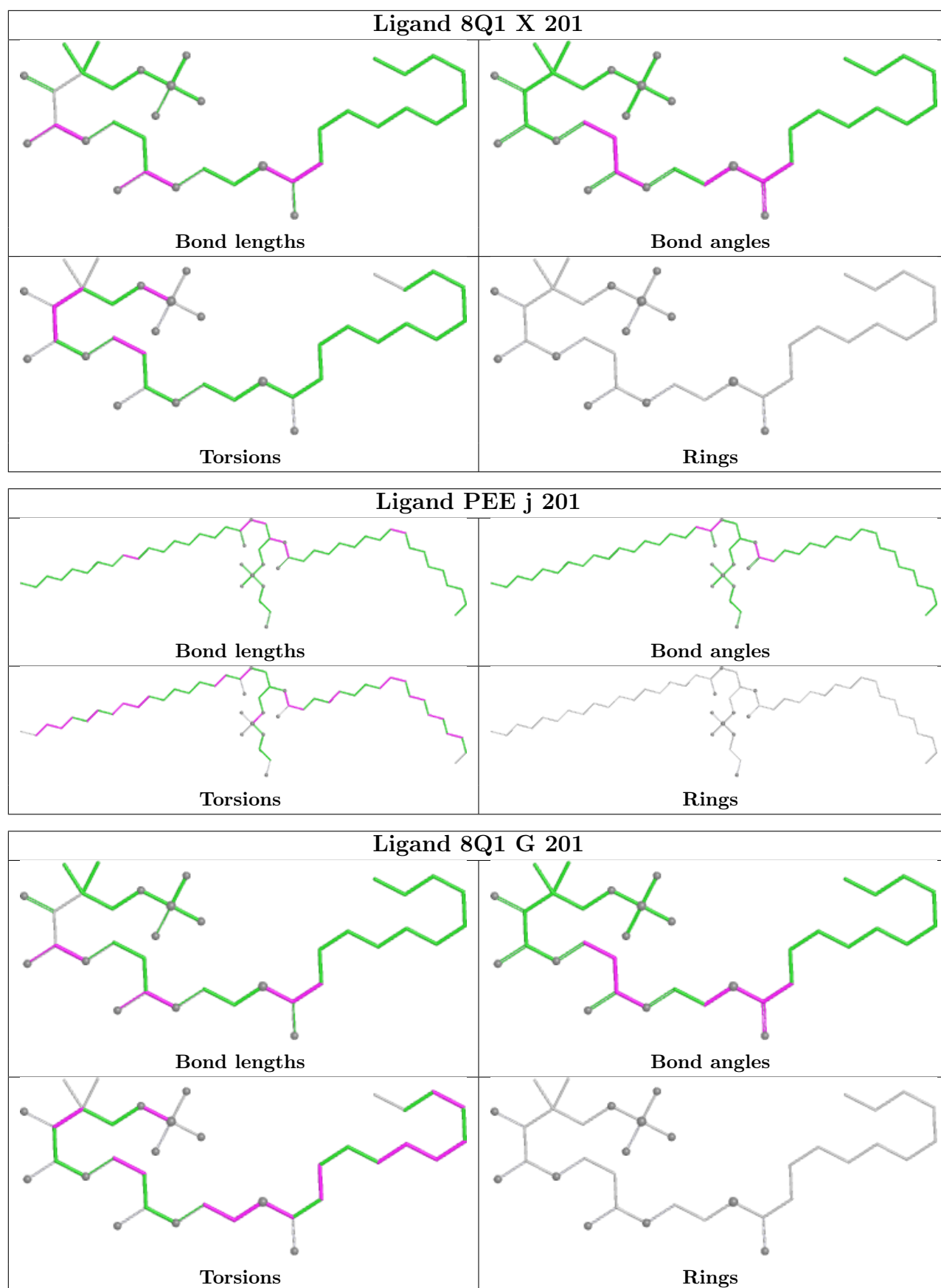


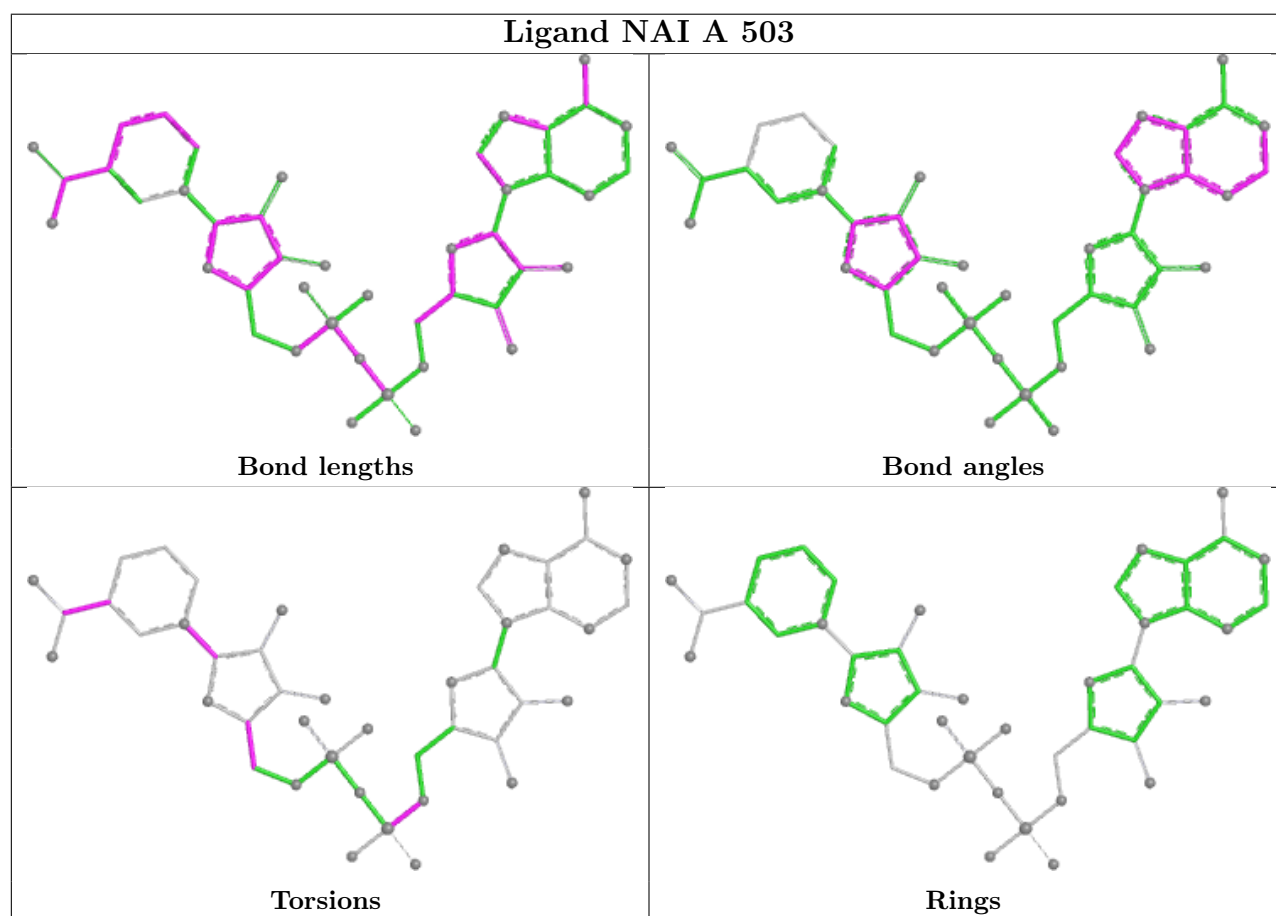
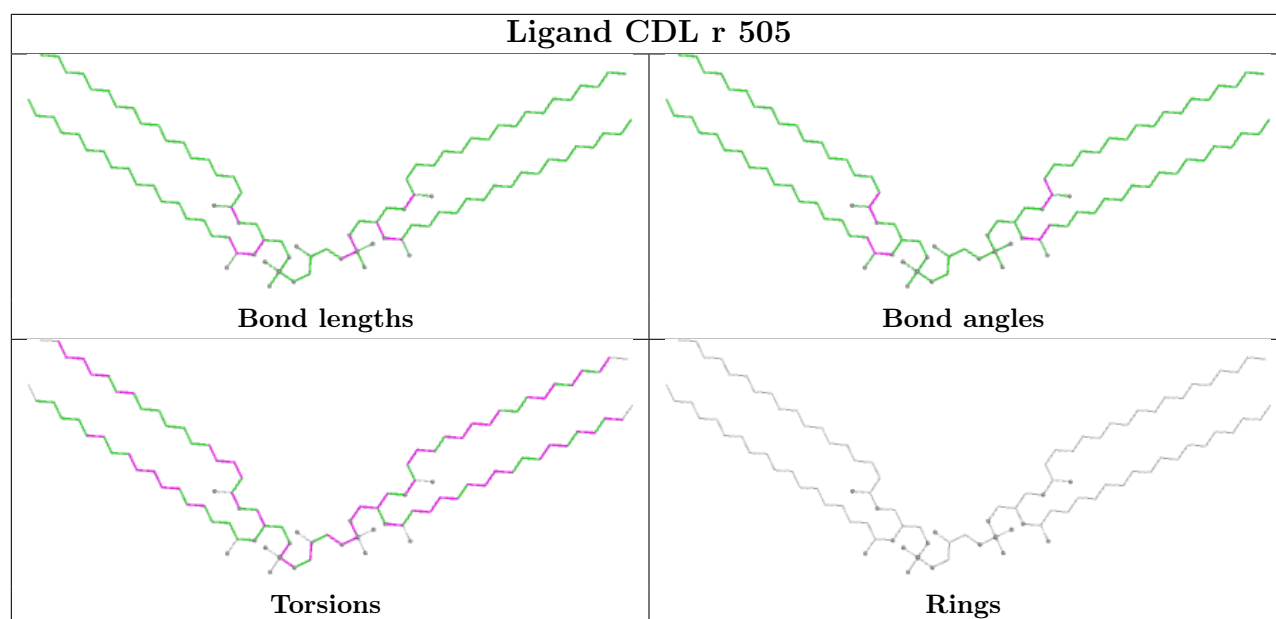


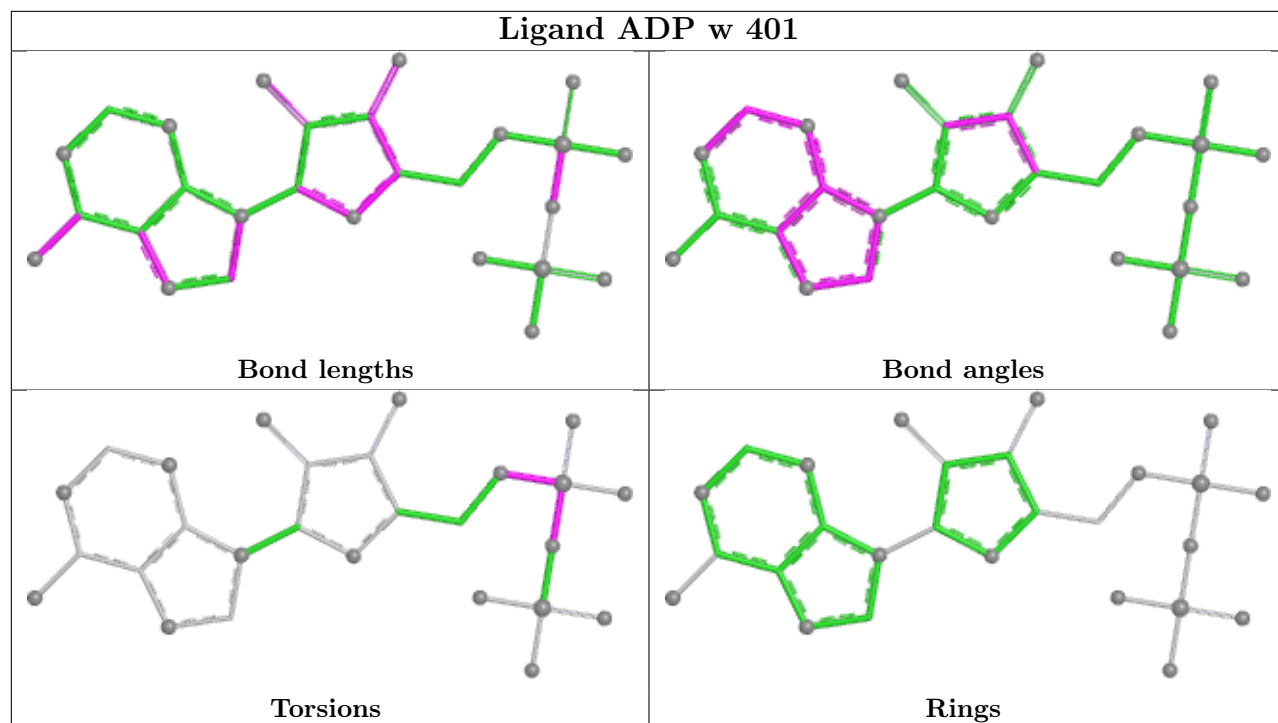


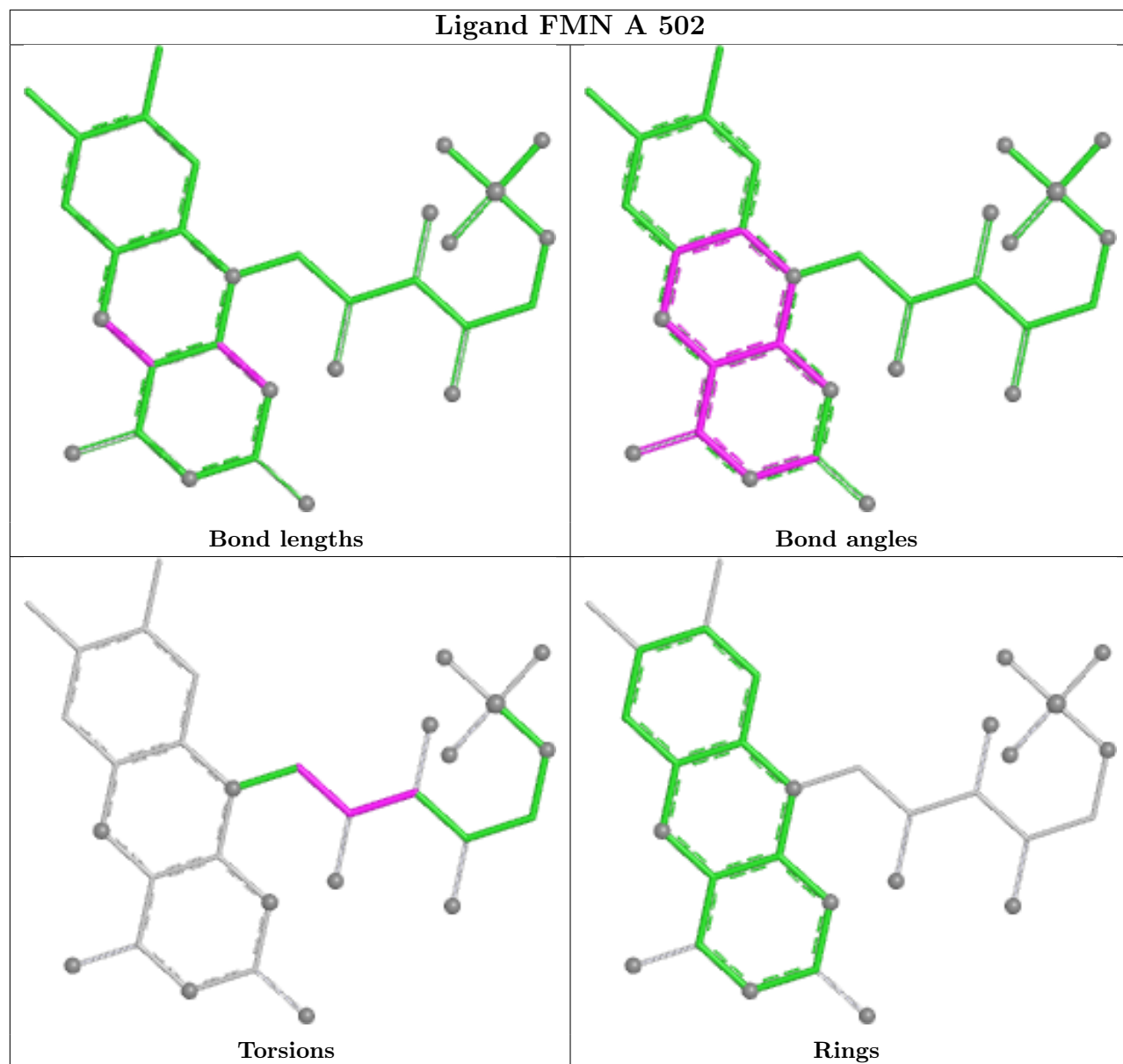


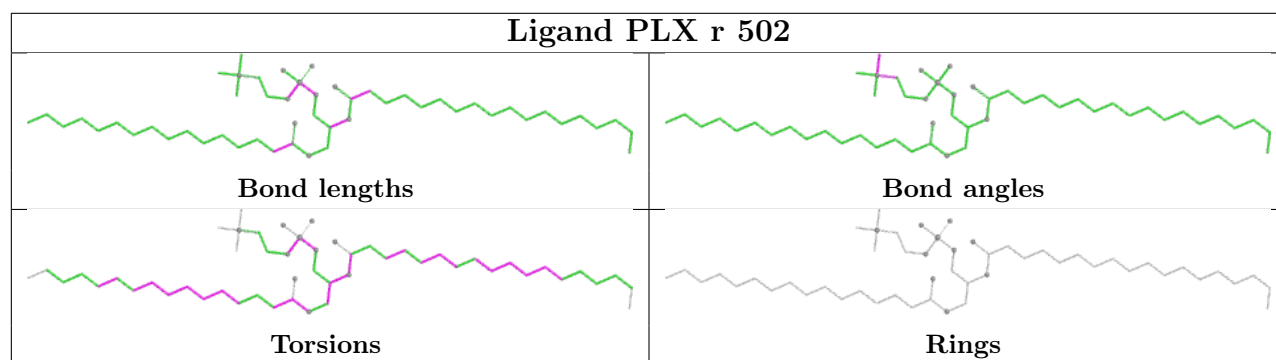
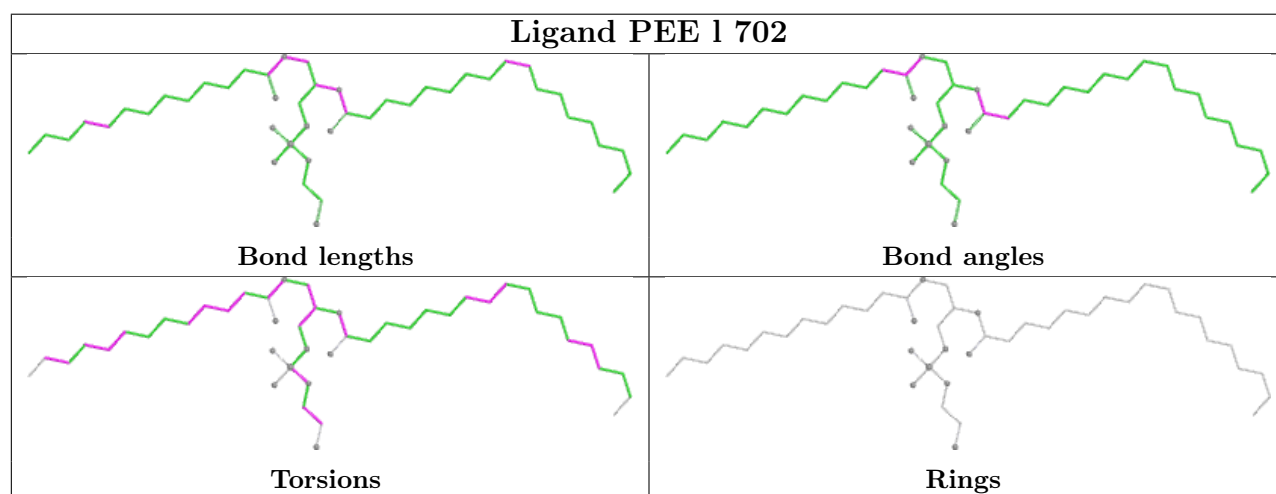
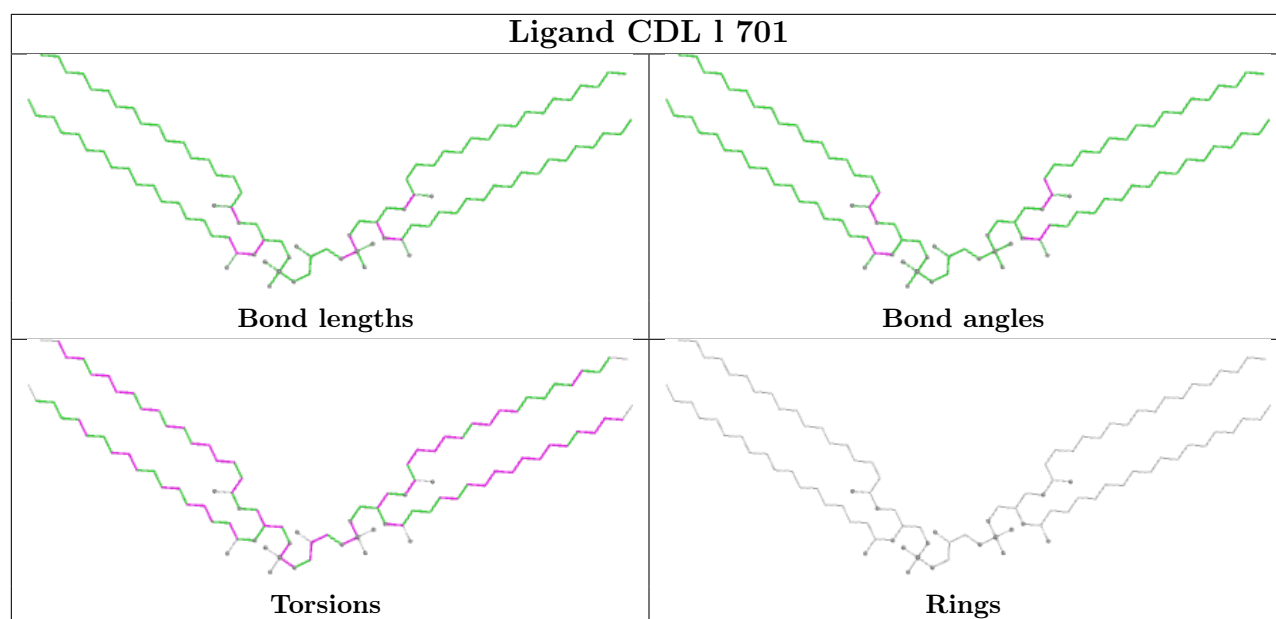


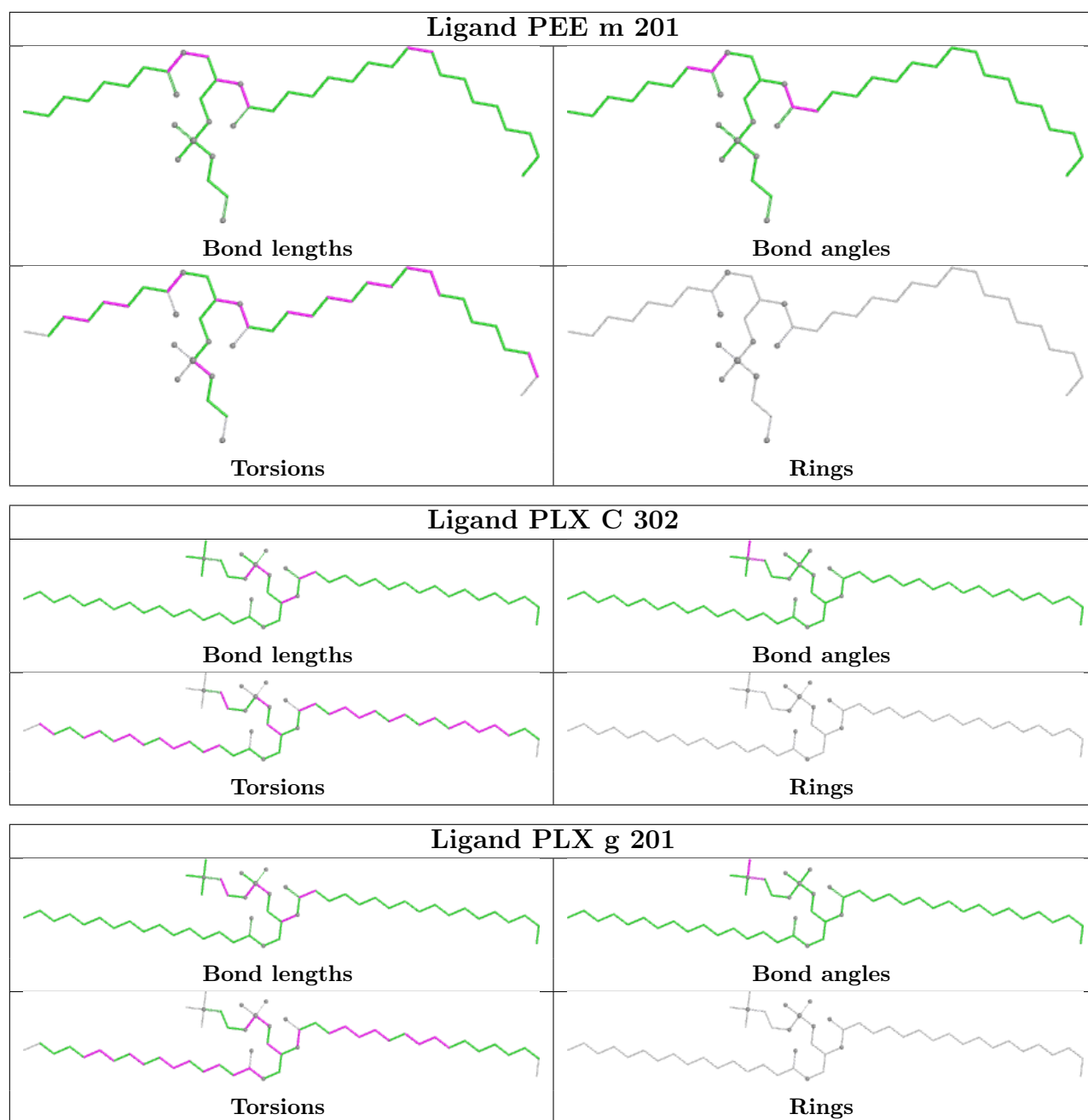












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

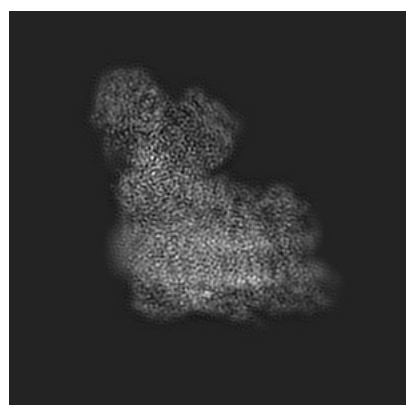
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32271. These allow visual inspection of the internal detail of the map and identification of artifacts.

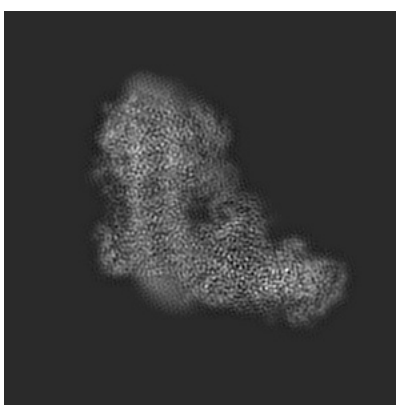
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

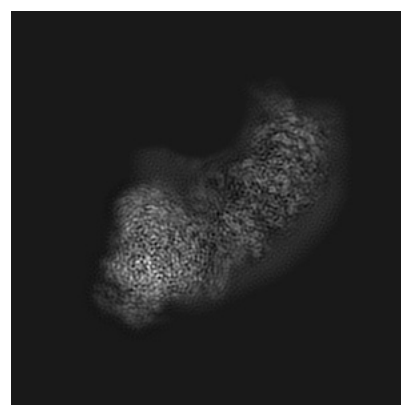
6.1.1 Primary map



X



Y

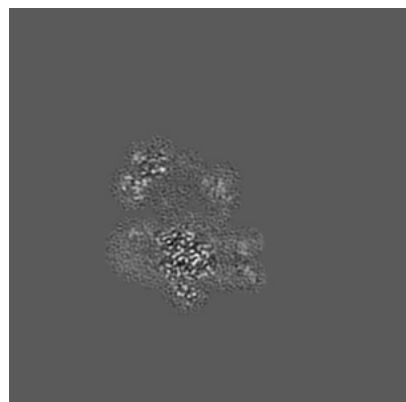


Z

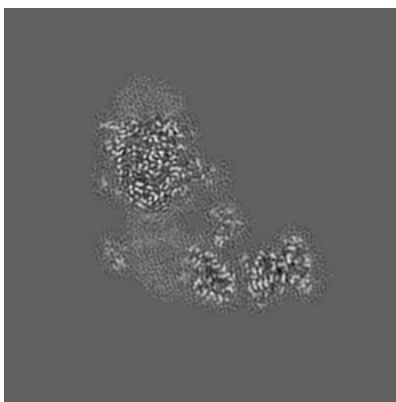
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

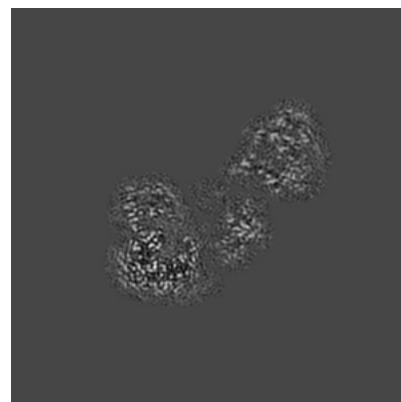
6.2.1 Primary map



X Index: 155



Y Index: 155

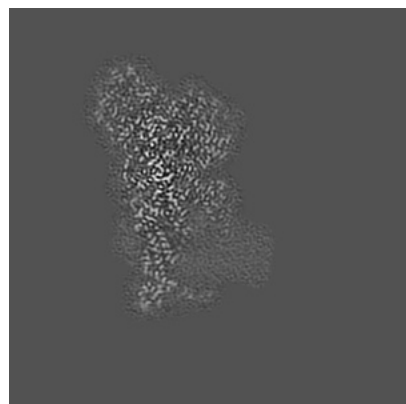


Z Index: 155

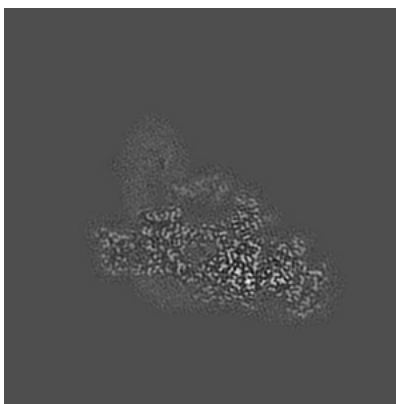
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

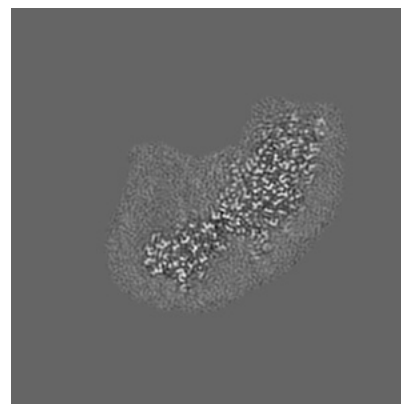
6.3.1 Primary map



X Index: 107



Y Index: 115

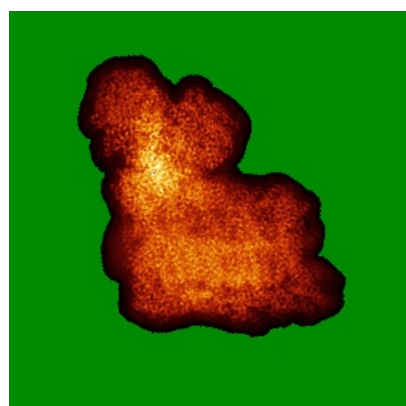


Z Index: 126

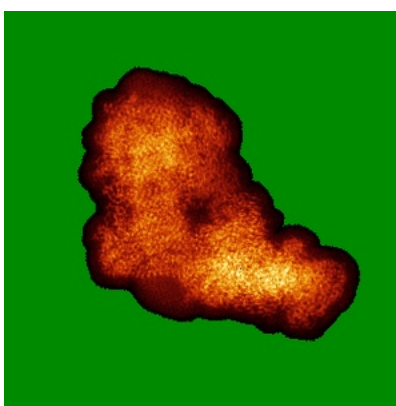
The images above show the largest variance slices of the map in three orthogonal directions.

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

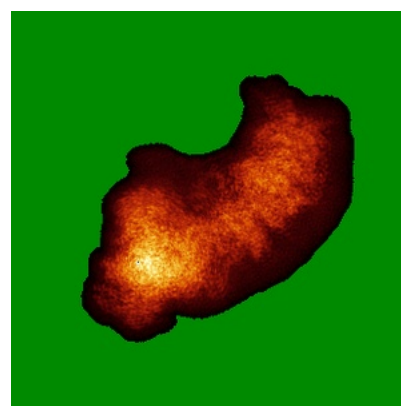
6.4.1 Primary map



X



Y

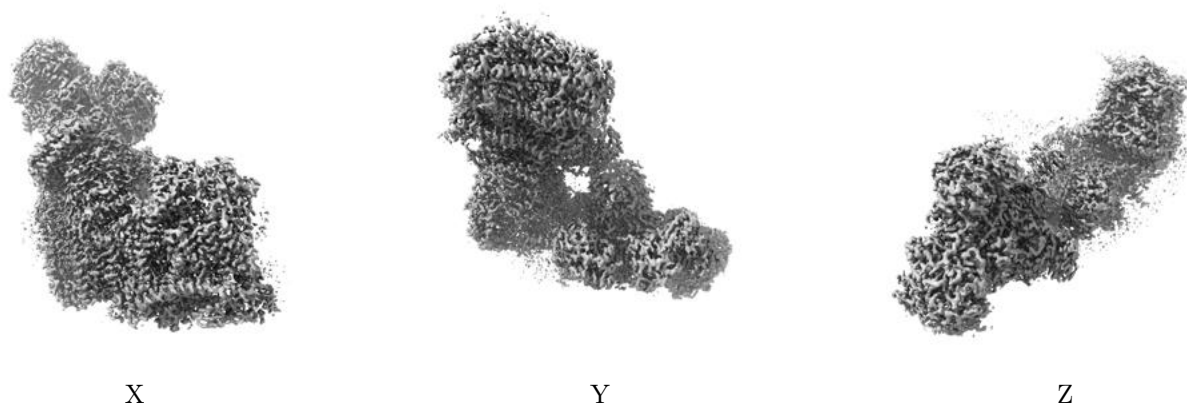


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

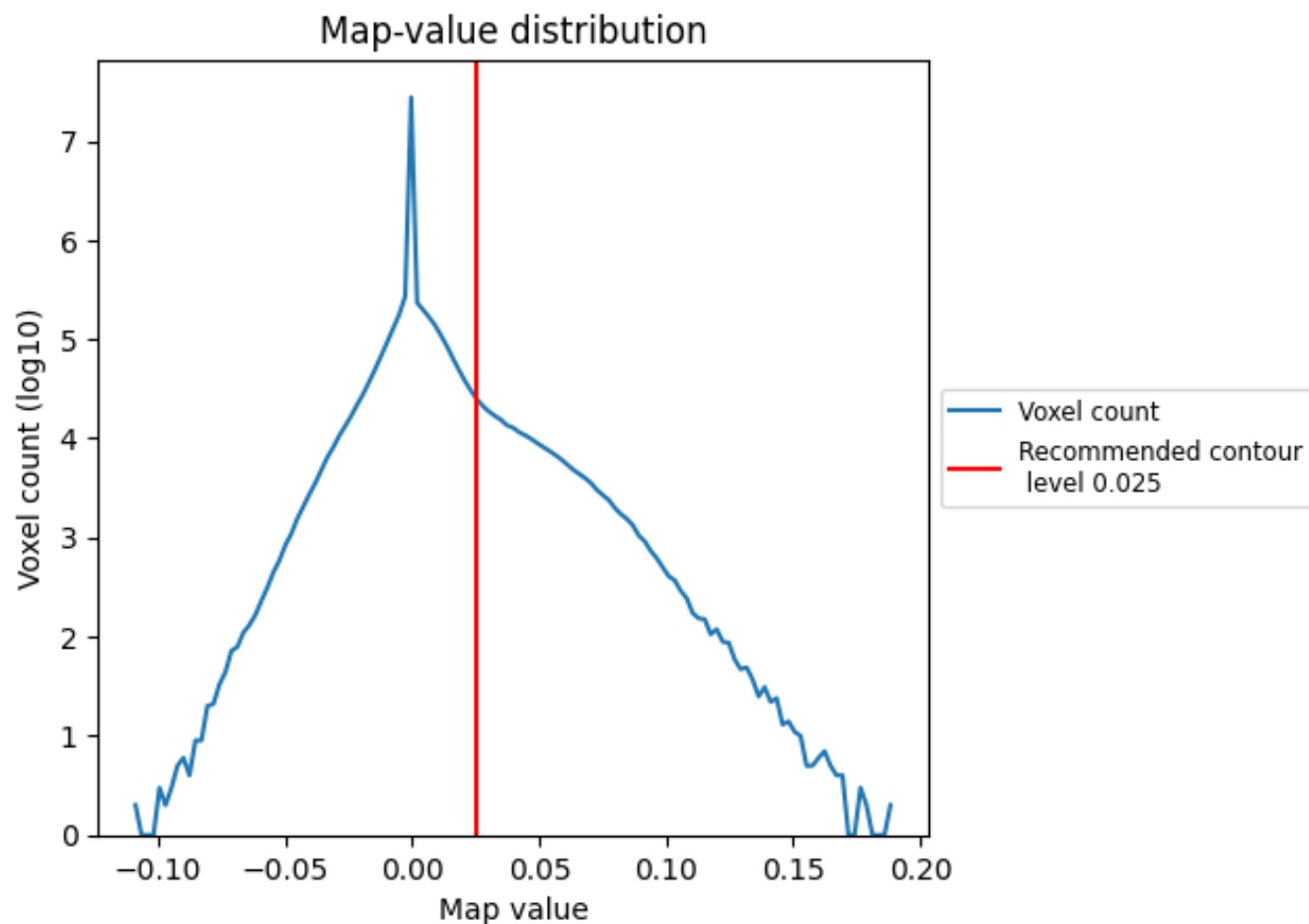
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

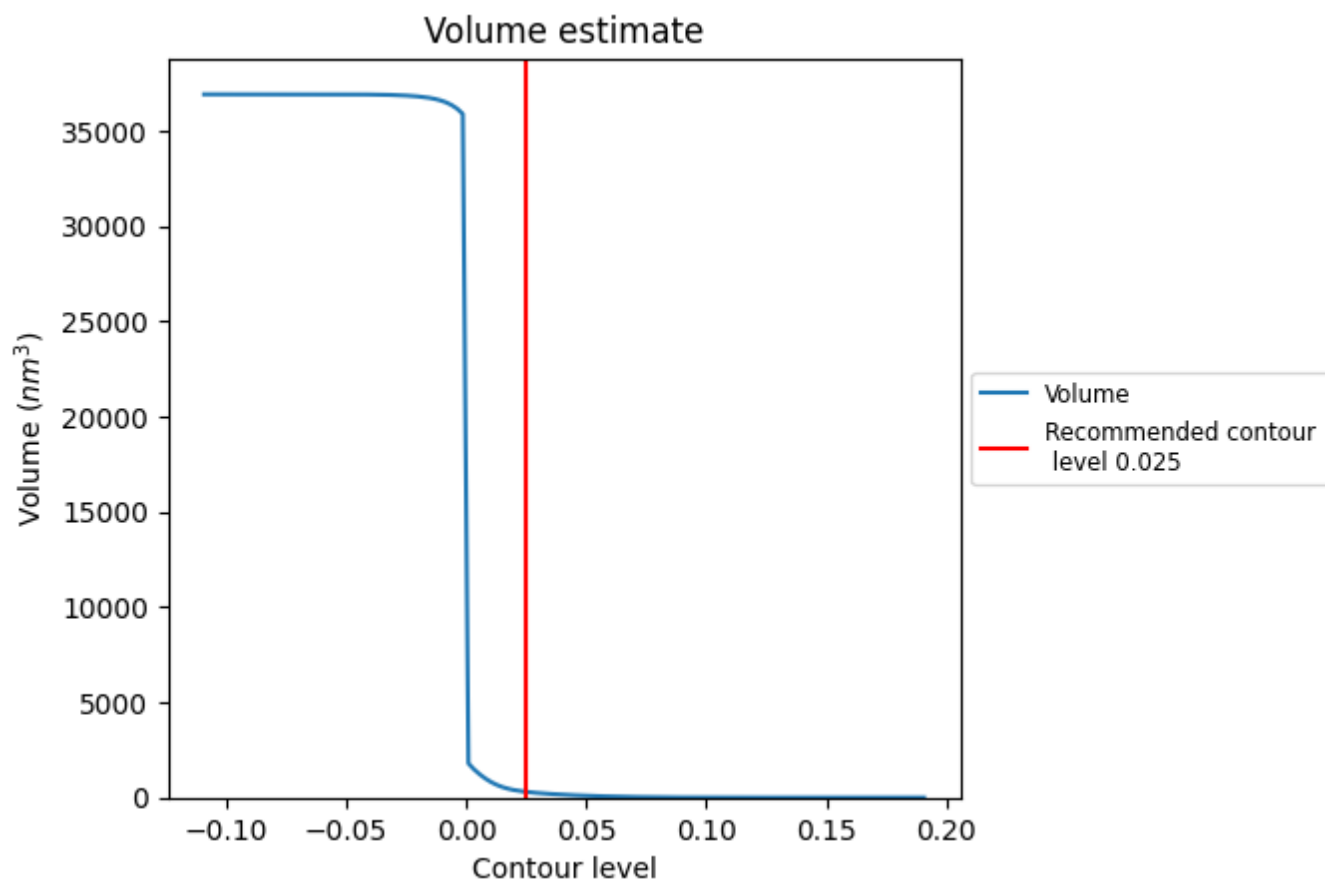
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

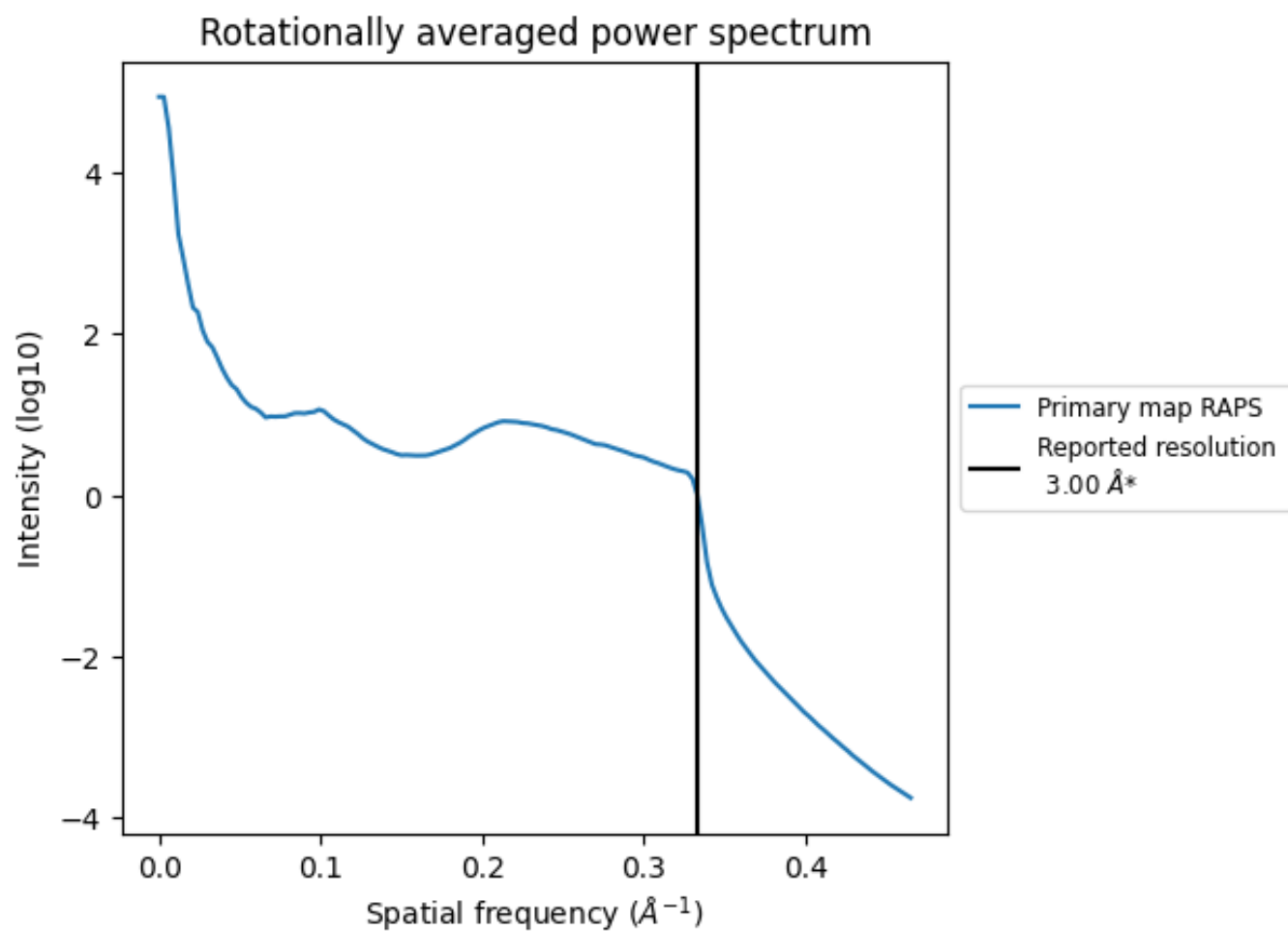
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 301 nm³; this corresponds to an approximate mass of 272 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

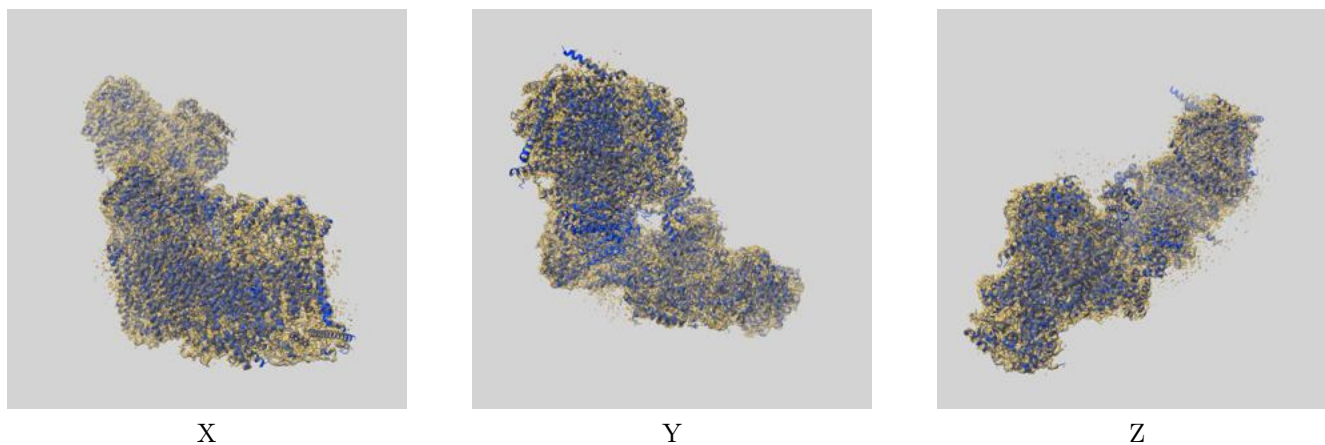
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

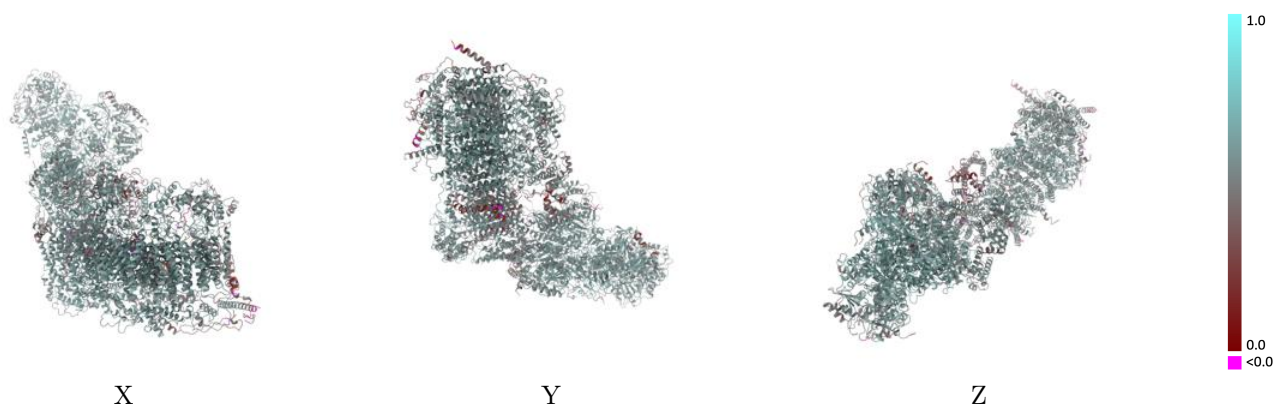
This section contains information regarding the fit between EMDB map EMD-32271 and PDB model 7W35. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



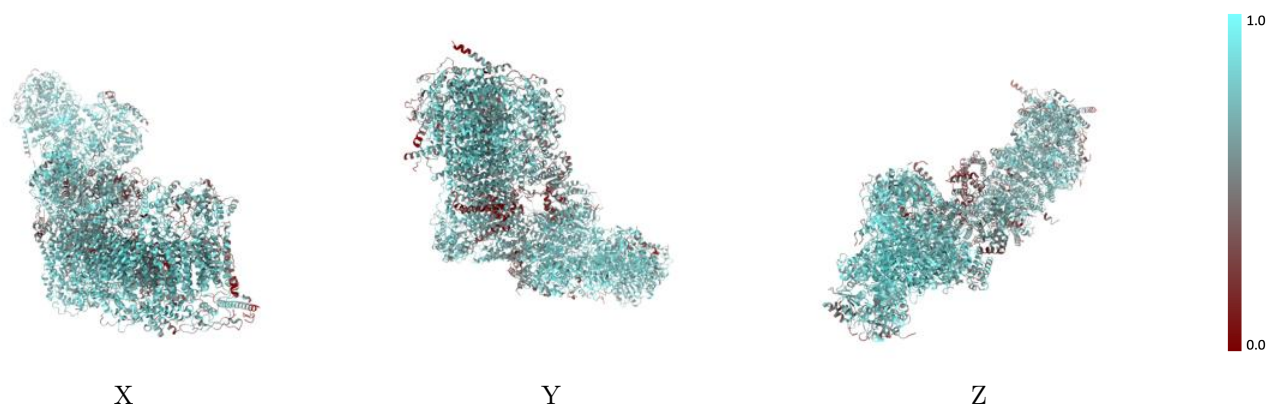
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



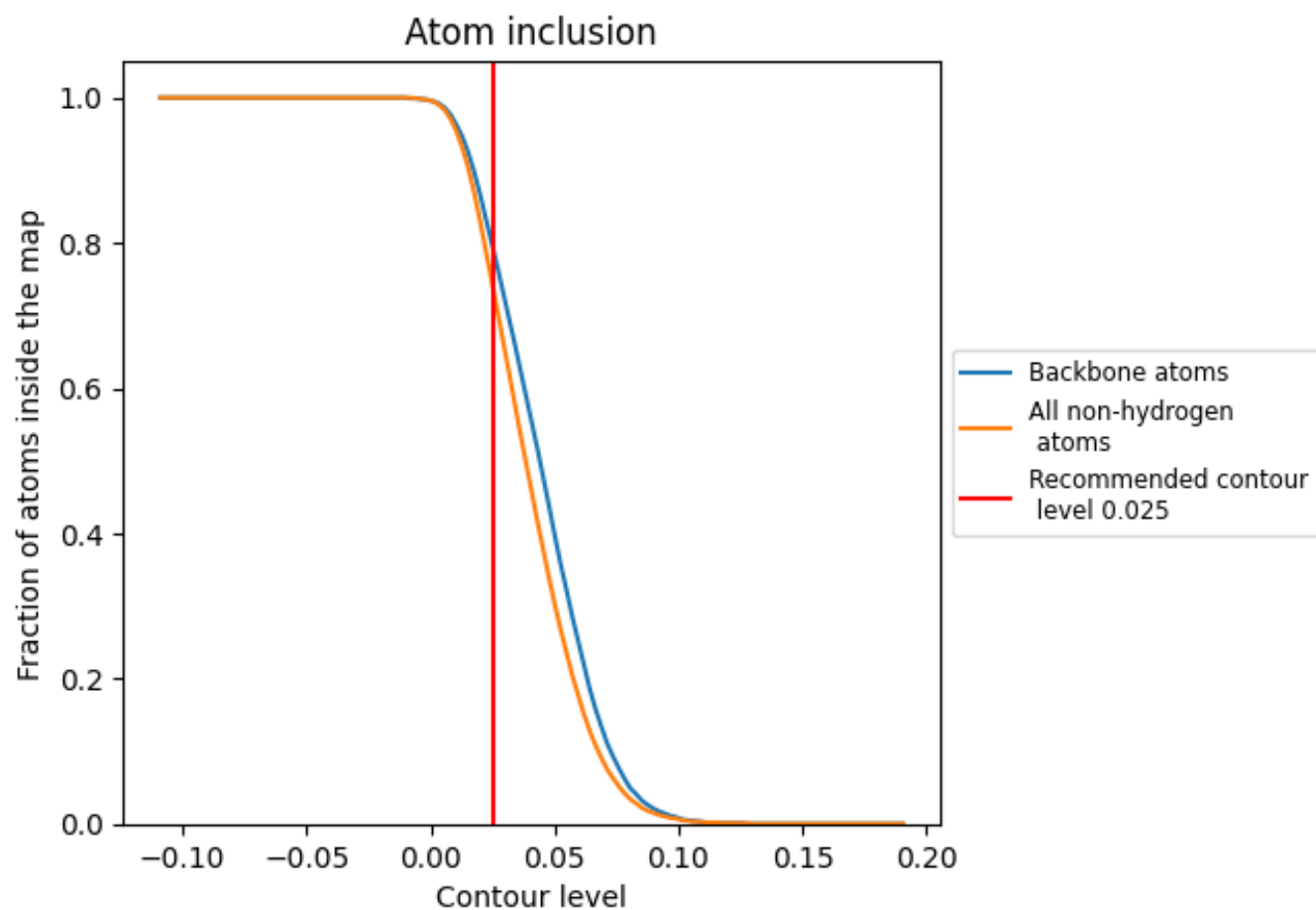
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.5590
A	 0.7610	 0.5630
B	 0.8920	 0.6160
C	 0.8610	 0.6070
E	 0.7410	 0.5610
F	 0.6560	 0.5040
G	 0.3420	 0.3570
H	 0.6860	 0.5320
I	 0.6550	 0.5400
J	 0.7280	 0.5500
K	 0.6540	 0.5420
L	 0.8380	 0.5940
M	 0.8370	 0.5910
N	 0.6750	 0.5580
O	 0.7010	 0.5470
P	 0.8850	 0.6100
Q	 0.8490	 0.6040
S	 0.8510	 0.5950
T	 0.7310	 0.5760
U	 0.7280	 0.5440
V	 0.3540	 0.3940
W	 0.7870	 0.5730
X	 0.6130	 0.5080
Y	 0.5570	 0.4510
Z	 0.4980	 0.4390
a	 0.7720	 0.5730
b	 0.5890	 0.4880
c	 0.7400	 0.5570
d	 0.7230	 0.5490
e	 0.6790	 0.5370
f	 0.6500	 0.5160
g	 0.7990	 0.5800
h	 0.7770	 0.5740
i	 0.8230	 0.5970
j	 0.6420	 0.5190



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Chain	Atom inclusion	Q-score
k	 0.5970	 0.5060
l	 0.7550	 0.5660
m	 0.6160	 0.5270
n	 0.6470	 0.5170
o	 0.7100	 0.5550
p	 0.7200	 0.5520
r	 0.8140	 0.5920
s	 0.8140	 0.5810
u	 0.7750	 0.5730
v	 0.6100	 0.4830
w	 0.6170	 0.5310