



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 12:45 AM UTC

PDB ID : 7W4D / pdb_00007w4d
EMDB ID : EMD-32301
Title : Active state CI from Q1-NADH dataset, Subclass 2
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-27
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

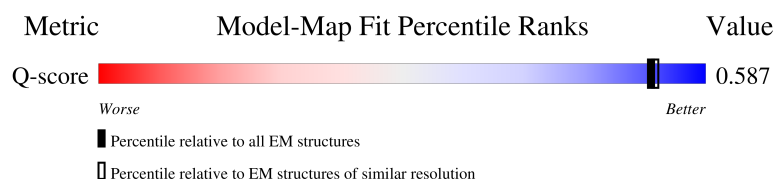
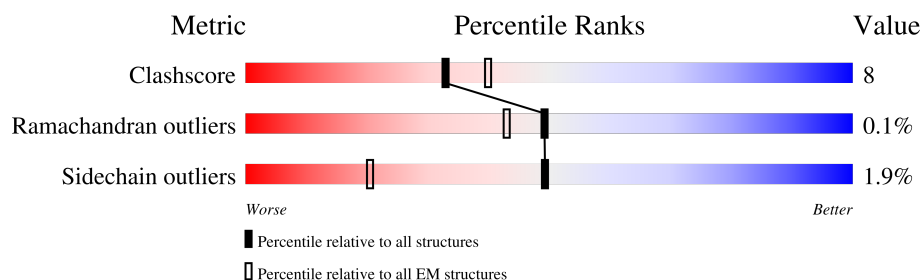
1 Overall quality at a glance

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	 77% 23%
2	B	176	 89% 11%
3	C	156	 82% 17%
4	E	115	 6% 76% 24%

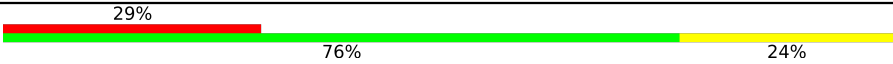
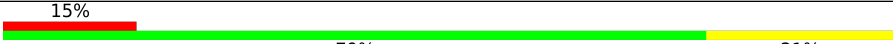
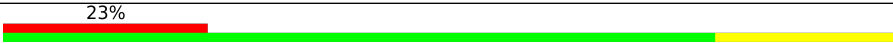
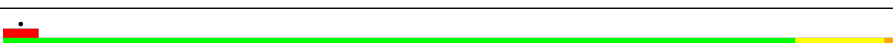
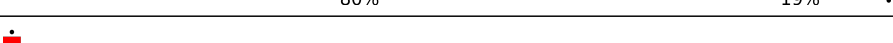
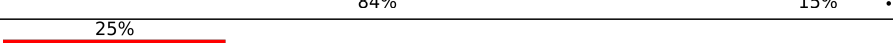
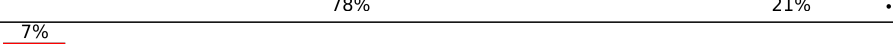
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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	C	301	-	-	X	-
50	CDL	l	702	-	-	X	-
55	UQ1	Q	501	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 68181 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	433	Total	C	N	O	S	0	0
			3330	2103	593	614	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
			968	618	179	166	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
			683	430	129	122	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
			703	453	104	141	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	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	43	Total	C	N	O	S	0	0
			366	228	68	69	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
			1671	1065	281	315	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	430	Total	C	N	O	S	0	0
			3459	2212	594	629	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
			566	364	103	94	5		

- 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
			1021	651	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	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	80	Total	C	N	O	S	0	0
			641	418	108	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	98	Total	C	N	O	S	0	0
			819	537	144	137	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	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	49	Total	C	N	O	0	0
			378	246	65	67		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	122	Total	C	N	O	S	0	0
			1005	653	174	172	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	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- 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	606	Total	C	N	O	S	0	0
			4816	3193	746	826	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	175	Total	C	N	O	S	0	0
			1292	863	188	228	13		

- 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
			1534	982	279	265	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	318	Total	C	N	O	S	0	0
			2508	1678	385	424	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
			1395	886	250	249	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
			1028	642	195	182	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.

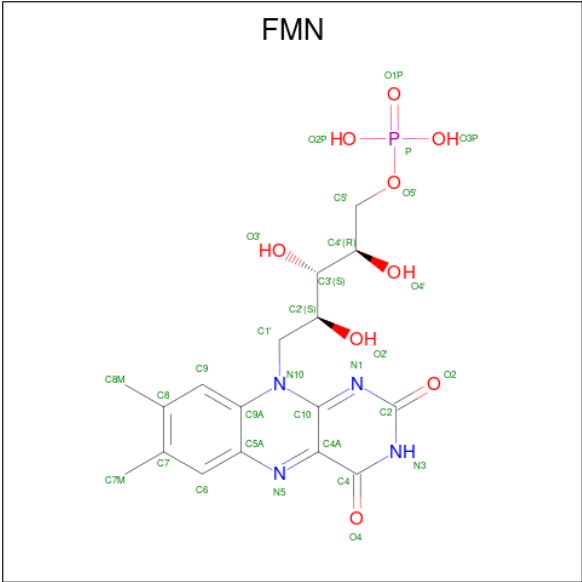
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

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



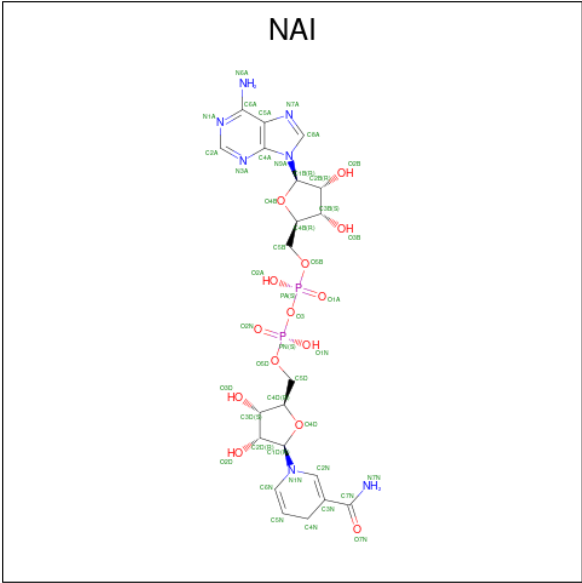
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- 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	

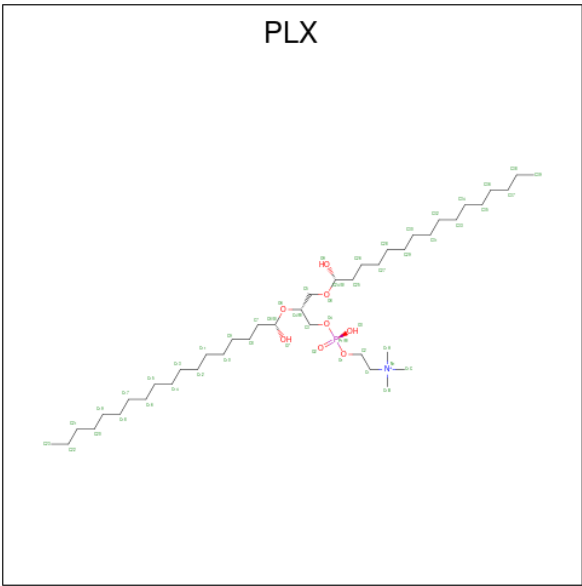
- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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

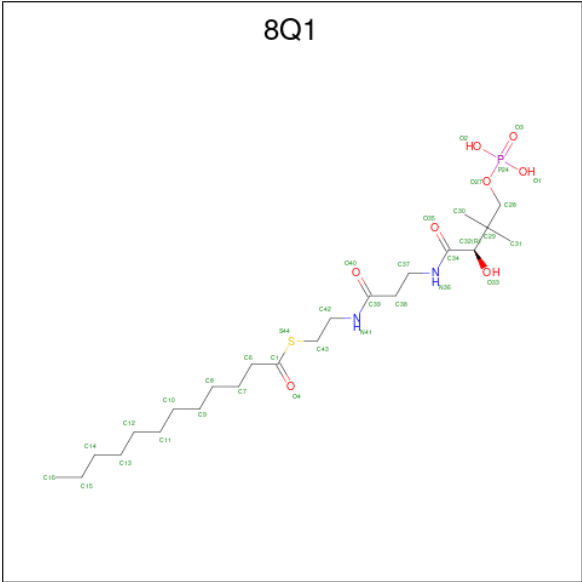
- Molecule 48 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,

11-TRIOL (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P).



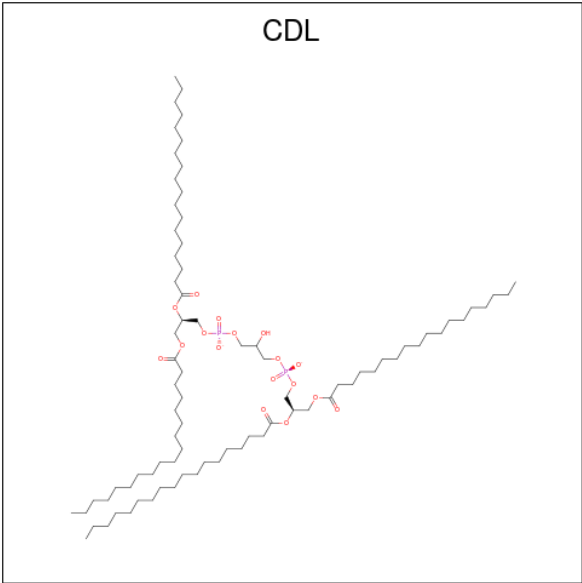
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42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

- Molecule 49 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
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 50 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



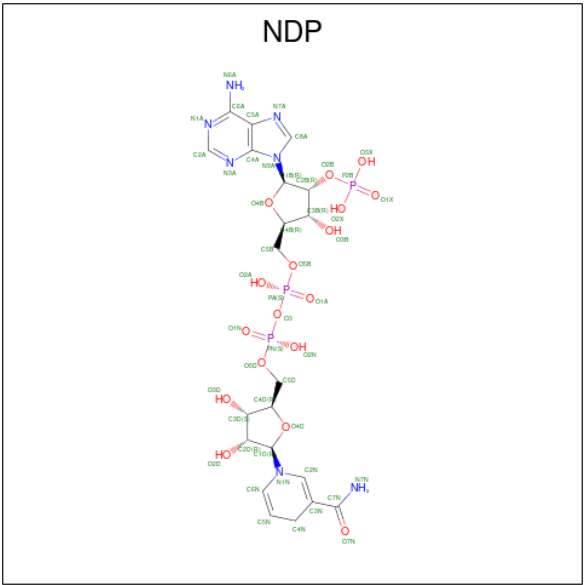
Mol	Chain	Residues	Atoms				AltConf
50	I	1	Total	C	O	P	0
			51	32	17	2	
50	V	1	Total	C	O	P	0
			94	75	17	2	

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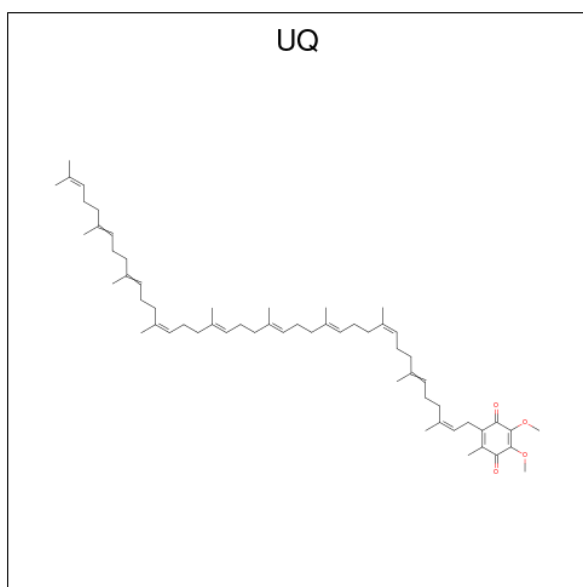
Mol	Chain	Residues	Atoms				AltConf
50	V	1	Total	C	O	P	0
			100	81	17	2	
50	b	1	Total	C	O	P	0
			100	81	17	2	
50	k	1	Total	C	O	P	0
			94	75	17	2	
50	l	1	Total	C	O	P	0
			99	80	17	2	
50	l	1	Total	C	O	P	0
			100	81	17	2	
50	n	1	Total	C	O	P	0
			55	36	17	2	
50	r	1	Total	C	O	P	0
			100	81	17	2	
50	s	1	Total	C	O	P	0
			89	70	17	2	

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



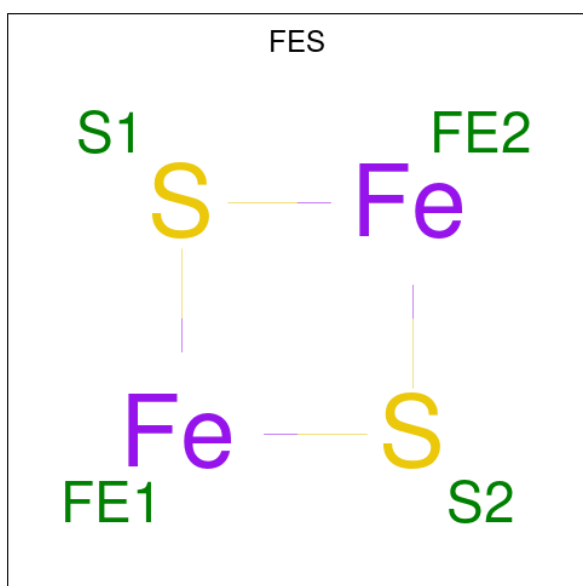
Mol	Chain	Residues	Atoms					AltConf
51	J	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 52 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄).



Mol	Chain	Residues	Atoms			AltConf
52	J	1	Total	C	O	0
			33	29	4	
52	s	1	Total	C	O	0
			38	34	4	

- Molecule 53 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

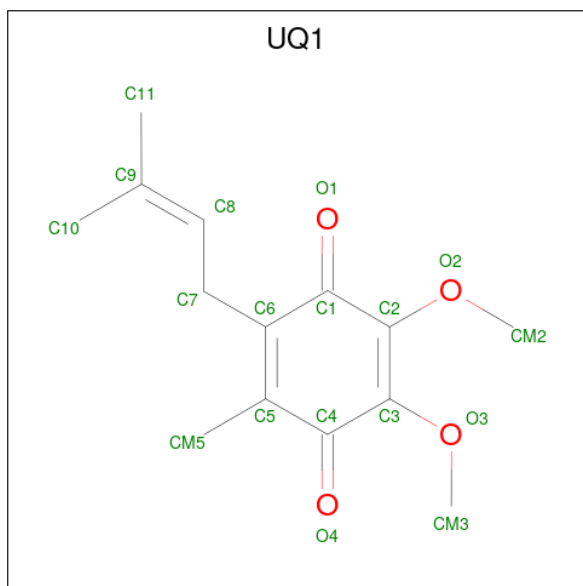


Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	Fe	S	0
			4	2	2	
53	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 55 is UBIQUINONE-1 (CCD ID: UQ1) (formula: C₁₄H₁₈O₄).

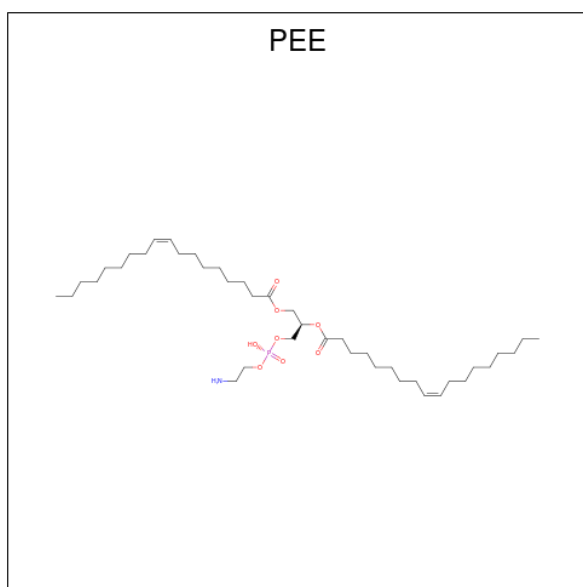


Mol	Chain	Residues	Atoms			AltConf
55	Q	1	Total	C	O	0
			18	14	4	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

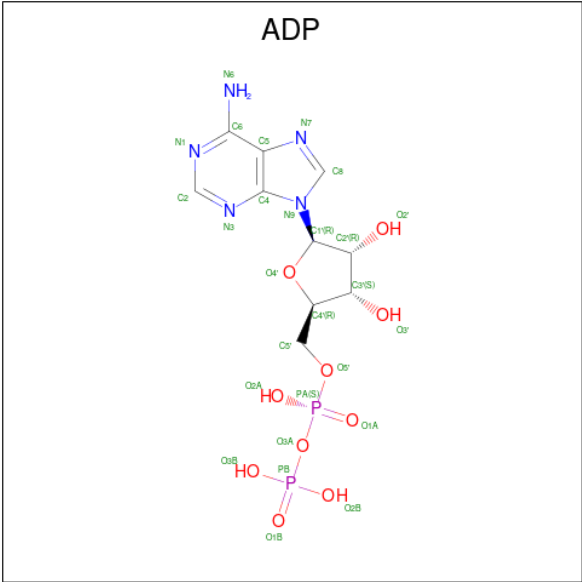
Mol	Chain	Residues	Atoms		AltConf
56	T	1	Total	Zn	0
			1	1	

- Molecule 57 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
57	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
57	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
57	j	1	Total	C	N	O	P	0
			47	37	1	8	1	
57	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
57	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
57	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
57	l	1	Total	C	N	O	P	0
			51	41	1	8	1	
57	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
57	r	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 58 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

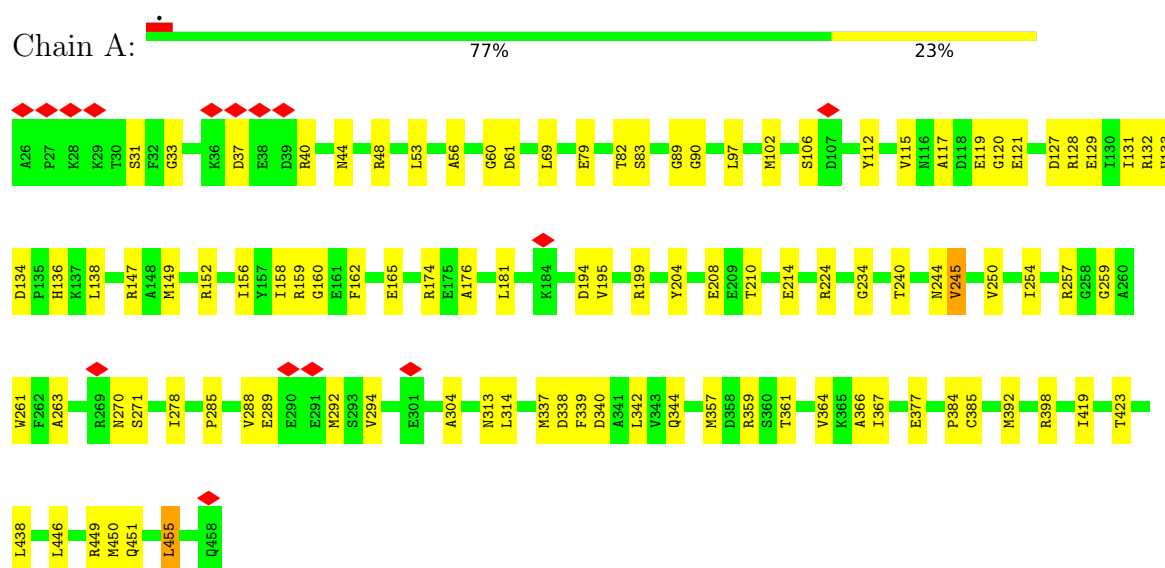


Mol	Chain	Residues	Atoms					AltConf
58	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

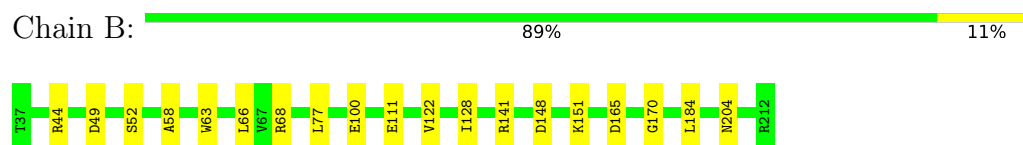
3 Residue-property plots

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.

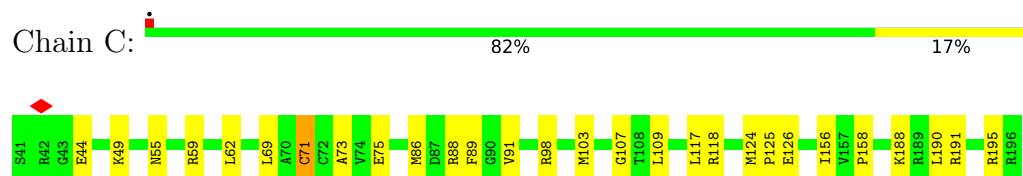
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



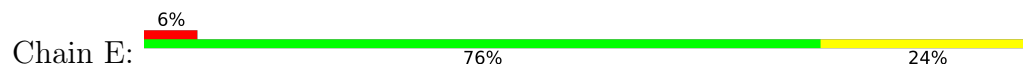
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



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

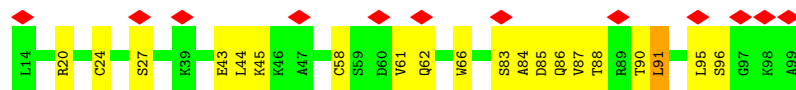
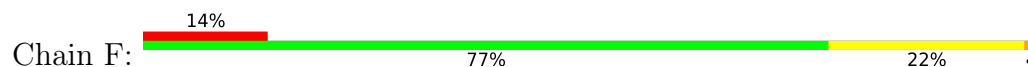


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

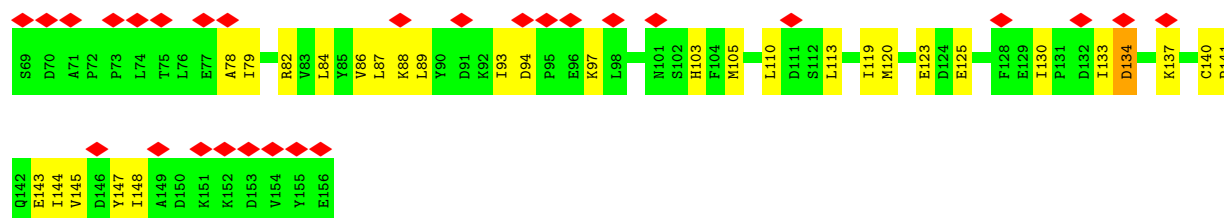




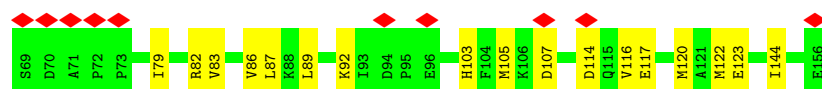
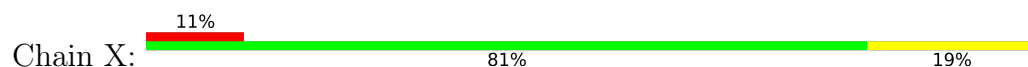
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



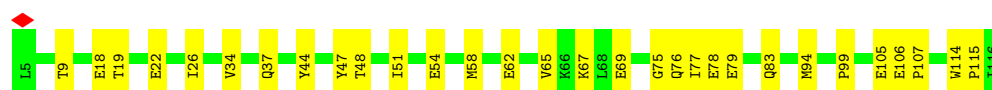
- Molecule 6: Acyl carrier protein



- Molecule 6: Acyl carrier protein



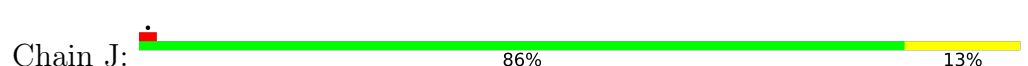
- Molecule 7: Complex I subunit B13

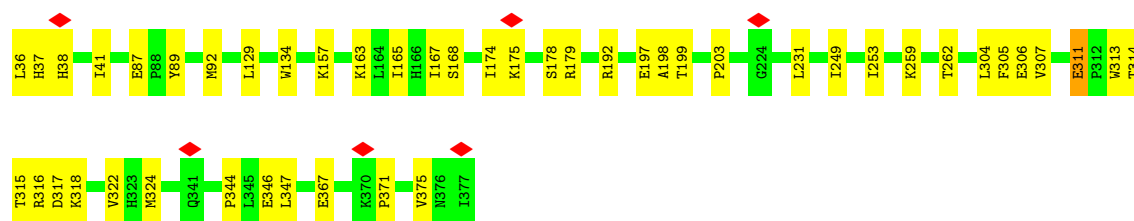


- Molecule 8: Complex I-B14.5a

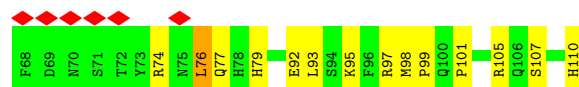


- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial

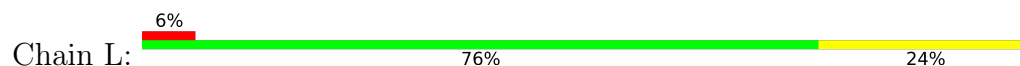




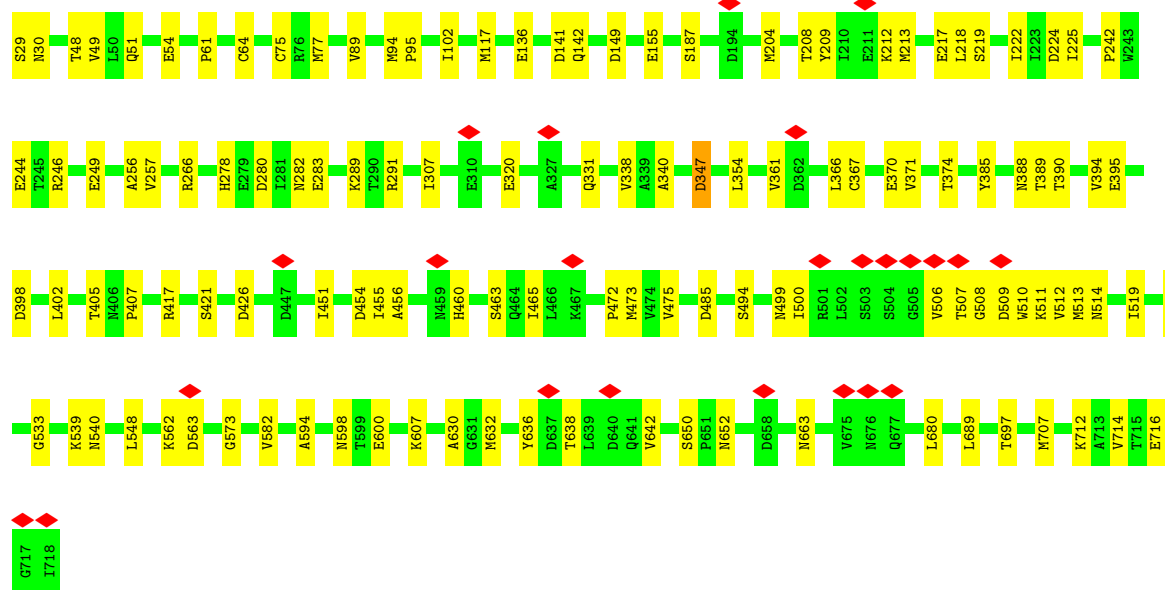
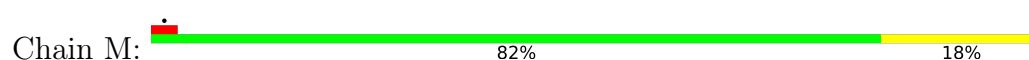
• Molecule 10: Complex I-9kD



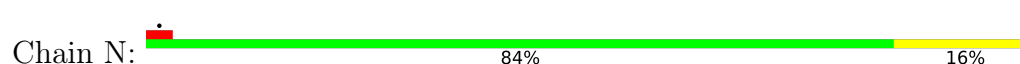
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

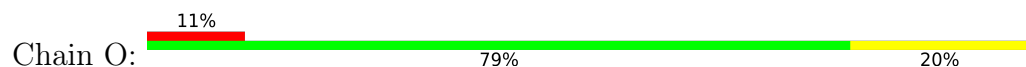


• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

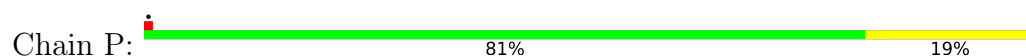




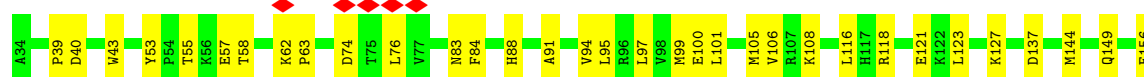
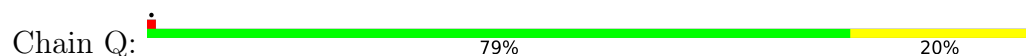
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: Complex I-30kD



- Molecule 16: Complex I-49kD



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



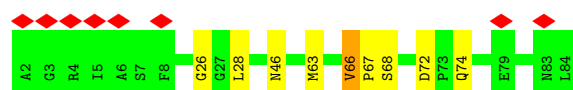
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain T:  86% 14%



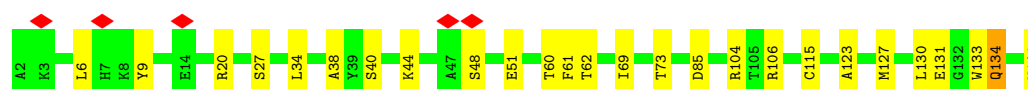
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U:  10% 89% 10%



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

Chain V:  81% 18%



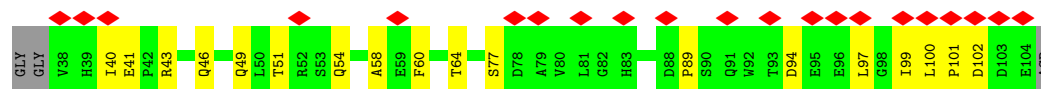
- Molecule 21: Complex I-B16.6

Chain W:  6% 78% 22%



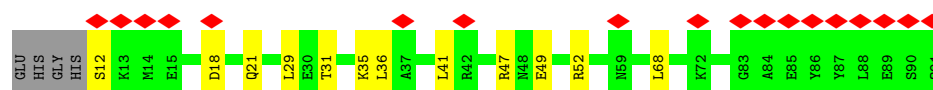
- Molecule 22: Complex I-AGGG

Chain Y:  30% 70% 26%



- Molecule 23: Complex I-B12

Chain Z:  21% 81% 14% 5%

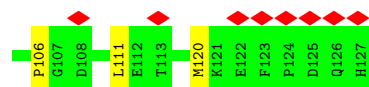
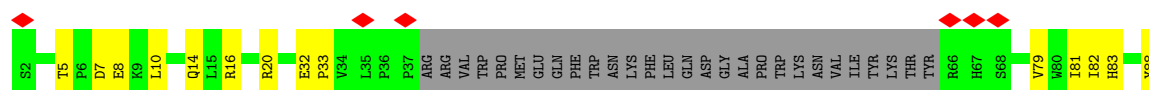


- Molecule 24: Complex I-SGDH

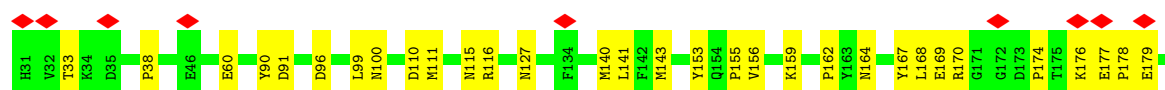
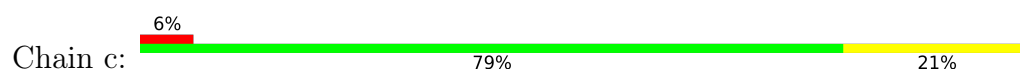
Chain a:  76% 23%



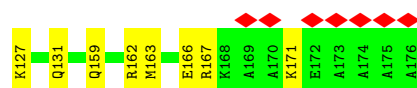
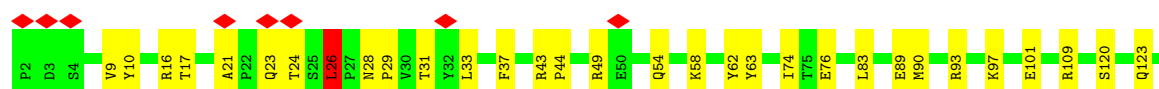
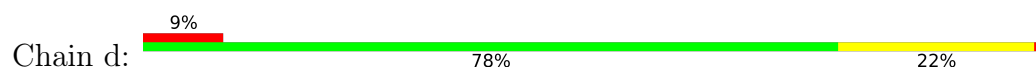
• Molecule 25: Complex I-B17



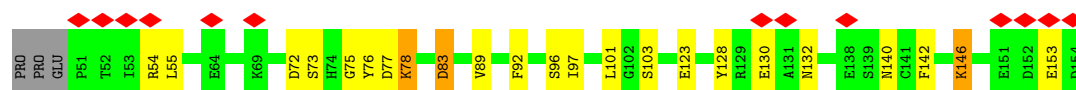
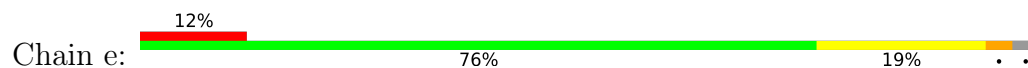
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



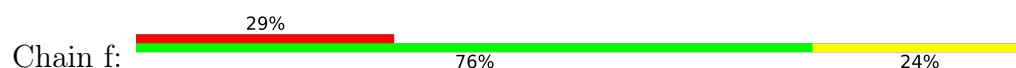
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

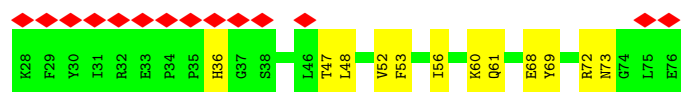


• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

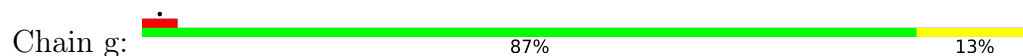


• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

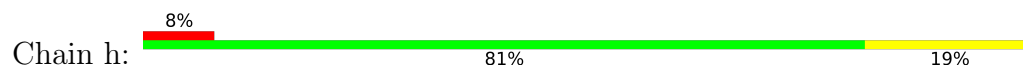




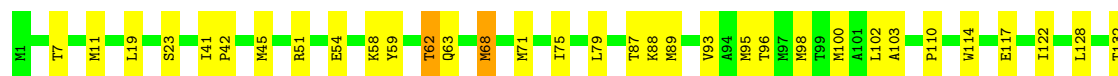
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



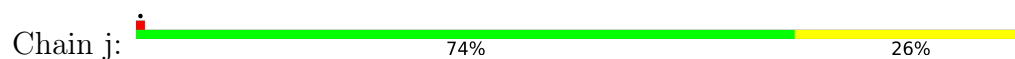
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



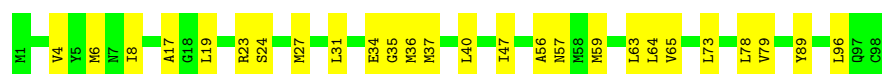
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



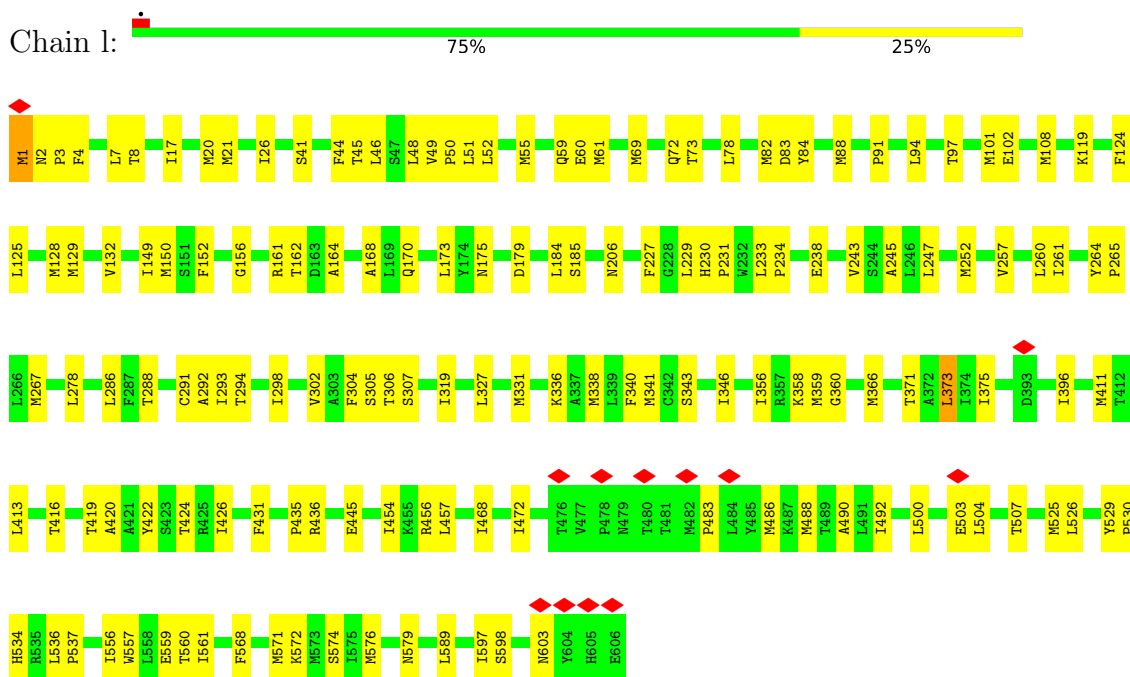
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3



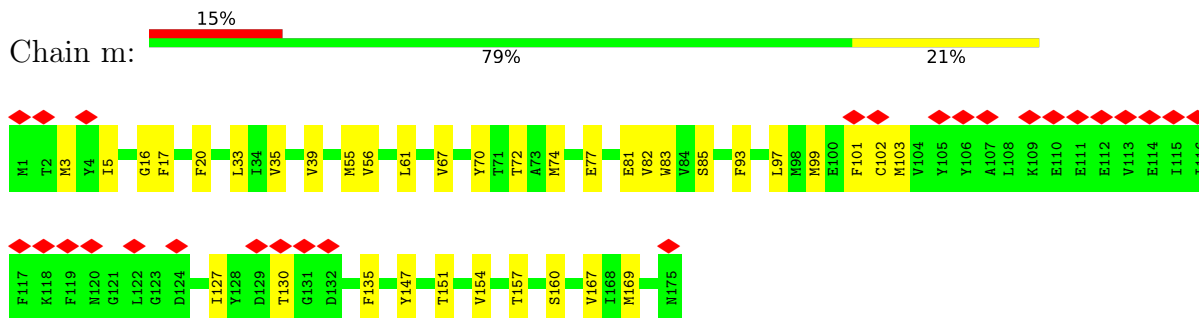
- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L



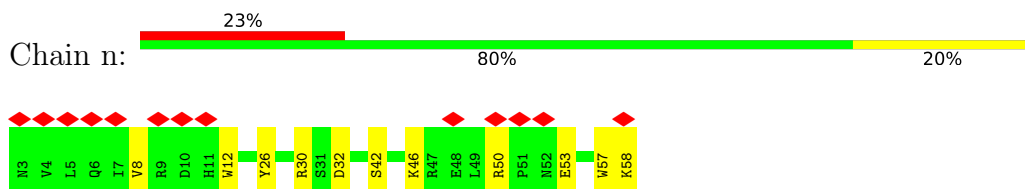
- Molecule 35: NADH-ubiquinone oxidoreductase chain 5



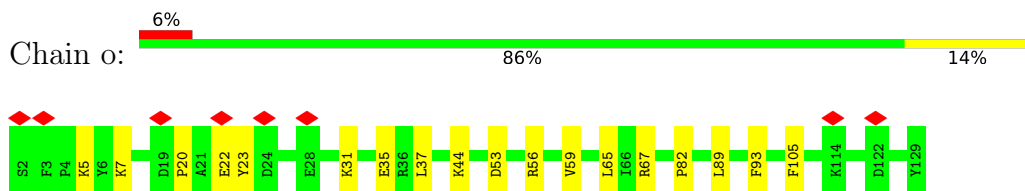
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



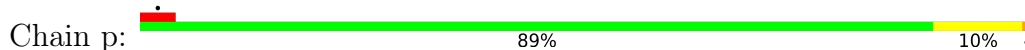
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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



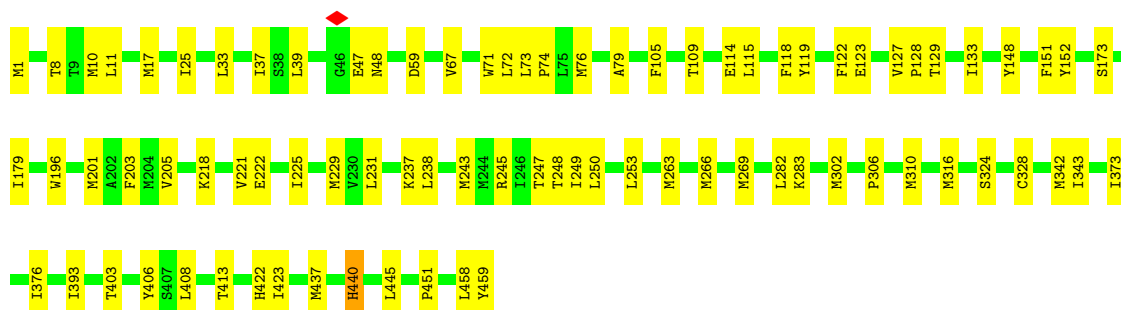
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9





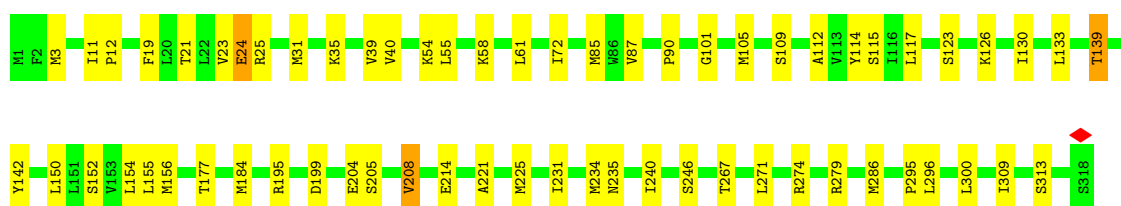
- Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 82% 18%



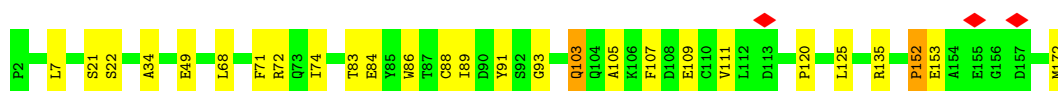
- Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain s: 80% 19%



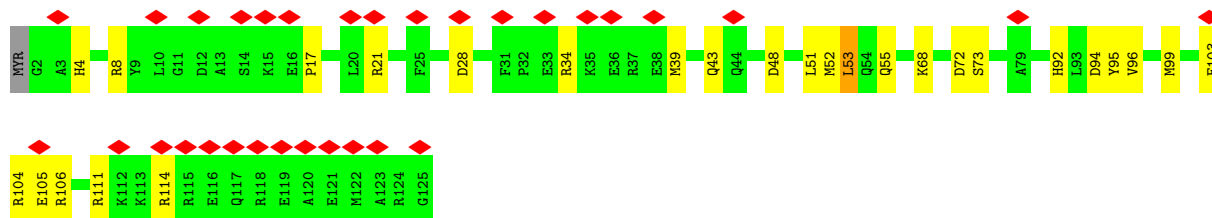
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 84% 15%

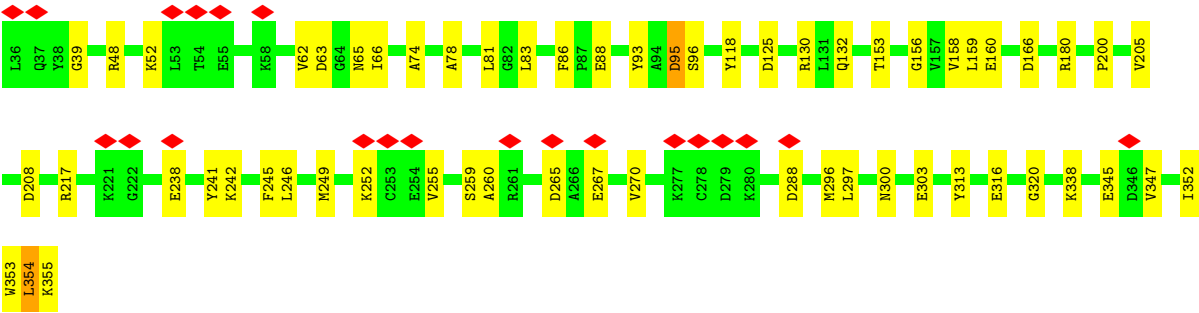
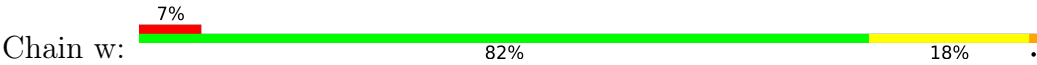


- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 25% 78% 21%



- 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	42194	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	0.202	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0314	Depositor
Map size (Å)	333.7616, 333.7616, 333.7616	wwPDB
Map dimensions	304, 304, 304	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UQ, ADP, ZN, CDL, 2MR, FMN, FES, NAI, NDP, PLX, MG, SF4, 8Q1, UQ1, PEE

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	0.15	0/3406	0.33	0/4603
2	B	0.14	0/1443	0.30	0/1952
3	C	0.15	0/1279	0.32	0/1730
4	E	0.23	0/992	0.49	1/1336 (0.1%)
5	F	0.21	0/694	0.47	0/935
6	G	0.17	0/705	0.40	0/956
6	X	0.15	0/715	0.31	0/967
7	H	0.16	0/929	0.38	0/1258
8	I	0.15	0/798	0.41	0/1079
9	J	0.14	0/2828	0.33	0/3834
10	K	0.14	0/377	0.34	0/509
11	L	0.17	0/1039	0.46	1/1403 (0.1%)
12	M	0.14	0/5384	0.37	0/7295
13	N	0.17	0/1245	0.37	1/1694 (0.1%)
14	O	0.20	0/1711	0.39	1/2328 (0.0%)
15	P	0.15	0/1789	0.34	0/2436
16	Q	0.18	0/3538	0.38	1/4796 (0.0%)
17	S	0.15	0/581	0.37	0/781
18	T	0.14	0/755	0.35	0/1018
19	U	0.12	0/664	0.28	0/912
20	V	0.13	0/1042	0.26	0/1411
21	W	0.20	0/1198	0.44	0/1617
22	Y	0.17	0/610	0.42	0/836
23	Z	0.12	0/660	0.32	0/892
24	a	0.17	0/1184	0.32	0/1603
25	b	0.15	0/844	0.37	0/1149
26	c	0.16	0/1371	0.39	0/1875
27	d	0.20	0/1494	0.50	4/2015 (0.2%)
28	e	0.17	0/891	0.37	0/1210
29	f	0.14	0/386	0.31	0/523
30	g	0.14	0/1036	0.32	0/1401
31	h	0.14	0/889	0.32	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.20	0/2773	0.39	0/3768
33	j	0.19	0/938	0.41	0/1281
34	k	0.19	0/759	0.34	0/1029
35	l	0.17	0/4947	0.38	0/6728
36	m	0.18	0/1325	0.39	0/1800
37	n	0.14	0/491	0.28	0/663
38	o	0.16	0/1092	0.32	0/1481
39	p	0.17	0/1590	0.43	2/2155 (0.1%)
40	r	0.18	0/3723	0.36	0/5078
41	s	0.20	0/2581	0.41	0/3529
42	u	0.16	0/1433	0.35	0/1934
43	v	0.16	0/1052	0.39	0/1411
44	w	0.15	0/2642	0.33	0/3580
All	All	0.17	0/67823	0.37	11/91981 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	73	LYS	N-CA-C	6.98	118.97	111.36
39	p	144	THR	CA-C-N	6.51	127.09	120.38
39	p	144	THR	C-N-CA	6.51	127.09	120.38
27	d	21	ALA	CA-C-N	-6.45	112.87	119.83
27	d	21	ALA	C-N-CA	-6.45	112.87	119.83
13	N	143	PRO	CA-N-CD	-6.17	103.37	112.00
16	Q	187	VAL	N-CA-C	5.59	115.79	110.53
4	E	110	THR	N-CA-C	5.37	117.22	111.36
14	O	213	ILE	O-C-N	5.32	127.16	121.10
27	d	26	LEU	CA-C-N	5.09	124.86	119.76
27	d	26	LEU	C-N-CA	5.09	124.86	119.76

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	3330	0	3292	72	0
2	B	1412	0	1363	16	0
3	C	1248	0	1254	22	0
4	E	968	0	973	21	0
5	F	683	0	696	23	0
6	G	693	0	671	25	0
6	X	703	0	693	12	0
7	H	910	0	950	20	0
8	I	780	0	808	17	0
9	J	2751	0	2773	29	0
10	K	366	0	338	16	0
11	L	1016	0	1016	22	0
12	M	5296	0	5326	71	0
13	N	1204	0	1162	17	0
14	O	1671	0	1673	32	0
15	P	1738	0	1693	26	0
16	Q	3459	0	3396	66	0
17	S	566	0	561	19	0
18	T	741	0	702	7	0
19	U	643	0	642	7	0
20	V	1021	0	1025	19	0
21	W	1167	0	1155	25	0
22	Y	584	0	529	13	0
23	Z	641	0	620	7	0
24	a	1151	0	1164	29	0
25	b	819	0	835	13	0
26	c	1315	0	1208	30	0
27	d	1461	0	1429	41	0
28	e	867	0	817	20	0
29	f	378	0	356	9	0
30	g	1005	0	999	15	0
31	h	867	0	871	14	0
32	i	2710	0	2874	76	0
33	j	914	0	951	32	0
34	k	748	0	799	26	0
35	l	4816	0	4955	105	0
36	m	1292	0	1261	32	0
37	n	479	0	486	13	0
38	o	1062	0	1072	18	0
39	p	1534	0	1470	14	0
40	r	3631	0	3839	58	0
41	s	2508	0	2607	50	0
42	u	1395	0	1372	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	v	1028	0	982	34	0
44	w	2582	0	2531	36	0
45	A	8	0	0	1	0
45	B	16	0	0	0	0
45	C	8	0	0	2	0
45	M	16	0	0	0	0
46	A	31	0	19	3	0
47	A	44	0	27	5	0
48	C	52	0	88	0	0
48	a	52	0	88	1	0
48	g	52	0	88	4	0
48	j	104	0	176	3	0
48	r	104	0	176	10	0
49	G	35	0	0	4	0
49	X	35	0	0	0	0
50	I	51	0	46	1	0
50	V	194	0	294	12	0
50	b	100	0	156	5	0
50	k	94	0	141	9	0
50	l	199	0	307	40	0
50	n	55	0	54	0	0
50	r	100	0	156	7	0
50	s	89	0	125	4	0
51	J	48	0	25	1	0
52	J	33	0	39	2	0
52	s	38	0	47	2	0
53	M	4	0	0	0	0
53	O	4	0	0	0	0
54	M	1	0	0	0	0
55	Q	18	0	18	10	0
56	T	1	0	0	0	0
57	W	41	0	59	1	0
57	i	47	0	71	2	0
57	j	139	0	212	10	0
57	l	137	0	205	10	0
57	r	51	0	82	4	0
58	w	27	0	11	1	0
All	All	68181	0	68899	1151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (1151) 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)
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.23
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.69	1.12
5:F:84:ALA:HA	5:F:87:VAL:CG2	1.87	1.05
50:l:702:CDL:CA6	50:l:702:CDL:H542	1.93	0.99
16:Q:185:MET:CE	55:Q:501:UQ1:HM32	1.94	0.97
50:l:702:CDL:H542	50:l:702:CDL:HA62	1.47	0.95
5:F:84:ALA:O	5:F:87:VAL:HG23	1.67	0.94
50:l:702:CDL:H811	50:l:702:CDL:H612	1.54	0.89
16:Q:185:MET:HE2	55:Q:501:UQ1:HM32	1.51	0.89
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.56	0.88
50:l:702:CDL:H221	50:l:702:CDL:C66	2.04	0.87
24:a:137:MET:HE1	37:n:42:SER:HB3	1.54	0.86
11:L:62:THR:HG23	11:L:72:ILE:HD13	1.57	0.86
17:S:52:ARG:HG2	17:S:52:ARG:HH11	1.39	0.86
7:H:94:MET:HE3	7:H:99:PRO:HG3	1.56	0.85
16:Q:185:MET:CE	55:Q:501:UQ1:HM23	2.05	0.85
50:l:702:CDL:C66	50:l:702:CDL:H622	2.07	0.84
8:I:40:LYS:HB3	21:W:7:LYS:H	1.41	0.83
5:F:83:SER:O	5:F:87:VAL:HG22	1.79	0.83
34:k:6:MET:HB3	36:m:103:MET:HE1	1.62	0.81
50:l:702:CDL:H452	40:r:445:LEU:HB3	1.63	0.81
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.63	0.81
16:Q:185:MET:HE1	55:Q:501:UQ1:HM23	1.64	0.80
32:i:68:MET:HE1	34:k:37:MET:HE2	1.64	0.80
5:F:95:LEU:HD23	5:F:95:LEU:O	1.82	0.79
7:H:18:GLU:HG2	7:H:19:THR:HG23	1.63	0.79
35:l:150:MET:HE3	35:l:150:MET:HA	1.65	0.79
27:d:26:LEU:HD12	27:d:26:LEU:H	1.46	0.79
50:l:702:CDL:C31	50:l:702:CDL:H742	2.13	0.79
17:S:12:MET:HE2	41:s:23:VAL:HG21	1.65	0.79
32:i:87:THR:HG22	32:i:88:LYS:H	1.46	0.79
44:w:267:GLU:N	44:w:267:GLU:OE2	2.15	0.79
1:A:451:GLN:HE22	1:A:455:LEU:CD2	1.95	0.78
7:H:34:VAL:HA	7:H:37:GLN:NE2	1.97	0.78
43:v:51:LEU:O	43:v:52:MET:HG2	1.84	0.78
27:d:167:ARG:HH21	28:e:153:GLU:HG3	1.48	0.78
43:v:92:HIS:O	43:v:96:VAL:HG23	1.83	0.77
5:F:84:ALA:CA	5:F:87:VAL:CG2	2.62	0.77
40:r:263:MET:HA	40:r:263:MET:HE3	1.66	0.77
16:Q:345:SER:HB2	21:W:19:ILE:HD12	1.67	0.76
5:F:91:LEU:HD13	5:F:91:LEU:O	1.83	0.76
7:H:106:GLU:HG3	7:H:107:PRO:HD2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:116:ARG:HG2	57:l:704:PEE:H49	1.68	0.76
5:F:84:ALA:HA	5:F:87:VAL:HG22	1.67	0.76
16:Q:185:MET:HE2	55:Q:501:UQ1:CM3	2.16	0.76
35:l:331:MET:HE1	35:l:468:ILE:HD12	1.68	0.75
16:Q:208:GLU:OE2	16:Q:221:ARG:NH2	2.20	0.75
22:Y:94:ASP:OD1	22:Y:99:ILE:HG12	1.87	0.75
26:c:162:PRO:HG3	43:v:39:MET:HE2	1.69	0.74
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.20	0.74
6:X:122:MET:HE3	6:X:144:ILE:HD13	1.68	0.74
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.68	0.74
50:l:702:CDL:H612	50:l:702:CDL:H791	1.69	0.74
27:d:159:GLN:O	27:d:163:MET:HG3	1.87	0.74
36:m:82:VAL:HG21	50:s:401:CDL:HB31	1.68	0.74
16:Q:404:LYS:HE3	16:Q:455:ASP:OD1	1.87	0.73
5:F:84:ALA:HA	5:F:87:VAL:HG21	1.66	0.73
5:F:84:ALA:O	5:F:87:VAL:CG2	2.37	0.72
50:l:702:CDL:H742	50:l:702:CDL:H311	1.71	0.72
50:r:504:CDL:H201	50:r:504:CDL:H351	1.71	0.72
7:H:83:GLN:HG3	15:P:104:THR:HG22	1.71	0.72
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.22	0.72
7:H:94:MET:HE3	7:H:99:PRO:CG	2.20	0.71
22:Y:60:PHE:O	22:Y:64:THR:HG23	1.90	0.71
21:W:93:GLU:O	21:W:97:ILE:HG13	1.90	0.71
40:r:39:LEU:HD11	48:r:503:PLX:H321	1.71	0.70
27:d:24:THR:HG23	43:v:73:SER:HA	1.73	0.70
36:m:81:GLU:N	36:m:81:GLU:OE2	2.24	0.70
44:w:39:GLY:HA2	44:w:296:MET:HE1	1.73	0.70
11:L:109:ASN:ND2	11:L:111:LEU:O	2.23	0.69
16:Q:99:MET:HE3	16:Q:101:LEU:HD21	1.74	0.69
50:l:702:CDL:H542	50:l:702:CDL:HA61	1.74	0.69
5:F:84:ALA:CA	5:F:87:VAL:HG22	2.20	0.69
4:E:71:ALA:O	49:G:201:8Q1:C37	2.41	0.69
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.74	0.69
28:e:77:ASP:OD1	28:e:78:LYS:N	2.25	0.69
32:i:89:MET:HE1	32:i:98:MET:HE3	1.74	0.69
33:j:5:LEU:HG	41:s:3:MET:HE1	1.74	0.69
1:A:244:ASN:ND2	46:A:502:FMN:O2	2.25	0.69
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.25	0.69
41:s:184:MET:HE1	41:s:296:LEU:HB3	1.75	0.69
10:K:97:ARG:C	10:K:98:MET:HE2	2.18	0.68
1:A:451:GLN:HE22	1:A:455:LEU:HD23	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:69:MET:HE3	40:r:451:PRO:HG2	1.75	0.68
17:S:59:ARG:HH11	17:S:59:ARG:HG2	1.57	0.68
41:s:19:PHE:O	41:s:23:VAL:HG23	1.93	0.67
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.28	0.67
26:c:162:PRO:CG	43:v:39:MET:HE2	2.25	0.67
6:G:78:ALA:O	6:G:82:ARG:HG3	1.94	0.67
8:I:103:ARG:HH11	8:I:103:ARG:HG2	1.59	0.67
26:c:156:VAL:HG12	43:v:99:MET:HG2	1.76	0.67
50:l:702:CDL:HA62	50:l:702:CDL:C54	2.23	0.67
24:a:134:GLU:OE1	37:n:57:TRP:NE1	2.22	0.67
1:A:234:GLY:HA3	1:A:240:THR:HG22	1.77	0.66
6:X:122:MET:CE	6:X:144:ILE:HD13	2.25	0.66
2:B:204:ASN:HD21	13:N:93:MET:HE1	1.60	0.66
3:C:126:GLU:OE1	33:j:33:LYS:NZ	2.28	0.66
16:Q:84:PHE:HB3	16:Q:97:LEU:HB3	1.76	0.66
33:j:58:VAL:HG11	41:s:286:MET:SD	2.36	0.66
40:r:342:MET:HE3	40:r:413:THR:HB	1.75	0.66
14:O:38:LEU:O	14:O:124:ARG:NH2	2.28	0.66
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.76	0.66
32:i:142:LEU:HB3	32:i:194:LEU:HD21	1.76	0.66
16:Q:185:MET:HE3	55:Q:501:UQ1:HM23	1.77	0.66
50:l:702:CDL:H742	50:l:702:CDL:H312	1.77	0.66
40:r:302:MET:HE2	40:r:302:MET:HA	1.78	0.66
38:o:65:LEU:HD11	40:r:343:ILE:HD11	1.78	0.65
11:L:78:ARG:HD2	12:M:607:LYS:HE2	1.78	0.65
12:M:61:PRO:HB2	12:M:77:MET:HG3	1.79	0.65
17:S:52:ARG:HG2	17:S:52:ARG:NH1	2.07	0.65
1:A:451:GLN:NE2	1:A:455:LEU:HD23	2.11	0.65
15:P:68:ILE:HG22	15:P:69:LEU:HG	1.79	0.65
21:W:90:ASN:ND2	21:W:123:GLU:O	2.30	0.65
24:a:137:MET:HG2	27:d:83:LEU:HD22	1.77	0.65
33:j:6:THR:HG21	41:s:87:VAL:HG11	1.78	0.65
29:f:48:LEU:O	29:f:52:VAL:HG23	1.97	0.65
16:Q:304:LYS:NZ	16:Q:316:PHE:O	2.29	0.65
41:s:24:GLU:OE1	41:s:274:ARG:NH1	2.29	0.64
1:A:285:PRO:O	14:O:222:ARG:NH2	2.30	0.64
33:j:61:THR:HG21	33:j:105:GLU:OE1	1.97	0.64
35:l:119:LYS:NZ	50:l:702:CDL:OA3	2.28	0.64
26:c:115:ASN:OD1	35:l:162:THR:HG23	1.98	0.64
26:c:186:ILE:HB	43:v:34:ARG:HH21	1.63	0.64
27:d:26:LEU:HD12	27:d:26:LEU:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:64:LEU:HD12	36:m:55:MET:HE3	1.79	0.64
50:l:702:CDL:H432	50:l:702:CDL:H602	1.80	0.64
1:A:37:ASP:OD1	1:A:37:ASP:N	2.30	0.64
4:E:70:ASN:ND2	49:G:201:8Q1:O4	2.30	0.64
12:M:331:GLN:NE2	12:M:630:ALA:O	2.30	0.64
16:Q:375:MET:HE3	16:Q:379:ILE:HG13	1.78	0.64
26:c:179:GLU:OE2	26:c:179:GLU:N	2.19	0.64
34:k:59:MET:HE1	34:k:63:LEU:HD12	1.78	0.64
37:n:50:ARG:HB2	37:n:53:GLU:HG2	1.80	0.64
5:F:95:LEU:HD23	5:F:95:LEU:C	2.23	0.64
41:s:205:SER:OG	41:s:279:ARG:NH2	2.31	0.64
57:j:203:PEE:H13	41:s:72:ILE:HD13	1.80	0.63
16:Q:259:GLU:OE2	21:W:23:ARG:NH1	2.30	0.63
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.81	0.63
14:O:59:ASN:ND2	14:O:89:GLN:OE1	2.32	0.63
10:K:76:LEU:HD13	10:K:79:HIS:CD2	2.33	0.63
33:j:1:MET:HA	33:j:4:MET:HE3	1.80	0.63
1:A:44:ASN:ND2	1:A:133:HIS:O	2.32	0.63
4:E:30:ARG:O	4:E:34:GLU:HG2	1.98	0.63
50:k:101:CDL:H801	36:m:99:MET:HE1	1.81	0.63
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.27	0.63
15:P:123:GLN:CD	15:P:123:GLN:H	2.07	0.62
13:N:88:ARG:HG3	13:N:93:MET:HE2	1.80	0.62
20:V:85:ASP:HB3	20:V:130:LEU:HD21	1.80	0.62
35:l:227:PHE:O	35:l:230:HIS:ND1	2.30	0.62
35:l:373:LEU:HD22	35:l:431:PHE:CE2	2.34	0.62
34:k:31:LEU:HD21	36:m:67:VAL:HG11	1.80	0.62
44:w:62:VAL:HG12	44:w:205:VAL:HB	1.81	0.62
3:C:71:CYS:HB2	45:C:301:SF4:S4	2.39	0.62
5:F:24:CYS:N	5:F:58:CYS:SG	2.72	0.62
5:F:84:ALA:C	5:F:87:VAL:CG2	2.73	0.62
32:i:87:THR:CG2	32:i:88:LYS:H	2.13	0.62
12:M:512:VAL:O	12:M:514:ASN:ND2	2.33	0.61
35:l:420:ALA:O	35:l:424:THR:HG22	1.99	0.61
33:j:108:GLN:HB2	36:m:169:MET:HE1	1.82	0.61
1:A:337:MET:HA	1:A:337:MET:HE2	1.81	0.61
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.39	0.61
4:E:59:GLY:O	4:E:63:VAL:HG23	2.00	0.61
14:O:113:TYR:O	14:O:117:THR:HG23	2.00	0.61
40:r:225:ILE:HG13	40:r:229:MET:HE2	1.82	0.61
5:F:83:SER:OG	5:F:86:GLN:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:l:702:CDL:H312	50:l:702:CDL:C74	2.31	0.61
41:s:221:ALA:O	41:s:225:MET:HG2	1.99	0.61
27:d:26:LEU:H	27:d:26:LEU:CD1	2.14	0.61
9:J:192:ARG:NH1	9:J:198:ALA:O	2.33	0.61
12:M:289:LYS:HA	12:M:707:MET:HE1	1.83	0.61
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.82	0.61
21:W:91:LEU:HD22	42:u:7:LEU:HD12	1.83	0.60
9:J:306:GLU:OE1	9:J:316:ARG:NH1	2.34	0.60
1:A:138:LEU:HD13	1:A:245:VAL:HG23	1.83	0.60
38:o:56:ARG:NH2	40:r:422:HIS:O	2.34	0.60
1:A:214:GLU:OE2	11:L:175:LYS:NZ	2.28	0.60
16:Q:442:HIS:HB3	16:Q:446:ASP:HB2	1.84	0.60
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.30	0.60
32:i:278:MET:O	32:i:282:MET:HG3	2.01	0.60
50:l:702:CDL:H612	50:l:702:CDL:C81	2.30	0.60
5:F:20:ARG:HB2	5:F:66:TRP:HB2	1.84	0.60
41:s:195:ARG:HD3	41:s:231:ILE:CD1	2.31	0.60
44:w:125:ASP:O	44:w:130:ARG:NH2	2.35	0.60
12:M:51:GLN:HA	12:M:54:GLU:HG2	1.83	0.60
2:B:111:GLU:O	2:B:141:ARG:NH1	2.35	0.60
20:V:131:GLU:O	57:r:501:PEE:N	2.35	0.60
21:W:143:TYR:O	57:W:201:PEE:N	2.35	0.60
1:A:119:GLU:O	1:A:159:ARG:NH1	2.34	0.60
3:C:73:ALA:HB1	55:Q:501:UQ1:H112	1.82	0.60
34:k:65:VAL:HG11	36:m:157:THR:HG23	1.83	0.60
35:l:286:LEU:HD22	35:l:411:MET:SD	2.41	0.60
44:w:132:GLN:NE2	44:w:166:ASP:OD1	2.34	0.60
24:a:131:LYS:NZ	37:n:32:ASP:OD2	2.27	0.59
27:d:43:ARG:HB3	27:d:44:PRO:HD3	1.84	0.59
4:E:40:TYR:HB3	6:G:120:MET:HE1	1.84	0.59
35:l:60:GLU:HG2	35:l:83:ASP:HA	1.84	0.59
12:M:456:ALA:O	12:M:499:ASN:ND2	2.34	0.59
35:l:338:MET:HB2	35:l:457:LEU:HB3	1.85	0.59
40:r:119:TYR:O	40:r:123:GLU:HG2	2.03	0.59
32:i:154:MET:HE3	32:i:154:MET:HA	1.84	0.59
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.83	0.59
6:G:79:ILE:HG22	6:G:145:VAL:HG12	1.84	0.59
12:M:77:MET:HE2	12:M:117:MET:HE2	1.85	0.59
12:M:347:ASP:OD1	12:M:347:ASP:N	2.35	0.59
28:e:128:TYR:CE1	28:e:132:ASN:OD1	2.56	0.59
32:i:42:PRO:HG3	36:m:167:VAL:HG13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:302:VAL:O	35:l:306:THR:HG23	2.03	0.59
40:r:306:PRO:O	40:r:310:MET:HG3	2.03	0.59
50:k:101:CDL:H222	50:k:101:CDL:H332	1.85	0.59
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.85	0.59
35:l:500:LEU:HD23	50:l:703:CDL:H562	1.84	0.59
9:J:315:THR:HG23	9:J:318:LYS:H	1.67	0.59
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.83	0.59
25:b:81:ILE:HG23	57:l:705:PEE:H58	1.85	0.59
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.85	0.59
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.36	0.58
24:a:106:VAL:HG23	37:n:50:ARG:HH21	1.68	0.58
26:c:127:ASN:HD21	38:o:7:LYS:HE3	1.68	0.58
32:i:100:MET:HE1	35:l:598:SER:HB3	1.85	0.58
50:r:504:CDL:H401	50:r:504:CDL:H221	1.85	0.58
30:g:15:PHE:HB2	48:g:201:PLX:H6	1.86	0.58
1:A:337:MET:HE2	1:A:342:LEU:HD11	1.85	0.58
7:H:9:THR:O	7:H:76:GLN:NE2	2.36	0.58
24:a:114:LYS:HB2	27:d:63:TYR:CE1	2.37	0.58
41:s:24:GLU:OE2	41:s:271:LEU:HD22	2.02	0.58
1:A:37:ASP:OD2	14:O:236:GLU:HB2	2.03	0.58
6:G:134:ASP:HA	6:G:137:LYS:HE2	1.85	0.58
42:u:88:CYS:SG	42:u:89:ILE:N	2.76	0.58
12:M:217:GLU:HG2	12:M:218:LEU:HG	1.84	0.58
40:r:403:THR:HA	40:r:406:TYR:CE2	2.38	0.58
16:Q:53:TYR:OH	32:i:295:ARG:NH2	2.36	0.58
41:s:112:ALA:O	41:s:115:SER:OG	2.20	0.58
44:w:48:ARG:HG3	44:w:288:ASP:OD2	2.04	0.58
30:g:36:MET:HE1	48:g:201:PLX:H393	1.86	0.58
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.69	0.57
16:Q:216:ARG:NH1	16:Q:243:ASP:OD2	2.35	0.57
17:S:12:MET:CE	41:s:23:VAL:HG21	2.34	0.57
20:V:48:SER:HB3	20:V:51:GLU:OE2	2.02	0.57
12:M:208:THR:HG21	12:M:212:LYS:HB3	1.86	0.57
32:i:236:LYS:NZ	32:i:314:LYS:O	2.31	0.57
33:j:106:TRP:HD1	33:j:106:TRP:O	1.86	0.57
12:M:49:VAL:HG13	12:M:102:ILE:HD12	1.85	0.57
12:M:256:ALA:O	12:M:598:ASN:ND2	2.38	0.57
50:V:202:CDL:H762	50:V:202:CDL:H622	1.84	0.57
31:h:102:GLU:OE1	31:h:103:ASP:N	2.34	0.57
35:l:288:THR:HG21	35:l:307:SER:HB3	1.86	0.57
44:w:78:ALA:HB2	44:w:158:VAL:HG11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:300:ASN:OD1	44:w:303:GLU:HB2	2.04	0.57
27:d:24:THR:CG2	43:v:73:SER:CB	2.82	0.57
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.38	0.57
12:M:472:PRO:O	12:M:510:TRP:NE1	2.30	0.57
14:O:54:ASP:OD1	14:O:100:LYS:NZ	2.38	0.57
1:A:446:LEU:O	1:A:450:MET:HG3	2.05	0.57
16:Q:121:GLU:HG2	16:Q:422:CYS:O	2.04	0.57
17:S:59:ARG:HG2	17:S:59:ARG:NH1	2.20	0.57
5:F:84:ALA:C	5:F:87:VAL:HG22	2.29	0.57
26:c:169:GLU:OE1	43:v:43:GLN:NE2	2.38	0.57
32:i:68:MET:HE1	34:k:37:MET:HG2	1.87	0.57
44:w:297:LEU:HD12	44:w:297:LEU:O	2.05	0.57
10:K:95:LYS:HD2	10:K:95:LYS:O	2.05	0.56
35:l:128:MET:HE3	35:l:132:VAL:HG23	1.86	0.56
41:s:21:THR:HG21	52:s:402:UQ:H13	1.86	0.56
42:u:105:ALA:O	42:u:109:GLU:HG3	2.05	0.56
5:F:91:LEU:HD13	5:F:91:LEU:C	2.29	0.56
11:L:78:ARG:NH2	11:L:148:GLU:OE1	2.38	0.56
14:O:134:VAL:HG12	14:O:186:VAL:HG22	1.87	0.56
27:d:24:THR:CG2	43:v:73:SER:HA	2.34	0.56
35:l:69:MET:CE	40:r:451:PRO:HG2	2.34	0.56
37:n:30:ARG:HG2	37:n:30:ARG:HH11	1.70	0.56
4:E:17:VAL:HG21	11:L:55:VAL:HG22	1.87	0.56
16:Q:83:ASN:HB2	33:j:38:GLU:HG3	1.86	0.56
1:A:79:GLU:O	1:A:83:SER:OG	2.22	0.56
6:G:134:ASP:HB3	6:G:147:TYR:HE2	1.71	0.56
27:d:101:GLU:HA	27:d:101:GLU:OE2	2.06	0.56
44:w:246:LEU:HD12	44:w:255:VAL:HG11	1.88	0.56
1:A:60:GLY:HA2	14:O:241:PRO:HA	1.87	0.56
6:X:123:GLU:OE1	39:p:25:ARG:NH2	2.34	0.56
1:A:112:TYR:O	1:A:240:THR:HA	2.06	0.56
25:b:83:HIS:HE1	35:l:1:MET:HB3	1.71	0.56
34:k:59:MET:CE	34:k:63:LEU:HD12	2.36	0.56
35:l:291:CYS:SG	35:l:526:LEU:HA	2.45	0.56
1:A:119:GLU:HG3	1:A:127:ASP:HB2	1.87	0.56
9:J:36:LEU:HD23	9:J:41:ILE:HG12	1.88	0.56
21:W:85:GLN:OE1	31:h:105:ARG:NH1	2.36	0.56
3:C:98:ARG:NH2	33:j:35:SER:O	2.38	0.56
16:Q:106:VAL:HG21	16:Q:447:VAL:HG21	1.87	0.56
32:i:258:SER:HB2	32:i:336:VAL:HG12	1.88	0.56
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:43:THR:HA	15:P:47:ILE:HD12	1.88	0.55
32:i:186:HIS:O	32:i:190:MET:HE3	2.07	0.55
24:a:135:LYS:NZ	37:n:32:ASP:OD1	2.30	0.55
50:b:201:CDL:H752	50:b:201:CDL:H191	1.89	0.55
26:c:143:MET:HE2	26:c:143:MET:HA	1.87	0.55
1:A:357:MET:HB3	1:A:361:THR:HG21	1.88	0.55
26:c:38:PRO:HD3	38:o:67:ARG:HG2	1.88	0.55
11:L:62:THR:HG23	11:L:72:ILE:CD1	2.34	0.55
50:l:702:CDL:H811	50:l:702:CDL:C61	2.34	0.55
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.39	0.55
44:w:208:ASP:OD2	44:w:242:LYS:NZ	2.40	0.55
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.30	0.55
15:P:147:THR:HB	15:P:153:ILE:HD11	1.87	0.55
32:i:246:VAL:HG11	50:r:504:CDL:H392	1.87	0.55
40:r:10:MET:HE2	40:r:10:MET:HA	1.88	0.55
23:Z:31:THR:O	23:Z:35:LYS:HG2	2.06	0.55
27:d:89:GLU:O	27:d:93:ARG:HG2	2.06	0.55
38:o:20:PRO:HB3	39:p:65:ARG:HH12	1.70	0.55
1:A:102:MET:HE2	1:A:149:MET:HB3	1.88	0.55
1:A:134:ASP:N	1:A:134:ASP:OD1	2.39	0.55
14:O:166:ASP:HB3	14:O:168:LEU:HD22	1.89	0.55
23:Z:29:LEU:HD11	23:Z:49:GLU:HB2	1.88	0.54
40:r:1:MET:O	40:r:1:MET:HG3	2.08	0.54
20:V:38:ALA:HA	50:k:101:CDL:H232	1.88	0.54
39:p:35:ASP:OD1	39:p:36:LYS:N	2.39	0.54
31:h:18:MET:HE3	34:k:56:ALA:HA	1.88	0.54
32:i:122:ILE:O	32:i:176:ARG:NH1	2.40	0.54
1:A:40:ARG:NH2	1:A:289:GLU:O	2.38	0.54
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.88	0.54
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.90	0.54
24:a:166:GLY:O	24:a:170:GLN:NE2	2.41	0.54
30:g:92:MET:O	30:g:96:VAL:HG23	2.07	0.54
35:l:21:MET:HE3	35:l:26:ILE:HG21	1.89	0.54
26:c:60:GLU:OE1	26:c:60:GLU:N	2.41	0.54
33:j:51:PHE:HD2	41:s:133:LEU:HD12	1.72	0.54
40:r:306:PRO:HB3	40:r:458:LEU:HD12	1.90	0.54
43:v:17:PRO:HB3	43:v:105:GLU:HG2	1.89	0.54
2:B:58:ALA:HB1	21:W:35:MET:CE	2.38	0.54
20:V:40:SER:HA	50:V:201:CDL:HB61	1.90	0.54
50:l:702:CDL:H591	50:l:702:CDL:H332	1.90	0.54
42:u:107:PHE:O	42:u:111:VAL:HG22	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:111:ARG:HG2	43:v:114:ARG:HH21	1.73	0.54
44:w:62:VAL:HG21	44:w:74:ALA:HB2	1.89	0.54
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.41	0.54
35:l:8:THR:HG21	35:l:82:MET:HG3	1.90	0.54
17:S:31:ASN:ND2	17:S:36:LYS:HB2	2.24	0.53
20:V:141:VAL:O	24:a:169:TYR:OH	2.22	0.53
50:V:201:CDL:H581	32:i:110:PRO:HB3	1.89	0.53
32:i:103:ALA:HB2	32:i:157:MET:HE1	1.89	0.53
35:l:78:LEU:HD11	50:l:702:CDL:H261	1.89	0.53
35:l:161:ARG:NH2	35:l:238:GLU:OE1	2.29	0.53
2:B:100:GLU:O	2:B:170:GLY:N	2.36	0.53
10:K:76:LEU:HD13	10:K:79:HIS:HD2	1.73	0.53
14:O:44:THR:HG22	14:O:46:GLU:H	1.72	0.53
18:T:64:GLU:OE2	18:T:64:GLU:HA	2.07	0.53
20:V:106:ARG:HA	20:V:106:ARG:NE	2.23	0.53
34:k:4:VAL:O	34:k:8:ILE:HG12	2.09	0.53
35:l:371:THR:O	35:l:375:ILE:HG13	2.08	0.53
7:H:105:GLU:HB3	15:P:89:HIS:NE2	2.23	0.53
16:Q:105:MET:HE2	33:j:115:GLU:OE2	2.08	0.53
35:l:7:LEU:HD22	35:l:46:LEU:HD11	1.90	0.53
50:l:702:CDL:C31	50:l:702:CDL:C74	2.86	0.53
3:C:44:GLU:HG2	3:C:195:ARG:HH21	1.73	0.53
40:r:17:MET:HE1	50:r:504:CDL:H562	1.91	0.53
1:A:270:ASN:ND2	1:A:338:ASP:OD2	2.41	0.53
9:J:313:TRP:CD1	52:J:402:UQ:H8	2.43	0.53
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.90	0.53
16:Q:372:LYS:NZ	18:T:94:GLY:O	2.32	0.53
17:S:35:GLU:HG2	42:u:93:GLY:H	1.73	0.53
28:e:97:ILE:O	28:e:101:LEU:HB2	2.09	0.53
35:l:557:TRP:O	35:l:561:ILE:HG23	2.09	0.53
40:r:237:LYS:HD2	40:r:316:MET:HG2	1.90	0.53
41:s:101:GLY:O	41:s:105:MET:HG2	2.08	0.53
12:M:389:THR:O	12:M:390:THR:OG1	2.23	0.53
21:W:103:ASP:OD1	21:W:103:ASP:N	2.41	0.53
10:K:93:LEU:HD23	10:K:97:ARG:CZ	2.38	0.53
6:X:117:GLU:OE2	39:p:45:ARG:NH1	2.41	0.53
29:f:69:TYR:CE1	29:f:73:ASN:ND2	2.73	0.53
30:g:18:ASN:O	30:g:21:ARG:HG3	2.09	0.53
6:G:103:HIS:HE1	6:G:105:MET:CG	2.21	0.53
6:G:103:HIS:HE1	6:G:105:MET:HB2	1.73	0.52
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.40	0.52
32:i:243:LEU:HD23	50:r:504:CDL:H361	1.91	0.52
40:r:133:ILE:HD11	40:r:231:LEU:HD11	1.91	0.52
1:A:89:GLY:O	47:A:503:NAI:H2N	2.09	0.52
6:G:82:ARG:O	6:G:86:VAL:HG23	2.09	0.52
34:k:64:LEU:HD11	36:m:56:VAL:HG23	1.91	0.52
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.91	0.52
10:K:105:ARG:NH2	12:M:426:ASP:OD2	2.42	0.52
32:i:95:MET:HE3	32:i:148:SER:OG	2.09	0.52
40:r:221:VAL:HG22	40:r:283:LYS:HB3	1.91	0.52
2:B:184:LEU:HD23	11:L:112:MET:HG3	1.92	0.52
50:V:202:CDL:HB4	38:o:82:PRO:HB2	1.91	0.52
41:s:21:THR:O	41:s:25:ARG:HG2	2.09	0.52
1:A:210:THR:HB	1:A:224:ARG:HG2	1.91	0.52
8:I:103:ARG:HG2	8:I:103:ARG:NH1	2.23	0.52
35:l:260:LEU:HD22	35:l:267:MET:HE3	1.92	0.52
35:l:419:THR:HA	35:l:422:TYR:CE2	2.44	0.52
44:w:65:ASN:HD22	44:w:238:GLU:HG3	1.73	0.52
44:w:259:SER:OG	44:w:260:ALA:N	2.43	0.52
6:G:144:ILE:O	6:G:148:ILE:HG13	2.08	0.52
11:L:62:THR:CG2	11:L:72:ILE:HD13	2.35	0.52
13:N:78:ASP:OD2	13:N:80:SER:OG	2.28	0.52
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.45	0.52
16:Q:242:ASP:OD1	16:Q:242:ASP:N	2.42	0.52
57:i:401:PEE:H37	57:i:401:PEE:H60	1.90	0.52
40:r:79:ALA:HB3	40:r:229:MET:HE1	1.92	0.52
41:s:156:MET:HE1	41:s:177:THR:HG21	1.90	0.52
4:E:36:TYR:CE1	6:G:113:LEU:HD13	2.45	0.52
9:J:249:ILE:O	9:J:253:ILE:HG12	2.08	0.52
31:h:18:MET:HE1	34:k:59:MET:HB2	1.92	0.52
32:i:88:LYS:HG2	32:i:148:SER:HB3	1.92	0.52
57:l:705:PEE:H2	48:r:503:PLX:H21	1.92	0.52
44:w:118:TYR:OH	58:w:401:ADP:O2'	2.27	0.52
7:H:19:THR:O	7:H:19:THR:OG1	2.23	0.52
12:M:394:VAL:HG22	12:M:473:MET:HE1	1.92	0.52
32:i:87:THR:HG22	32:i:88:LYS:N	2.20	0.52
14:O:46:GLU:OE1	14:O:46:GLU:N	2.43	0.52
38:o:105:PHE:CD2	40:r:263:MET:HE1	2.45	0.52
6:G:134:ASP:HB3	6:G:147:TYR:CE2	2.45	0.52
31:h:69:ARG:O	31:h:73:MET:HG3	2.10	0.52
41:s:139:THR:HA	41:s:142:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:83:LEU:HD22	44:w:156:GLY:HA3	1.91	0.52
2:B:58:ALA:HB1	21:W:35:MET:HE3	1.92	0.51
16:Q:100:GLU:HB2	16:Q:108:LYS:HB3	1.92	0.51
22:Y:43:ARG:HB3	22:Y:46:GLN:HB2	1.93	0.51
30:g:106:LYS:HE2	30:g:107:ASP:OD1	2.11	0.51
50:l:702:CDL:H791	50:l:702:CDL:C61	2.40	0.51
40:r:218:LYS:O	40:r:222:GLU:HG2	2.10	0.51
40:r:373:ILE:HA	40:r:376:ILE:HD12	1.92	0.51
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.93	0.51
28:e:54:ARG:NH2	44:w:313:TYR:O	2.42	0.51
41:s:152:SER:HA	41:s:155:LEU:HD12	1.91	0.51
12:M:278:HIS:CE1	12:M:280:ASP:HB2	2.45	0.51
13:N:21:ARG:NH1	13:N:21:ARG:HG2	2.25	0.51
35:l:293:ILE:HG13	35:l:294:THR:HG23	1.92	0.51
1:A:337:MET:CE	1:A:342:LEU:HD11	2.41	0.51
17:S:69:ILE:HD13	42:u:71:PHE:HB3	1.91	0.51
22:Y:89:PRO:HB3	43:v:103:GLU:HG2	1.91	0.51
26:c:162:PRO:CB	43:v:39:MET:HE2	2.40	0.51
43:v:21:ARG:HG3	43:v:21:ARG:HH11	1.73	0.51
11:L:131:LYS:NZ	11:L:149:GLU:OE2	2.39	0.51
12:M:513:MET:HE3	12:M:514:ASN:H	1.76	0.51
50:b:201:CDL:H532	57:l:705:PEE:H61	1.92	0.51
6:G:123:GLU:HG2	6:G:130:ILE:HG13	1.92	0.51
16:Q:40:ASP:OD1	16:Q:40:ASP:N	2.40	0.51
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.46	0.51
25:b:16:ARG:HG2	25:b:20:ARG:NH1	2.26	0.51
31:h:32:ARG:NH2	31:h:66:CYS:O	2.43	0.51
35:l:17:ILE:HA	35:l:20:MET:HE3	1.92	0.51
35:l:41:SER:O	35:l:45:THR:HG23	2.11	0.51
12:M:451:ILE:HA	12:M:454:ASP:OD2	2.10	0.51
19:U:46:ASN:OD1	21:W:58:ARG:NH2	2.43	0.51
27:d:24:THR:CG2	43:v:73:SER:HB3	2.41	0.51
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.46	0.51
33:j:86:THR:O	33:j:90:MET:HG2	2.10	0.51
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.46	0.51
1:A:392:MET:HE2	1:A:419:ILE:CD1	2.40	0.51
9:J:375:VAL:HG23	9:J:375:VAL:O	2.11	0.51
6:X:82:ARG:O	6:X:86:VAL:HG23	2.10	0.51
40:r:201:MET:O	40:r:205:VAL:HG12	2.11	0.51
20:V:34:LEU:HD11	50:k:101:CDL:H441	1.92	0.51
50:l:702:CDL:H652	57:l:705:PEE:H30	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:O	1:A:132:ARG:HG2	2.10	0.50
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.44	0.50
17:S:51:ASP:OD2	42:u:22:SER:OG	2.27	0.50
41:s:11:ILE:HB	41:s:12:PRO:HD3	1.93	0.50
44:w:93:TYR:O	44:w:96:SER:OG	2.27	0.50
16:Q:256:ASP:OD1	16:Q:338:ARG:NH2	2.40	0.50
17:S:1:MET:O	17:S:4:GLU:HG3	2.12	0.50
48:g:201:PLX:H332	32:i:342:ALA:HB3	1.93	0.50
34:k:19:LEU:HD22	34:k:36:MET:HE1	1.93	0.50
35:l:346:ILE:HD11	35:l:431:PHE:HE1	1.76	0.50
39:p:136:GLU:OE2	39:p:167:TRP:NE1	2.42	0.50
3:C:55:ASN:O	3:C:59:ARG:HG2	2.11	0.50
11:L:79:ILE:HG12	11:L:99:MET:HG3	1.93	0.50
34:k:79:VAL:HG22	36:m:74:MET:HE1	1.94	0.50
6:G:103:HIS:HE1	6:G:105:MET:CB	2.25	0.50
12:M:370:GLU:HG3	12:M:519:ILE:HG13	1.92	0.50
28:e:103:SER:HA	48:r:503:PLX:H271	1.92	0.50
29:f:69:TYR:CD1	29:f:73:ASN:ND2	2.80	0.50
40:r:59:ASP:HB2	40:r:245:ARG:HH22	1.76	0.50
16:Q:39:PRO:HB3	16:Q:43:TRP:CD1	2.45	0.50
27:d:109:ARG:NH1	28:e:130:GLU:OE2	2.40	0.50
27:d:163:MET:HA	27:d:166:GLU:HG2	1.92	0.50
41:s:85:MET:HE1	41:s:109:SER:HB3	1.93	0.50
1:A:90:GLY:HA3	47:A:503:NAI:H1D	1.93	0.50
17:S:35:GLU:HG2	42:u:93:GLY:N	2.27	0.50
50:I:201:CDL:H512	50:I:201:CDL:H722	1.91	0.50
16:Q:189:THR:HG21	55:Q:501:UQ1:HM21	1.93	0.50
36:m:35:VAL:O	36:m:39:VAL:HG22	2.12	0.50
26:c:91:ASP:O	38:o:44:LYS:NZ	2.45	0.50
33:j:94:LEU:HD13	36:m:154:VAL:HG13	1.94	0.50
34:k:17:ALA:HB2	50:k:101:CDL:H811	1.94	0.50
40:r:282:LEU:HD13	40:r:342:MET:HG3	1.94	0.50
44:w:200:PRO:HG3	44:w:252:LYS:HD3	1.92	0.50
8:I:12:ARG:HB3	8:I:20:LEU:HD12	1.92	0.50
26:c:96:ASP:N	26:c:96:ASP:OD1	2.43	0.50
35:l:51:LEU:HG	35:l:55:MET:HE3	1.94	0.50
35:l:503:GLU:O	35:l:507:THR:HG23	2.12	0.50
41:s:150:LEU:O	41:s:154:LEU:HD12	2.11	0.50
1:A:159:ARG:NH2	14:O:176:CYS:O	2.45	0.49
2:B:77:LEU:HD13	41:s:31:MET:HE3	1.93	0.49
9:J:179:ARG:HH11	9:J:179:ARG:HB2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:81:LEU:HD21	44:w:270:VAL:HG13	1.92	0.49
2:B:128:ILE:O	15:P:231:ARG:NH2	2.45	0.49
26:c:170:ARG:HG2	43:v:53:LEU:HD13	1.94	0.49
37:n:42:SER:O	37:n:46:LYS:HB2	2.12	0.49
38:o:31:LYS:O	38:o:35:GLU:HG3	2.12	0.49
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.94	0.49
8:I:70:MET:O	8:I:70:MET:SD	2.70	0.49
9:J:87:GLU:HG3	9:J:89:TYR:H	1.76	0.49
15:P:152:PRO:HB3	15:P:177:PHE:HD2	1.78	0.49
16:Q:184:ILE:HG21	16:Q:207:ARG:HG3	1.94	0.49
50:l:702:CDL:HA62	50:l:702:CDL:C52	2.42	0.49
50:l:702:CDL:H122	50:l:702:CDL:OA9	2.12	0.49
9:J:178:SER:OG	9:J:317:ASP:OD1	2.28	0.49
12:M:573:GLY:HA3	13:N:137:TRP:CD1	2.47	0.49
32:i:258:SER:OG	32:i:333:SER:O	2.28	0.49
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.94	0.49
15:P:64:TYR:O	15:P:68:ILE:HD13	2.13	0.49
21:W:74:LEU:O	21:W:78:GLU:HG3	2.13	0.49
32:i:322:GLN:H	32:i:322:GLN:CD	2.20	0.49
35:l:97:THR:O	35:l:101:MET:HG3	2.13	0.49
41:s:90:PRO:HD2	41:s:240:ILE:HD13	1.94	0.49
43:v:52:MET:HB2	43:v:55:GLN:HG3	1.95	0.49
32:i:96:THR:O	32:i:100:MET:HG3	2.12	0.49
33:j:105:GLU:HA	36:m:169:MET:HE2	1.94	0.49
35:l:534:HIS:CD2	57:l:704:PEE:H13	2.47	0.49
4:E:120:SER:O	4:E:124:VAL:HG22	2.13	0.49
12:M:367:CYS:HB3	12:M:533:GLY:O	2.12	0.49
17:S:63:THR:HG23	42:u:21:SER:HB2	1.95	0.49
24:a:78:THR:HG21	28:e:96:SER:HA	1.95	0.49
35:l:44:PHE:HB2	35:l:94:LEU:HB3	1.94	0.49
3:C:103:MET:HB2	3:C:124:MET:HE1	1.95	0.49
5:F:61:VAL:HG23	5:F:62:GLN:H	1.77	0.49
21:W:121:MET:HE2	21:W:136:ALA:HB1	1.93	0.49
32:i:7:THR:HG22	32:i:11:MET:HE3	1.94	0.49
35:l:298:ILE:O	35:l:302:VAL:HG23	2.13	0.49
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.29	0.49
12:M:539:LYS:HE3	12:M:540:ASN:ND2	2.27	0.49
33:j:8:LEU:O	33:j:12:THR:OG1	2.25	0.49
41:s:235:ASN:ND2	41:s:267:THR:HA	2.28	0.49
42:u:83:THR:HA	42:u:86:TRP:CD1	2.48	0.49
44:w:353:TRP:CE3	44:w:354:LEU:HD12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:95:LEU:C	5:F:95:LEU:CD2	2.86	0.49
12:M:89:VAL:HB	12:M:94:MET:HE3	1.95	0.48
6:X:103:HIS:CE1	6:X:105:MET:HB2	2.48	0.48
35:l:556:ILE:O	35:l:560:THR:OG1	2.29	0.48
12:M:340:ALA:HB3	12:M:366:LEU:HD23	1.94	0.48
18:T:32:SER:OG	18:T:36:GLU:O	2.28	0.48
41:s:126:LYS:O	41:s:130:ILE:HG12	2.13	0.48
41:s:313:SER:O	41:s:313:SER:OG	2.24	0.48
16:Q:55:THR:OG1	16:Q:57:GLU:OE1	2.30	0.48
31:h:38:LYS:O	31:h:42:GLU:HG3	2.13	0.48
36:m:101:PHE:C	36:m:101:PHE:CD1	2.91	0.48
40:r:122:PHE:HD1	40:r:238:LEU:HD13	1.78	0.48
8:I:58:ASP:OD1	8:I:61:ARG:HB2	2.13	0.48
22:Y:100:LEU:HD13	22:Y:101:PRO:HD2	1.95	0.48
32:i:155:LEU:HD22	32:i:278:MET:HE2	1.93	0.48
1:A:160:GLY:O	1:A:199:ARG:NH2	2.46	0.48
7:H:114:TRP:CD2	7:H:115:PRO:HA	2.49	0.48
17:S:37:ARG:HG2	17:S:48:MET:HE2	1.96	0.48
32:i:222:SER:O	32:i:224:ALA:N	2.47	0.48
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.47	0.48
4:E:70:ASN:O	49:G:201:8Q1:C38	2.62	0.48
6:G:140:CYS:SG	6:G:143:GLU:HG3	2.54	0.48
12:M:208:THR:HA	14:O:110:MET:HE2	1.95	0.48
12:M:338:VAL:HG21	12:M:361:VAL:HG11	1.96	0.48
15:P:75:GLN:HB3	15:P:87:PHE:CD1	2.49	0.48
26:c:169:GLU:CD	26:c:169:GLU:H	2.21	0.48
36:m:82:VAL:HG22	36:m:83:TRP:H	1.77	0.48
1:A:392:MET:HE2	1:A:419:ILE:HD12	1.95	0.48
19:U:26:GLY:HA3	57:j:202:PEE:H37	1.96	0.48
6:X:89:LEU:HD22	23:Z:47:ARG:C	2.38	0.48
26:c:90:TYR:HE2	26:c:100:ASN:HD21	1.62	0.48
28:e:55:LEU:HD21	44:w:320:GLY:CA	2.44	0.48
28:e:72:ASP:OD1	28:e:72:ASP:N	2.39	0.48
33:j:71:LEU:O	36:m:147:TYR:OH	2.24	0.48
12:M:385:TYR:OH	12:M:527:ASP:OD1	2.24	0.48
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.96	0.48
35:l:341:MET:HE2	35:l:454:ILE:HG12	1.95	0.48
35:l:359:MET:O	35:l:436:ARG:NH2	2.47	0.48
57:r:501:PEE:H29	57:r:501:PEE:H71	1.95	0.48
9:J:168:SER:O	9:J:203:PRO:HD2	2.13	0.48
12:M:509:ASP:OD1	12:M:509:ASP:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:66:LEU:HD11	42:u:74:ILE:HG22	1.95	0.48
21:W:51:MET:HA	41:s:313:SER:HB2	1.96	0.48
27:d:24:THR:HG23	43:v:73:SER:CB	2.44	0.48
32:i:93:VAL:HG22	35:l:603:ASN:OD1	2.13	0.48
8:I:66:PRO:HB2	15:P:77:GLN:HG2	1.95	0.47
20:V:61:PHE:HD2	20:V:104:ARG:HH21	1.62	0.47
24:a:149:LEU:HD22	30:g:92:MET:HE1	1.95	0.47
35:l:170:GLN:NE2	57:l:704:PEE:O1P	2.47	0.47
38:o:37:LEU:HD12	39:p:8:ALA:CA	2.44	0.47
38:o:53:ASP:HB3	38:o:56:ARG:HB2	1.95	0.47
39:p:49:ASP:OD1	39:p:49:ASP:C	2.57	0.47
42:u:34:ALA:HB2	42:u:120:PRO:HG3	1.95	0.47
2:B:44:ARG:HG3	2:B:44:ARG:HH11	1.79	0.47
7:H:65:VAL:O	7:H:69:GLU:HG3	2.14	0.47
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.96	0.47
1:A:33:GLY:HA3	1:A:294:VAL:HG23	1.94	0.47
1:A:82:THR:HG23	1:A:259:GLY:HA3	1.95	0.47
1:A:128:ARG:O	1:A:131:ILE:HG22	2.14	0.47
2:B:49:ASP:OD1	2:B:52:SER:OG	2.23	0.47
19:U:63:MET:HB2	19:U:66:VAL:HG12	1.95	0.47
3:C:118:ARG:NH1	3:C:156:ILE:O	2.42	0.47
50:b:201:CDL:H772	50:b:201:CDL:H212	1.97	0.47
32:i:322:GLN:N	32:i:322:GLN:OE1	2.47	0.47
35:l:156:GLY:HA2	35:l:164:ALA:HB1	1.96	0.47
36:m:82:VAL:HG12	36:m:85:SER:HB3	1.95	0.47
38:o:22:GLU:O	38:o:22:GLU:OE1	2.32	0.47
43:v:28:ASP:OD1	43:v:34:ARG:HB2	2.15	0.47
1:A:340:ASP:O	1:A:344:GLN:HG2	2.14	0.47
13:N:85:GLU:HG2	13:N:86:TRP:N	2.29	0.47
16:Q:268:TRP:O	16:Q:272:THR:OG1	2.26	0.47
24:a:168:TRP:HB3	30:g:3:MET:HG3	1.97	0.47
40:r:248:THR:HG23	40:r:249:ILE:HG23	1.96	0.47
35:l:78:LEU:HD11	50:l:702:CDL:C26	2.44	0.47
40:r:201:MET:HE2	57:r:501:PEE:H78	1.96	0.47
1:A:119:GLU:CG	1:A:127:ASP:HB2	2.45	0.47
4:E:62:LYS:HD2	4:E:66:MET:HE3	1.97	0.47
11:L:71:HIS:CE1	11:L:120:PRO:HD2	2.50	0.47
12:M:390:THR:HA	12:M:600:GLU:HG2	1.97	0.47
12:M:506:VAL:HG12	12:M:508:GLY:H	1.78	0.47
14:O:156:LEU:HB3	14:O:158:ILE:HG12	1.96	0.47
27:d:24:THR:HG23	43:v:73:SER:CA	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:97:LYS:NZ	40:r:47:GLU:OE2	2.36	0.47
35:l:206:ASN:N	35:l:206:ASN:OD1	2.39	0.47
35:l:356:ILE:HA	35:l:359:MET:SD	2.55	0.47
44:w:95:ASP:OD1	44:w:95:ASP:N	2.45	0.47
14:O:213:ILE:HA	14:O:214:PRO:HD3	1.71	0.47
15:P:154:GLU:OE1	15:P:180:ASN:ND2	2.47	0.47
25:b:88:TYR:CE2	27:d:49:ARG:HG2	2.50	0.47
29:f:69:TYR:HE1	29:f:73:ASN:HD22	1.58	0.47
12:M:402:LEU:HD23	12:M:475:VAL:HB	1.97	0.47
50:l:702:CDL:H641	48:r:503:PLX:C11	2.44	0.47
8:I:54:TYR:CZ	16:Q:362:LYS:HD2	2.49	0.47
12:M:136:GLU:HG2	12:M:242:PRO:HG3	1.95	0.47
27:d:23:GLN:HB2	43:v:72:ASP:HB3	1.97	0.47
32:i:322:GLN:CD	32:i:322:GLN:N	2.73	0.47
40:r:73:LEU:HA	40:r:76:MET:HE2	1.97	0.47
40:r:105:PHE:O	40:r:109:THR:OG1	2.22	0.47
9:J:134:TRP:CZ2	9:J:311:GLU:HG3	2.50	0.46
10:K:93:LEU:HD23	10:K:97:ARG:NH2	2.30	0.46
10:K:98:MET:HE2	10:K:98:MET:N	2.30	0.46
16:Q:99:MET:HE1	16:Q:444:LEU:HD21	1.96	0.46
33:j:60:ILE:HD11	36:m:70:TYR:OH	2.15	0.46
33:j:106:TRP:CD1	33:j:106:TRP:C	2.93	0.46
57:j:202:PEE:H35	57:j:202:PEE:H30	1.81	0.46
42:u:68:LEU:O	42:u:72:ARG:HG3	2.15	0.46
6:G:133:ILE:O	6:G:134:ASP:HB2	2.15	0.46
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.50	0.46
24:a:160:MET:HE2	30:g:95:TYR:CD1	2.51	0.46
26:c:159:LYS:HE2	43:v:94:ASP:OD2	2.15	0.46
27:d:28:ASN:O	27:d:31:THR:HG22	2.15	0.46
30:g:51:ARG:NH2	32:i:322:GLN:CG	2.78	0.46
33:j:90:MET:SD	36:m:151:THR:HG23	2.56	0.46
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.96	0.46
35:l:568:PHE:O	35:l:572:LYS:HG2	2.15	0.46
2:B:44:ARG:HG3	2:B:44:ARG:NH1	2.30	0.46
6:G:103:HIS:CE1	6:G:105:MET:HB2	2.50	0.46
12:M:485:ASP:CG	12:M:680:LEU:HD12	2.40	0.46
21:W:10:MET:HE3	21:W:10:MET:HB3	1.84	0.46
21:W:121:MET:HE3	36:m:130:THR:HB	1.97	0.46
22:Y:97:LEU:HD21	43:v:104:ARG:HA	1.98	0.46
29:f:60:LYS:HB2	29:f:60:LYS:HE2	1.58	0.46
3:C:89:PHE:HA	41:s:39:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:58:ALA:HB1	35:l:371:THR:HG21	1.97	0.46
28:e:128:TYR:HE1	28:e:132:ASN:OD1	1.97	0.46
35:l:173:LEU:HD13	57:l:704:PEE:H15	1.98	0.46
40:r:342:MET:HE3	40:r:413:THR:CB	2.43	0.46
3:C:188:LYS:HB3	3:C:191:ARG:NH1	2.31	0.46
3:C:190:LEU:HD22	57:j:201:PEE:H13	1.96	0.46
4:E:127:ASP:OD2	11:L:104:ARG:NH1	2.49	0.46
5:F:91:LEU:C	5:F:91:LEU:CD1	2.89	0.46
32:i:246:VAL:HG21	50:r:504:CDL:H362	1.98	0.46
1:A:250:VAL:O	1:A:254:ILE:HD13	2.16	0.46
13:N:78:ASP:H	13:N:81:MET:HE2	1.81	0.46
50:V:201:CDL:OB6	35:l:576:MET:HE2	2.16	0.46
27:d:171:LYS:HB3	27:d:171:LYS:HE2	1.70	0.46
32:i:51:ARG:HG2	34:k:96:LEU:HD21	1.97	0.46
35:l:366:MET:HA	35:l:445:GLU:OE2	2.15	0.46
35:l:413:LEU:O	35:l:416:THR:HG22	2.15	0.46
37:n:30:ARG:HG2	37:n:30:ARG:NH1	2.30	0.46
3:C:109:LEU:HD13	3:C:117:LEU:HD13	1.96	0.46
9:J:174:ILE:HG23	9:J:175:LYS:HD3	1.96	0.46
12:M:257:VAL:O	12:M:598:ASN:ND2	2.48	0.46
12:M:650:SER:OG	12:M:652:ASN:OD1	2.34	0.46
20:V:123:ALA:O	20:V:127:MET:HG3	2.16	0.46
37:n:8:VAL:O	37:n:12:TRP:HB3	2.16	0.46
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.51	0.46
6:G:147:TYR:CD1	6:G:147:TYR:C	2.94	0.46
7:H:54:GLU:O	7:H:58:MET:HG3	2.15	0.46
15:P:101:ARG:O	15:P:109:LYS:NZ	2.49	0.46
26:c:110:ASP:OD1	26:c:110:ASP:N	2.48	0.46
27:d:37:PHE:CE1	35:l:3:PRO:HB3	2.51	0.46
29:f:68:GLU:OE2	29:f:72:ARG:HG3	2.16	0.46
32:i:54:GLU:HG2	34:k:96:LEU:HD12	1.96	0.46
48:j:204:PLX:H282	48:j:204:PLX:H251	1.64	0.46
4:E:22:SER:HB3	4:E:27:GLU:HB2	1.98	0.46
16:Q:203:MET:HE2	16:Q:258:LEU:CD1	2.45	0.46
16:Q:203:MET:HE2	16:Q:258:LEU:HD12	1.97	0.46
6:X:79:ILE:O	6:X:83:VAL:HG23	2.16	0.46
33:j:69:ILE:O	33:j:73:LEU:HG	2.16	0.46
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.51	0.46
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.51	0.46
3:C:126:GLU:HG2	9:J:89:TYR:OH	2.15	0.46
13:N:144:TYR:HD1	13:N:144:TYR:H	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:156:GLU:OE1	16:Q:171:ARG:NH2	2.47	0.46
16:Q:334:VAL:HA	16:Q:337:MET:HE3	1.98	0.46
6:X:116:VAL:O	6:X:120:MET:HG3	2.16	0.46
24:a:157:ARG:HD3	30:g:3:MET:SD	2.56	0.46
36:m:3:MET:HB3	36:m:5:ILE:HD13	1.97	0.46
4:E:66:MET:HG3	49:G:201:8Q1:C11	2.46	0.45
13:N:77:VAL:HA	13:N:81:MET:HE2	1.98	0.45
32:i:71:MET:HE2	32:i:71:MET:HA	1.98	0.45
35:l:1:MET:O	35:l:1:MET:HG2	2.16	0.45
35:l:61:MET:HE3	35:l:61:MET:HB2	1.82	0.45
50:l:702:CDL:OA9	50:l:702:CDL:H331	2.15	0.45
40:r:310:MET:HE3	40:r:459:TYR:HA	1.98	0.45
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.72	0.45
9:J:163:LYS:NZ	9:J:253:ILE:O	2.36	0.45
9:J:231:LEU:HD23	9:J:231:LEU:HA	1.83	0.45
12:M:388:ASN:ND2	12:M:513:MET:O	2.36	0.45
16:Q:94:VAL:HG21	16:Q:116:LEU:HB2	1.98	0.45
32:i:98:MET:HE2	32:i:98:MET:HB2	1.85	0.45
32:i:258:SER:CB	32:i:336:VAL:HG12	2.46	0.45
36:m:61:LEU:O	41:s:114:TYR:OH	2.33	0.45
1:A:174:ARG:NH1	10:K:92:GLU:OE2	2.49	0.45
1:A:278:ILE:HG21	1:A:304:ALA:HB2	1.98	0.45
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.98	0.45
48:g:201:PLX:H12	31:h:2:PRO:HD2	1.97	0.45
36:m:93:PHE:CE2	36:m:97:LEU:HD11	2.52	0.45
8:I:34:ARG:HA	8:I:34:ARG:HD2	1.87	0.45
14:O:199:LYS:H	14:O:199:LYS:HG3	1.62	0.45
16:Q:185:MET:HE3	55:Q:501:UQ1:CM2	2.45	0.45
23:Z:18:ASP:O	23:Z:21:GLN:HG2	2.17	0.45
24:a:83:ALA:O	24:a:87:THR:HG23	2.17	0.45
26:c:140:MET:HE1	35:l:411:MET:SD	2.56	0.45
32:i:58:LYS:NZ	32:i:117:GLU:HG2	2.31	0.45
35:l:72:GLN:NE2	40:r:458:LEU:O	2.49	0.45
40:r:203:PHE:HB2	40:r:243:MET:HG3	1.99	0.45
12:M:371:VAL:HG22	12:M:533:GLY:HA2	1.98	0.45
32:i:89:MET:HG2	32:i:95:MET:HE2	1.98	0.45
50:s:401:CDL:H771	50:s:401:CDL:H801	1.81	0.45
1:A:117:ALA:HB3	1:A:158:ILE:HA	1.97	0.45
1:A:451:GLN:HE22	1:A:455:LEU:HD21	1.78	0.45
8:I:92:LYS:HA	8:I:92:LYS:HE2	1.98	0.45
16:Q:206:GLU:O	16:Q:210:MET:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:62:THR:HG21	32:i:114:TRP:CD1	2.51	0.45
34:k:23:ARG:NE	50:k:101:CDL:OB4	2.39	0.45
3:C:88:ARG:O	41:s:39:VAL:HG12	2.17	0.45
16:Q:158:LEU:HD23	16:Q:158:LEU:HA	1.85	0.45
30:g:52:ARG:NH2	44:w:338:LYS:O	2.49	0.45
30:g:106:LYS:HA	30:g:106:LYS:HD2	1.69	0.45
38:o:37:LEU:HD12	39:p:8:ALA:HA	1.99	0.45
1:A:176:ALA:HA	1:A:181:LEU:HD12	1.99	0.45
4:E:35:LEU:HD21	4:E:86:GLY:HA3	1.99	0.45
12:M:64:CYS:HB3	12:M:75:CYS:HB3	1.99	0.45
12:M:209:TYR:O	14:O:41:HIS:HB3	2.17	0.45
16:Q:58:THR:HG21	35:l:579:ASN:ND2	2.32	0.45
16:Q:444:LEU:HD23	16:Q:444:LEU:HA	1.77	0.45
24:a:186:THR:OG1	24:a:189:ASN:O	2.34	0.45
14:O:130:TYR:HA	14:O:189:ASN:ND2	2.32	0.45
35:l:468:ILE:O	35:l:472:ILE:HG23	2.17	0.45
39:p:55:LYS:HD3	39:p:55:LYS:N	2.32	0.45
17:S:50:ARG:O	17:S:54:ILE:HG23	2.17	0.45
50:V:201:CDL:H371	50:V:201:CDL:H341	1.62	0.45
35:l:48:LEU:O	35:l:52:LEU:HG	2.16	0.45
52:s:402:UQ:H152	52:s:402:UQ:H121	1.83	0.45
2:B:148:ASP:HB3	2:B:151:LYS:HB2	1.99	0.44
31:h:53:GLU:HG2	31:h:54:LYS:HG2	1.99	0.44
33:j:5:LEU:CG	41:s:3:MET:HE1	2.44	0.44
35:l:124:PHE:CE1	35:l:252:MET:HB2	2.53	0.44
37:n:26:TYR:CD1	37:n:26:TYR:C	2.95	0.44
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.98	0.44
1:A:69:LEU:HD22	1:A:147:ARG:HG2	2.00	0.44
1:A:292:MET:HE1	1:A:339:PHE:CE2	2.52	0.44
3:C:69:LEU:HB2	3:C:107:GLY:HA3	1.98	0.44
5:F:85:ASP:HA	5:F:88:THR:HG22	1.98	0.44
7:H:22:GLU:O	7:H:26:ILE:HD12	2.17	0.44
7:H:62:GLU:OE2	7:H:67:LYS:HE3	2.18	0.44
12:M:712:LYS:O	12:M:716:GLU:HG2	2.17	0.44
14:O:224:SER:OG	14:O:226:GLU:OE1	2.35	0.44
35:l:396:ILE:HG21	35:l:490:ALA:HB2	1.99	0.44
57:l:705:PEE:H60	57:l:705:PEE:H55	1.62	0.44
40:r:67:VAL:HG12	48:r:503:PLX:H382	1.98	0.44
4:E:118:PHE:CD1	4:E:118:PHE:C	2.94	0.44
16:Q:238:LEU:HD23	16:Q:238:LEU:HA	1.80	0.44
50:V:202:CDL:H552	50:V:202:CDL:H152	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:16:ARG:NH2	43:v:48:ASP:OD2	2.49	0.44
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.99	0.44
6:G:86:VAL:HG22	6:G:125:GLU:CD	2.43	0.44
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.48	0.44
24:a:184:LYS:C	24:a:186:THR:H	2.25	0.44
32:i:171:ASN:HB2	35:l:574:SER:OG	2.18	0.44
32:i:193:VAL:HB	32:i:266:ILE:HG23	1.99	0.44
50:l:702:CDL:H312	50:l:702:CDL:C73	2.46	0.44
44:w:88:GLU:N	44:w:160:GLU:HG3	2.32	0.44
1:A:195:VAL:O	10:K:97:ARG:NH1	2.41	0.44
9:J:165:ILE:HD13	9:J:199:THR:HB	2.00	0.44
16:Q:259:GLU:O	16:Q:263:THR:HG22	2.17	0.44
24:a:53:ARG:NH2	25:b:33:PRO:HD3	2.32	0.44
35:l:51:LEU:HD22	35:l:91:PRO:HG3	2.00	0.44
35:l:245:ALA:HB2	35:l:340:PHE:HB3	1.99	0.44
42:u:84:GLU:HG3	42:u:103:GLN:HG2	1.99	0.44
12:M:224:ASP:OD2	12:M:291:ARG:NH2	2.50	0.44
22:Y:40:ILE:HG23	22:Y:49:GLN:HB3	2.00	0.44
25:b:7:ASP:OD1	25:b:7:ASP:N	2.50	0.44
39:p:13:GLN:HG3	39:p:14:GLN:N	2.32	0.44
1:A:263:ALA:HA	1:A:271:SER:HB3	1.98	0.44
9:J:305:PHE:HD2	9:J:314:THR:HG22	1.82	0.44
10:K:107:SER:OG	10:K:110:HIS:ND1	2.44	0.44
12:M:117:MET:HE3	12:M:142:GLN:C	2.43	0.44
12:M:638:THR:O	12:M:642:VAL:HG23	2.18	0.44
24:a:184:LYS:HB3	31:h:30:PRO:HB3	2.00	0.44
26:c:167:TYR:CD2	26:c:178:PRO:HG3	2.53	0.44
40:r:324:SER:OG	40:r:440:HIS:NE2	2.32	0.44
42:u:172:MET:HE2	42:u:172:MET:HB3	1.85	0.44
1:A:48:ARG:NH1	14:O:226:GLU:OE1	2.50	0.44
4:E:16:SER:HA	11:L:52:LEU:HD13	1.99	0.44
26:c:168:LEU:HD11	26:c:174:PRO:HB3	1.99	0.44
35:l:84:TYR:CE1	35:l:88:MET:HG3	2.53	0.44
35:l:358:LYS:HG3	39:p:80:TYR:CE1	2.52	0.44
38:o:23:TYR:CD2	39:p:65:ARG:HG3	2.53	0.44
38:o:89:LEU:HD22	38:o:93:PHE:HE2	1.82	0.44
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.83	0.44
12:M:282:ASN:O	12:M:283:GLU:HG2	2.18	0.44
15:P:211:ARG:NH2	15:P:213:ASP:OD2	2.48	0.44
20:V:9:TYR:CD1	20:V:9:TYR:C	2.96	0.44
24:a:127:ASP:OD1	48:a:201:PLX:H12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:176:LYS:O	26:c:177:GLU:HG3	2.18	0.44
32:i:141:VAL:O	32:i:145:ILE:HG12	2.18	0.44
35:l:97:THR:HG22	35:l:101:MET:HE3	1.99	0.44
50:r:504:CDL:H782	50:r:504:CDL:H232	1.99	0.44
5:F:43:GLU:OE1	5:F:44:LEU:N	2.51	0.43
10:K:105:ARG:NH1	11:L:167:ASN:O	2.50	0.43
12:M:405:THR:HG23	12:M:407:PRO:HD3	1.99	0.43
12:M:562:LYS:O	12:M:563:ASP:OD1	2.36	0.43
15:P:65:VAL:HG11	15:P:86:ILE:HD13	1.99	0.43
16:Q:325:ASP:OD1	16:Q:325:ASP:N	2.50	0.43
18:T:84:ILE:HD12	18:T:85:SER:H	1.83	0.43
21:W:52:LYS:HE2	21:W:52:LYS:HB3	1.73	0.43
6:X:107:ASP:OD1	6:X:107:ASP:N	2.51	0.43
27:d:127:LYS:O	27:d:131:GLN:HG3	2.17	0.43
29:f:53:PHE:O	29:f:56:ILE:HG13	2.18	0.43
33:j:18:VAL:HG12	57:j:203:PEE:H16	1.99	0.43
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.53	0.43
48:r:502:PLX:H51	48:r:502:PLX:H6	1.43	0.43
41:s:114:TYR:HA	41:s:117:LEU:HB2	2.00	0.43
1:A:56:ALA:HB1	1:A:61:ASP:HB2	2.00	0.43
6:G:93:ILE:HD11	6:G:110:LEU:HD11	1.99	0.43
8:I:6:ARG:O	8:I:10:LEU:HG	2.18	0.43
12:M:307:ILE:HG22	12:M:582:VAL:HG22	2.00	0.43
12:M:460:HIS:O	12:M:463:SER:OG	2.33	0.43
13:N:85:GLU:HG2	13:N:86:TRP:H	1.83	0.43
16:Q:185:MET:HE1	55:Q:501:UQ1:HM32	1.91	0.43
50:k:101:CDL:H541	50:k:101:CDL:H571	1.80	0.43
48:r:502:PLX:H101	48:r:502:PLX:H72	1.52	0.43
1:A:129:GLU:OE1	14:O:225:CYS:HB3	2.19	0.43
13:N:21:ARG:HG2	13:N:21:ARG:HH11	1.82	0.43
16:Q:242:ASP:O	16:Q:246:GLU:HG2	2.19	0.43
33:j:56:PHE:O	33:j:60:ILE:HG13	2.18	0.43
33:j:102:LEU:HD21	41:s:295:PRO:HG3	2.00	0.43
33:j:106:TRP:O	33:j:106:TRP:CD1	2.70	0.43
35:l:457:LEU:HD23	35:l:457:LEU:HA	1.84	0.43
50:l:702:CDL:H751	50:l:702:CDL:H711	1.99	0.43
39:p:124:GLN:OE1	39:p:127:ARG:NH1	2.51	0.43
50:s:401:CDL:H322	50:s:401:CDL:HB61	2.00	0.43
44:w:65:ASN:ND2	44:w:238:GLU:HG3	2.33	0.43
9:J:174:ILE:HG23	9:J:175:LYS:HG2	2.00	0.43
20:V:48:SER:N	20:V:51:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:16:GLY:HA2	50:s:401:CDL:H791	1.99	0.43
41:s:204:GLU:HA	41:s:208:VAL:O	2.18	0.43
1:A:367:ILE:HG13	1:A:438:LEU:HD13	2.00	0.43
9:J:304:LEU:O	9:J:307:VAL:HG22	2.18	0.43
20:V:20:ARG:HG3	20:V:20:ARG:HH11	1.84	0.43
23:Z:36:LEU:HD12	23:Z:41:LEU:HB2	2.00	0.43
32:i:68:MET:CE	34:k:37:MET:HG2	2.48	0.43
32:i:270:MET:O	32:i:275:SER:HB3	2.18	0.43
35:l:2:ASN:ND2	35:l:61:MET:HE1	2.32	0.43
35:l:175:ASN:O	35:l:179:ASP:OD1	2.37	0.43
37:n:46:LYS:HB2	37:n:46:LYS:HE3	1.87	0.43
40:r:114:GLU:HG3	40:r:115:LEU:N	2.33	0.43
44:w:265:ASP:OD1	44:w:265:ASP:N	2.46	0.43
12:M:219:SER:O	12:M:222:ILE:HG12	2.18	0.43
19:U:63:MET:HB2	19:U:66:VAL:CG1	2.48	0.43
31:h:2:PRO:HA	32:i:140:SER:HB2	2.01	0.43
32:i:267:ILE:HG12	32:i:279:PRO:HB3	2.00	0.43
34:k:27:MET:HG2	34:k:78:LEU:HD11	2.01	0.43
1:A:313:ASN:OD1	1:A:359:ARG:HG3	2.18	0.43
7:H:75:GLY:O	7:H:79:GLU:CD	2.62	0.43
10:K:74:ARG:O	10:K:77:GLN:NE2	2.52	0.43
15:P:123:GLN:CD	15:P:123:GLN:N	2.74	0.43
20:V:69:ILE:HD13	20:V:69:ILE:HA	1.89	0.43
24:a:147:ALA:HB2	40:r:173:SER:HB2	2.01	0.43
48:j:205:PLX:H132	48:j:205:PLX:H161	1.40	0.43
40:r:328:CYS:HB3	40:r:437:MET:HE1	2.00	0.43
48:r:502:PLX:H22	48:r:502:PLX:H1C3	1.75	0.43
1:A:53:LEU:HD13	1:A:136:HIS:CE1	2.54	0.43
1:A:204:TYR:HB3	1:A:377:GLU:OE1	2.18	0.43
9:J:344:PRO:HG2	9:J:347:LEU:HG	2.01	0.43
12:M:511:LYS:HE3	12:M:663:ASN:HB2	2.01	0.43
33:j:87:MET:HE3	33:j:87:MET:HB3	1.88	0.43
35:l:2:ASN:O	35:l:4:PHE:N	2.51	0.43
1:A:250:VAL:O	1:A:254:ILE:CD1	2.67	0.43
5:F:45:LYS:HD2	5:F:45:LYS:HA	1.68	0.43
24:a:176:LYS:HE3	31:h:45:HIS:CD2	2.53	0.43
25:b:111:LEU:HD23	25:b:111:LEU:HA	1.81	0.43
35:l:483:PRO:HD2	35:l:486:MET:HE2	2.00	0.43
40:r:8:THR:O	40:r:11:LEU:HB2	2.19	0.43
44:w:86:PHE:HB2	44:w:159:LEU:HD23	2.01	0.43
6:G:119:ILE:O	6:G:123:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:26:LEU:HD13	13:N:55:PHE:CD2	2.54	0.43
24:a:134:GLU:HA	24:a:137:MET:HE3	2.01	0.43
27:d:24:THR:HG21	43:v:73:SER:HB3	2.00	0.43
28:e:146:LYS:NZ	28:e:146:LYS:HB3	2.34	0.43
50:l:702:CDL:H861	50:l:702:CDL:H581	2.01	0.43
7:H:44:TYR:CD2	7:H:94:MET:HG2	2.54	0.42
12:M:29:SER:OG	12:M:30:ASN:N	2.50	0.42
14:O:84:ASP:OD1	14:O:88:ARG:NH1	2.51	0.42
16:Q:123:LEU:O	16:Q:127:LYS:HG2	2.20	0.42
32:i:136:LEU:HD23	32:i:205:LEU:HD21	2.00	0.42
33:j:51:PHE:CD2	41:s:133:LEU:HD12	2.52	0.42
35:l:336:LYS:HD3	35:l:336:LYS:HA	1.83	0.42
41:s:123:SER:HB3	41:s:214:GLU:HG3	2.01	0.42
44:w:345:GLU:HB2	44:w:352:ILE:HD12	2.01	0.42
6:G:141:PRO:O	6:G:145:VAL:HG22	2.19	0.42
32:i:153:LEU:O	32:i:157:MET:HG3	2.18	0.42
32:i:291:TYR:HA	40:r:151:PHE:HZ	1.85	0.42
57:j:202:PEE:H48	57:j:202:PEE:H55	1.84	0.42
7:H:34:VAL:HA	7:H:37:GLN:HE21	1.81	0.42
12:M:244:GLU:CD	12:M:266:ARG:HD2	2.44	0.42
12:M:507:THR:HG22	12:M:507:THR:O	2.20	0.42
16:Q:137:ASP:OD1	16:Q:144:MET:HB3	2.20	0.42
22:Y:100:LEU:CD1	22:Y:101:PRO:HD2	2.50	0.42
50:b:201:CDL:H472	27:d:43:ARG:HH12	1.84	0.42
27:d:54:GLN:C	27:d:54:GLN:CD	2.87	0.42
32:i:89:MET:CE	32:i:98:MET:HE3	2.45	0.42
35:l:184:LEU:HB2	40:r:393:ILE:HG12	2.01	0.42
8:I:5:THR:HB	13:N:2:GLU:CD	2.44	0.42
9:J:165:ILE:HG13	9:J:253:ILE:HD11	2.01	0.42
16:Q:294:ARG:NH2	16:Q:401:GLU:OE1	2.46	0.42
18:T:71:ILE:HD12	18:T:71:ILE:HA	1.86	0.42
21:W:98:MET:HG2	21:W:104:TRP:CE2	2.53	0.42
33:j:20:ILE:HG12	48:j:204:PLX:H142	2.02	0.42
35:l:488:MET:O	35:l:492:ILE:HG12	2.19	0.42
40:r:122:PHE:CD2	40:r:123:GLU:OE2	2.73	0.42
4:E:101:THR:OG1	15:P:219:VAL:O	2.29	0.42
11:L:75:ARG:HD2	11:L:75:ARG:HA	1.77	0.42
20:V:133:TRP:CZ3	57:r:501:PEE:H51	2.54	0.42
24:a:130:GLU:HG2	24:a:131:LYS:N	2.34	0.42
35:l:150:MET:HA	35:l:150:MET:CE	2.43	0.42
50:l:703:CDL:H521	50:l:703:CDL:HB61	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:GLY:HA2	45:C:301:SF4:S1	2.59	0.42
50:b:201:CDL:H341	50:b:201:CDL:H372	1.87	0.42
50:l:702:CDL:HA62	50:l:702:CDL:H522	2.00	0.42
50:l:703:CDL:H751	50:l:703:CDL:H781	1.83	0.42
41:s:184:MET:HE1	41:s:296:LEU:CB	2.45	0.42
3:C:188:LYS:HB3	3:C:191:ARG:HH11	1.83	0.42
6:G:84:LEU:HG	6:G:88:LYS:HE3	2.00	0.42
6:G:94:ASP:CG	6:G:97:LYS:HG3	2.45	0.42
18:T:95:HIS:ND1	18:T:96:PRO:O	2.50	0.42
20:V:134:GLN:OE1	32:i:274:GLU:HG3	2.19	0.42
25:b:106:PRO:HG2	25:b:120:MET:HG3	2.02	0.42
30:g:2:THR:O	30:g:2:THR:OG1	2.38	0.42
32:i:79:LEU:HB2	34:k:47:ILE:CD1	2.50	0.42
57:j:202:PEE:H26	41:s:295:PRO:HB3	2.01	0.42
35:l:373:LEU:HD22	35:l:431:PHE:HE2	1.79	0.42
40:r:148:TYR:O	40:r:152:TYR:HB2	2.19	0.42
48:r:502:PLX:H111	48:r:502:PLX:H141	1.89	0.42
41:s:234:MET:HE2	41:s:234:MET:HA	2.02	0.42
44:w:62:VAL:HG23	44:w:62:VAL:O	2.19	0.42
1:A:115:VAL:HB	1:A:156:ILE:HG12	2.02	0.42
27:d:90:MET:HE1	40:r:48:ASN:HB3	2.01	0.42
32:i:19:LEU:O	32:i:23:SER:OG	2.24	0.42
32:i:271:THR:HG22	32:i:276:ILE:HD13	2.02	0.42
35:l:108:MET:HE3	35:l:108:MET:HB3	1.82	0.42
38:o:105:PHE:HD2	40:r:263:MET:HE1	1.84	0.42
44:w:65:ASN:OD1	44:w:66:ILE:N	2.43	0.42
1:A:152:ARG:CZ	10:K:101:PRO:HD3	2.50	0.42
14:O:149:LEU:HD11	14:O:173:GLU:OE1	2.19	0.42
15:P:145:THR:OG1	15:P:146:TYR:N	2.52	0.42
50:V:201:CDL:OB6	35:l:576:MET:CE	2.68	0.42
25:b:83:HIS:CE1	35:l:1:MET:HB3	2.53	0.42
30:g:106:LYS:HD2	30:g:107:ASP:H	1.85	0.42
32:i:68:MET:HE1	34:k:37:MET:CE	2.42	0.42
57:j:202:PEE:H29	41:s:295:PRO:HB3	2.01	0.42
35:l:302:VAL:O	35:l:305:SER:OG	2.29	0.42
4:E:19:PRO:HB3	11:L:53:ILE:HG21	2.01	0.42
12:M:689:LEU:HD12	12:M:689:LEU:HA	1.88	0.42
14:O:100:LYS:HD2	14:O:100:LYS:HA	1.79	0.42
40:r:72:LEU:O	40:r:76:MET:HG3	2.20	0.42
41:s:199:ASP:OD2	41:s:279:ARG:NH1	2.53	0.42
57:j:202:PEE:H67	57:j:202:PEE:H73	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:33:LEU:O	40:r:37:ILE:HG12	2.20	0.41
1:A:120:GLY:HA3	1:A:204:TYR:HD1	1.84	0.41
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.84	0.41
22:Y:41:GLU:OE2	23:Z:12:SER:N	2.53	0.41
25:b:5:THR:OG1	25:b:8:GLU:HG3	2.19	0.41
32:i:58:LYS:HZ3	32:i:117:GLU:HG2	1.85	0.41
32:i:59:TYR:O	32:i:63:GLN:HG2	2.19	0.41
32:i:311:MET:HE2	32:i:311:MET:HB2	1.88	0.41
50:l:702:CDL:H641	48:r:503:PLX:H102	2.02	0.41
42:u:91:TYR:CD1	42:u:91:TYR:C	2.98	0.41
9:J:259:LYS:HD3	9:J:259:LYS:HA	1.88	0.41
12:M:213:MET:HE1	12:M:714:VAL:HA	2.03	0.41
27:d:74:ILE:HG22	28:e:142:PHE:CE1	2.55	0.41
35:l:292:ALA:HB2	35:l:304:PHE:HB3	2.02	0.41
50:l:702:CDL:HA62	50:l:702:CDL:C53	2.49	0.41
40:r:127:VAL:HB	40:r:128:PRO:HD3	2.01	0.41
27:d:33:LEU:HD12	27:d:33:LEU:HA	1.87	0.41
32:i:192:ALA:HB1	32:i:282:MET:HE1	2.02	0.41
33:j:87:MET:HE1	41:s:309:ILE:HD11	2.02	0.41
1:A:257:ARG:HH21	1:A:261:TRP:NE1	2.19	0.41
28:e:73:SER:C	28:e:75:GLY:H	2.27	0.41
57:j:202:PEE:H49	57:j:202:PEE:H7	1.94	0.41
37:n:58:LYS:HB2	37:n:58:LYS:HE2	1.90	0.41
41:s:55:LEU:HD13	41:s:221:ALA:HB2	2.02	0.41
1:A:366:ALA:HA	14:O:141:MET:HE1	2.03	0.41
7:H:34:VAL:HA	7:H:37:GLN:HE22	1.82	0.41
7:H:76:GLN:O	7:H:78:GLU:N	2.54	0.41
15:P:190:ASP:OD1	15:P:191:TYR:N	2.52	0.41
25:b:10:LEU:O	25:b:14:GLN:HG3	2.21	0.41
26:c:168:LEU:O	27:d:123:GLN:HG3	2.21	0.41
27:d:10:TYR:OH	28:e:123:GLU:OE1	2.38	0.41
32:i:41:ILE:HG13	34:k:73:LEU:HD21	2.01	0.41
44:w:245:PHE:O	44:w:249:MET:HB2	2.21	0.41
12:M:204:MET:HE2	12:M:204:MET:HB3	1.80	0.41
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.50	0.41
14:O:155:LYS:HE2	14:O:206:ASP:OD1	2.20	0.41
14:O:196:LEU:HD13	14:O:201:ILE:HD13	2.02	0.41
15:P:115:THR:OG1	15:P:116:ALA:N	2.53	0.41
25:b:32:GLU:HB2	25:b:33:PRO:HD3	2.03	0.41
27:d:76:GLU:HG2	28:e:146:LYS:NZ	2.35	0.41
32:i:313:MET:HE3	32:i:313:MET:HB2	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:35:GLY:HA3	36:m:20:PHE:CZ	2.56	0.41
50:l:702:CDL:C66	50:l:702:CDL:C62	2.86	0.41
50:l:703:CDL:H201	50:l:703:CDL:H172	1.92	0.41
57:l:705:PEE:H25	57:l:705:PEE:H19	1.90	0.41
42:u:152:PRO:O	42:u:153:GLU:HB2	2.20	0.41
43:v:21:ARG:HG3	43:v:21:ARG:NH1	2.36	0.41
1:A:131:ILE:CG2	1:A:165:GLU:HB3	2.51	0.41
3:C:158:PRO:HB2	9:J:92:MET:HE3	2.03	0.41
7:H:47:TYR:O	7:H:51:ILE:HG23	2.20	0.41
12:M:77:MET:CE	12:M:117:MET:HE2	2.49	0.41
16:Q:282:ASP:OD2	16:Q:437:LYS:NZ	2.34	0.41
50:V:202:CDL:H391	50:V:202:CDL:H421	1.95	0.41
21:W:86:MET:HE3	21:W:124:LEU:HB3	2.01	0.41
22:Y:97:LEU:HD22	22:Y:99:ILE:HG23	2.03	0.41
24:a:95:GLU:OE1	24:a:115:HIS:HD2	2.04	0.41
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.20	0.41
35:l:125:LEU:O	35:l:129:MET:HG2	2.21	0.41
35:l:149:ILE:HD13	35:l:149:ILE:HA	1.86	0.41
44:w:217:ARG:HG2	44:w:217:ARG:HH11	1.86	0.41
1:A:152:ARG:NH2	10:K:99:PRO:O	2.53	0.41
47:A:503:NAI:H6N	47:A:503:NAI:H2D	1.77	0.41
4:E:119:LEU:HD12	4:E:119:LEU:HA	1.87	0.41
9:J:129:LEU:HD23	9:J:167:ILE:HG13	2.03	0.41
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.03	0.41
12:M:94:MET:HE2	12:M:94:MET:HB2	1.84	0.41
12:M:395:GLU:OE2	12:M:417:ARG:NH1	2.54	0.41
14:O:215:LYS:O	14:O:219:ARG:NH1	2.54	0.41
16:Q:88:HIS:HB3	16:Q:91:ALA:HB2	2.02	0.41
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.56	0.41
6:X:87:LEU:HD23	6:X:87:LEU:HA	1.88	0.41
6:X:92:LYS:HD3	6:X:114:ASP:OD2	2.20	0.41
22:Y:102:ASP:HA	43:v:111:ARG:HD3	2.02	0.41
24:a:97:GLU:OE2	27:d:62:TYR:CE1	2.73	0.41
24:a:102:PRO:HG2	24:a:105:TYR:HB3	2.03	0.41
24:a:115:HIS:HE1	24:a:117:ILE:HD12	1.85	0.41
27:d:24:THR:CG2	43:v:73:SER:CA	2.99	0.41
29:f:36:HIS:O	44:w:355:LYS:HE2	2.21	0.41
31:h:7:GLN:O	31:h:11:GLY:N	2.54	0.41
32:i:45:MET:HB3	32:i:45:MET:HE3	1.74	0.41
32:i:228:LEU:O	32:i:231:SER:OG	2.35	0.41
32:i:265:MET:HE2	32:i:343:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:291:TYR:CZ	57:i:401:PEE:H48	2.55	0.41
35:l:338:MET:HE2	35:l:338:MET:HB3	1.93	0.41
50:l:702:CDL:H432	50:l:702:CDL:C62	2.50	0.41
36:m:20:PHE:CE2	36:m:33:LEU:HD13	2.55	0.41
36:m:77:GLU:N	36:m:77:GLU:OE2	2.54	0.41
38:o:5:LYS:HD2	38:o:5:LYS:HA	1.81	0.41
43:v:68:LYS:HE3	43:v:68:LYS:HB3	1.78	0.41
43:v:103:GLU:OE1	43:v:106:ARG:NH1	2.54	0.41
44:w:52:LYS:HE2	44:w:153:THR:O	2.20	0.41
2:B:68:ARG:NE	16:Q:260:GLU:OE2	2.44	0.41
8:I:43:VAL:HG23	8:I:44:GLY:H	1.86	0.41
9:J:157:LYS:NZ	9:J:197:GLU:OE1	2.52	0.41
13:N:55:PHE:CZ	13:N:58:ARG:HG3	2.56	0.41
15:P:161:LYS:HA	15:P:161:LYS:HD3	1.69	0.41
17:S:40:HIS:N	17:S:44:GLN:OE1	2.53	0.41
19:U:28:LEU:HD13	19:U:28:LEU:HA	1.91	0.41
19:U:67:PRO:HB3	19:U:72:ASP:HB2	2.02	0.41
20:V:44:LYS:HA	20:V:44:LYS:HD3	1.92	0.41
21:W:32:GLY:HA2	21:W:35:MET:HE2	2.02	0.41
25:b:82:ILE:HD13	25:b:82:ILE:HA	1.82	0.41
26:c:111:MET:O	26:c:111:MET:HG2	2.21	0.41
32:i:252:GLY:HA3	32:i:290:LEU:HD13	2.03	0.41
35:l:571:MET:HE2	35:l:571:MET:HB3	2.00	0.41
41:s:54:LYS:HE3	41:s:54:LYS:HB3	1.95	0.41
52:J:402:UQ:HM53	52:J:402:UQ:H72	1.81	0.40
50:V:202:CDL:H392	50:V:202:CDL:H361	1.92	0.40
50:V:202:CDL:H811	50:V:202:CDL:H842	1.89	0.40
33:j:33:LYS:HD3	41:s:61:LEU:HD21	2.03	0.40
35:l:230:HIS:N	35:l:231:PRO:HD3	2.36	0.40
1:A:194:ASP:OD2	10:K:98:MET:HG2	2.21	0.40
3:C:62:LEU:O	3:C:91:VAL:HA	2.21	0.40
13:N:64:TYR:CD1	13:N:81:MET:HE3	2.55	0.40
14:O:44:THR:HG22	14:O:46:GLU:N	2.35	0.40
16:Q:392:PRO:HA	16:Q:393:PRO:HD3	1.96	0.40
17:S:18:ILE:HD13	17:S:18:ILE:HA	1.88	0.40
20:V:34:LEU:HD23	20:V:34:LEU:HA	1.90	0.40
50:V:202:CDL:H792	50:V:202:CDL:H761	1.64	0.40
23:Z:52:ARG:HD3	35:l:435:PRO:O	2.21	0.40
32:i:7:THR:HG22	32:i:11:MET:CE	2.52	0.40
50:l:702:CDL:H202	50:l:702:CDL:H231	1.74	0.40
40:r:71:TRP:O	40:r:74:PRO:HD2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:118:PHE:O	40:r:122:PHE:HB3	2.21	0.40
3:C:75:GLU:OE1	16:Q:221:ARG:NH1	2.55	0.40
6:G:89:LEU:HD12	6:G:89:LEU:HA	1.85	0.40
11:L:99:MET:HE2	11:L:126:LEU:HD12	2.02	0.40
13:N:42:ASP:HB3	13:N:44:TYR:H	1.86	0.40
14:O:185:MET:HE2	14:O:185:MET:HB2	1.90	0.40
16:Q:62:LYS:HE2	16:Q:63:PRO:HD2	2.03	0.40
16:Q:74:ASP:OD1	16:Q:74:ASP:N	2.39	0.40
16:Q:342:ARG:HD2	21:W:21:TYR:CZ	2.55	0.40
27:d:162:ARG:NH1	28:e:140:ASN:OD1	2.54	0.40
28:e:92:PHE:O	28:e:96:SER:HB2	2.21	0.40
32:i:128:LEU:O	32:i:132:THR:OG1	2.22	0.40
32:i:321:LYS:HD3	32:i:321:LYS:HA	1.86	0.40
33:j:70:ALA:HB1	36:m:55:MET:SD	2.61	0.40
34:k:24:SER:HB3	34:k:89:TYR:CD1	2.57	0.40
35:l:233:LEU:HB3	35:l:234:PRO:HD3	2.02	0.40
35:l:243:VAL:HG13	35:l:247:LEU:HD13	2.03	0.40
39:p:108:HIS:HB3	39:p:111:GLU:HG3	2.02	0.40
1:A:364:VAL:HB	1:A:449:ARG:NH2	2.37	0.40
6:G:87:LEU:CD1	6:G:141:PRO:HG3	2.51	0.40
8:I:66:PRO:HB3	15:P:79:SER:HA	2.04	0.40
8:I:70:MET:HG3	15:P:66:ALA:CB	2.51	0.40
19:U:67:PRO:HG3	19:U:74:GLN:C	2.46	0.40
21:W:68:ARG:HD2	36:m:135:PHE:CD2	2.56	0.40
22:Y:51:THR:O	22:Y:54:GLN:HG2	2.21	0.40
24:a:96:ALA:HB3	27:d:63:TYR:HD1	1.87	0.40
26:c:141:LEU:HD23	26:c:141:LEU:HA	1.95	0.40
32:i:102:LEU:HD13	32:i:142:LEU:HG	2.04	0.40
50:k:101:CDL:H131	35:l:589:LEU:HD21	2.03	0.40
35:l:257:VAL:O	35:l:261:ILE:HG13	2.22	0.40
3:C:49:LYS:HD3	3:C:49:LYS:HA	1.85	0.40
4:E:28:ALA:HB1	4:E:79:VAL:HG11	2.02	0.40
12:M:48:THR:HA	12:M:95:PRO:HA	2.03	0.40
20:V:62:THR:HG23	20:V:104:ARG:HG2	2.03	0.40
26:c:155:PRO:HD3	43:v:4:HIS:CE1	2.56	0.40
27:d:9:VAL:O	27:d:109:ARG:NH2	2.52	0.40
27:d:28:ASN:HA	27:d:29:PRO:HD2	1.94	0.40
31:h:74:LYS:HB3	31:h:74:LYS:HE3	2.00	0.40
32:i:75:ILE:HD12	34:k:40:LEU:HD22	2.04	0.40
50:k:101:CDL:H592	50:k:101:CDL:H782	2.02	0.40
35:l:278:LEU:HD13	35:l:319:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:504:LEU:HD23	35:l:504:LEU:HA	1.90	0.40
40:r:266:MET:O	40:r:269:MET:HG2	2.20	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	431/433 (100%)	421 (98%)	10 (2%)	0	100	100
2	B	174/176 (99%)	171 (98%)	3 (2%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
6	G	86/88 (98%)	80 (93%)	5 (6%)	1 (1%)	10	40
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	101 (92%)	8 (7%)	1 (1%)	14	48
8	I	93/112 (83%)	80 (86%)	13 (14%)	0	100	100
9	J	340/342 (99%)	325 (96%)	14 (4%)	1 (0%)	36	70
10	K	41/43 (95%)	40 (98%)	1 (2%)	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	22 (3%)	0	100	100
13	N	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
14	O	215/217 (99%)	198 (92%)	17 (8%)	0	100	100
15	P	206/208 (99%)	198 (96%)	8 (4%)	0	100	100
16	Q	427/430 (99%)	413 (97%)	14 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	T	94/96 (98%)	93 (99%)	1 (1%)	0	100	100
19	U	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
20	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
21	W	140/142 (99%)	134 (96%)	6 (4%)	0	100	100
22	Y	65/70 (93%)	61 (94%)	4 (6%)	0	100	100
23	Z	78/84 (93%)	75 (96%)	3 (4%)	0	100	100
24	a	136/140 (97%)	133 (98%)	3 (2%)	0	100	100
25	b	94/126 (75%)	86 (92%)	8 (8%)	0	100	100
26	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
27	d	173/175 (99%)	170 (98%)	3 (2%)	0	100	100
28	e	102/107 (95%)	96 (94%)	6 (6%)	0	100	100
29	f	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
30	g	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	327 (95%)	18 (5%)	0	100	100
33	j	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
34	k	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
35	l	604/606 (100%)	583 (96%)	21 (4%)	0	100	100
36	m	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
37	n	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
38	o	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
39	p	176/178 (99%)	166 (94%)	9 (5%)	1 (1%)	21	56
40	r	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
41	s	316/318 (99%)	306 (97%)	9 (3%)	1 (0%)	36	70
42	u	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	56
43	v	122/125 (98%)	114 (93%)	8 (7%)	0	100	100
44	w	318/320 (99%)	305 (96%)	13 (4%)	0	100	100
All	All	8175/8326 (98%)	7857 (96%)	312 (4%)	6 (0%)	49	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	G	134	ASP

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Mol	Chain	Res	Type
41	s	208	VAL
9	J	38	HIS
7	H	77	ILE
42	u	152	PRO
39	p	174	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	346/346 (100%)	339 (98%)	7 (2%)	48	76
2	B	151/151 (100%)	151 (100%)	0	100	100
3	C	132/132 (100%)	130 (98%)	2 (2%)	57	80
4	E	106/107 (99%)	105 (99%)	1 (1%)	70	85
5	F	74/76 (97%)	70 (95%)	4 (5%)	20	53
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	79/81 (98%)	79 (100%)	0	100	100
7	H	99/99 (100%)	98 (99%)	1 (1%)	68	84
8	I	87/97 (90%)	85 (98%)	2 (2%)	44	74
9	J	296/296 (100%)	292 (99%)	4 (1%)	59	80
10	K	42/42 (100%)	41 (98%)	1 (2%)	43	73
11	L	113/113 (100%)	110 (97%)	3 (3%)	39	71
12	M	580/580 (100%)	567 (98%)	13 (2%)	45	74
13	N	130/130 (100%)	127 (98%)	3 (2%)	44	74
14	O	183/183 (100%)	180 (98%)	3 (2%)	55	79
15	P	190/190 (100%)	189 (100%)	1 (0%)	81	89
16	Q	370/370 (100%)	364 (98%)	6 (2%)	55	79
17	S	57/58 (98%)	54 (95%)	3 (5%)	20	54
18	T	79/79 (100%)	76 (96%)	3 (4%)	29	63
19	U	69/69 (100%)	67 (97%)	2 (3%)	37	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	V	101/101 (100%)	95 (94%)	6 (6%)	18	50
21	W	122/123 (99%)	119 (98%)	3 (2%)	42	72
22	Y	62/63 (98%)	61 (98%)	1 (2%)	55	79
23	Z	62/65 (95%)	61 (98%)	1 (2%)	55	79
24	a	121/122 (99%)	120 (99%)	1 (1%)	73	86
25	b	90/119 (76%)	89 (99%)	1 (1%)	65	83
26	c	141/141 (100%)	137 (97%)	4 (3%)	38	70
27	d	155/155 (100%)	151 (97%)	4 (3%)	40	72
28	e	96/99 (97%)	93 (97%)	3 (3%)	35	68
29	f	36/45 (80%)	35 (97%)	1 (3%)	38	70
30	g	108/109 (99%)	106 (98%)	2 (2%)	50	76
31	h	93/93 (100%)	91 (98%)	2 (2%)	45	74
32	i	311/311 (100%)	303 (97%)	8 (3%)	40	72
33	j	100/100 (100%)	99 (99%)	1 (1%)	68	84
34	k	85/85 (100%)	83 (98%)	2 (2%)	43	73
35	l	540/540 (100%)	528 (98%)	12 (2%)	45	74
36	m	129/141 (92%)	125 (97%)	4 (3%)	35	68
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	113/113 (100%)	113 (100%)	0	100	100
39	p	159/159 (100%)	158 (99%)	1 (1%)	78	88
40	r	410/410 (100%)	404 (98%)	6 (2%)	57	80
41	s	275/275 (100%)	269 (98%)	6 (2%)	45	74
42	u	152/153 (99%)	151 (99%)	1 (1%)	76	86
43	v	104/111 (94%)	103 (99%)	1 (1%)	68	84
44	w	281/283 (99%)	276 (98%)	5 (2%)	51	77
All	All	7158/7249 (99%)	7023 (98%)	135 (2%)	49	76

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	97	LEU
1	A	106	SER

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Mol	Chain	Res	Type
1	A	245	VAL
1	A	288	VAL
1	A	314	LEU
1	A	455	LEU
3	C	71	CYS
3	C	86	MET
4	E	68	MET
5	F	27	SER
5	F	90	THR
5	F	91	LEU
5	F	96	SER
7	H	48	THR
8	I	29	GLN
8	I	90	THR
9	J	311	GLU
9	J	322	VAL
9	J	324	MET
9	J	367	GLU
10	K	76	LEU
11	L	77	VAL
11	L	86	ASN
11	L	117	THR
12	M	187	SER
12	M	249	GLU
12	M	347	ASP
12	M	374	THR
12	M	398	ASP
12	M	421	SER
12	M	455	ILE
12	M	465	ILE
12	M	494	SER
12	M	500	ILE
12	M	632	MET
12	M	636	TYR
12	M	697	THR
13	N	4	VAL
13	N	96	ASP
13	N	104	THR
14	O	44	THR
14	O	144	ASN
14	O	235	THR
15	P	128	ILE

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Mol	Chain	Res	Type
16	Q	76	LEU
16	Q	217	VAL
16	Q	242	ASP
16	Q	272	THR
16	Q	308	TYR
16	Q	345	SER
17	S	6	LEU
17	S	11	VAL
17	S	47	LEU
18	T	31	THR
18	T	39	THR
18	T	104	LYS
19	U	66	VAL
19	U	68	SER
20	V	6	LEU
20	V	27	SER
20	V	60	THR
20	V	73	THR
20	V	115	CYS
20	V	134	GLN
21	W	34	SER
21	W	96	ILE
21	W	109	SER
22	Y	77	SER
23	Z	68	LEU
24	a	148	GLU
25	b	79	VAL
26	c	33	THR
26	c	99	LEU
26	c	164	ASN
26	c	182	VAL
27	d	17	THR
27	d	26	LEU
27	d	58	LYS
27	d	120	SER
28	e	78	LYS
28	e	83	ASP
28	e	146	LYS
29	f	61	GLN
30	g	98	SER
30	g	113	GLU
31	h	70	GLN

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Mol	Chain	Res	Type
31	h	91	LYS
32	i	62	THR
32	i	68	MET
32	i	223	SER
32	i	229	SER
32	i	271	THR
32	i	280	THR
32	i	335	LEU
32	i	336	VAL
33	j	46	SER
34	k	34	GLU
34	k	57	ASN
35	l	1	MET
35	l	59	GLN
35	l	73	THR
35	l	185	SER
35	l	229	LEU
35	l	327	LEU
35	l	343	SER
35	l	373	LEU
35	l	426	ILE
35	l	525	MET
35	l	559	GLU
35	l	597	ILE
36	m	72	THR
36	m	102	CYS
36	m	127	ILE
36	m	160	SER
39	p	13	GLN
40	r	129	THR
40	r	179	ILE
40	r	247	THR
40	r	253	LEU
40	r	408	LEU
40	r	440	HIS
41	s	24	GLU
41	s	35	LYS
41	s	40	VAL
41	s	139	THR
41	s	246	SER
41	s	300	LEU
42	u	103	GLN

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Mol	Chain	Res	Type
43	v	53	LEU
44	w	63	ASP
44	w	95	ASP
44	w	241	TYR
44	w	347	VAL
44	w	354	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	393	ASN
1	A	451	GLN
4	E	58	GLN
5	F	86	GLN
6	G	142	GLN
7	H	37	GLN
9	J	122	HIS
9	J	376	ASN
10	K	79	HIS
11	L	71	HIS
11	L	86	ASN
12	M	39	GLN
12	M	74	ASN
12	M	123	ASN
12	M	425	ASN
12	M	460	HIS
12	M	540	ASN
12	M	598	ASN
12	M	604	GLN
12	M	669	ASN
12	M	688	GLN
13	N	112	ASN
14	O	90	ASN
14	O	189	ASN
14	O	246	GLN
15	P	55	HIS
15	P	77	GLN
15	P	131	ASN
15	P	228	GLN
16	Q	223	HIS
16	Q	233	HIS

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Mol	Chain	Res	Type
16	Q	265	ASN
16	Q	339	GLN
17	S	61	HIS
18	T	101	ASN
18	T	120	GLN
21	W	76	GLN
6	X	101	ASN
23	Z	21	GLN
24	a	115	HIS
25	b	13	GLN
26	c	127	ASN
27	d	23	GLN
27	d	54	GLN
27	d	107	GLN
27	d	131	GLN
28	e	86	ASN
29	f	61	GLN
30	g	99	HIS
31	h	45	HIS
32	i	63	GLN
32	i	134	GLN
32	i	172	GLN
34	k	57	ASN
34	k	92	ASN
35	l	34	ASN
35	l	72	GLN
35	l	165	ASN
35	l	194	ASN
35	l	321	GLN
35	l	452	ASN
35	l	579	ASN
37	n	6	GLN
38	o	117	GLN
39	p	169	HIS
40	r	51	ASN
40	r	81	GLN
40	r	139	GLN
41	s	235	ASN
42	u	30	HIS
42	u	163	HIS
44	w	111	ASN
44	w	323	GLN

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Mol	Chain	Res	Type
44	w	344	ASN

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	2.01	1 (10%)	5,13,15	6.01	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	5.76	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	12.30	130.75	119.48
16	Q	118	2MR	CD-NE-CZ	3.96	130.79	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.40	130.95	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 2 are monoatomic - leaving 43 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$
58	ADP	w	401	-	28,29,29	3.20	9 (32%)	43,45,45	1.90	9 (20%)
50	CDL	l	703	-	99,99,99	1.11	9 (9%)	105,111,111	0.95	5 (4%)
55	UQ1	Q	501	-	18,18,18	2.35	6 (33%)	24,25,25	2.16	7 (29%)
50	CDL	V	202	-	99,99,99	1.11	8 (8%)	105,111,111	0.89	4 (3%)
57	PEE	l	705	-	45,45,50	1.24	6 (13%)	48,50,55	1.05	2 (4%)
52	UQ	s	402	-	38,38,63	3.65	12 (31%)	48,49,79	2.74	16 (33%)
48	PLX	r	502	-	51,51,51	1.21	5 (9%)	53,59,59	0.65	1 (1%)
57	PEE	j	203	-	40,40,50	1.17	4 (10%)	43,45,55	1.07	3 (6%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
50	CDL	r	504	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
57	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
45	SF4	C	301	3	0,12,12	-	-	-	-	-
49	8Q1	X	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.65	6 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
50	CDL	l	702	-	98,98,99	0.93	4 (4%)	104,110,111	1.09	5 (4%)
53	FES	M	803	12	0,4,4	-	-	-		
57	PEE	W	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.03	2 (4%)
52	UQ	J	402	-	33,33,63	3.51	9 (27%)	42,43,79	2.74	14 (33%)
57	PEE	l	701	-	39,39,50	1.34	6 (15%)	42,44,55	1.10	3 (7%)
47	NAI	A	503	-	47,48,48	4.01	22 (46%)	64,73,73	1.71	12 (18%)
48	PLX	g	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.66	1 (1%)
45	SF4	A	501	1	0,12,12	-	-	-		
45	SF4	M	802	12	0,12,12	-	-	-		
48	PLX	a	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.62	1 (1%)
46	FMN	A	502	-	33,33,33	1.08	2 (6%)	48,50,50	1.29	8 (16%)
50	CDL	s	401	-	88,88,99	1.16	8 (9%)	94,100,111	0.91	4 (4%)
48	PLX	r	503	-	51,51,51	1.22	5 (9%)	53,59,59	0.59	1 (1%)
50	CDL	k	101	-	93,93,99	1.14	8 (8%)	99,105,111	0.87	4 (4%)
45	SF4	B	302	2	0,12,12	-	-	-		
50	CDL	V	201	-	93,93,99	1.14	9 (9%)	99,105,111	0.91	5 (5%)
57	PEE	j	202	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
50	CDL	n	101	-	54,54,99	1.38	8 (14%)	60,66,111	1.09	4 (6%)
57	PEE	l	704	-	50,50,50	1.18	6 (12%)	53,55,55	0.94	2 (3%)
48	PLX	j	205	-	51,51,51	1.21	4 (7%)	53,59,59	0.65	1 (1%)
48	PLX	j	204	-	51,51,51	1.20	4 (7%)	53,59,59	0.64	2 (3%)
50	CDL	b	201	-	99,99,99	1.12	9 (9%)	105,111,111	0.88	4 (3%)
51	NDP	J	401	-	51,52,52	4.30	25 (49%)	71,80,80	2.20	12 (16%)
57	PEE	j	201	-	46,46,50	1.23	6 (13%)	49,51,55	0.95	2 (4%)
48	PLX	C	302	-	51,51,51	1.20	4 (7%)	53,59,59	0.68	1 (1%)
45	SF4	M	801	12	0,12,12	-	-	-		
49	8Q1	G	201	6	32,34,34	1.60	5 (15%)	39,43,43	1.81	6 (15%)
53	FES	O	301	14	0,4,4	-	-	-		
57	PEE	i	401	-	46,46,50	1.23	6 (13%)	49,51,55	1.04	2 (4%)
50	CDL	I	201	-	50,50,99	1.41	9 (18%)	56,62,111	1.15	4 (7%)

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
58	ADP	w	401	-	-	5/16/32/32	0/3/3/3
50	CDL	l	703	-	-	65/110/110/110	-
55	UQ1	Q	501	-	-	4/9/33/33	0/1/1/1
50	CDL	V	202	-	-	58/110/110/110	-
57	PEE	l	705	-	-	17/49/49/54	-
52	UQ	s	402	-	-	12/33/57/87	0/1/1/1
48	PLX	r	502	-	-	29/55/55/55	-
57	PEE	j	203	-	-	22/44/44/54	-
45	SF4	B	301	2	-	-	0/6/5/5
50	CDL	r	504	-	-	56/110/110/110	-
57	PEE	r	501	-	-	24/54/54/54	-
45	SF4	C	301	3	-	-	0/6/5/5
49	8Q1	X	201	-	-	11/41/41/41	-
50	CDL	l	702	-	-	41/109/109/110	-
57	PEE	W	201	-	-	17/44/44/54	-
57	PEE	l	701	-	-	21/43/43/54	-
52	UQ	J	402	-	-	8/27/51/87	0/1/1/1
53	FES	M	803	12	-	-	0/1/1/1
47	NAI	A	503	-	-	8/29/72/72	0/5/5/5
48	PLX	g	201	-	-	29/55/55/55	-
45	SF4	A	501	1	-	-	0/6/5/5
45	SF4	M	802	12	-	-	0/6/5/5
48	PLX	a	201	-	-	26/55/55/55	-
46	FMN	A	502	-	-	10/18/18/18	0/3/3/3
50	CDL	s	401	-	-	47/99/99/110	-
48	PLX	r	503	-	-	30/55/55/55	-
50	CDL	k	101	-	-	47/104/104/110	-
50	CDL	V	201	-	-	55/104/104/110	-
57	PEE	j	202	-	-	24/54/54/54	-
45	SF4	B	302	2	-	-	0/6/5/5
50	CDL	n	101	-	-	26/65/65/110	-
57	PEE	l	704	-	-	29/54/54/54	-
48	PLX	j	205	-	-	24/55/55/55	-
48	PLX	j	204	-	-	32/55/55/55	-
50	CDL	b	201	-	-	62/110/110/110	-
51	NDP	J	401	-	-	4/34/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PEE	j	201	-	-	27/50/50/54	-
48	PLX	C	302	-	-	26/55/55/55	-
45	SF4	M	801	12	-	-	0/6/5/5
49	8Q1	G	201	6	-	16/41/41/41	-
53	FES	O	301	14	-	-	0/1/1/1
57	PEE	i	401	-	-	23/50/50/54	-
50	CDL	I	201	-	-	31/61/61/110	-

All (257) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-13.31	1.23	1.53
51	J	401	NDP	O4D-C4D	10.84	1.69	1.45
47	A	503	NAI	C3D-C4D	-10.34	1.26	1.53
52	s	402	UQ	C18-C19	10.04	1.56	1.33
51	J	401	NDP	C3D-C4D	-9.93	1.27	1.53
52	J	402	UQ	C18-C19	9.87	1.55	1.33
52	s	402	UQ	C13-C14	9.62	1.55	1.33
52	J	402	UQ	C13-C14	9.49	1.54	1.33
52	s	402	UQ	C23-C24	9.46	1.54	1.33
52	s	402	UQ	C8-C9	9.41	1.54	1.33
52	J	402	UQ	C8-C9	9.38	1.54	1.33
47	A	503	NAI	O4B-C1B	9.37	1.63	1.42
58	w	401	ADP	C3'-C4'	-8.96	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.31	1.26	1.45
51	J	401	NDP	O4B-C4B	-7.90	1.27	1.45
58	w	401	ADP	O4'-C4'	7.87	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.71	1.29	1.53
52	J	402	UQ	C23-C24	7.50	1.54	1.32
51	J	401	NDP	C2N-C3N	7.43	1.55	1.35
47	A	503	NAI	C2B-C1B	-7.35	1.30	1.53
51	J	401	NDP	C6N-C5N	7.35	1.55	1.33
52	s	402	UQ	C28-C29	7.32	1.54	1.32
55	Q	501	UQ1	C8-C9	7.09	1.53	1.32
47	A	503	NAI	O4D-C4D	7.02	1.60	1.45
58	w	401	ADP	PA-O3A	6.76	1.66	1.59
51	J	401	NDP	PN-O3	6.60	1.66	1.59
47	A	503	NAI	PA-O3	6.34	1.66	1.59
47	A	503	NAI	C2D-C3D	6.00	1.69	1.53
51	J	401	NDP	P2B-O2B	5.98	1.70	1.59
51	J	401	NDP	C6A-N6A	5.76	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	PA-O3	5.72	1.65	1.59
47	A	503	NAI	O4D-C1D	5.58	1.54	1.42
47	A	503	NAI	PN-O3	5.48	1.65	1.59
58	w	401	ADP	C6-N6	5.43	1.48	1.34
51	J	401	NDP	C3B-C4B	5.34	1.66	1.53
47	A	503	NAI	C7N-N7N	5.31	1.48	1.33
47	A	503	NAI	C4N-C3N	-5.25	1.40	1.50
51	J	401	NDP	C6N-N1N	5.14	1.49	1.37
49	X	201	8Q1	C39-N41	5.09	1.45	1.33
49	X	201	8Q1	C34-N36	5.07	1.45	1.33
47	A	503	NAI	C6A-N6A	5.04	1.47	1.34
51	J	401	NDP	O4D-C1D	-4.99	1.30	1.42
49	G	201	8Q1	C39-N41	4.99	1.45	1.33
49	G	201	8Q1	C34-N36	4.88	1.45	1.33
51	J	401	NDP	O4B-C1B	4.75	1.53	1.42
51	J	401	NDP	C1B-N9A	-4.61	1.33	1.46
58	w	401	ADP	O4'-C1'	-4.56	1.31	1.42
47	A	503	NAI	O2B-C2B	4.33	1.53	1.43
50	l	702	CDL	OB8-CB7	4.30	1.45	1.33
50	l	702	CDL	OA8-CA7	4.28	1.45	1.33
50	l	702	CDL	OA6-CA5	4.15	1.46	1.34
50	l	702	CDL	OB6-CB5	4.09	1.45	1.34
51	J	401	NDP	O2D-C2D	-3.97	1.33	1.43
51	J	401	NDP	C7N-N7N	3.87	1.44	1.33
57	l	701	PEE	C18-C19	3.84	1.53	1.31
57	W	201	PEE	C18-C19	3.83	1.53	1.31
57	r	501	PEE	C18-C19	3.83	1.53	1.31
57	j	201	PEE	C18-C19	3.83	1.53	1.31
57	l	704	PEE	C18-C19	3.82	1.53	1.31
57	j	203	PEE	C18-C19	3.82	1.53	1.31
57	j	202	PEE	C18-C19	3.81	1.53	1.31
57	l	705	PEE	C18-C19	3.81	1.53	1.31
57	i	401	PEE	C18-C19	3.79	1.53	1.31
57	r	501	PEE	C39-C38	3.73	1.52	1.31
57	l	701	PEE	C39-C38	3.73	1.52	1.31
57	j	201	PEE	C39-C38	3.73	1.52	1.31
57	l	705	PEE	C39-C38	3.73	1.52	1.31
57	j	202	PEE	C39-C38	3.72	1.52	1.31
57	i	401	PEE	C39-C38	3.71	1.52	1.31
57	l	704	PEE	C39-C38	3.68	1.52	1.31
47	A	503	NAI	C7N-C3N	3.61	1.56	1.48
50	I	201	CDL	OA8-CA7	3.50	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	V	201	CDL	OA8-CA7	3.49	1.43	1.33
50	n	101	CDL	OA8-CA7	3.46	1.43	1.33
50	b	201	CDL	OA8-CA7	3.43	1.43	1.33
50	k	101	CDL	OA8-CA7	3.43	1.43	1.33
50	l	703	CDL	OA8-CA7	3.42	1.43	1.33
50	r	504	CDL	OA8-CA7	3.42	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.40	1.40	1.49
50	V	202	CDL	OA8-CA7	3.40	1.43	1.33
46	A	502	FMN	C4A-N5	3.38	1.38	1.30
50	s	401	CDL	OA8-CA7	3.36	1.43	1.33
58	w	401	ADP	C8-N9	-3.34	1.31	1.37
50	k	101	CDL	OA6-CA5	3.25	1.43	1.34
58	w	401	ADP	O2'-C2'	-3.15	1.35	1.43
51	J	401	NDP	C8A-N9A	-3.14	1.32	1.37
50	r	504	CDL	OB6-CB5	3.13	1.43	1.34
50	V	201	CDL	OA6-CA5	3.10	1.43	1.34
50	b	201	CDL	OB6-CB5	3.09	1.43	1.34
50	s	401	CDL	OB6-CB5	3.06	1.42	1.34
50	r	504	CDL	OB8-CB7	3.05	1.42	1.33
50	k	101	CDL	OB6-CB5	3.05	1.42	1.34
50	l	703	CDL	OA6-CA5	3.03	1.42	1.34
50	s	401	CDL	OA6-CA5	3.02	1.42	1.34
51	J	401	NDP	C5A-N7A	-3.02	1.33	1.39
50	b	201	CDL	OB8-CB7	3.01	1.42	1.33
50	l	703	CDL	OB8-CB7	3.00	1.42	1.33
50	n	101	CDL	OB6-CB5	2.99	1.42	1.34
50	I	201	CDL	OB8-CB7	2.98	1.42	1.33
50	V	202	CDL	OB6-CB5	2.98	1.42	1.34
50	n	101	CDL	OB8-CB7	2.97	1.42	1.33
50	l	703	CDL	OB6-CB5	2.97	1.42	1.34
50	n	101	CDL	OA6-CA5	2.97	1.42	1.34
50	k	101	CDL	OB8-CB7	2.96	1.42	1.33
51	J	401	NDP	C7N-C3N	2.96	1.55	1.48
50	V	201	CDL	OB8-CB7	2.96	1.42	1.33
50	r	504	CDL	OA6-CA5	2.96	1.42	1.34
50	b	201	CDL	OA6-CA5	2.95	1.42	1.34
50	s	401	CDL	OB8-CB7	2.95	1.41	1.33
50	V	202	CDL	OB8-CB7	2.94	1.41	1.33
51	J	401	NDP	O3D-C3D	2.94	1.50	1.43
58	w	401	ADP	O3'-C3'	2.94	1.50	1.43
48	g	201	PLX	O6-C4	-2.94	1.40	1.44
50	I	201	CDL	OA6-CA5	2.94	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	I	201	CDL	OB6-CB5	2.92	1.42	1.34
48	C	302	PLX	O6-C4	-2.92	1.40	1.44
50	V	202	CDL	OA6-CA5	2.89	1.42	1.34
50	V	201	CDL	OB6-CB4	-2.86	1.39	1.46
48	a	201	PLX	O6-C4	-2.86	1.41	1.44
52	J	402	UQ	C6-C1	2.76	1.54	1.46
55	Q	501	UQ1	C6-C1	2.71	1.54	1.46
47	A	503	NAI	C8A-N9A	-2.69	1.33	1.37
57	j	201	PEE	O2-C2	-2.66	1.40	1.46
57	i	401	PEE	O2-C2	-2.65	1.40	1.46
48	r	503	PLX	O6-C4	-2.65	1.41	1.44
48	r	502	PLX	O6-C4	-2.64	1.41	1.44
50	V	202	CDL	OA6-CA4	-2.64	1.40	1.46
50	r	504	CDL	OA6-CA4	-2.61	1.40	1.46
48	j	205	PLX	O6-C4	-2.60	1.41	1.44
50	b	201	CDL	OA6-CA4	-2.60	1.40	1.46
57	j	202	PEE	O2-C2	-2.59	1.40	1.46
48	j	204	PLX	O6-C4	-2.59	1.41	1.44
57	r	501	PEE	O2-C2	-2.58	1.40	1.46
50	n	101	CDL	OA6-CA4	-2.58	1.40	1.46
49	G	201	8Q1	O40-C39	-2.57	1.18	1.23
52	s	402	UQ	C6-C1	2.57	1.53	1.46
57	j	202	PEE	O3-C30	2.56	1.40	1.33
57	j	203	PEE	O2-C2	-2.55	1.40	1.46
51	J	401	NDP	O2B-C2B	2.54	1.52	1.44
50	s	401	CDL	OA6-CA4	-2.52	1.40	1.46
57	j	203	PEE	O3-C30	2.52	1.40	1.33
50	I	201	CDL	OA6-CA4	-2.52	1.40	1.46
57	W	201	PEE	O2-C2	-2.52	1.40	1.46
57	l	705	PEE	O2-C2	-2.51	1.40	1.46
57	l	701	PEE	O3-C30	2.51	1.40	1.33
57	l	701	PEE	O2-C2	-2.50	1.40	1.46
57	l	704	PEE	O2-C2	-2.50	1.40	1.46
49	G	201	8Q1	O35-C34	-2.49	1.18	1.23
57	l	704	PEE	O3-C30	2.47	1.40	1.33
57	l	705	PEE	O3-C30	2.46	1.40	1.33
48	j	205	PLX	C7-C6	2.46	1.55	1.50
46	A	502	FMN	C10-N1	2.45	1.38	1.33
50	I	201	CDL	OB6-CB4	-2.44	1.40	1.46
57	j	201	PEE	O3-C30	2.43	1.40	1.33
47	A	503	NAI	PN-O5D	2.43	1.68	1.59
49	X	201	8Q1	C1-S44	2.42	1.82	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	r	503	PLX	C7-C6	2.42	1.55	1.50
57	W	201	PEE	O3-C30	2.41	1.40	1.33
57	i	401	PEE	O3-C30	2.40	1.40	1.33
58	w	401	ADP	C5-N7	-2.39	1.34	1.39
50	l	703	CDL	OA6-CA4	-2.39	1.41	1.46
48	a	201	PLX	C7-C6	2.39	1.55	1.50
47	A	503	NAI	C5B-C4B	2.37	1.58	1.51
47	A	503	NAI	C6N-C5N	2.37	1.40	1.33
57	r	501	PEE	O3-C30	2.36	1.40	1.33
50	l	703	CDL	OB6-CB4	-2.35	1.41	1.46
52	s	402	UQ	C7-C8	2.35	1.54	1.50
49	X	201	8Q1	O35-C34	-2.34	1.18	1.23
48	r	502	PLX	C7-C6	2.34	1.55	1.50
51	J	401	NDP	C2D-C3D	2.34	1.59	1.53
47	A	503	NAI	O3B-C3B	-2.34	1.37	1.43
50	n	101	CDL	OB6-CB4	-2.34	1.41	1.46
57	l	705	PEE	O2-C10	2.33	1.40	1.34
50	V	202	CDL	OB6-CB4	-2.33	1.41	1.46
50	V	201	CDL	PB2-OB2	2.33	1.68	1.59
57	l	701	PEE	O2-C10	2.33	1.40	1.34
48	g	201	PLX	C7-C6	2.32	1.55	1.50
57	l	704	PEE	O2-C10	2.32	1.40	1.34
49	X	201	8Q1	C6-C1	2.32	1.53	1.50
49	G	201	8Q1	C1-S44	2.32	1.81	1.76
48	j	204	PLX	C7-C6	2.31	1.55	1.50
55	Q	501	UQ1	O2-CM2	-2.31	1.40	1.45
57	W	201	PEE	O2-C10	2.30	1.40	1.34
50	V	201	CDL	PB2-OB5	2.28	1.68	1.59
57	r	501	PEE	O2-C10	2.28	1.40	1.34
52	J	402	UQ	C7-C8	2.27	1.54	1.50
50	b	201	CDL	OB6-CB4	-2.26	1.41	1.46
50	V	202	CDL	PB2-OB2	2.26	1.68	1.59
48	j	205	PLX	P1-O4	2.26	1.68	1.59
57	j	201	PEE	O3-C3	-2.26	1.40	1.45
50	V	201	CDL	OA6-CA4	-2.26	1.41	1.46
50	b	201	CDL	PB2-OB5	2.25	1.68	1.59
50	l	703	CDL	PB2-OB5	2.25	1.68	1.59
57	j	201	PEE	O2-C10	2.25	1.40	1.34
50	k	101	CDL	OB6-CB4	-2.25	1.41	1.46
52	s	402	UQ	O1-C1	-2.24	1.18	1.23
50	r	504	CDL	PB2-OB2	2.24	1.68	1.59
50	b	201	CDL	PB2-OB2	2.24	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	r	502	PLX	P1-O4	2.24	1.68	1.59
50	n	101	CDL	PB2-OB5	2.24	1.68	1.59
57	r	501	PEE	O3-C3	-2.24	1.40	1.45
50	n	101	CDL	PB2-OB2	2.24	1.68	1.59
49	X	201	8Q1	O40-C39	-2.24	1.18	1.23
57	i	401	PEE	O2-C10	2.24	1.40	1.34
50	k	101	CDL	PB2-OB5	2.24	1.68	1.59
50	s	401	CDL	OB6-CB4	-2.23	1.41	1.46
50	k	101	CDL	PB2-OB2	2.23	1.68	1.59
50	s	401	CDL	PB2-OB2	2.22	1.68	1.59
57	j	202	PEE	O2-C10	2.22	1.40	1.34
50	r	504	CDL	PB2-OB5	2.22	1.68	1.59
50	V	202	CDL	PB2-OB5	2.22	1.68	1.59
48	C	302	PLX	C7-C6	2.22	1.55	1.50
57	j	203	PEE	O2-C10	2.20	1.40	1.34
50	r	504	CDL	OB6-CB4	-2.19	1.41	1.46
48	a	201	PLX	P1-O4	2.18	1.67	1.59
52	J	402	UQ	C21-C19	2.18	1.55	1.51
57	i	401	PEE	O3-C3	-2.18	1.40	1.45
50	l	703	CDL	PB2-OB2	2.17	1.67	1.59
52	J	402	UQ	O4-C4	-2.17	1.18	1.23
55	Q	501	UQ1	O3-CM3	-2.17	1.40	1.45
50	s	401	CDL	PB2-OB5	2.16	1.67	1.59
48	g	201	PLX	P1-O4	2.16	1.67	1.59
50	I	201	CDL	PB2-OB5	2.16	1.67	1.59
51	J	401	NDP	O7N-C7N	-2.15	1.19	1.24
52	s	402	UQ	O4-C4	-2.15	1.18	1.23
57	l	704	PEE	O3-C3	-2.15	1.40	1.45
48	r	503	PLX	P1-O4	2.14	1.67	1.59
48	j	205	PLX	P1-O1	2.14	1.67	1.59
50	I	201	CDL	PB2-OB2	2.13	1.67	1.59
51	J	401	NDP	PA-O5B	2.13	1.67	1.59
48	j	204	PLX	P1-O4	2.13	1.67	1.59
48	r	502	PLX	C25-C24	2.13	1.55	1.50
57	l	701	PEE	O3-C3	-2.12	1.40	1.45
50	k	101	CDL	OA6-CA4	-2.12	1.41	1.46
50	V	201	CDL	OB6-CB5	2.12	1.40	1.34
57	W	201	PEE	O3-C3	-2.11	1.40	1.45
48	r	502	PLX	P1-O1	2.11	1.67	1.59
57	l	705	PEE	O3-C3	-2.11	1.40	1.45
52	s	402	UQ	C21-C19	2.09	1.55	1.51
55	Q	501	UQ1	O1-C1	-2.09	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	J	402	UQ	O3-CM3	-2.09	1.40	1.45
47	A	503	NAI	C5A-N7A	-2.09	1.35	1.39
48	j	204	PLX	P1-O1	2.08	1.67	1.59
48	C	302	PLX	P1-O4	2.08	1.67	1.59
52	s	402	UQ	C5-C4	2.08	1.54	1.47
48	C	302	PLX	P1-O1	2.07	1.67	1.59
50	V	201	CDL	C11-CA5	2.07	1.56	1.50
48	g	201	PLX	P1-O1	2.07	1.67	1.59
48	r	503	PLX	P1-O1	2.06	1.67	1.59
48	r	503	PLX	C1-C2	2.06	1.57	1.51
48	a	201	PLX	P1-O1	2.06	1.67	1.59
55	Q	501	UQ1	O4-C4	-2.06	1.18	1.23
50	b	201	CDL	C11-CA5	2.06	1.56	1.50
52	s	402	UQ	O3-CM3	-2.05	1.40	1.45
50	l	703	CDL	C11-CA5	2.05	1.56	1.50
50	I	201	CDL	C11-CA5	2.03	1.56	1.50
57	j	202	PEE	O3-C3	-2.02	1.40	1.45

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	402	UQ	C7-C8-C9	-7.88	113.26	126.83
51	J	401	NDP	C1D-N1N-C2N	-7.87	108.18	121.14
52	s	402	UQ	C7-C8-C9	-7.51	113.89	126.83
51	J	401	NDP	C3N-C2N-N1N	-7.32	112.46	123.20
49	G	201	8Q1	C6-C1-S44	7.05	121.80	113.40
52	J	402	UQ	C17-C18-C19	-6.54	112.64	127.62
52	J	402	UQ	C12-C13-C14	-6.50	112.74	127.62
52	s	402	UQ	C22-C23-C24	-6.20	113.44	127.62
51	J	401	NDP	C6N-N1N-C2N	-6.07	112.83	119.32
52	s	402	UQ	C12-C13-C14	-5.94	114.03	127.62
52	s	402	UQ	C17-C18-C19	-5.91	114.10	127.62
49	X	201	8Q1	C6-C1-S44	5.90	120.44	113.40
51	J	401	NDP	C1D-N1N-C6N	-5.54	109.06	120.77
51	J	401	NDP	C5A-C4A-N3A	-5.40	119.28	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.36	119.33	126.72
58	w	401	ADP	C5-C4-N3	-5.28	119.44	126.72
55	Q	501	UQ1	C7-C6-C1	5.12	124.46	118.52
55	Q	501	UQ1	C7-C6-C5	-4.59	117.03	124.89
49	G	201	8Q1	O4-C1-C6	-4.59	118.69	123.98
55	Q	501	UQ1	C7-C8-C9	-4.57	114.32	127.25
52	s	402	UQ	C27-C28-C29	-4.57	112.42	127.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	J	402	UQ	C22-C23-C24	-4.53	112.53	127.64
58	w	401	ADP	N3-C2-N1	-4.52	121.74	128.58
52	s	402	UQ	C10-C9-C8	-4.48	112.13	123.63
50	l	703	CDL	OA6-CA5-C11	4.47	121.15	111.48
50	l	702	CDL	OA6-CA5-C11	4.44	121.09	111.48
47	A	503	NAI	N3A-C2A-N1A	-4.44	121.87	128.58
52	J	402	UQ	C20-C19-C18	-4.42	112.29	123.63
50	V	201	CDL	OB6-CB5-C51	4.39	120.97	111.48
52	J	402	UQ	C10-C9-C8	-4.32	112.52	123.63
52	J	402	UQ	C15-C14-C13	-4.28	112.63	123.63
57	j	203	PEE	O2-C10-C11	4.20	120.58	111.48
58	w	401	ADP	N3-C4-N9	4.19	134.28	127.17
57	l	705	PEE	O2-C10-C11	4.16	120.49	111.48
50	b	201	CDL	OB6-CB5-C51	4.13	120.42	111.48
51	J	401	NDP	N3A-C2A-N1A	-4.12	122.35	128.58
52	s	402	UQ	C15-C14-C13	-4.07	113.17	123.63
50	l	703	CDL	OB6-CB5-C51	4.06	120.27	111.48
49	X	201	8Q1	C37-C38-C39	4.04	119.11	112.39
57	W	201	PEE	O2-C10-C11	4.03	120.20	111.48
52	s	402	UQ	C25-C24-C23	-4.02	113.31	123.63
50	k	101	CDL	OB6-CB5-C51	3.99	120.10	111.48
50	r	504	CDL	OB6-CB5-C51	3.98	120.10	111.48
57	l	701	PEE	O2-C10-C11	3.98	120.10	111.48
50	l	702	CDL	OB6-CB5-C51	3.96	120.05	111.48
50	s	401	CDL	OB6-CB5-C51	3.95	120.03	111.48
50	V	202	CDL	OA6-CA5-C11	3.95	120.03	111.48
57	i	401	PEE	O2-C10-C11	3.94	120.01	111.48
57	r	501	PEE	O2-C10-C11	3.94	120.01	111.48
50	b	201	CDL	OA6-CA5-C11	3.92	119.97	111.48
50	V	202	CDL	OB6-CB5-C51	3.92	119.97	111.48
52	s	402	UQ	C20-C19-C18	-3.90	113.61	123.63
52	J	402	UQ	C21-C19-C18	-3.88	112.46	121.17
50	n	101	CDL	OA6-CA5-C11	3.87	119.86	111.48
52	J	402	UQ	C16-C14-C13	-3.86	112.51	121.17
50	V	201	CDL	OA6-CA5-C11	3.85	119.81	111.48
50	I	201	CDL	OA6-CA5-C11	3.84	119.79	111.48
47	A	503	NAI	N3A-C4A-N9A	3.84	133.70	127.17
50	s	401	CDL	OA6-CA5-C11	3.81	119.73	111.48
51	J	401	NDP	N3A-C4A-N9A	3.80	133.63	127.17
50	I	201	CDL	OB6-CB5-C51	3.78	119.66	111.48
50	n	101	CDL	OB6-CB5-C51	3.77	119.63	111.48
52	s	402	UQ	C26-C24-C23	-3.75	112.75	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	j	202	PEE	O2-C10-C11	3.69	119.46	111.48
49	X	201	8Q1	O4-C1-C6	-3.67	119.74	123.98
47	A	503	NAI	C2A-N3A-C4A	3.67	120.79	111.83
50	r	504	CDL	OA6-CA5-C11	3.66	119.39	111.48
57	l	704	PEE	O2-C10-C11	3.59	119.24	111.48
58	w	401	ADP	N9-C8-N7	-3.57	108.87	113.94
52	s	402	UQ	C21-C19-C18	-3.56	113.18	121.17
51	J	401	NDP	C2A-N3A-C4A	3.53	120.45	111.83
58	w	401	ADP	C2-N3-C4	3.47	120.32	111.83
46	A	502	FMN	C4-N3-C2	-3.45	119.51	125.64
52	s	402	UQ	C16-C14-C13	-3.45	113.42	121.17
57	j	201	PEE	O2-C10-C11	3.43	118.90	111.48
47	A	503	NAI	N9A-C8A-N7A	-3.38	109.15	113.94
47	A	503	NAI	C5A-N7A-C8A	3.37	108.75	103.45
47	A	503	NAI	C4A-C5A-N7A	-3.37	106.73	110.58
58	w	401	ADP	C4-N9-C8	3.30	109.20	105.74
52	J	402	UQ	C26-C24-C23	-3.30	112.76	122.66
52	s	402	UQ	C30-C29-C28	-3.29	112.79	122.66
52	s	402	UQ	C31-C29-C28	-3.28	112.81	122.66
52	J	402	UQ	C11-C9-C8	-3.26	113.85	121.17
52	J	402	UQ	C25-C24-C23	-3.23	112.98	122.66
52	s	402	UQ	C11-C9-C8	-3.19	114.00	121.17
58	w	401	ADP	C5-N7-C8	3.17	108.44	103.45
51	J	401	NDP	C4A-C5A-N7A	-3.16	106.97	110.58
50	k	101	CDL	OA6-CA5-C11	3.12	118.24	111.48
49	G	201	8Q1	C37-C38-C39	3.12	117.59	112.39
50	l	702	CDL	OA8-CA7-C31	3.09	121.27	111.83
51	J	401	NDP	N9A-C8A-N7A	-3.08	109.57	113.94
55	Q	501	UQ1	C10-C9-C8	-3.01	113.63	122.66
47	A	503	NAI	C4D-O4D-C1D	-2.99	102.86	109.47
51	J	401	NDP	C5A-N7A-C8A	2.95	108.09	103.45
58	w	401	ADP	C4-C5-N7	-2.94	107.22	110.58
47	A	503	NAI	C3D-C2D-C1D	2.93	107.01	101.46
50	l	702	CDL	OB8-CB7-C71	2.93	120.77	111.83
57	i	401	PEE	O3-C30-C31	2.91	120.70	111.83
50	k	101	CDL	OB8-CB7-C71	2.88	120.62	111.83
50	n	101	CDL	OA8-CA7-C31	2.86	119.84	111.15
50	I	201	CDL	OA8-CA7-C31	2.84	120.49	111.83
57	j	202	PEE	O3-C30-C31	2.82	120.44	111.83
57	l	704	PEE	O3-C30-C31	2.78	120.32	111.83
50	I	201	CDL	OB8-CB7-C71	2.78	120.30	111.83
50	l	703	CDL	OB8-CB7-C71	2.77	120.28	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	V	201	CDL	OB8-CB7-C71	2.77	120.28	111.83
46	A	502	FMN	C4A-C4-N3	2.76	120.29	113.25
57	j	203	PEE	O3-C30-C31	2.76	120.25	111.83
50	k	101	CDL	OA8-CA7-C31	2.75	120.22	111.83
50	r	504	CDL	OB8-CB7-C71	2.73	120.16	111.83
50	l	703	CDL	OA8-CA7-C31	2.73	120.14	111.83
50	b	201	CDL	OB8-CB7-C71	2.72	120.13	111.83
57	l	705	PEE	O3-C30-C31	2.72	120.12	111.83
52	J	402	UQ	C7-C6-C5	-2.71	120.24	124.89
50	n	101	CDL	OB8-CB7-C71	2.71	120.10	111.83
57	l	701	PEE	O3-C30-C31	2.71	120.10	111.83
57	W	201	PEE	O3-C30-C31	2.71	120.09	111.83
50	s	401	CDL	OA8-CA7-C31	2.70	120.08	111.83
50	V	202	CDL	OB8-CB7-C71	2.69	120.05	111.83
50	r	504	CDL	OA8-CA7-C31	2.69	120.05	111.83
47	A	503	NAI	C2D-C3D-C4D	2.69	107.81	102.61
50	b	201	CDL	OA8-CA7-C31	2.68	120.00	111.83
46	A	502	FMN	C5A-C9A-N10	2.66	120.37	117.97
50	V	201	CDL	OB6-CB5-OB7	-2.65	117.51	123.70
55	Q	501	UQ1	C11-C9-C8	-2.65	114.71	122.66
57	r	501	PEE	O3-C30-C31	2.64	119.89	111.83
52	s	402	UQ	CM5-C5-C6	-2.62	120.14	124.45
57	j	201	PEE	O3-C30-C31	2.59	119.75	111.83
46	A	502	FMN	O4-C4-C4A	-2.59	119.69	126.53
50	V	202	CDL	OA8-CA7-C31	2.59	119.73	111.83
48	g	201	PLX	C1A-N1-C1	2.57	120.11	109.91
50	l	702	CDL	CA4-OA6-CA5	-2.54	111.72	117.80
47	A	503	NAI	C4A-N9A-C8A	2.54	108.40	105.74
50	V	201	CDL	OA8-CA7-C31	2.54	119.58	111.83
52	J	402	UQ	CM5-C5-C6	-2.50	120.34	124.45
49	G	201	8Q1	O4-C1-S44	-2.50	119.50	122.68
49	G	201	8Q1	C38-C39-N41	2.49	120.89	116.34
55	Q	501	UQ1	CM5-C5-C6	-2.47	120.38	124.45
57	j	203	PEE	C2-O2-C10	-2.46	111.91	117.80
48	r	502	PLX	C1A-N1-C1	2.46	119.68	109.91
46	A	502	FMN	C4A-C10-N10	2.43	119.96	116.48
51	J	401	NDP	C4A-N9A-C8A	2.41	108.27	105.74
50	s	401	CDL	OB8-CB7-C71	2.39	119.12	111.83
48	j	205	PLX	C1A-N1-C1	2.37	119.33	109.91
55	Q	501	UQ1	C6-C5-C4	2.36	121.03	119.17
48	a	201	PLX	C1A-N1-C1	2.36	119.28	109.91
48	j	204	PLX	C1A-N1-C1	2.35	119.24	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	r	503	PLX	C1A-N1-C1	2.34	119.22	109.91
57	l	701	PEE	C20-C19-C18	-2.34	112.33	126.42
48	C	302	PLX	C1A-N1-C1	2.33	119.19	109.91
50	l	703	CDL	CB4-OB6-CB5	-2.33	112.22	117.80
46	A	502	FMN	C4A-C10-N1	-2.29	118.99	124.59
47	A	503	NAI	C6N-N1N-C2N	2.28	121.76	119.32
49	X	201	8Q1	O4-C1-S44	-2.25	119.82	122.68
46	A	502	FMN	C9A-C5A-N5	-2.23	120.09	122.45
49	G	201	8Q1	C43-S44-C1	2.12	108.12	101.84
46	A	502	FMN	C10-C4A-N5	-2.10	120.53	124.81
49	X	201	8Q1	C43-S44-C1	2.08	108.00	101.84
49	X	201	8Q1	C32-C34-N36	2.03	120.34	116.48
48	j	204	PLX	C2-C1-N1	-2.03	109.30	115.82
58	w	401	ADP	C4'-O4'-C1'	-2.01	105.03	109.47

There are no chirality outliers.

All (966) 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	C3'-C4'-C5'-O5'
46	A	502	FMN	O4'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O1P
46	A	502	FMN	C5'-O5'-P-O2P
47	A	503	NAI	PN-O3-PA-O5B
48	C	302	PLX	O7-C6-C7-C8
48	C	302	PLX	C2-O1-P1-O2
48	C	302	PLX	N1-C1-C2-O1
48	a	201	PLX	O7-C6-O6-C4
48	a	201	PLX	C3-O4-P1-O1
48	a	201	PLX	C3-O4-P1-O3
48	a	201	PLX	N1-C1-C2-O1
48	a	201	PLX	O9-C24-O8-C5
48	a	201	PLX	O9-C24-C25-C26
48	g	201	PLX	C3-O4-P1-O2
48	g	201	PLX	C2-O1-P1-O4
48	g	201	PLX	C2-O1-P1-O2
48	g	201	PLX	C2-O1-P1-O3
48	g	201	PLX	C25-C24-O8-C5
48	j	204	PLX	O7-C6-O6-C4
48	j	204	PLX	C3-O4-P1-O3

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Mol	Chain	Res	Type	Atoms
48	j	204	PLX	C2-O1-P1-O4
48	j	204	PLX	C2-O1-P1-O2
48	j	204	PLX	N1-C1-C2-O1
48	j	204	PLX	O8-C24-C25-C26
48	j	204	PLX	O9-C24-C25-C26
48	j	205	PLX	O7-C6-C7-C8
48	j	205	PLX	O9-C24-O8-C5
48	r	502	PLX	O7-C6-C7-C8
48	r	502	PLX	C5-C4-O6-C6
48	r	502	PLX	O9-C24-C25-C26
48	r	503	PLX	O9-C24-O8-C5
48	r	503	PLX	O9-C24-C25-C26
49	G	201	8Q1	O4-C1-S44-C43
49	G	201	8Q1	C6-C1-S44-C43
49	G	201	8Q1	C28-C29-C32-C34
49	G	201	8Q1	C28-C29-C32-O33
49	G	201	8Q1	C30-C29-C32-C34
49	G	201	8Q1	C30-C29-C32-O33
49	G	201	8Q1	C31-C29-C32-C34
49	G	201	8Q1	C29-C32-C34-N36
49	G	201	8Q1	C29-C32-C34-O35
49	G	201	8Q1	O33-C32-C34-N36
49	X	201	8Q1	C1-C6-C7-C8
49	X	201	8Q1	O4-C1-S44-C43
49	X	201	8Q1	C6-C1-S44-C43
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
50	I	201	CDL	CA2-OA2-PA1-OA5
50	I	201	CDL	OA5-CA3-CA4-OA6
50	I	201	CDL	CB2-OB2-PB2-OB3
50	I	201	CDL	CB2-OB2-PB2-OB4
50	I	201	CDL	CB2-OB2-PB2-OB5
50	I	201	CDL	CB3-OB5-PB2-OB2
50	I	201	CDL	CB3-OB5-PB2-OB3
50	I	201	CDL	CB3-OB5-PB2-OB4
50	V	201	CDL	CB2-OB2-PB2-OB3
50	V	201	CDL	CB2-OB2-PB2-OB5
50	V	201	CDL	CB3-OB5-PB2-OB3
50	V	201	CDL	CB3-OB5-PB2-OB4
50	V	202	CDL	CA2-OA2-PA1-OA4
50	V	202	CDL	CA2-OA2-PA1-OA5
50	V	202	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
50	V	202	CDL	CB3-OB5-PB2-OB2
50	V	202	CDL	CB3-OB5-PB2-OB4
50	V	202	CDL	OB5-CB3-CB4-OB6
50	b	201	CDL	CB2-C1-CA2-OA2
50	b	201	CDL	CA2-C1-CB2-OB2
50	b	201	CDL	CA2-OA2-PA1-OA3
50	b	201	CDL	CB2-OB2-PB2-OB3
50	b	201	CDL	CB2-OB2-PB2-OB4
50	b	201	CDL	CB2-OB2-PB2-OB5
50	b	201	CDL	OB7-CB5-OB6-CB4
50	b	201	CDL	C51-CB5-OB6-CB4
50	k	101	CDL	CA3-OA5-PA1-OA2
50	k	101	CDL	CA3-OA5-PA1-OA3
50	k	101	CDL	CA3-OA5-PA1-OA4
50	k	101	CDL	OA5-CA3-CA4-OA6
50	l	702	CDL	CA2-OA2-PA1-OA3
50	l	702	CDL	CA3-OA5-PA1-OA2
50	l	702	CDL	CA3-OA5-PA1-OA3
50	l	702	CDL	CB2-OB2-PB2-OB3
50	l	702	CDL	CB2-OB2-PB2-OB4
50	l	702	CDL	CB2-OB2-PB2-OB5
50	l	702	CDL	CB3-OB5-PB2-OB2
50	l	702	CDL	CB3-OB5-PB2-OB3
50	l	702	CDL	CB3-OB5-PB2-OB4
50	l	703	CDL	CB2-C1-CA2-OA2
50	l	703	CDL	CA3-OA5-PA1-OA2
50	l	703	CDL	CA3-OA5-PA1-OA3
50	l	703	CDL	CA3-OA5-PA1-OA4
50	l	703	CDL	CB2-OB2-PB2-OB3
50	l	703	CDL	CB2-OB2-PB2-OB4
50	l	703	CDL	CB2-OB2-PB2-OB5
50	l	703	CDL	CB3-OB5-PB2-OB4
50	n	101	CDL	CA3-OA5-PA1-OA2
50	n	101	CDL	CA3-OA5-PA1-OA3
50	n	101	CDL	CA3-OA5-PA1-OA4
50	n	101	CDL	CB2-OB2-PB2-OB3
50	n	101	CDL	CB2-OB2-PB2-OB5
50	r	504	CDL	CA3-OA5-PA1-OA2
50	r	504	CDL	CA3-OA5-PA1-OA3
50	r	504	CDL	CB3-OB5-PB2-OB2
50	r	504	CDL	CB3-OB5-PB2-OB3
50	r	504	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
50	r	504	CDL	C51-CB5-OB6-CB4
50	s	401	CDL	CB2-OB2-PB2-OB3
50	s	401	CDL	CB2-OB2-PB2-OB4
50	s	401	CDL	CB2-OB2-PB2-OB5
50	s	401	CDL	CB3-OB5-PB2-OB2
50	s	401	CDL	CB3-OB5-PB2-OB3
52	J	402	UQ	C7-C8-C9-C10
52	J	402	UQ	C17-C18-C19-C21
52	s	402	UQ	C7-C8-C9-C11
52	s	402	UQ	C17-C18-C19-C21
52	s	402	UQ	C22-C23-C24-C26
52	s	402	UQ	C23-C24-C26-C27
55	Q	501	UQ1	C1-C6-C7-C8
55	Q	501	UQ1	C5-C6-C7-C8
57	W	201	PEE	C4-O4P-P-O3P
57	W	201	PEE	C4-O4P-P-O1P
57	i	401	PEE	O4-C10-O2-C2
57	i	401	PEE	C4-O4P-P-O3P
57	i	401	PEE	C4-O4P-P-O1P
57	j	201	PEE	C1-O3P-P-O1P
57	j	201	PEE	C1-O3P-P-O4P
57	j	202	PEE	C1-O3P-P-O1P
57	j	203	PEE	C1-O3P-P-O2P
57	j	203	PEE	C1-O3P-P-O1P
57	j	203	PEE	C1-O3P-P-O4P
57	j	203	PEE	C4-O4P-P-O2P
57	j	203	PEE	O4P-C4-C5-N
57	l	701	PEE	C1-O3P-P-O2P
57	l	701	PEE	C1-O3P-P-O4P
57	l	701	PEE	C4-O4P-P-O3P
57	l	704	PEE	C11-C10-O2-C2
57	l	704	PEE	O4-C10-O2-C2
57	l	704	PEE	C4-O4P-P-O3P
57	l	704	PEE	C4-O4P-P-O2P
57	l	705	PEE	O4P-C4-C5-N
57	r	501	PEE	C4-O4P-P-O3P
57	r	501	PEE	C4-O4P-P-O2P
58	w	401	ADP	C5'-O5'-PA-O2A
58	w	401	ADP	C5'-O5'-PA-O3A
58	w	401	ADP	O4'-C4'-C5'-O5'
50	s	401	CDL	OA9-CA7-OA8-CA6
55	Q	501	UQ1	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
50	s	401	CDL	C31-CA7-OA8-CA6
57	i	401	PEE	O5-C30-O3-C3
57	j	202	PEE	O5-C30-O3-C3
50	r	504	CDL	OB7-CB5-OB6-CB4
57	i	401	PEE	C31-C30-O3-C3
57	j	202	PEE	C31-C30-O3-C3
57	i	401	PEE	C11-C10-O2-C2
57	l	701	PEE	O5-C30-O3-C3
52	s	402	UQ	C18-C19-C21-C22
52	J	402	UQ	C22-C23-C24-C26
50	l	703	CDL	OB9-CB7-OB8-CB6
50	l	703	CDL	C71-CB7-OB8-CB6
52	J	402	UQ	C12-C13-C14-C15
52	s	402	UQ	C7-C8-C9-C10
57	l	701	PEE	C17-C18-C19-C20
57	l	701	PEE	O4-C10-O2-C2
48	j	204	PLX	C25-C26-C27-C28
50	I	201	CDL	O1-C1-CA2-OA2
50	I	201	CDL	O1-C1-CB2-OB2
50	V	201	CDL	O1-C1-CA2-OA2
50	b	201	CDL	O1-C1-CA2-OA2
50	l	703	CDL	O1-C1-CA2-OA2
50	l	703	CDL	O1-C1-CB2-OB2
50	n	101	CDL	O1-C1-CA2-OA2
50	r	504	CDL	O1-C1-CA2-OA2
57	l	701	PEE	C31-C30-O3-C3
50	V	201	CDL	C11-CA5-OA6-CA4
50	V	202	CDL	C51-CB5-OB6-CB4
57	l	701	PEE	C11-C10-O2-C2
48	j	205	PLX	C13-C14-C15-C16
50	V	201	CDL	C11-C12-C13-C14
47	A	503	NAI	C3D-C4D-C5D-O5D
52	J	402	UQ	C15-C14-C16-C17
52	J	402	UQ	C20-C19-C21-C22
52	J	402	UQ	C12-C11-C9-C8
52	s	402	UQ	C13-C14-C16-C17
50	V	201	CDL	OA7-CA5-OA6-CA4
52	s	402	UQ	C14-C16-C17-C18
48	r	502	PLX	C11-C12-C13-C14
52	s	402	UQ	C27-C28-C29-C31
57	j	202	PEE	C17-C18-C19-C20
57	l	705	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
57	j	203	PEE	C11-C10-O2-C2
50	V	201	CDL	CB2-C1-CA2-OA2
50	V	201	CDL	C31-CA7-OA8-CA6
50	V	202	CDL	C31-CA7-OA8-CA6
50	l	702	CDL	C31-CA7-OA8-CA6
57	W	201	PEE	C31-C30-O3-C3
48	r	502	PLX	C7-C8-C9-C10
50	V	201	CDL	C62-C63-C64-C65
48	g	201	PLX	C2-C1-N1-C1B
48	g	201	PLX	C2-C1-N1-C1A
48	r	502	PLX	C9-C10-C11-C12
50	l	702	CDL	C58-C59-C60-C61
50	V	201	CDL	OA9-CA7-OA8-CA6
48	C	302	PLX	C25-C26-C27-C28
50	s	401	CDL	CB7-C71-C72-C73
50	V	201	CDL	C59-C60-C61-C62
57	l	705	PEE	C11-C10-O2-C2
50	l	703	CDL	C37-C38-C39-C40
50	V	202	CDL	OB6-CB4-CB6-OB8
50	l	703	CDL	OA6-CA4-CA6-OA8
51	J	401	NDP	C2D-C1D-N1N-C6N
50	s	401	CDL	CA7-C31-C32-C33
50	l	702	CDL	OA9-CA7-OA8-CA6
50	l	703	CDL	C75-C76-C77-C78
51	J	401	NDP	O4D-C4D-C5D-O5D
50	l	703	CDL	C51-C52-C53-C54
50	V	202	CDL	OB7-CB5-OB6-CB4
50	I	201	CDL	CA7-C31-C32-C33
50	k	101	CDL	CA7-C31-C32-C33
50	l	703	CDL	CB7-C71-C72-C73
57	W	201	PEE	O5-C30-O3-C3
50	V	202	CDL	CA5-C11-C12-C13
50	s	401	CDL	CB5-C51-C52-C53
50	V	202	CDL	OA9-CA7-OA8-CA6
50	l	702	CDL	C32-C33-C34-C35
50	I	201	CDL	C51-C52-C53-C54
50	V	201	CDL	O1-C1-CB2-OB2
50	V	202	CDL	O1-C1-CB2-OB2
50	b	201	CDL	O1-C1-CB2-OB2
50	r	504	CDL	CB5-C51-C52-C53
57	j	203	PEE	O4-C10-O2-C2
50	l	703	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
50	n	101	CDL	C75-C76-C77-C78
57	l	705	PEE	C21-C22-C23-C24
57	l	704	PEE	C33-C34-C35-C36
50	l	703	CDL	OB7-CB5-OB6-CB4
57	l	705	PEE	O4-C10-O2-C2
50	I	201	CDL	CB2-C1-CA2-OA2
50	V	201	CDL	CA2-C1-CB2-OB2
50	V	202	CDL	CA2-C1-CB2-OB2
50	l	703	CDL	CA2-C1-CB2-OB2
50	n	101	CDL	CB2-C1-CA2-OA2
50	r	504	CDL	CB2-C1-CA2-OA2
57	l	704	PEE	C31-C30-O3-C3
47	A	503	NAI	O4D-C4D-C5D-O5D
58	w	401	ADP	C3'-C4'-C5'-O5'
48	C	302	PLX	O6-C6-C7-C8
48	a	201	PLX	O8-C24-C25-C26
48	r	502	PLX	O6-C6-C7-C8
50	s	401	CDL	C51-CB5-OB6-CB4
50	l	703	CDL	C35-C36-C37-C38
50	s	401	CDL	OB7-CB5-OB6-CB4
50	b	201	CDL	C34-C35-C36-C37
50	r	504	CDL	CA7-C31-C32-C33
50	r	504	CDL	C74-C75-C76-C77
50	V	201	CDL	C1-CB2-OB2-PB2
57	l	705	PEE	C39-C40-C41-C42
57	l	704	PEE	O5-C30-O3-C3
50	s	401	CDL	C14-C15-C16-C17
48	a	201	PLX	C34-C35-C36-C37
48	C	302	PLX	C28-C29-C30-C31
48	g	201	PLX	C9-C10-C11-C12
48	j	204	PLX	C31-C32-C33-C34
48	j	205	PLX	C12-C13-C14-C15
48	j	205	PLX	C34-C35-C36-C37
49	X	201	8Q1	C12-C13-C14-C15
50	b	201	CDL	C51-C52-C53-C54
50	r	504	CDL	C41-C42-C43-C44
50	r	504	CDL	C83-C84-C85-C86
50	s	401	CDL	C59-C60-C61-C62
57	r	501	PEE	C37-C38-C39-C40
48	a	201	PLX	C12-C13-C14-C15
48	r	502	PLX	C11-C10-C9-C8
50	V	201	CDL	C55-C56-C57-C58

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Mol	Chain	Res	Type	Atoms
50	V	202	CDL	C42-C43-C44-C45
50	V	202	CDL	C59-C60-C61-C62
50	r	504	CDL	C14-C15-C16-C17
50	r	504	CDL	C34-C35-C36-C37
50	r	504	CDL	C57-C58-C59-C60
48	C	302	PLX	C10-C11-C12-C13
48	g	201	PLX	C11-C10-C9-C8
48	r	503	PLX	C14-C15-C16-C17
50	V	201	CDL	C31-C32-C33-C34
50	V	201	CDL	C37-C38-C39-C40
50	l	703	CDL	C72-C73-C74-C75
50	r	504	CDL	C43-C44-C45-C46
57	j	202	PEE	C11-C12-C13-C14
48	C	302	PLX	C14-C15-C16-C17
48	j	204	PLX	C27-C28-C29-C30
48	j	205	PLX	C30-C31-C32-C33
50	k	101	CDL	C52-C53-C54-C55
50	V	201	CDL	CA7-C31-C32-C33
48	a	201	PLX	C31-C32-C33-C34
50	V	202	CDL	C40-C41-C42-C43
48	j	205	PLX	C14-C15-C16-C17
57	j	201	PEE	C32-C33-C34-C35
50	V	201	CDL	C51-CB5-OB6-CB4
48	j	205	PLX	C33-C34-C35-C36
50	k	101	CDL	C75-C76-C77-C78
50	s	401	CDL	O1-C1-CB2-OB2
50	I	201	CDL	CB5-C51-C52-C53
48	r	503	PLX	C10-C11-C12-C13
50	V	201	CDL	C34-C35-C36-C37
50	l	703	CDL	C15-C16-C17-C18
50	s	401	CDL	C32-C33-C34-C35
57	j	203	PEE	C13-C14-C15-C16
57	r	501	PEE	C14-C15-C16-C17
48	C	302	PLX	C33-C34-C35-C36
48	g	201	PLX	C28-C29-C30-C31
50	n	101	CDL	CA5-C11-C12-C13
50	n	101	CDL	CB5-C51-C52-C53
50	b	201	CDL	C54-C55-C56-C57
50	b	201	CDL	C61-C62-C63-C64
50	n	101	CDL	C55-C56-C57-C58
50	r	504	CDL	C60-C61-C62-C63
52	J	402	UQ	C19-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
50	V	202	CDL	C12-C13-C14-C15
50	l	703	CDL	C11-C12-C13-C14
50	s	401	CDL	C73-C74-C75-C76
57	j	202	PEE	C12-C13-C14-C15
48	a	201	PLX	C27-C28-C29-C30
48	j	205	PLX	C9-C10-C11-C12
48	r	503	PLX	C30-C31-C32-C33
50	k	101	CDL	C11-C12-C13-C14
50	s	401	CDL	C35-C36-C37-C38
57	l	704	PEE	C11-C12-C13-C14
57	r	501	PEE	C20-C21-C22-C23
48	a	201	PLX	C13-C14-C15-C16
48	j	204	PLX	C13-C14-C15-C16
48	r	503	PLX	C25-C26-C27-C28
48	r	503	PLX	C29-C30-C31-C32
57	j	202	PEE	C22-C23-C24-C25
57	j	202	PEE	C40-C41-C42-C43
57	j	203	PEE	C12-C13-C14-C15
48	g	201	PLX	C2-C1-N1-C1C
48	g	201	PLX	C27-C28-C29-C30
48	r	502	PLX	C28-C29-C30-C31
50	n	101	CDL	C52-C53-C54-C55
50	n	101	CDL	C73-C74-C75-C76
50	V	201	CDL	C53-C54-C55-C56
57	j	202	PEE	C31-C32-C33-C34
57	r	501	PEE	C31-C32-C33-C34
50	I	201	CDL	C51-CB5-OB6-CB4
57	j	201	PEE	C11-C10-O2-C2
57	j	202	PEE	C36-C37-C38-C39
48	g	201	PLX	C33-C34-C35-C36
50	k	101	CDL	C73-C74-C75-C76
48	r	502	PLX	C27-C28-C29-C30
57	l	701	PEE	C31-C32-C33-C34
50	b	201	CDL	C52-C53-C54-C55
50	n	101	CDL	C56-C57-C58-C59
57	i	401	PEE	C21-C22-C23-C24
48	C	302	PLX	C11-C10-C9-C8
50	V	202	CDL	C14-C15-C16-C17
57	r	501	PEE	C33-C34-C35-C36
48	a	201	PLX	C25-C26-C27-C28
50	V	201	CDL	C71-C72-C73-C74
50	k	101	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
57	j	203	PEE	C23-C24-C25-C26
48	C	302	PLX	C11-C12-C13-C14
50	b	201	CDL	C21-C22-C23-C24
50	k	101	CDL	C20-C21-C22-C23
50	k	101	CDL	C21-C22-C23-C24
50	r	504	CDL	C75-C76-C77-C78
57	r	501	PEE	C40-C41-C42-C43
50	b	201	CDL	CB5-C51-C52-C53
48	r	502	PLX	C30-C31-C32-C33
48	r	503	PLX	C11-C12-C13-C14
50	k	101	CDL	C15-C16-C17-C18
57	j	203	PEE	C11-C12-C13-C14
50	I	201	CDL	C11-C12-C13-C14
50	l	703	CDL	C14-C15-C16-C17
50	r	504	CDL	C84-C85-C86-C87
48	a	201	PLX	C14-C15-C16-C17
48	r	502	PLX	C33-C34-C35-C36
50	b	201	CDL	C60-C61-C62-C63
50	k	101	CDL	CA5-C11-C12-C13
50	b	201	CDL	C32-C33-C34-C35
57	l	701	PEE	C18-C19-C20-C21
50	k	101	CDL	C32-C33-C34-C35
50	b	201	CDL	C11-CA5-OA6-CA4
50	l	703	CDL	C11-CA5-OA6-CA4
50	s	401	CDL	C11-CA5-OA6-CA4
57	W	201	PEE	C11-C10-O2-C2
57	r	501	PEE	C11-C10-O2-C2
50	l	702	CDL	CA5-C11-C12-C13
50	l	703	CDL	OA7-CA5-OA6-CA4
50	s	401	CDL	OA7-CA5-OA6-CA4
57	r	501	PEE	O4-C10-O2-C2
57	j	201	PEE	C42-C43-C44-C45
57	i	401	PEE	C19-C20-C21-C22
48	g	201	PLX	C30-C31-C32-C33
48	r	503	PLX	C11-C10-C9-C8
48	j	205	PLX	C7-C8-C9-C10
48	j	204	PLX	C29-C30-C31-C32
48	r	502	PLX	C13-C14-C15-C16
50	V	202	CDL	C39-C40-C41-C42
50	k	101	CDL	C34-C35-C36-C37
52	s	402	UQ	C12-C11-C9-C10
48	j	204	PLX	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
50	b	201	CDL	C17-C18-C19-C20
48	r	503	PLX	C27-C28-C29-C30
50	V	201	CDL	C75-C76-C77-C78
50	V	202	CDL	C83-C84-C85-C86
50	s	401	CDL	C52-C53-C54-C55
48	r	503	PLX	C13-C14-C15-C16
50	k	101	CDL	C36-C37-C38-C39
50	V	201	CDL	OB7-CB5-OB6-CB4
57	j	201	PEE	O4-C10-O2-C2
50	s	401	CDL	OA5-CA3-CA4-OA6
48	j	205	PLX	C25-C26-C27-C28
48	g	201	PLX	C14-C15-C16-C17
50	V	202	CDL	C37-C38-C39-C40
50	k	101	CDL	C82-C83-C84-C85
50	n	101	CDL	CB7-C71-C72-C73
50	l	703	CDL	C40-C41-C42-C43
50	k	101	CDL	OB6-CB4-CB6-OB8
50	r	504	CDL	OA6-CA4-CA6-OA8
50	V	201	CDL	C56-C57-C58-C59
50	s	401	CDL	C75-C76-C77-C78
50	k	101	CDL	C71-CB7-OB8-CB6
50	V	202	CDL	C17-C18-C19-C20
50	V	202	CDL	C75-C76-C77-C78
57	j	202	PEE	C41-C42-C43-C44
50	r	504	CDL	C62-C63-C64-C65
50	l	703	CDL	C32-C33-C34-C35
48	g	201	PLX	C32-C33-C34-C35
48	j	204	PLX	C30-C31-C32-C33
50	k	101	CDL	C35-C36-C37-C38
50	k	101	CDL	C76-C77-C78-C79
50	l	703	CDL	C55-C56-C57-C58
50	I	201	CDL	C71-C72-C73-C74
48	j	204	PLX	C7-C8-C9-C10
48	a	201	PLX	C29-C30-C31-C32
57	W	201	PEE	C22-C23-C24-C25
57	r	501	PEE	C17-C18-C19-C20
50	V	201	CDL	C44-C45-C46-C47
57	l	704	PEE	C44-C45-C46-C47
50	r	504	CDL	C55-C56-C57-C58
50	V	201	CDL	C40-C41-C42-C43
50	b	201	CDL	C53-C54-C55-C56
50	n	101	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
50	r	504	CDL	C77-C78-C79-C80
48	g	201	PLX	C10-C11-C12-C13
50	V	201	CDL	C58-C59-C60-C61
50	V	202	CDL	C32-C33-C34-C35
50	l	702	CDL	C16-C17-C18-C19
50	r	504	CDL	C23-C24-C25-C26
49	G	201	8Q1	O33-C32-C34-O35
57	j	201	PEE	C13-C14-C15-C16
50	k	101	CDL	C14-C15-C16-C17
50	k	101	CDL	C37-C38-C39-C40
57	W	201	PEE	C13-C14-C15-C16
57	j	203	PEE	C19-C20-C21-C22
57	r	501	PEE	C15-C16-C17-C18
48	r	503	PLX	C28-C29-C30-C31
50	V	202	CDL	C34-C35-C36-C37
50	k	101	CDL	C71-C72-C73-C74
50	l	703	CDL	C39-C40-C41-C42
50	I	201	CDL	OA5-CA3-CA4-CA6
50	V	202	CDL	OB5-CB3-CB4-CB6
50	k	101	CDL	OA5-CA3-CA4-CA6
50	I	201	CDL	OB7-CB5-OB6-CB4
57	W	201	PEE	O4-C10-O2-C2
50	V	201	CDL	C33-C34-C35-C36
50	V	201	CDL	C54-C55-C56-C57
57	l	701	PEE	C32-C33-C34-C35
50	b	201	CDL	C22-C23-C24-C25
57	l	704	PEE	C30-C31-C32-C33
50	b	201	CDL	C35-C36-C37-C38
50	b	201	CDL	C58-C59-C60-C61
57	l	705	PEE	C34-C35-C36-C37
50	V	201	CDL	CA3-CA4-CA6-OA8
50	V	202	CDL	CB3-CB4-CB6-OB8
50	k	101	CDL	CB3-CB4-CB6-OB8
50	l	703	CDL	CA3-CA4-CA6-OA8
50	r	504	CDL	CA3-CA4-CA6-OA8
57	W	201	PEE	C1-C2-C3-O3
57	j	201	PEE	C1-C2-C3-O3
57	j	203	PEE	C1-C2-C3-O3
50	b	201	CDL	C55-C56-C57-C58
50	r	504	CDL	C52-C53-C54-C55
50	s	401	CDL	C51-C52-C53-C54
57	j	201	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
57	l	704	PEE	C19-C20-C21-C22
48	g	201	PLX	C15-C16-C17-C18
50	V	202	CDL	C60-C61-C62-C63
50	b	201	CDL	C23-C24-C25-C26
50	s	401	CDL	C71-C72-C73-C74
57	r	501	PEE	C22-C23-C24-C25
50	b	201	CDL	C31-CA7-OA8-CA6
50	b	201	CDL	C71-CB7-OB8-CB6
50	r	504	CDL	C71-CB7-OB8-CB6
50	n	101	CDL	C74-C75-C76-C77
50	b	201	CDL	C62-C63-C64-C65
50	s	401	CDL	C17-C18-C19-C20
57	W	201	PEE	C21-C22-C23-C24
57	r	501	PEE	C10-C11-C12-C13
50	k	101	CDL	OB9-CB7-OB8-CB6
49	X	201	8Q1	C7-C8-C9-C10
48	a	201	PLX	C15-C16-C17-C18
48	j	205	PLX	C10-C11-C12-C13
48	r	503	PLX	C18-C19-C20-C21
50	r	504	CDL	C71-C72-C73-C74
48	j	204	PLX	C33-C34-C35-C36
50	b	201	CDL	C11-C12-C13-C14
50	r	504	CDL	C76-C77-C78-C79
50	l	702	CDL	C38-C39-C40-C41
50	r	504	CDL	C13-C14-C15-C16
50	s	401	CDL	C11-C12-C13-C14
50	V	201	CDL	CA6-CA4-OA6-CA5
50	b	201	CDL	C37-C38-C39-C40
57	j	202	PEE	C19-C20-C21-C22
48	r	502	PLX	C16-C17-C18-C19
48	r	502	PLX	C12-C13-C14-C15
50	s	401	CDL	C55-C56-C57-C58
57	W	201	PEE	C17-C18-C19-C20
57	i	401	PEE	C11-C12-C13-C14
57	l	704	PEE	O3P-C1-C2-O2
49	X	201	8Q1	C11-C12-C13-C14
57	j	202	PEE	C21-C22-C23-C24
50	V	202	CDL	C71-CB7-OB8-CB6
57	l	704	PEE	C40-C41-C42-C43
57	l	701	PEE	C11-C12-C13-C14
50	s	401	CDL	C37-C38-C39-C40
50	s	401	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
49	X	201	8Q1	C11-C10-C9-C8
50	V	201	CDL	C14-C15-C16-C17
50	V	202	CDL	C64-C65-C66-C67
48	j	204	PLX	C10-C11-C12-C13
50	b	201	CDL	C57-C58-C59-C60
48	C	302	PLX	O6-C4-C5-O8
48	r	502	PLX	O6-C4-C5-O8
57	l	701	PEE	O2-C2-C3-O3
48	C	302	PLX	C7-C8-C9-C10
48	r	503	PLX	C7-C8-C9-C10
50	V	201	CDL	C73-C74-C75-C76
57	l	704	PEE	C24-C25-C26-C27
48	g	201	PLX	C17-C18-C19-C20
48	j	205	PLX	C19-C20-C21-C22
57	W	201	PEE	C23-C24-C25-C26
57	W	201	PEE	C15-C16-C17-C18
49	G	201	8Q1	C31-C29-C32-O33
50	k	101	CDL	C84-C85-C86-C87
48	C	302	PLX	C13-C14-C15-C16
50	I	201	CDL	C71-CB7-OB8-CB6
48	j	204	PLX	C14-C15-C16-C17
57	l	705	PEE	C20-C21-C22-C23
57	r	501	PEE	C21-C22-C23-C24
57	j	201	PEE	C44-C45-C46-C47
50	I	201	CDL	C72-C73-C74-C75
50	s	401	CDL	C84-C85-C86-C87
50	l	702	CDL	C71-C72-C73-C74
57	l	705	PEE	C11-C12-C13-C14
50	b	201	CDL	OA7-CA5-OA6-CA4
48	g	201	PLX	C12-C13-C14-C15
50	l	703	CDL	C61-C62-C63-C64
50	r	504	CDL	C32-C33-C34-C35
50	r	504	CDL	C35-C36-C37-C38
48	g	201	PLX	C25-C26-C27-C28
48	j	204	PLX	O4-C3-C4-C5
50	b	201	CDL	OA5-CA3-CA4-CA6
50	l	703	CDL	OB5-CB3-CB4-CB6
50	s	401	CDL	OA5-CA3-CA4-CA6
50	b	201	CDL	C71-C72-C73-C74
50	l	703	CDL	C73-C74-C75-C76
50	r	504	CDL	C64-C65-C66-C67
50	I	201	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
50	V	201	CDL	C64-C65-C66-C67
57	j	203	PEE	C31-C32-C33-C34
50	b	201	CDL	C33-C34-C35-C36
50	b	201	CDL	OB9-CB7-OB8-CB6
50	r	504	CDL	OB9-CB7-OB8-CB6
50	r	504	CDL	C37-C38-C39-C40
48	r	503	PLX	C31-C32-C33-C34
50	b	201	CDL	OA9-CA7-OA8-CA6
50	V	202	CDL	C76-C77-C78-C79
50	l	703	CDL	C33-C34-C35-C36
48	a	201	PLX	C3-C4-C5-O8
48	j	204	PLX	C3-C4-C5-O8
48	j	205	PLX	C3-C4-C5-O8
48	r	503	PLX	C3-C4-C5-O8
57	l	704	PEE	C31-C32-C33-C34
49	X	201	8Q1	C13-C14-C15-C16
57	j	203	PEE	C32-C33-C34-C35
48	C	302	PLX	C26-C27-C28-C29
48	r	502	PLX	C25-C26-C27-C28
57	j	201	PEE	C41-C42-C43-C44
50	V	202	CDL	OB9-CB7-OB8-CB6
50	k	101	CDL	C44-C45-C46-C47
50	V	202	CDL	C31-C32-C33-C34
50	k	101	CDL	C53-C54-C55-C56
50	V	202	CDL	C73-C74-C75-C76
50	s	401	CDL	OB6-CB4-CB6-OB8
57	j	203	PEE	O2-C2-C3-O3
48	C	302	PLX	C31-C32-C33-C34
48	j	205	PLX	C29-C30-C31-C32
50	k	101	CDL	C80-C81-C82-C83
57	j	202	PEE	C34-C35-C36-C37
48	r	502	PLX	O8-C24-C25-C26
48	j	205	PLX	C11-C12-C13-C14
57	l	704	PEE	C23-C24-C25-C26
50	V	202	CDL	C55-C56-C57-C58
57	r	501	PEE	C23-C24-C25-C26
48	g	201	PLX	C36-C37-C38-C39
50	l	702	CDL	C24-C25-C26-C27
50	b	201	CDL	C76-C77-C78-C79
50	l	703	CDL	C44-C45-C46-C47
50	n	101	CDL	C71-C72-C73-C74
50	b	201	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
46	A	502	FMN	O2'-C2'-C3'-C4'
50	I	201	CDL	CA2-C1-CB2-OB2
50	V	202	CDL	CB2-C1-CA2-OA2
50	b	201	CDL	C82-C83-C84-C85
57	W	201	PEE	C19-C20-C21-C22
50	k	101	CDL	C13-C14-C15-C16
50	r	504	CDL	C11-C12-C13-C14
57	l	704	PEE	C42-C43-C44-C45
46	A	502	FMN	C1'-C2'-C3'-O3'
50	V	201	CDL	OA5-CA3-CA4-CA6
57	j	201	PEE	O3P-C1-C2-C3
50	k	101	CDL	C39-C40-C41-C42
50	k	101	CDL	C38-C39-C40-C41
50	s	401	CDL	C36-C37-C38-C39
50	b	201	CDL	C64-C65-C66-C67
50	V	202	CDL	C63-C64-C65-C66
50	l	702	CDL	C12-C13-C14-C15
50	l	702	CDL	C82-C83-C84-C85
51	J	401	NDP	C3D-C4D-C5D-O5D
50	I	201	CDL	OB9-CB7-OB8-CB6
50	I	201	CDL	C52-C53-C54-C55
57	j	201	PEE	C14-C15-C16-C17
50	b	201	CDL	C36-C37-C38-C39
50	l	703	CDL	C80-C81-C82-C83
50	s	401	CDL	C12-C13-C14-C15
57	l	701	PEE	C35-C36-C37-C38
50	l	703	CDL	C62-C63-C64-C65
50	r	504	CDL	C59-C60-C61-C62
57	r	501	PEE	C41-C42-C43-C44
48	j	204	PLX	O4-C3-C4-O6
50	V	201	CDL	OA5-CA3-CA4-OA6
50	b	201	CDL	OA5-CA3-CA4-OA6
50	s	401	CDL	OB5-CB3-CB4-OB6
57	j	201	PEE	C12-C13-C14-C15
57	l	705	PEE	C1-C2-C3-O3
50	b	201	CDL	C31-C32-C33-C34
50	r	504	CDL	C33-C34-C35-C36
57	l	704	PEE	C14-C15-C16-C17
50	r	504	CDL	C44-C45-C46-C47
48	j	205	PLX	O6-C4-C5-O8
50	l	703	CDL	OB6-CB4-CB6-OB8
57	W	201	PEE	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
57	j	201	PEE	O2-C2-C3-O3
57	j	202	PEE	C35-C36-C37-C38
48	C	302	PLX	C27-C28-C29-C30
50	V	201	CDL	C72-C73-C74-C75
50	l	703	CDL	C82-C83-C84-C85
50	n	101	CDL	C51-C52-C53-C54
50	r	504	CDL	C12-C13-C14-C15
50	V	202	CDL	C54-C55-C56-C57
48	j	204	PLX	C24-C25-C26-C27
50	V	202	CDL	C71-C72-C73-C74
50	l	702	CDL	C61-C62-C63-C64
50	l	702	CDL	C36-C37-C38-C39
57	l	705	PEE	C13-C14-C15-C16
47	A	503	NAI	C3B-C4B-C5B-O5B
48	g	201	PLX	C7-C8-C9-C10
57	l	705	PEE	C32-C33-C34-C35
50	V	202	CDL	O1-C1-CA2-OA2
48	r	503	PLX	C32-C33-C34-C35
48	j	205	PLX	C28-C29-C30-C31
50	l	703	CDL	C12-C13-C14-C15
48	C	302	PLX	C25-C24-O8-C5
48	a	201	PLX	C25-C24-O8-C5
49	G	201	8Q1	N41-C42-C43-S44
50	b	201	CDL	CA5-C11-C12-C13
50	l	702	CDL	C81-C82-C83-C84
57	r	501	PEE	C36-C37-C38-C39
50	V	201	CDL	C52-C53-C54-C55
50	s	401	CDL	C82-C83-C84-C85
57	l	705	PEE	C15-C16-C17-C18
50	V	202	CDL	C33-C34-C35-C36
57	j	203	PEE	C22-C23-C24-C25
50	s	401	CDL	OB5-CB3-CB4-CB6
57	i	401	PEE	O3P-C1-C2-C3
57	l	704	PEE	O3P-C1-C2-C3
50	l	703	CDL	C13-C14-C15-C16
57	j	202	PEE	C37-C38-C39-C40
48	r	502	PLX	C14-C15-C16-C17
48	r	502	PLX	C31-C32-C33-C34
50	l	702	CDL	C31-C32-C33-C34
57	j	202	PEE	C44-C45-C46-C47
50	V	202	CDL	C1-CB2-OB2-PB2
50	r	504	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
48	r	503	PLX	C36-C37-C38-C39
50	l	703	CDL	OB5-CB3-CB4-OB6
57	j	201	PEE	O3P-C1-C2-O2
57	l	701	PEE	O3P-C1-C2-O2
48	C	302	PLX	C9-C10-C11-C12
50	l	702	CDL	C56-C57-C58-C59
57	l	704	PEE	C32-C33-C34-C35
50	l	703	CDL	C78-C79-C80-C81
50	s	401	CDL	C34-C35-C36-C37
50	k	101	CDL	C33-C34-C35-C36
57	r	501	PEE	C13-C14-C15-C16
48	a	201	PLX	O6-C4-C5-O8
48	r	503	PLX	O6-C4-C5-O8
57	l	705	PEE	O2-C2-C3-O3
48	r	502	PLX	C3-C4-C5-O8
49	G	201	8Q1	C43-C42-N41-C39
50	l	703	CDL	CB3-CB4-CB6-OB8
50	s	401	CDL	CB3-CB4-CB6-OB8
57	l	701	PEE	C1-C2-C3-O3
50	r	504	CDL	C15-C16-C17-C18
57	j	201	PEE	C31-C30-O3-C3
50	V	202	CDL	CA7-C31-C32-C33
48	r	503	PLX	C19-C20-C21-C22
57	j	201	PEE	O5-C30-O3-C3
50	V	202	CDL	C13-C14-C15-C16
48	C	302	PLX	C2-O1-P1-O4
48	C	302	PLX	C2-O1-P1-O3
48	a	201	PLX	C2-O1-P1-O2
48	g	201	PLX	C3-O4-P1-O1
48	g	201	PLX	C3-O4-P1-O3
48	j	204	PLX	C3-C4-O6-C6
48	j	204	PLX	C3-O4-P1-O1
48	j	204	PLX	C3-O4-P1-O2
48	j	204	PLX	C2-O1-P1-O3
48	r	502	PLX	C3-O4-P1-O1
48	r	502	PLX	C3-O4-P1-O2
48	r	502	PLX	C3-O4-P1-O3
48	r	502	PLX	C2-O1-P1-O4
48	r	502	PLX	C2-O1-P1-O3
48	r	503	PLX	C3-C4-O6-C6
48	r	503	PLX	C5-C4-O6-C6
48	r	503	PLX	C3-O4-P1-O1

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Mol	Chain	Res	Type	Atoms
48	r	503	PLX	C3-O4-P1-O2
48	r	503	PLX	C3-O4-P1-O3
50	I	201	CDL	CA3-OA5-PA1-OA3
50	V	201	CDL	CA3-OA5-PA1-OA3
50	V	201	CDL	CB2-OB2-PB2-OB4
50	V	201	CDL	CB3-OB5-PB2-OB2
50	V	202	CDL	CA3-OA5-PA1-OA2
50	V	202	CDL	CA3-OA5-PA1-OA3
50	b	201	CDL	CB3-OB5-PB2-OB3
50	k	101	CDL	CB2-OB2-PB2-OB4
50	l	702	CDL	CA3-OA5-PA1-OA4
50	l	703	CDL	CA2-OA2-PA1-OA5
50	l	703	CDL	CB3-OB5-PB2-OB2
50	l	703	CDL	CB3-OB5-PB2-OB3
50	n	101	CDL	CB2-OB2-PB2-OB4
50	n	101	CDL	CB3-OB5-PB2-OB2
50	n	101	CDL	CB3-OB5-PB2-OB3
50	r	504	CDL	CB2-OB2-PB2-OB3
50	r	504	CDL	CB2-OB2-PB2-OB4
50	r	504	CDL	CB2-OB2-PB2-OB5
57	i	401	PEE	C4-O4P-P-O2P
57	j	201	PEE	C1-O3P-P-O2P
57	j	201	PEE	C4-O4P-P-O2P
57	j	202	PEE	C1-O3P-P-O4P
57	j	202	PEE	C4-O4P-P-O1P
57	j	203	PEE	C4-O4P-P-O3P
57	j	203	PEE	C4-O4P-P-O1P
57	l	701	PEE	C4-O4P-P-O1P
57	W	201	PEE	C12-C13-C14-C15
50	k	101	CDL	CA4-CA3-OA5-PA1
50	r	504	CDL	C1-CB2-OB2-PB2
57	l	704	PEE	C10-C11-C12-C13
50	k	101	CDL	C23-C24-C25-C26
50	l	703	CDL	C18-C19-C20-C21
57	j	201	PEE	C30-C31-C32-C33
48	a	201	PLX	C16-C17-C18-C19
48	r	503	PLX	C33-C34-C35-C36
50	V	202	CDL	C81-C82-C83-C84
50	k	101	CDL	CA6-CA4-OA6-CA5
57	l	704	PEE	C3-C2-O2-C10
57	i	401	PEE	C24-C25-C26-C27
50	V	202	CDL	C84-C85-C86-C87

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Mol	Chain	Res	Type	Atoms
50	k	101	CDL	C58-C59-C60-C61
48	j	204	PLX	C11-C10-C9-C8
50	b	201	CDL	C43-C44-C45-C46
57	r	501	PEE	C32-C33-C34-C35
50	l	703	CDL	C20-C21-C22-C23
57	i	401	PEE	C38-C39-C40-C41
57	i	401	PEE	O3P-C1-C2-O2
50	s	401	CDL	C56-C57-C58-C59
47	A	503	NAI	O4B-C4B-C5B-O5B
50	V	202	CDL	C36-C37-C38-C39
50	k	101	CDL	C16-C17-C18-C19
50	b	201	CDL	C42-C43-C44-C45
48	j	204	PLX	O6-C4-C5-O8
50	V	201	CDL	OA6-CA4-CA6-OA8
50	r	504	CDL	OB6-CB4-CB6-OB8
50	V	201	CDL	C32-C31-CA7-OA8
46	A	502	FMN	O2'-C2'-C3'-O3'
57	l	704	PEE	C16-C17-C18-C19
57	i	401	PEE	C35-C36-C37-C38
48	C	302	PLX	C3-C4-C5-O8
57	l	704	PEE	C13-C14-C15-C16
57	i	401	PEE	C16-C17-C18-C19
57	l	704	PEE	C38-C39-C40-C41
48	j	204	PLX	C34-C35-C36-C37
48	r	503	PLX	C12-C13-C14-C15
48	r	503	PLX	O8-C24-C25-C26
50	l	703	CDL	C19-C20-C21-C22
50	V	201	CDL	CB7-C71-C72-C73
50	V	202	CDL	C82-C83-C84-C85
50	l	702	CDL	CA4-CA3-OA5-PA1
50	l	703	CDL	C64-C65-C66-C67
50	I	201	CDL	CB7-C71-C72-C73
50	l	703	CDL	C74-C75-C76-C77
57	W	201	PEE	C16-C17-C18-C19
57	j	203	PEE	C18-C19-C20-C21
57	i	401	PEE	C37-C38-C39-C40
50	V	201	CDL	C13-C14-C15-C16
50	V	201	CDL	C21-C22-C23-C24
50	l	702	CDL	C51-C52-C53-C54
50	V	202	CDL	C77-C78-C79-C80
50	s	401	CDL	C74-C75-C76-C77
57	l	704	PEE	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
57	l	704	PEE	O2-C2-C3-O3
49	X	201	8Q1	C10-C11-C12-C13
51	J	401	NDP	O4D-C1D-N1N-C6N
57	i	401	PEE	C2-C1-O3P-P
48	C	302	PLX	C16-C17-C18-C19
50	l	703	CDL	C32-C31-CA7-OA8
50	l	702	CDL	C55-C56-C57-C58
57	r	501	PEE	C16-C17-C18-C19
57	r	501	PEE	C38-C39-C40-C41
50	l	703	CDL	C38-C39-C40-C41
50	b	201	CDL	C39-C40-C41-C42
48	C	302	PLX	C19-C20-C21-C22
57	i	401	PEE	C18-C19-C20-C21
57	j	202	PEE	C38-C39-C40-C41
48	j	204	PLX	C36-C37-C38-C39
50	b	201	CDL	C59-C60-C61-C62
57	l	705	PEE	C2-C1-O3P-P
48	a	201	PLX	C7-C8-C9-C10
50	l	702	CDL	C80-C81-C82-C83
57	i	401	PEE	C14-C15-C16-C17
57	l	701	PEE	O3P-C1-C2-C3
48	a	201	PLX	C28-C29-C30-C31
57	l	701	PEE	C36-C37-C38-C39
50	b	201	CDL	C12-C13-C14-C15
47	A	503	NAI	O4D-C1D-N1N-C2N
47	A	503	NAI	C2N-C3N-C7N-N7N
48	r	503	PLX	C26-C27-C28-C29
50	k	101	CDL	C55-C56-C57-C58
50	V	201	CDL	C22-C23-C24-C25
47	A	503	NAI	C2D-C1D-N1N-C2N
57	l	705	PEE	C31-C32-C33-C34
50	k	101	CDL	C43-C44-C45-C46
57	j	201	PEE	C16-C17-C18-C19
48	g	201	PLX	O6-C6-C7-C8
48	g	201	PLX	O8-C24-C25-C26
48	j	205	PLX	O6-C6-C7-C8
50	s	401	CDL	C40-C41-C42-C43
52	s	402	UQ	C12-C13-C14-C15
57	j	201	PEE	C34-C35-C36-C37
52	s	402	UQ	C9-C11-C12-C13
48	C	302	PLX	O9-C24-C25-C26
49	G	201	8Q1	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
50	V	201	CDL	C60-C61-C62-C63
57	j	202	PEE	C13-C14-C15-C16
48	r	502	PLX	C29-C30-C31-C32
50	r	504	CDL	C72-C71-CB7-OB8
50	b	201	CDL	OB5-CB3-CB4-CB6
57	i	401	PEE	O2-C2-C3-O3
50	n	101	CDL	C32-C31-CA7-OA8
50	r	504	CDL	CB7-C71-C72-C73
50	V	202	CDL	C32-C31-CA7-OA8
57	l	701	PEE	C38-C39-C40-C41
50	l	702	CDL	C72-C73-C74-C75
57	j	203	PEE	C33-C34-C35-C36
46	A	502	FMN	C5'-O5'-P-O3P
57	j	203	PEE	C16-C17-C18-C19
57	l	701	PEE	C16-C17-C18-C19
50	V	201	CDL	CB5-C51-C52-C53
50	V	202	CDL	C78-C79-C80-C81
50	l	703	CDL	C76-C77-C78-C79
48	a	201	PLX	C11-C12-C13-C14
48	a	201	PLX	C32-C33-C34-C35
50	V	201	CDL	C35-C36-C37-C38
50	l	702	CDL	C37-C38-C39-C40
57	l	704	PEE	C2-C1-O3P-P
50	l	703	CDL	OA5-CA3-CA4-OA6
50	r	504	CDL	CB3-CB4-CB6-OB8
57	i	401	PEE	C1-C2-C3-O3
57	l	704	PEE	C1-C2-C3-O3
57	j	201	PEE	C36-C37-C38-C39
50	n	101	CDL	C32-C31-CA7-OA9
57	r	501	PEE	C5-C4-O4P-P
50	V	201	CDL	C17-C18-C19-C20
50	V	202	CDL	C74-C75-C76-C77
57	r	501	PEE	C39-C40-C41-C42
57	j	202	PEE	C16-C17-C18-C19
50	r	504	CDL	C79-C80-C81-C82
50	k	101	CDL	C54-C55-C56-C57
48	j	205	PLX	C7-C6-O6-C4
50	b	201	CDL	C32-C31-CA7-OA8
50	l	703	CDL	C22-C23-C24-C25
48	r	502	PLX	C34-C35-C36-C37
50	b	201	CDL	C18-C19-C20-C21
57	j	201	PEE	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
50	l	703	CDL	C71-C72-C73-C74
48	g	201	PLX	C16-C17-C18-C19
48	j	204	PLX	C28-C29-C30-C31
48	j	205	PLX	N1-C1-C2-O1
50	l	703	CDL	C52-C53-C54-C55
48	r	503	PLX	C24-C25-C26-C27
55	Q	501	UQ1	C7-C8-C9-C11
50	l	702	CDL	C72-C71-CB7-OB8
50	V	201	CDL	OB5-CB3-CB4-OB6
50	b	201	CDL	OB5-CB3-CB4-OB6
50	l	702	CDL	OB5-CB3-CB4-OB6
50	V	202	CDL	C52-C51-CB5-OB6
48	j	205	PLX	C24-C25-C26-C27
50	I	201	CDL	C12-C11-CA5-OA6
50	l	702	CDL	C12-C11-CA5-OA6
48	j	205	PLX	C25-C24-O8-C5
50	I	201	CDL	C72-C71-CB7-OB8
50	b	201	CDL	C12-C11-CA5-OA6
50	l	703	CDL	C72-C71-CB7-OB8
48	j	205	PLX	C36-C37-C38-C39
50	V	202	CDL	C44-C45-C46-C47
50	s	401	CDL	CA3-CA4-OA6-CA5
50	s	401	CDL	CA6-CA4-OA6-CA5
50	r	504	CDL	C73-C74-C75-C76
50	l	702	CDL	OA7-CA5-OA6-CA4
57	j	202	PEE	O3-C30-C31-C32
50	b	201	CDL	CA7-C31-C32-C33
50	s	401	CDL	C20-C21-C22-C23
50	I	201	CDL	C72-C71-CB7-OB9
50	l	702	CDL	C72-C71-CB7-OB9
48	a	201	PLX	O6-C6-C7-C8
48	r	502	PLX	C6-C7-C8-C9
50	n	101	CDL	C72-C73-C74-C75
50	r	504	CDL	CA5-C11-C12-C13
48	g	201	PLX	O9-C24-O8-C5
50	b	201	CDL	C44-C45-C46-C47
50	l	702	CDL	C12-C11-CA5-OA7
49	G	201	8Q1	C6-C7-C8-C9
50	l	702	CDL	C52-C51-CB5-OB6
50	V	202	CDL	C52-C51-CB5-OB7
48	j	204	PLX	C12-C13-C14-C15
50	k	101	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
50	b	201	CDL	C32-C31-CA7-OA9
57	i	401	PEE	C36-C37-C38-C39
48	C	302	PLX	C15-C16-C17-C18
57	j	202	PEE	O5-C30-C31-C32
50	r	504	CDL	C52-C51-CB5-OB6
57	j	201	PEE	C20-C21-C22-C23
50	l	702	CDL	C15-C16-C17-C18
50	s	401	CDL	C72-C71-CB7-OB8
50	l	703	CDL	C72-C71-CB7-OB9
50	l	703	CDL	OA5-CA3-CA4-CA6
50	I	201	CDL	C12-C11-CA5-OA7
50	b	201	CDL	C12-C11-CA5-OA7
50	k	101	CDL	C12-C11-CA5-OA6
50	l	702	CDL	C11-CA5-OA6-CA4
58	w	401	ADP	PB-O3A-PA-O2A
57	l	705	PEE	C38-C39-C40-C41
50	n	101	CDL	C52-C51-CB5-OB6
57	j	201	PEE	O3-C30-C31-C32
50	l	703	CDL	C41-C42-C43-C44

There are no ring outliers.

33 monomers are involved in 149 short contacts:

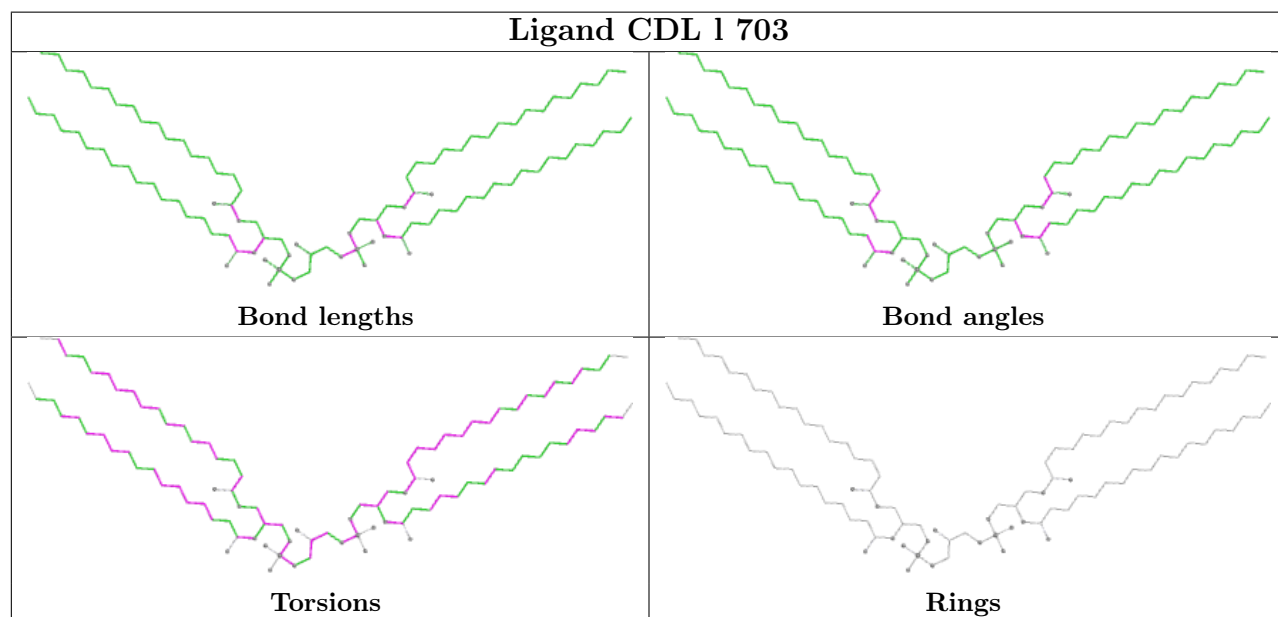
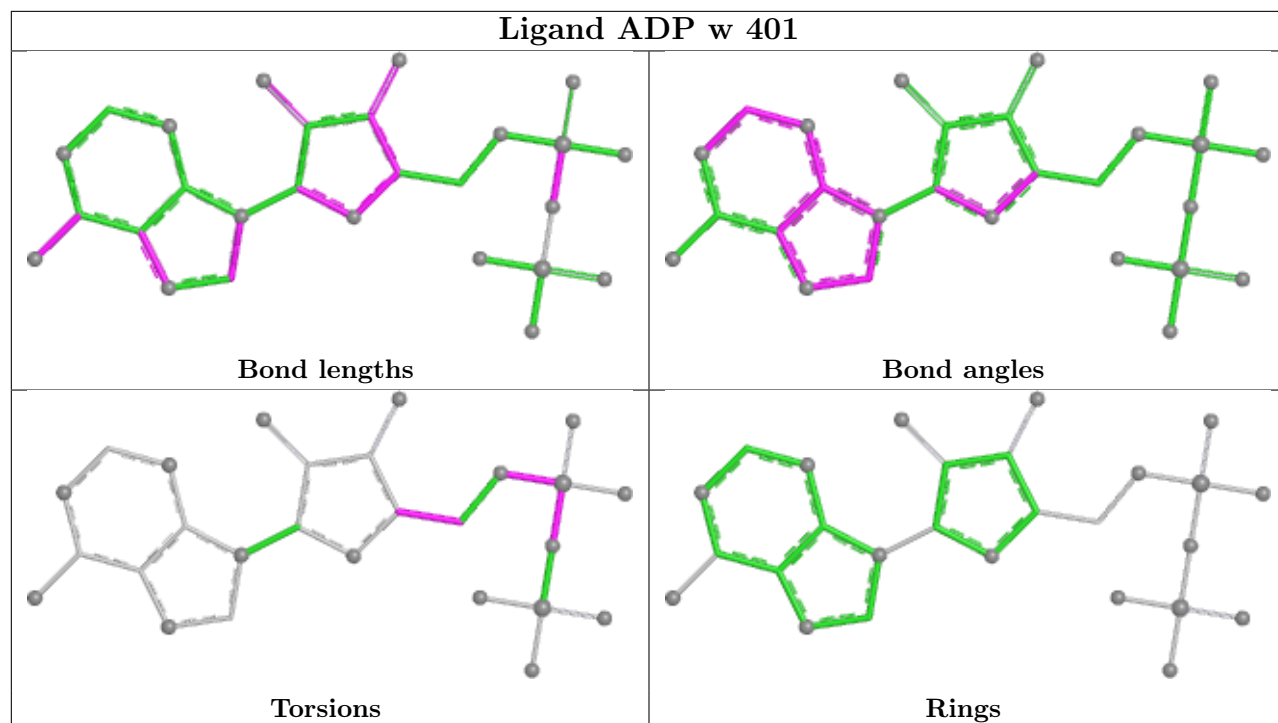
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	w	401	ADP	1	0
50	l	703	CDL	4	0
55	Q	501	UQ1	10	0
50	V	202	CDL	7	0
57	l	705	PEE	6	0
52	s	402	UQ	2	0
48	r	502	PLX	4	0
57	j	203	PEE	2	0
50	r	504	CDL	7	0
57	r	501	PEE	4	0
45	C	301	SF4	2	0
50	l	702	CDL	36	0
57	W	201	PEE	1	0
52	J	402	UQ	2	0
47	A	503	NAI	5	0
48	g	201	PLX	4	0
45	A	501	SF4	1	0
48	a	201	PLX	1	0

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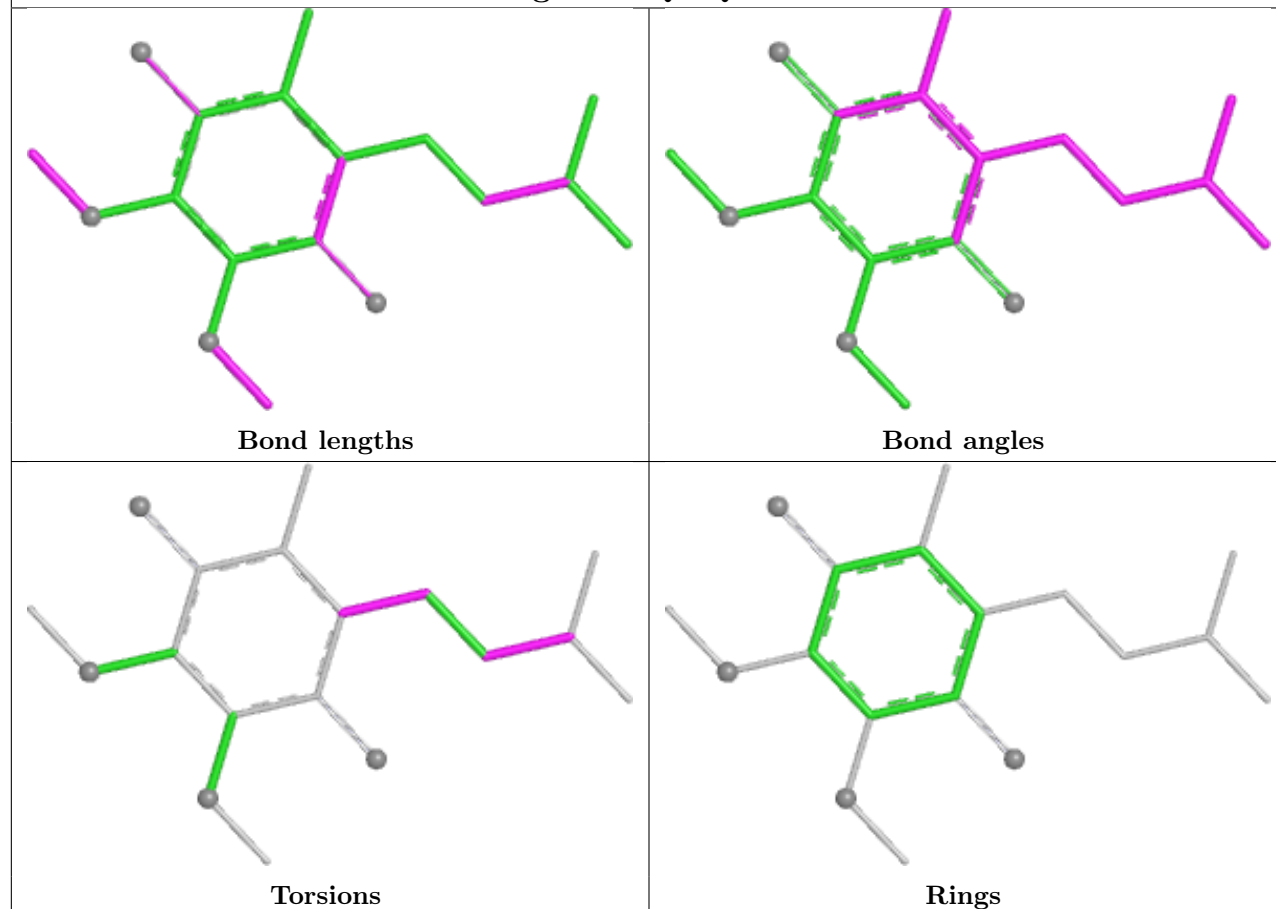
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	502	FMN	3	0
50	s	401	CDL	4	0
48	r	503	PLX	6	0
50	k	101	CDL	9	0
50	V	201	CDL	5	0
57	j	202	PEE	7	0
57	l	704	PEE	4	0
48	j	205	PLX	1	0
48	j	204	PLX	2	0
50	b	201	CDL	5	0
51	J	401	NDP	1	0
57	j	201	PEE	1	0
49	G	201	8Q1	4	0
57	i	401	PEE	2	0
50	I	201	CDL	1	0

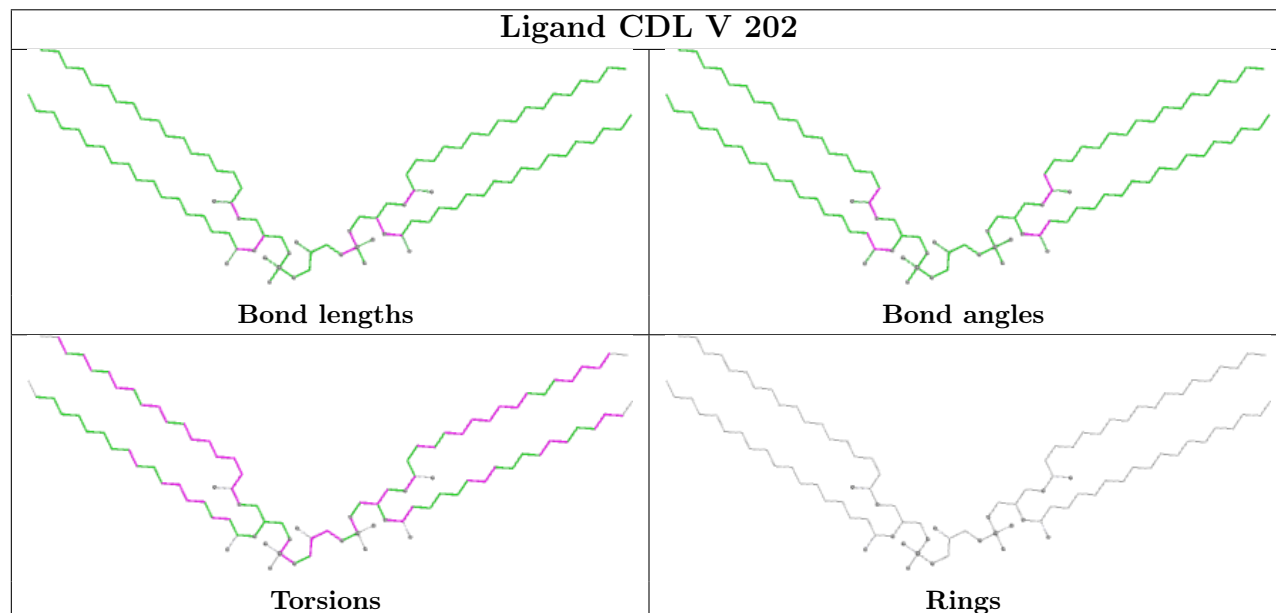
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

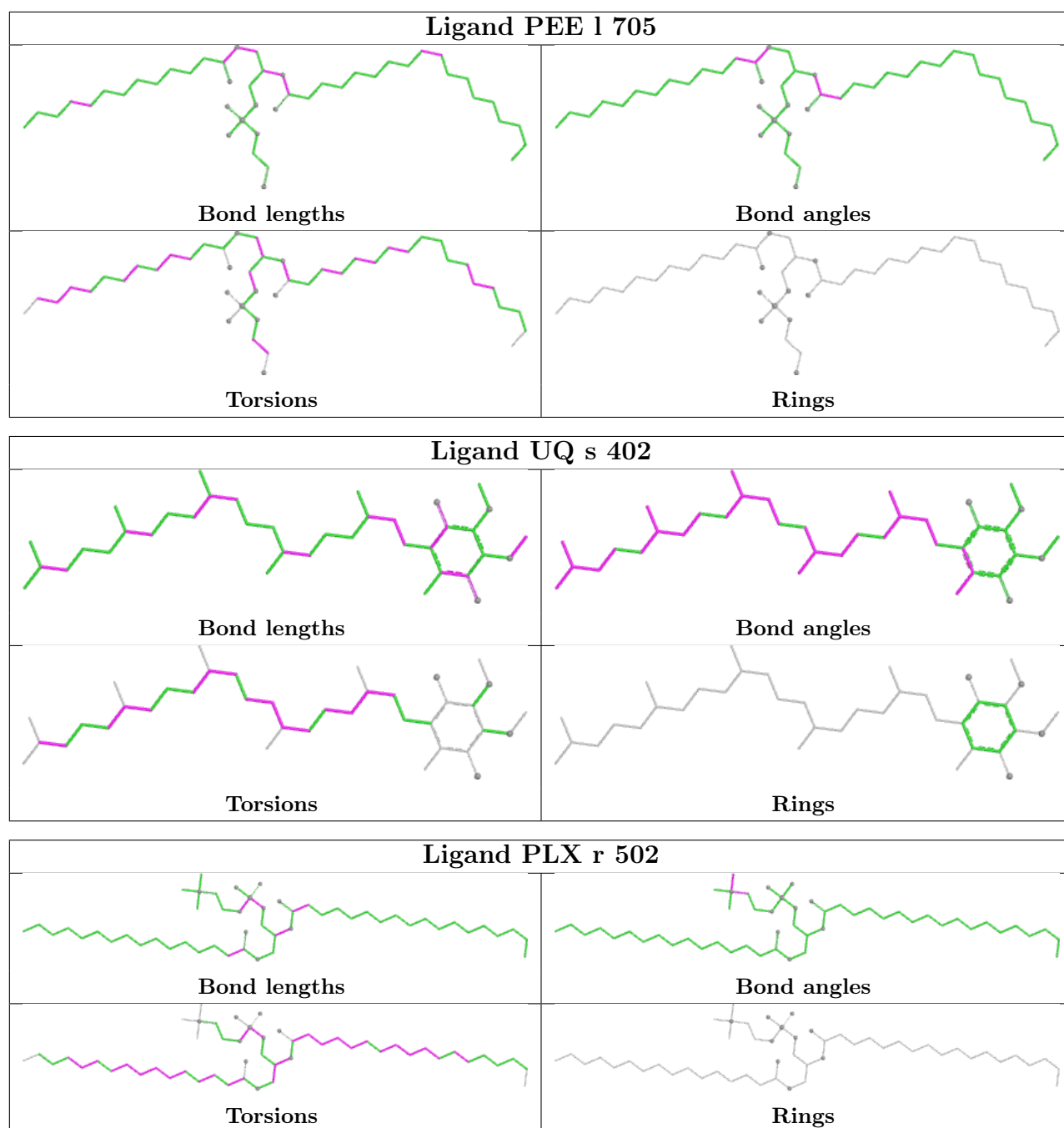


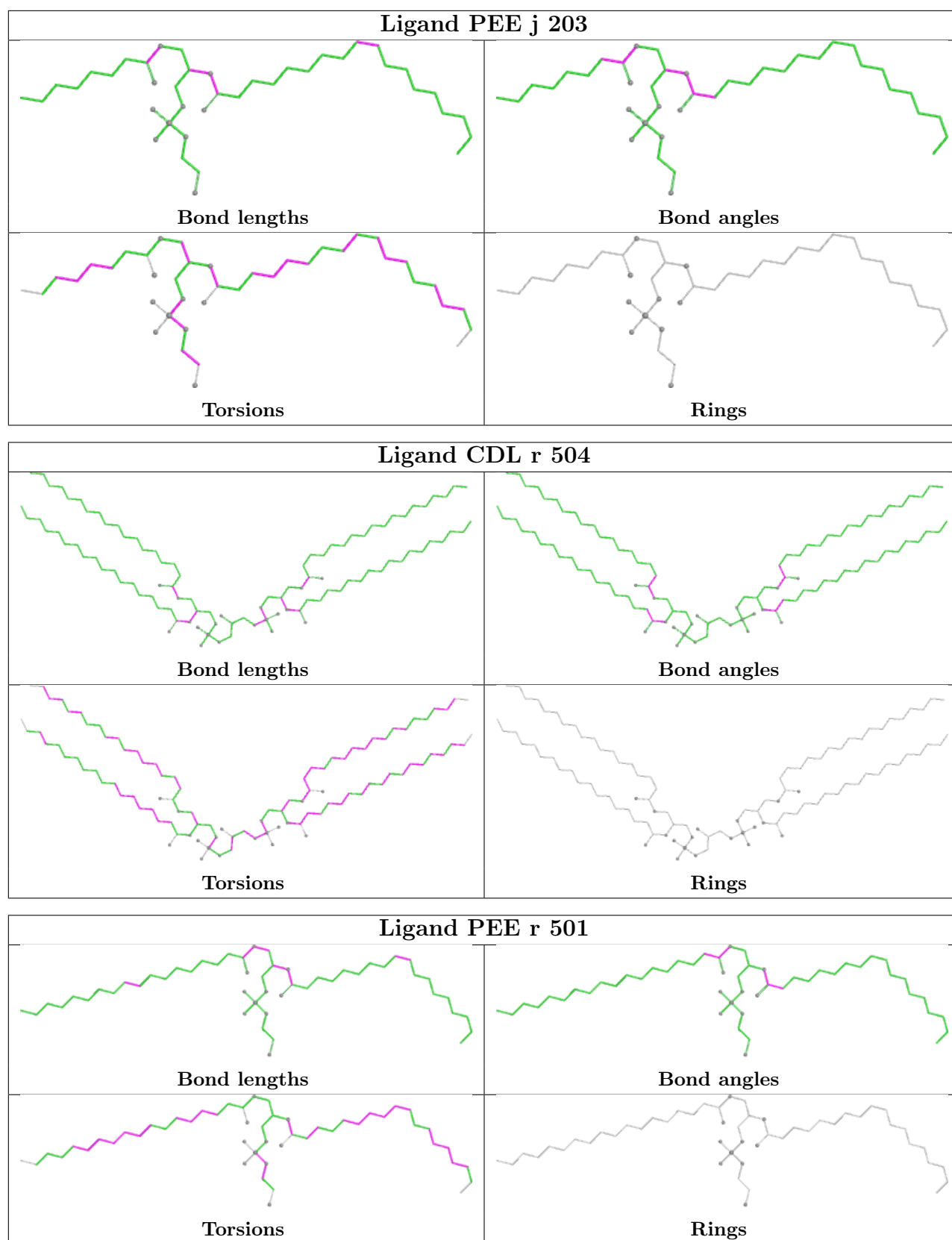
Ligand UQ1 Q 501

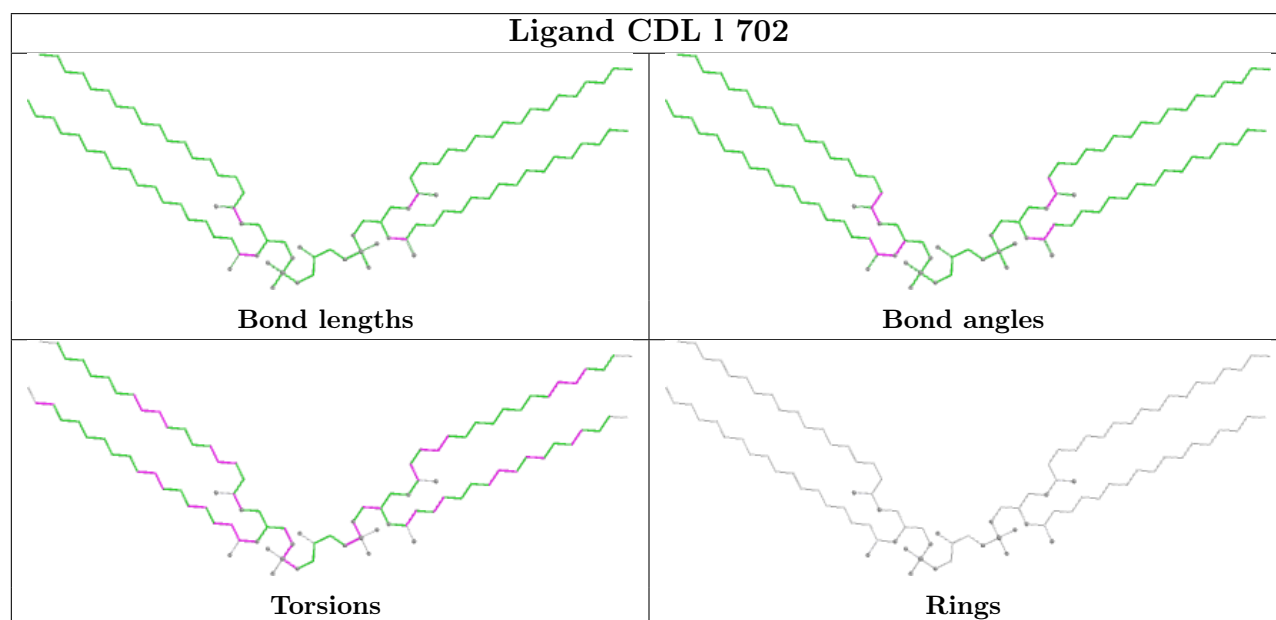
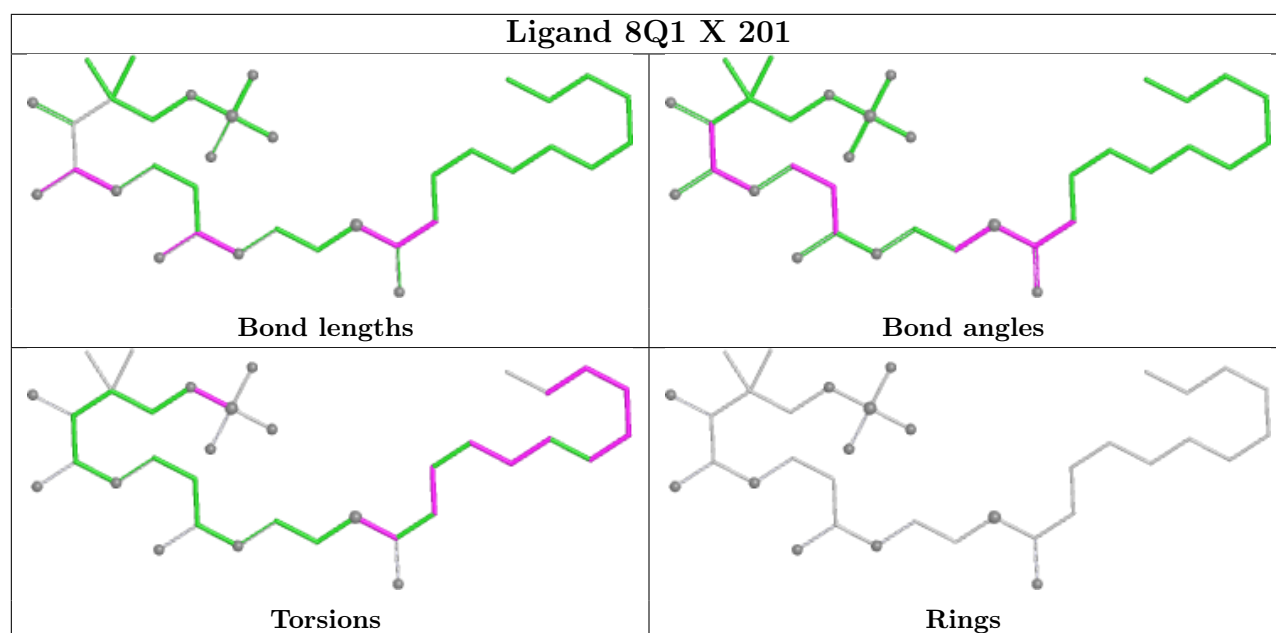


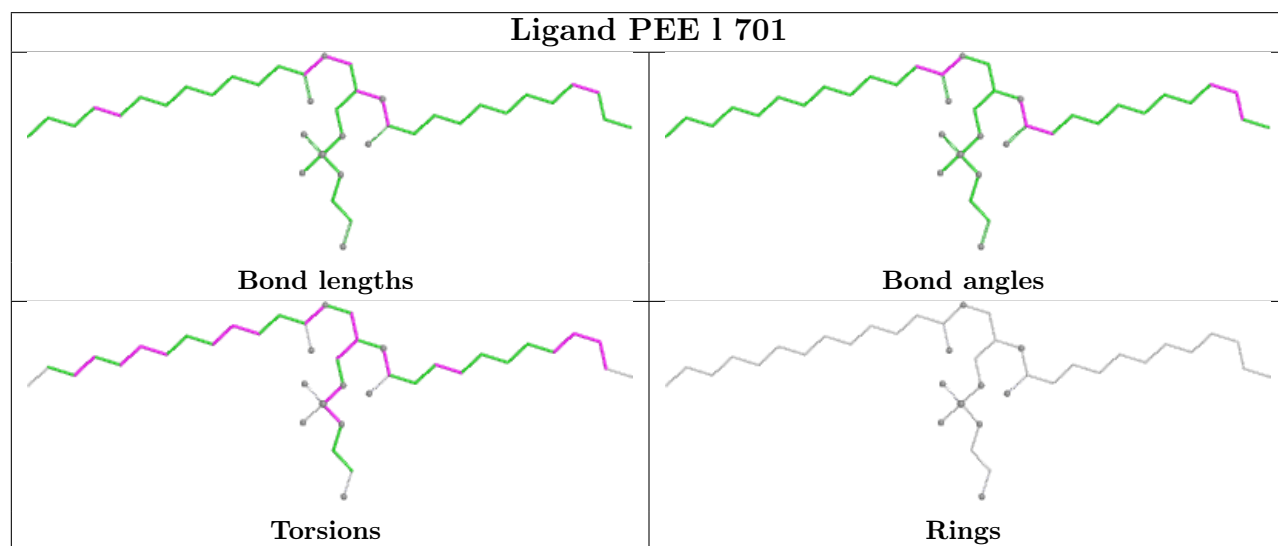
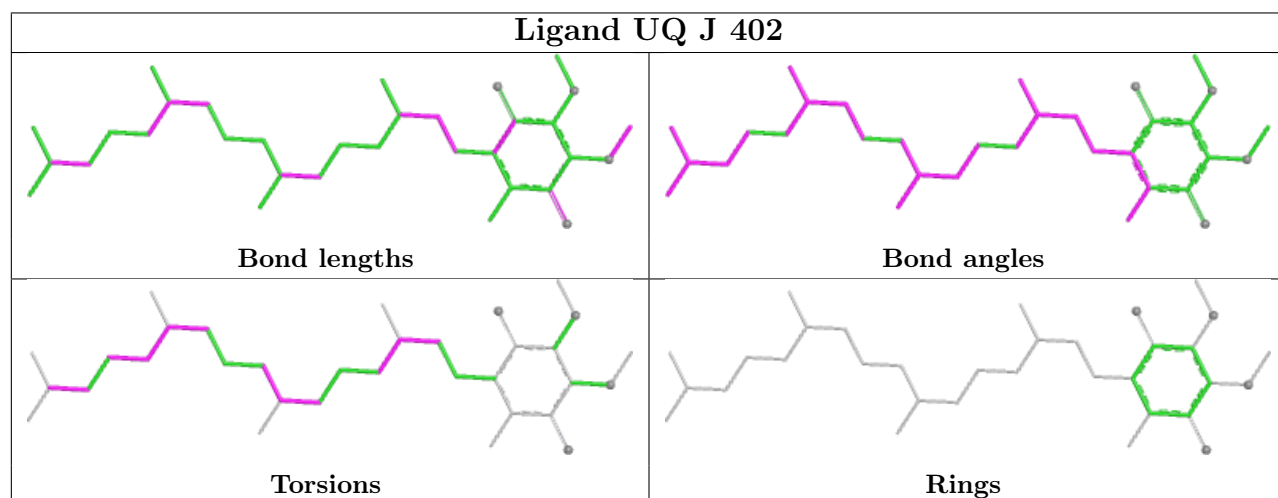
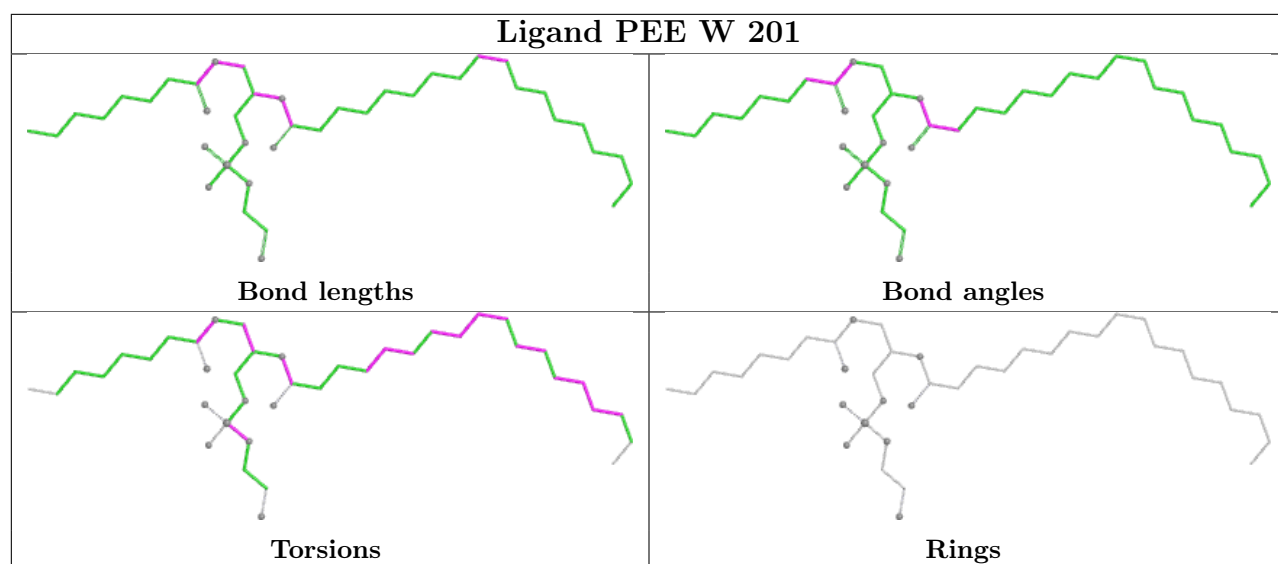
Ligand CDL V 202

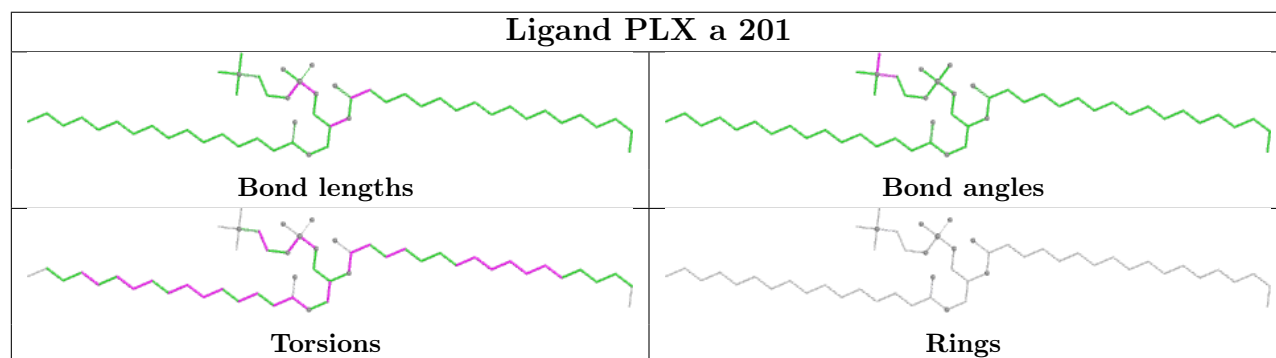
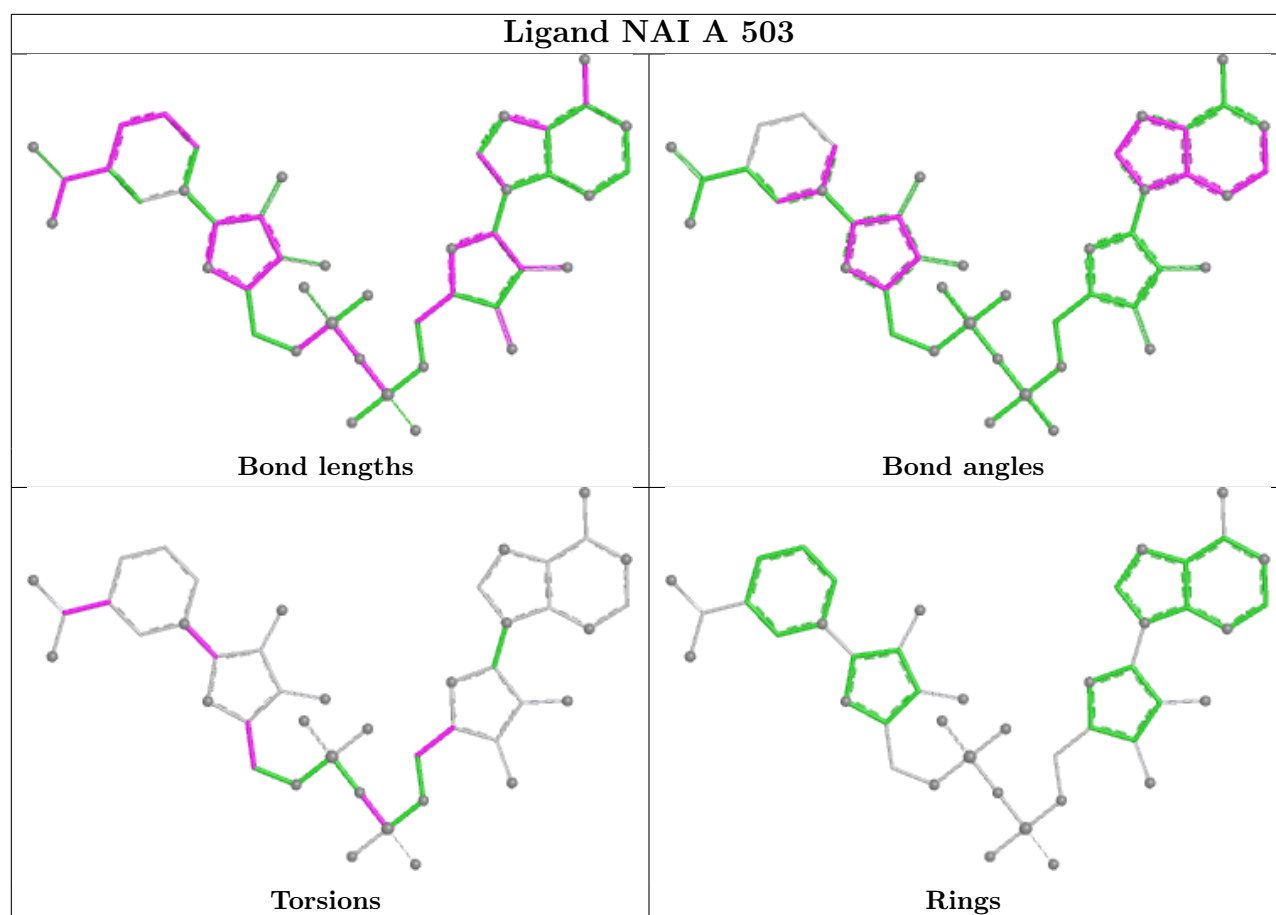


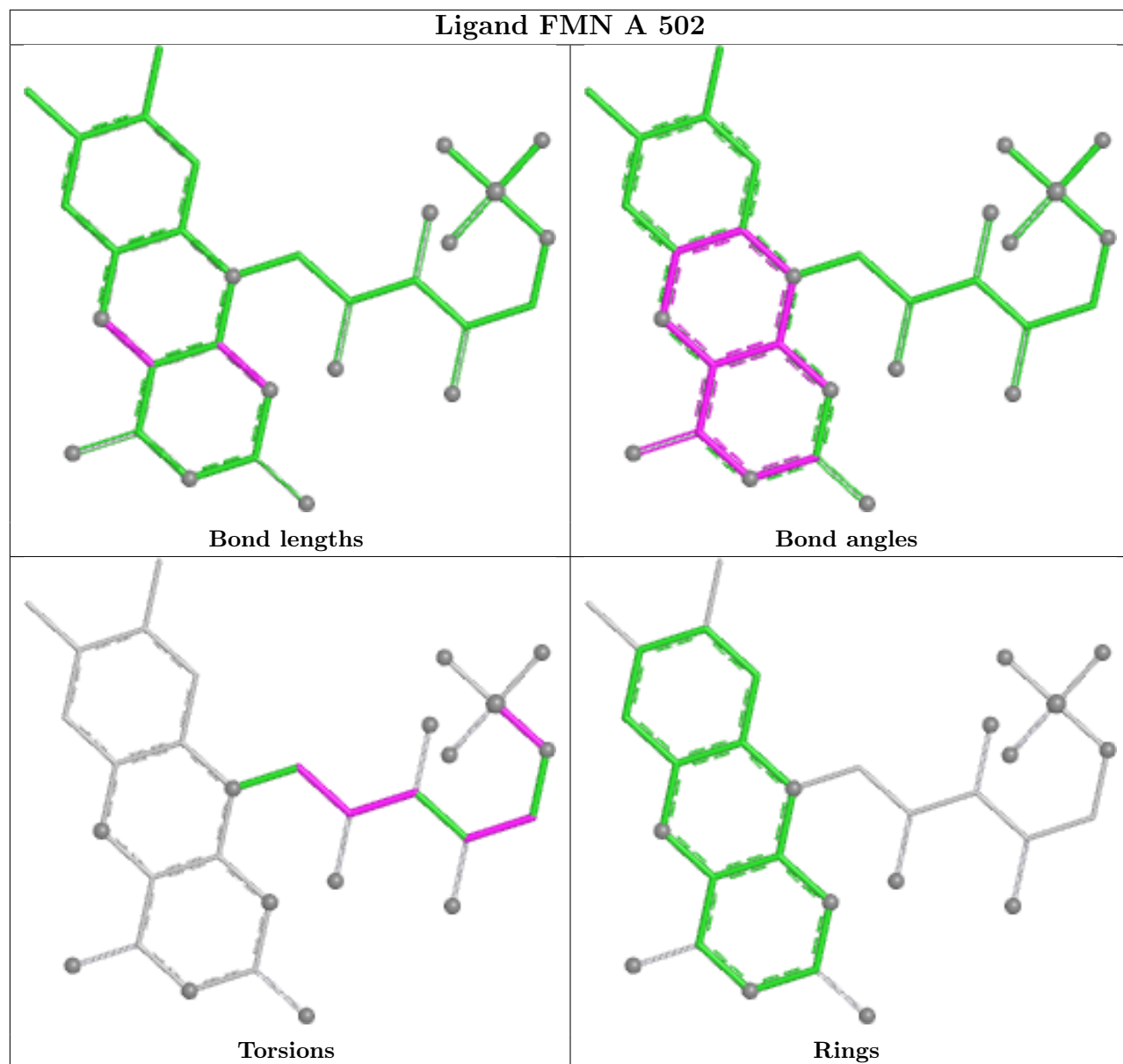


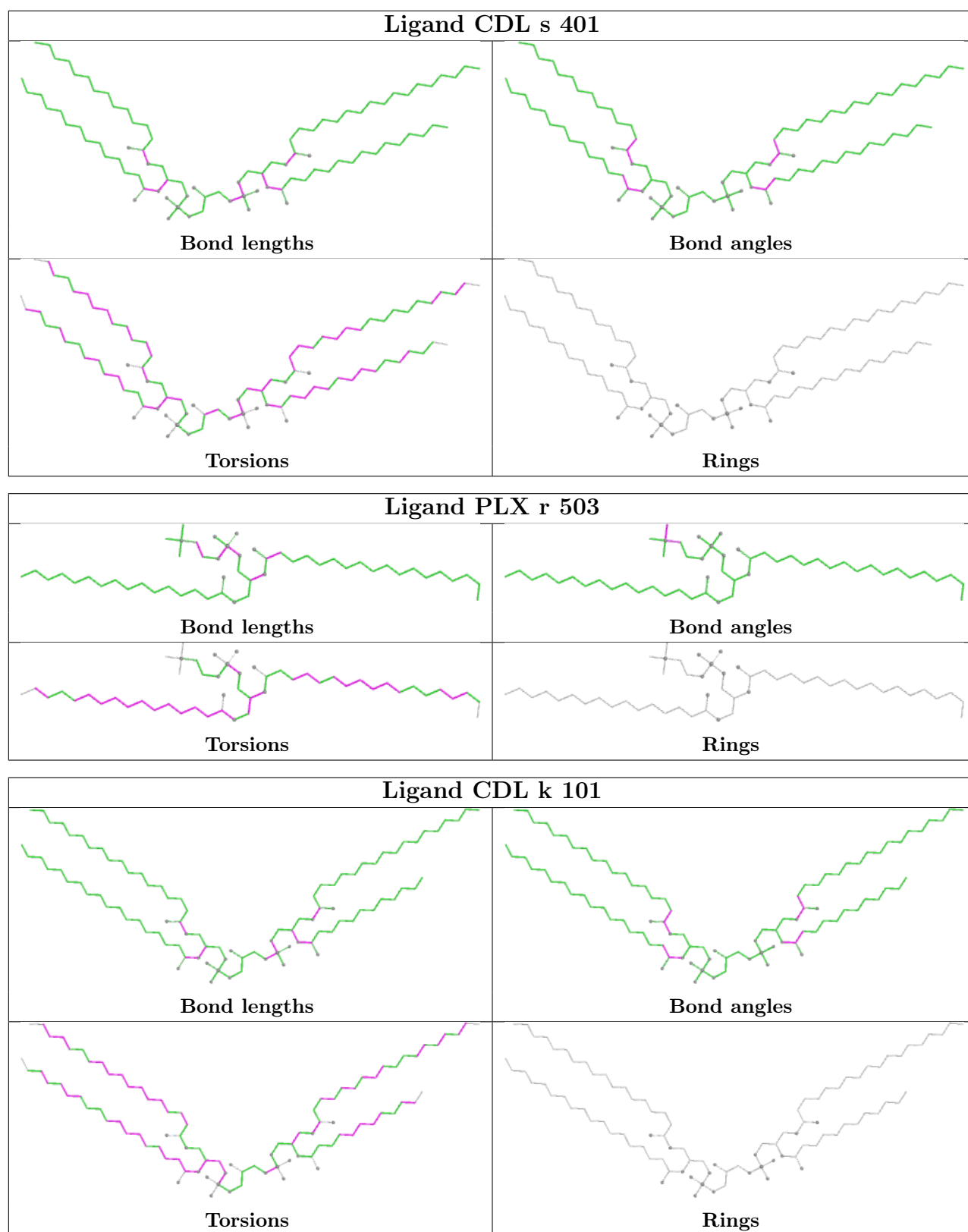


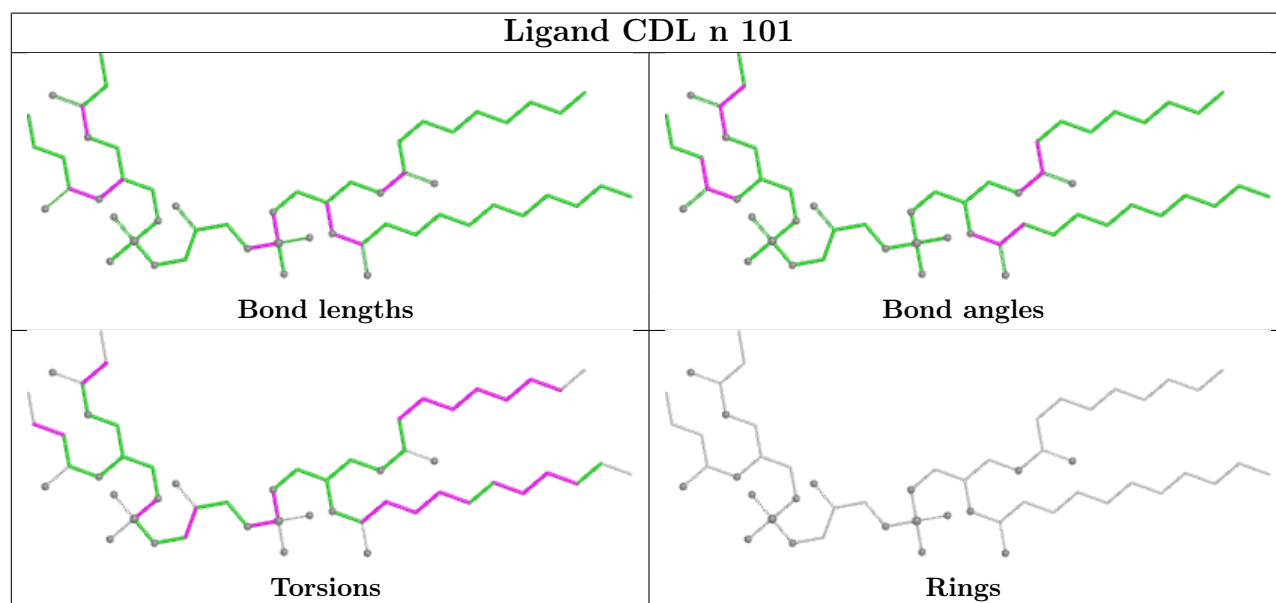
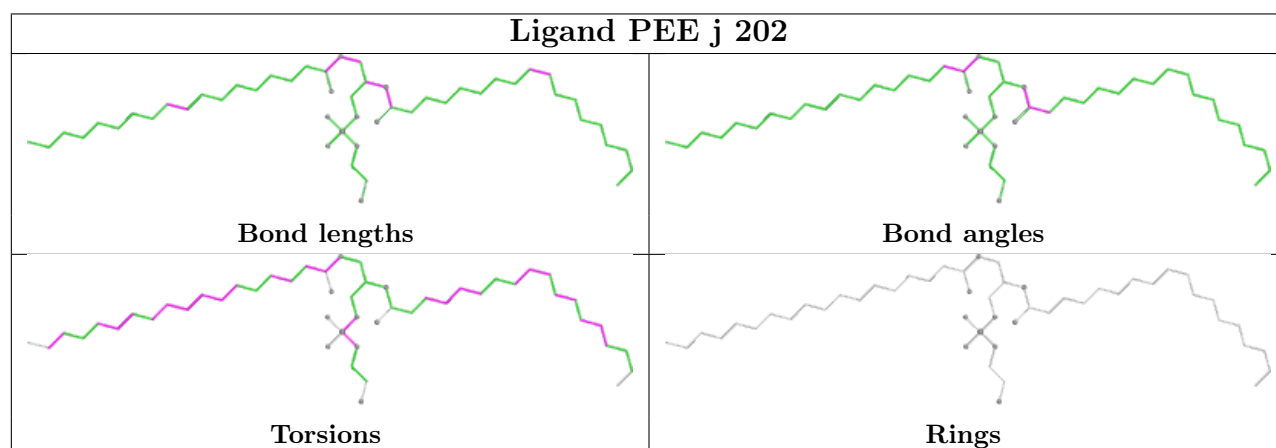
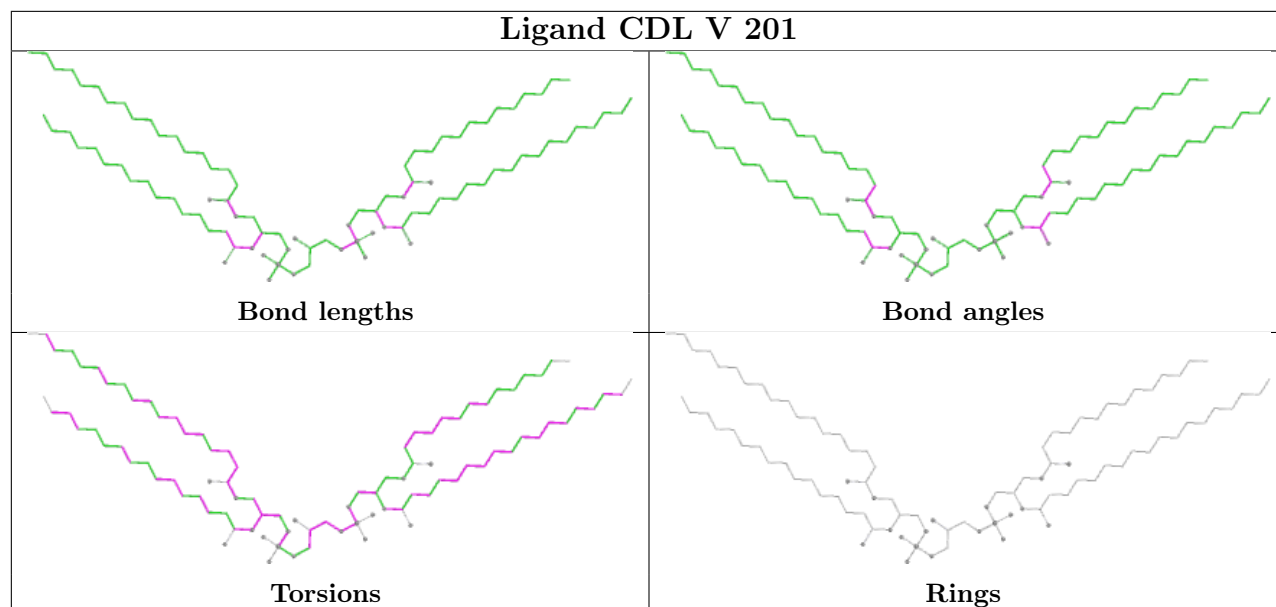


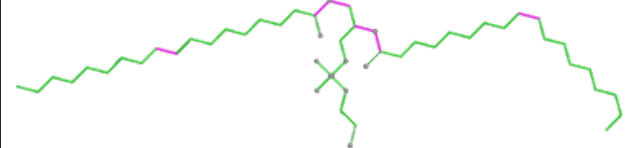
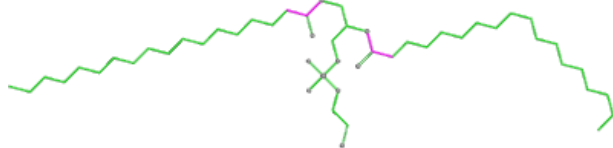
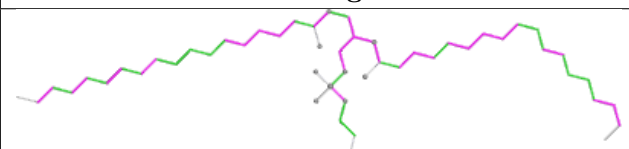
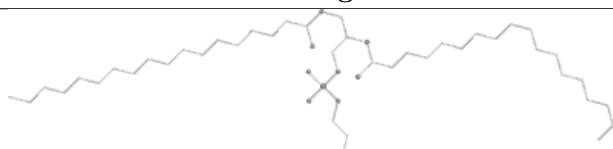
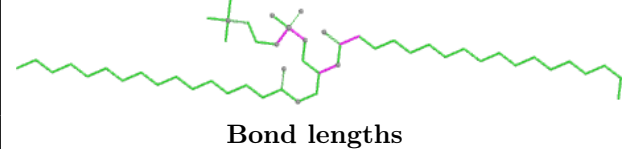
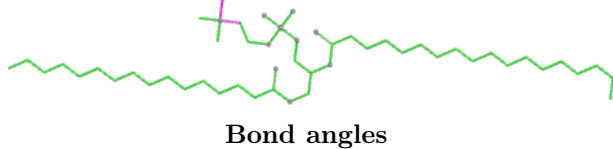
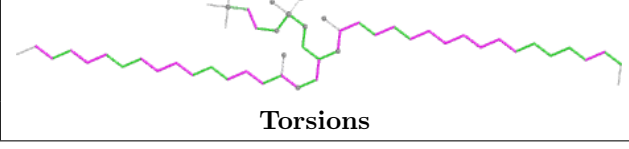
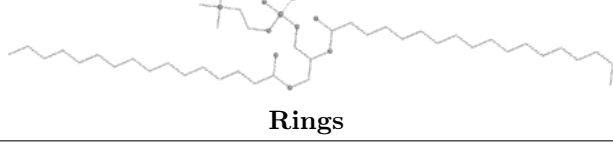
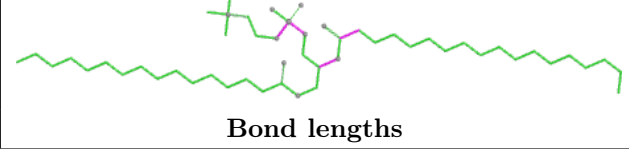
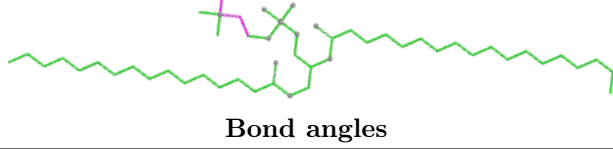
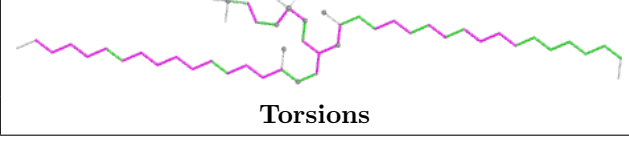
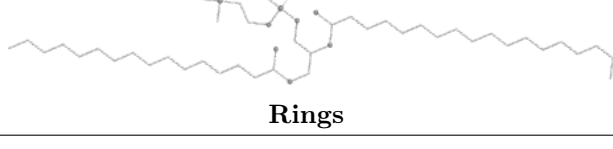


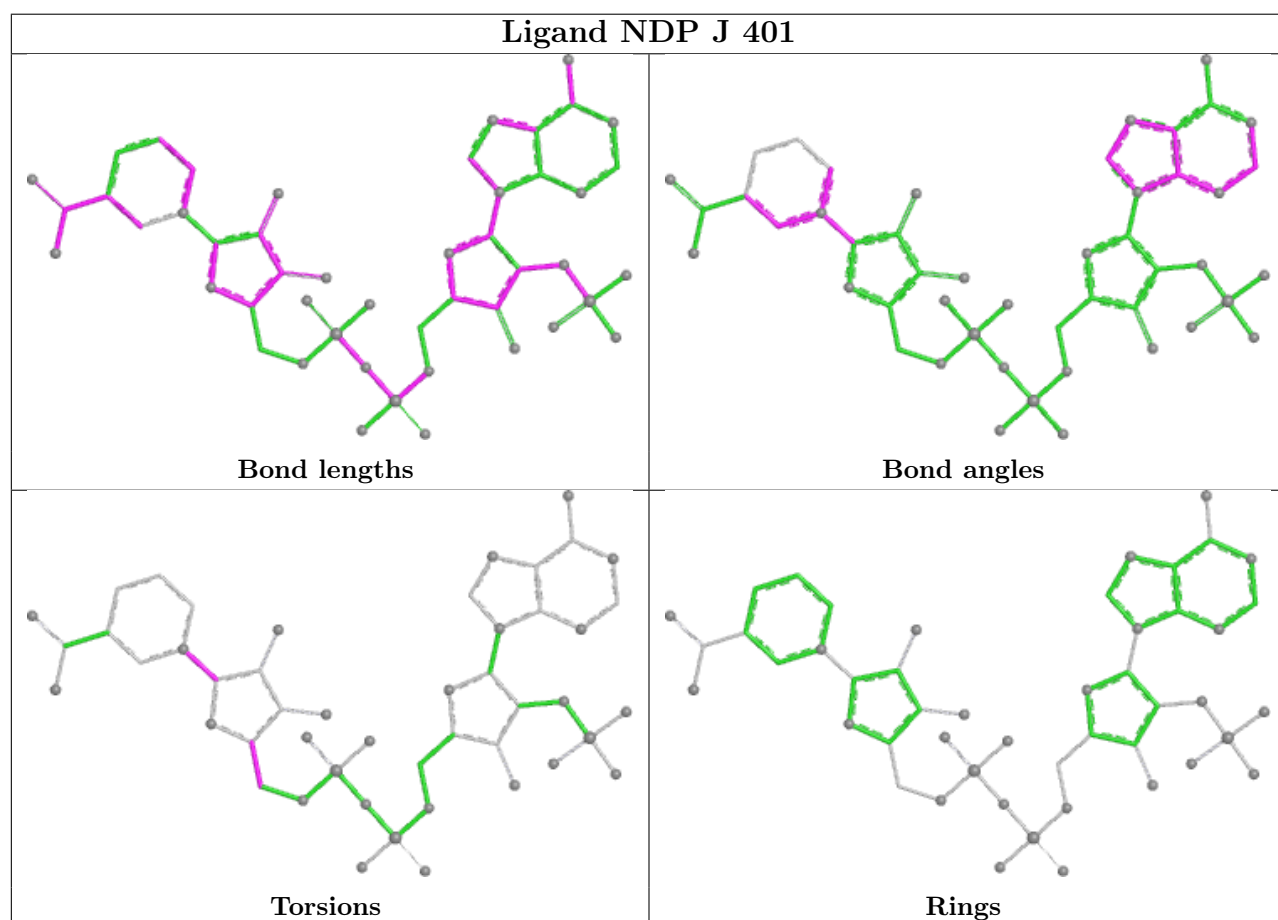
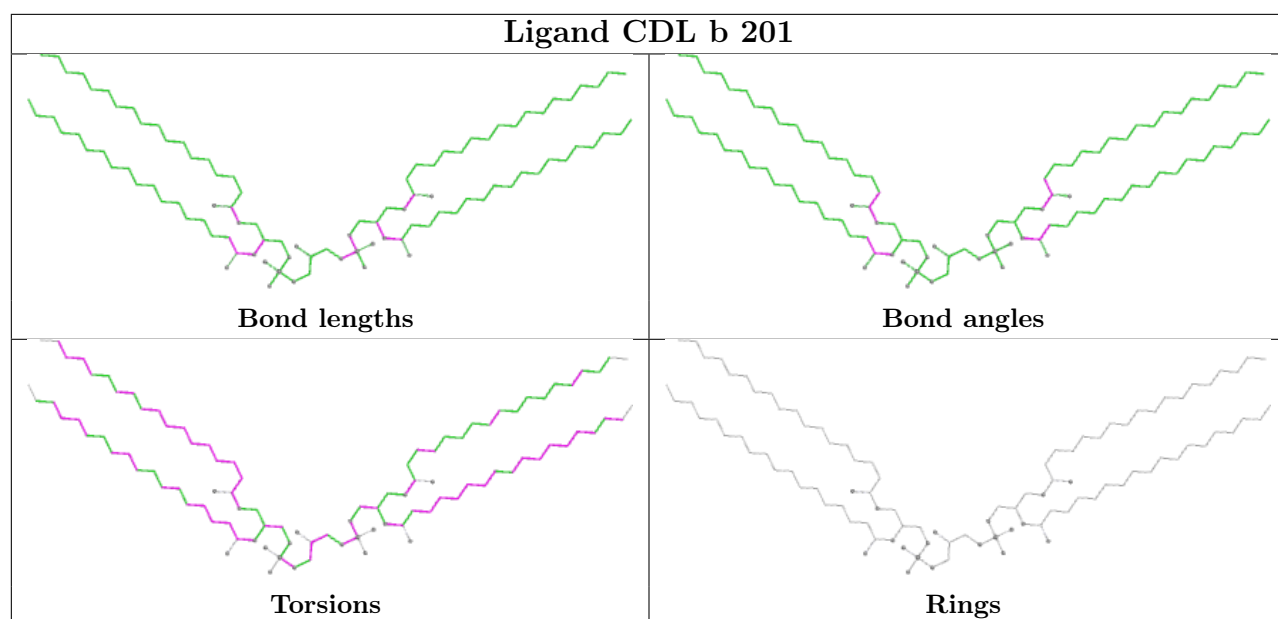


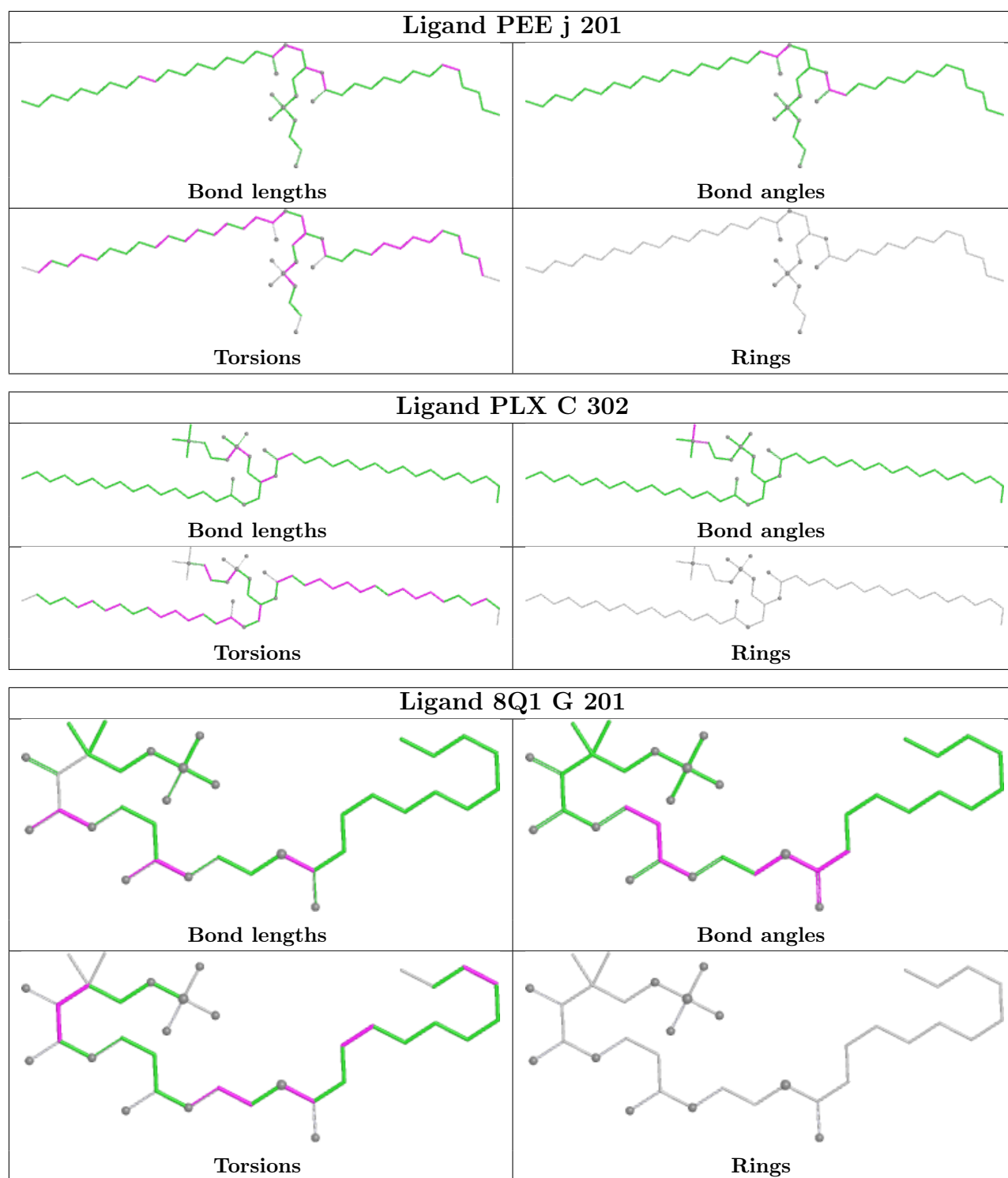


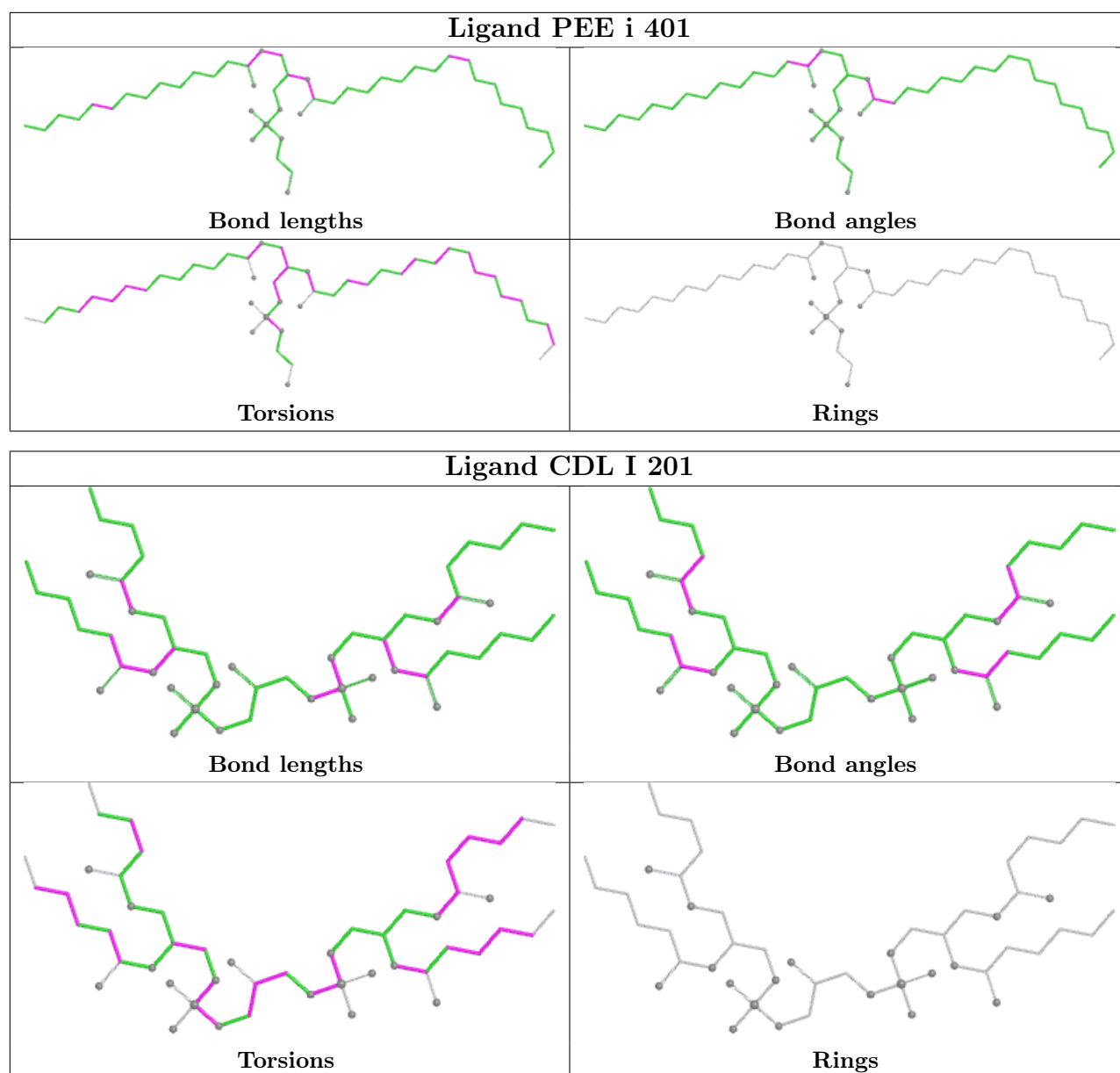




Ligand PEE l 704	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PLX j 205	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PLX j 204	
 Bond lengths	 Bond angles
 Torsions	 Rings







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.

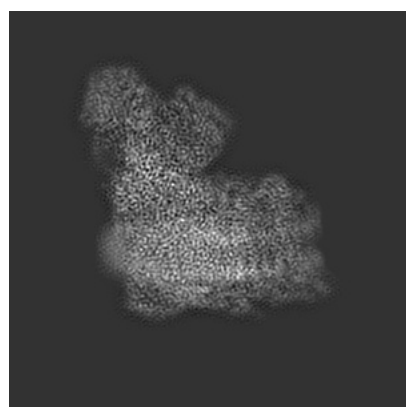
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32301. These allow visual inspection of the internal detail of the map and identification of artifacts.

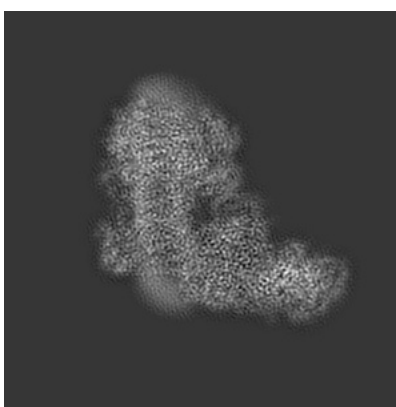
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

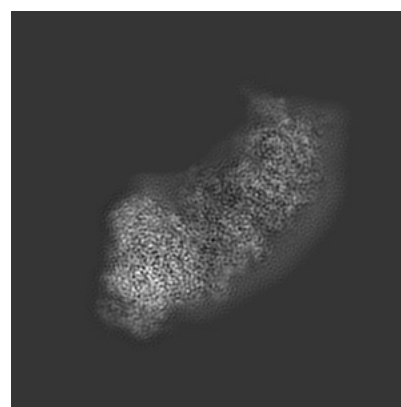
6.1.1 Primary map



X



Y

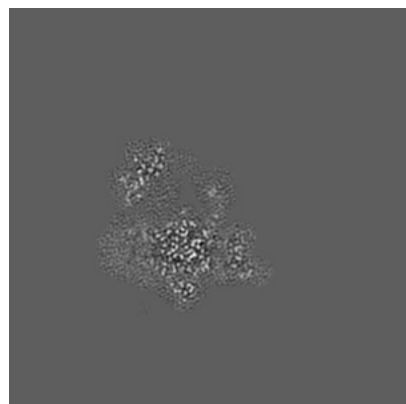


Z

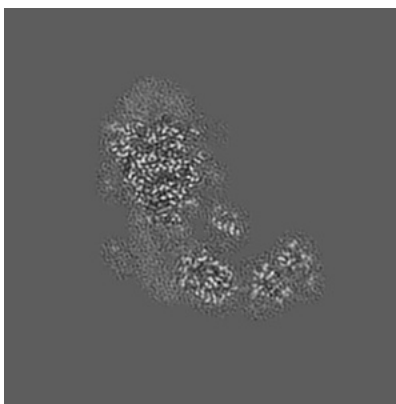
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

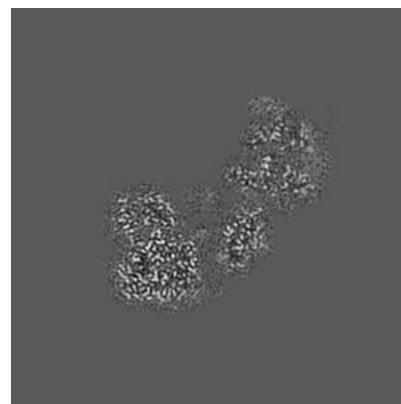
6.2.1 Primary map



X Index: 152



Y Index: 152

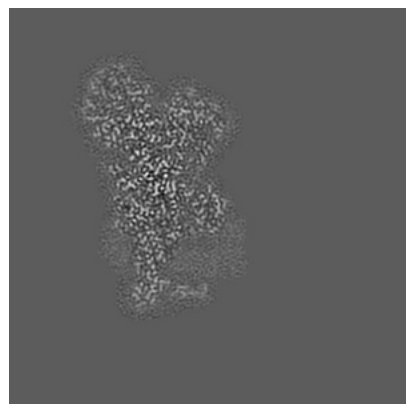


Z Index: 152

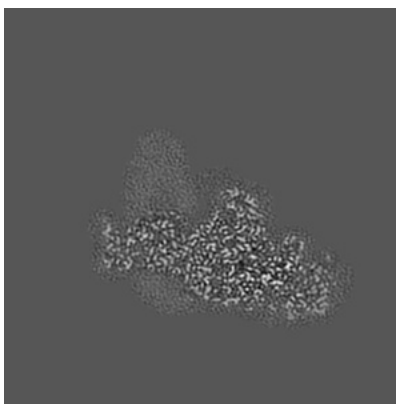
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

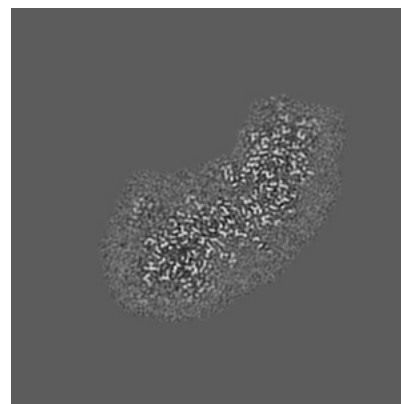
6.3.1 Primary map



X Index: 106



Y Index: 100

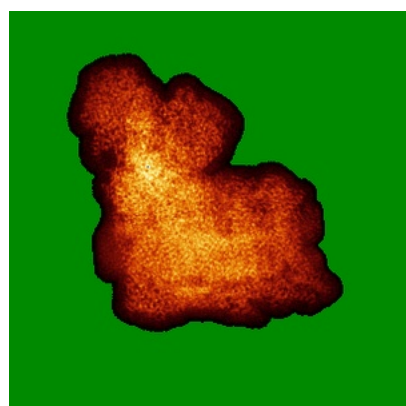


Z Index: 133

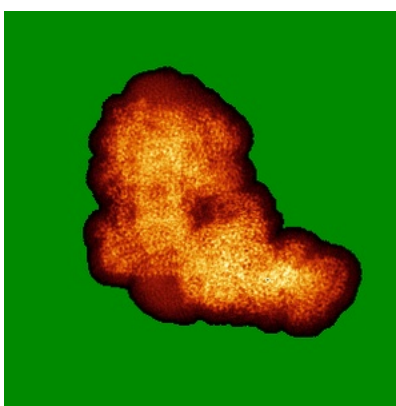
The images above show the largest variance slices of the map in three orthogonal directions.

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

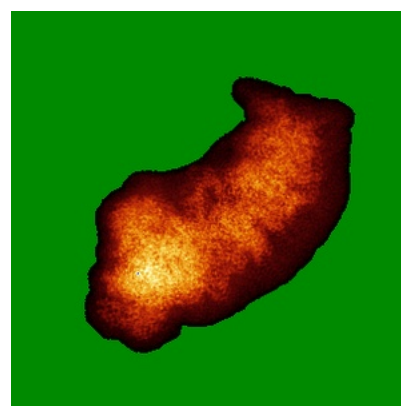
6.4.1 Primary map



X



Y

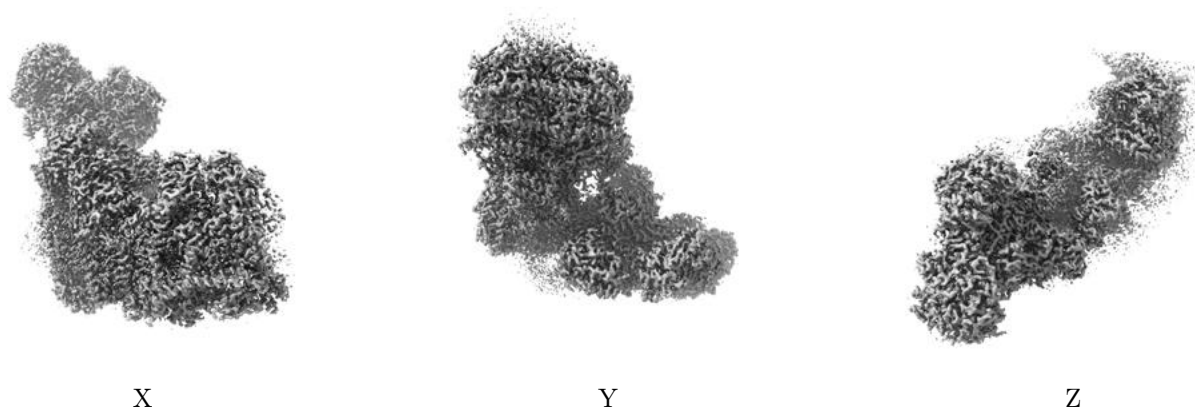


Z

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 0.0314. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

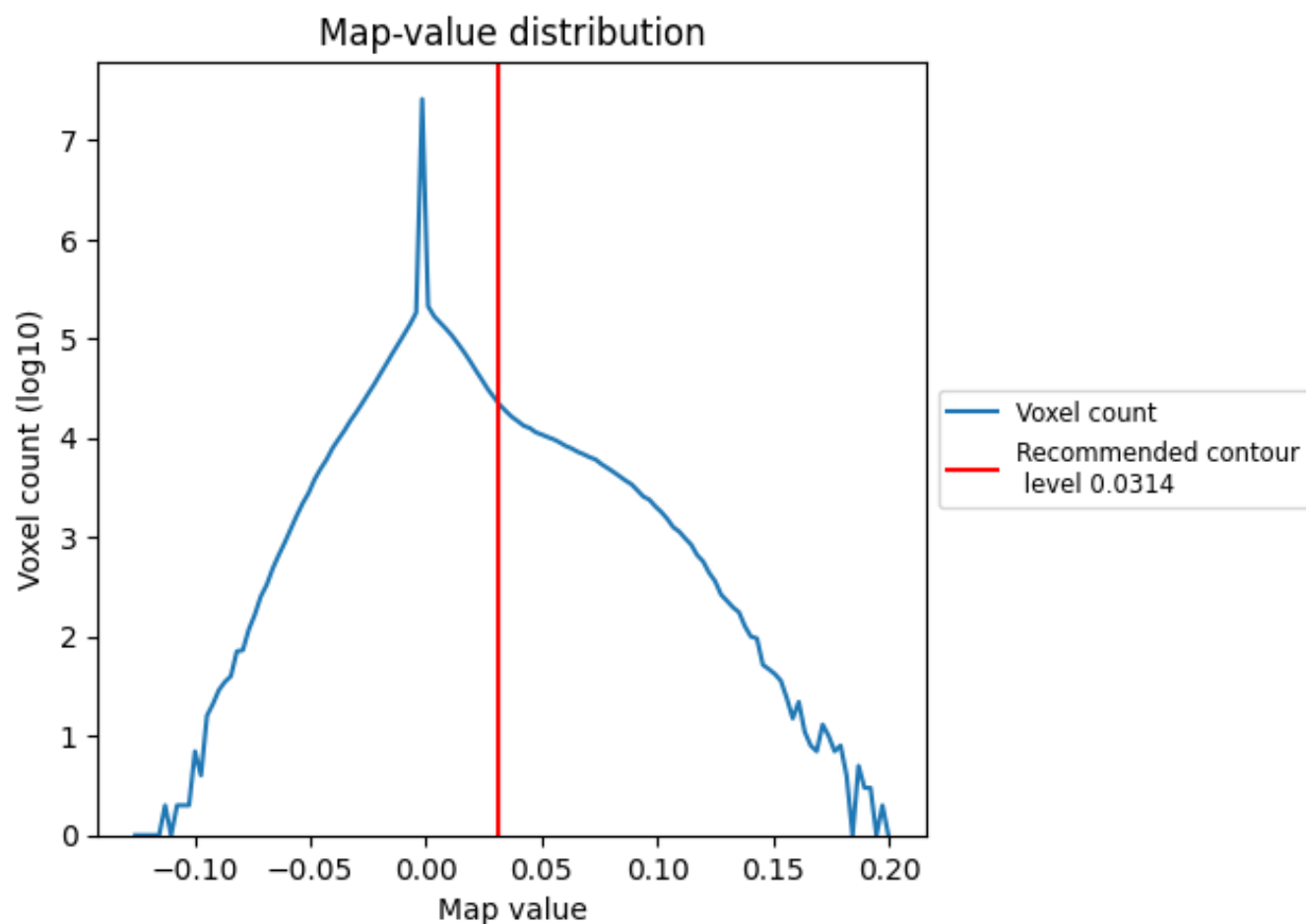
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

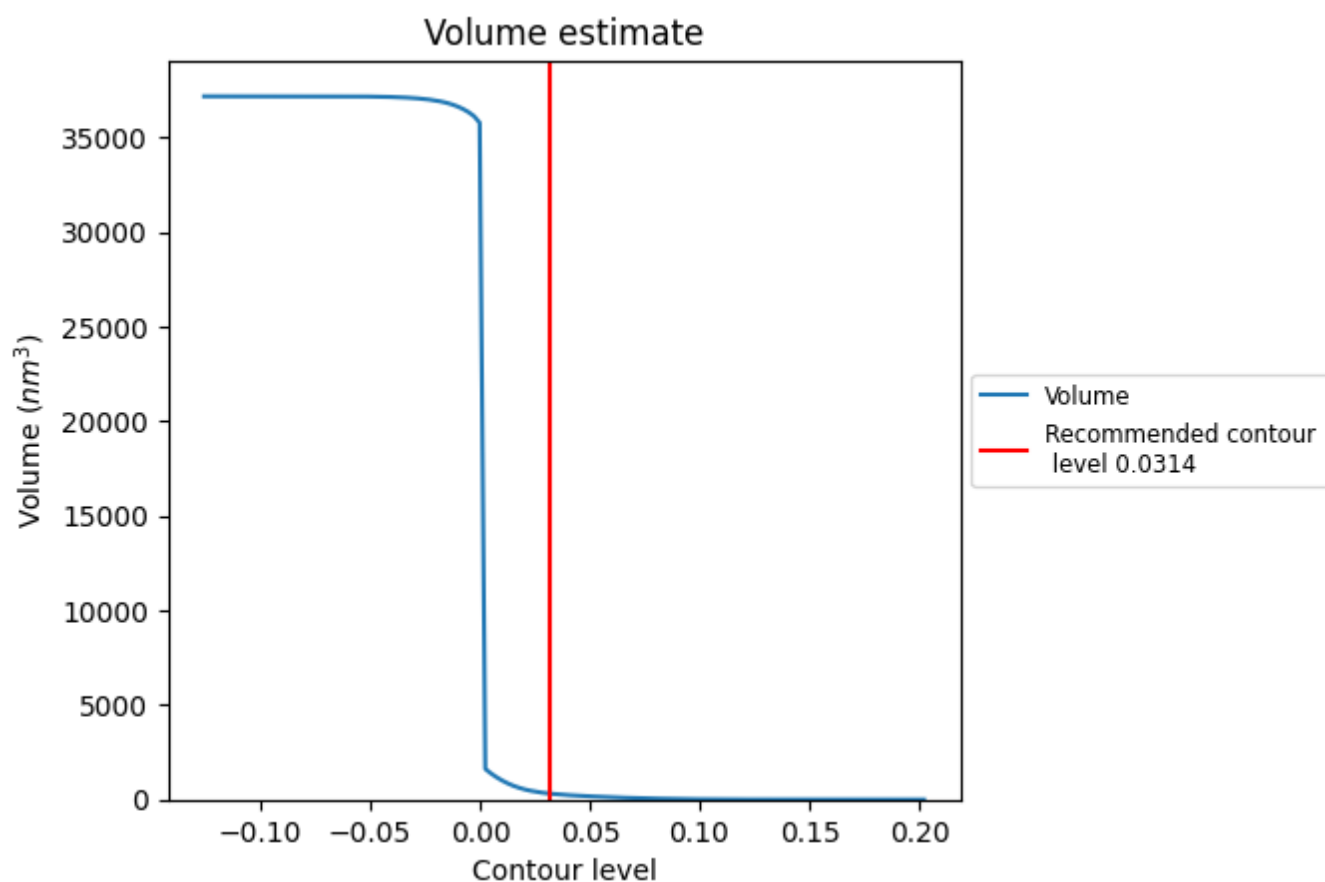
This section contains the results of statistical analysis of the map.

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.

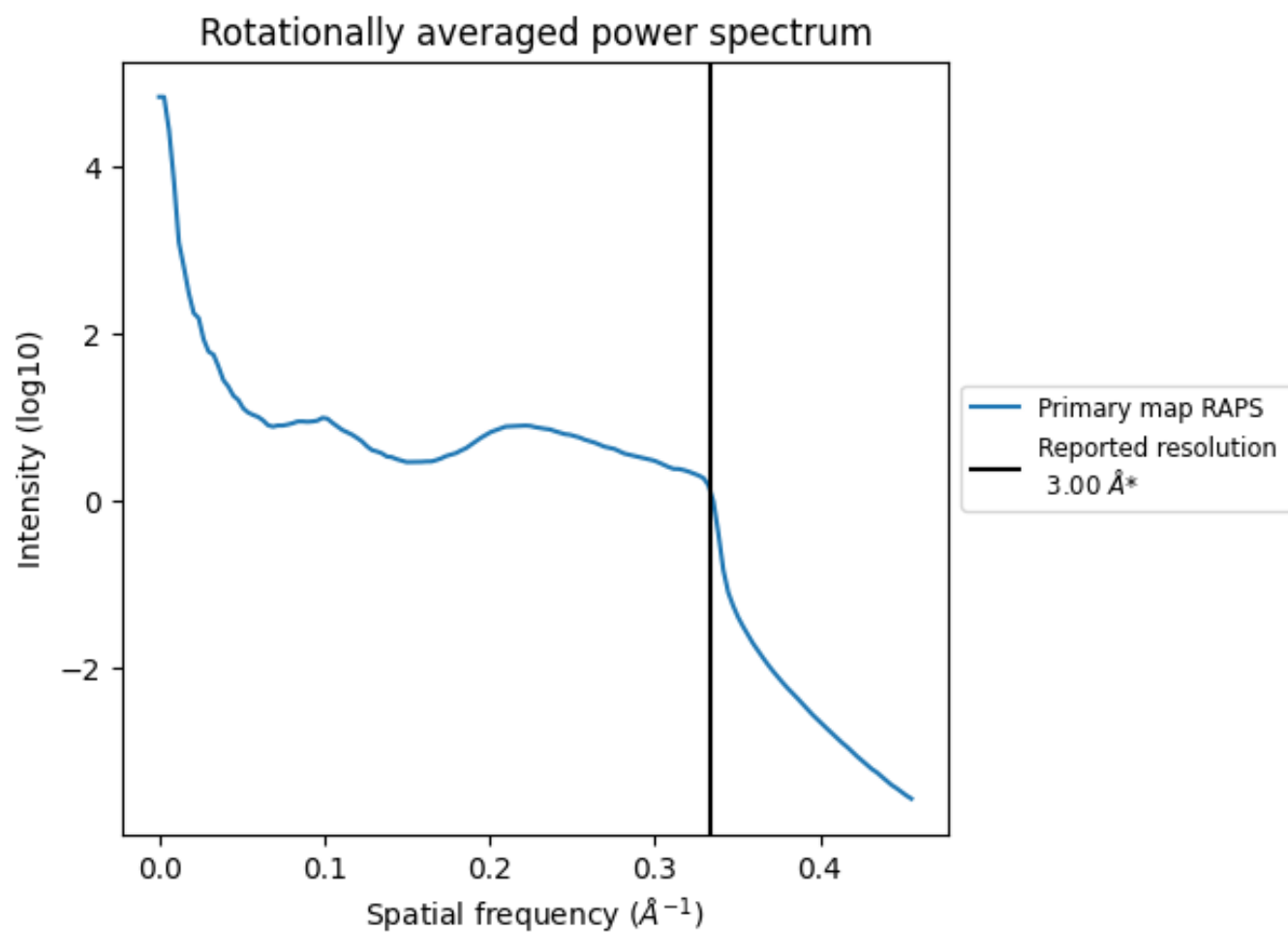
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 322 nm³; this corresponds to an approximate mass of 291 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

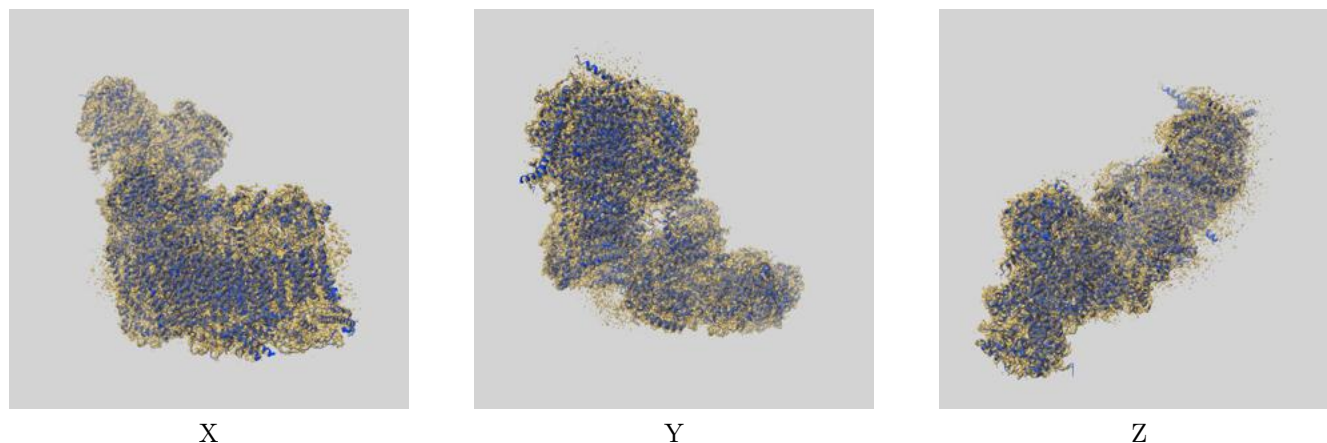
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

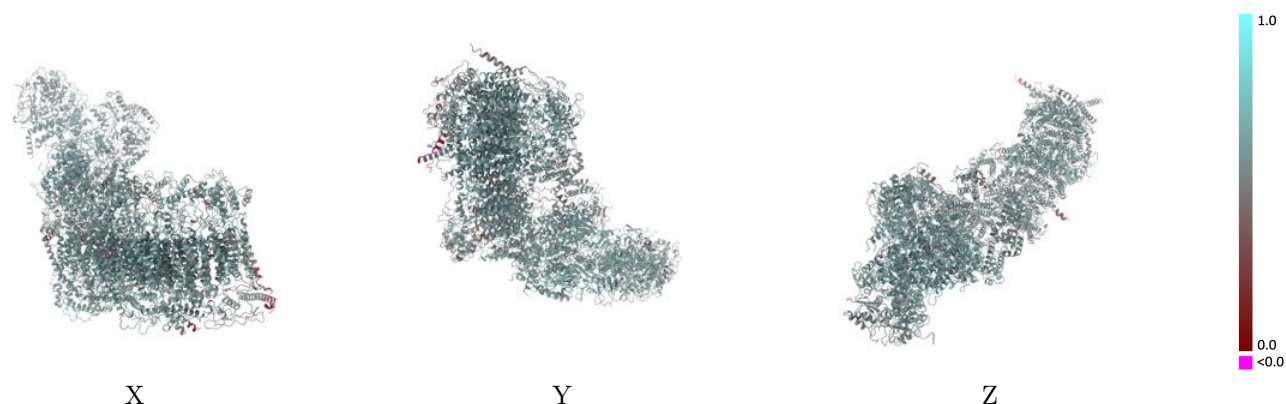
This section contains information regarding the fit between EMDB map EMD-32301 and PDB model 7W4D. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



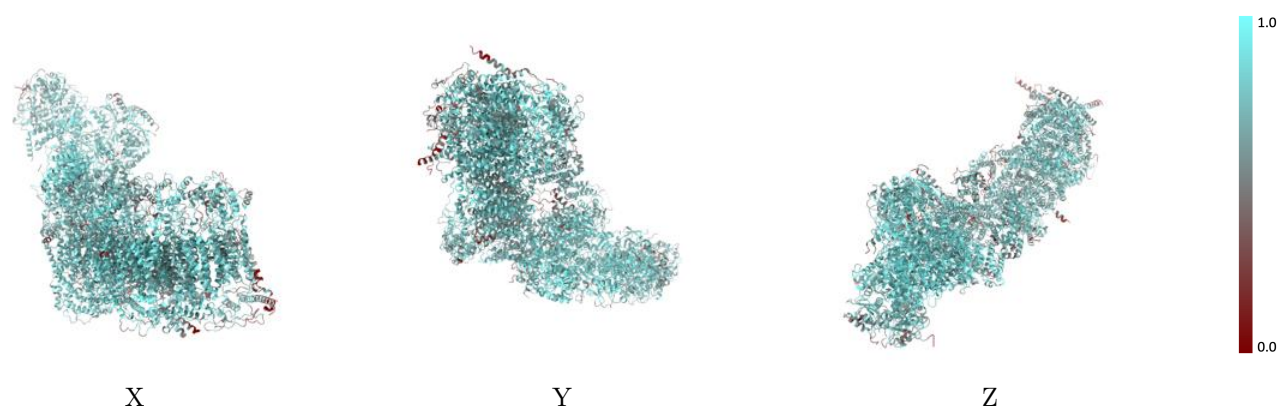
The images above show the 3D surface view of the map at the recommended contour level 0.0314 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



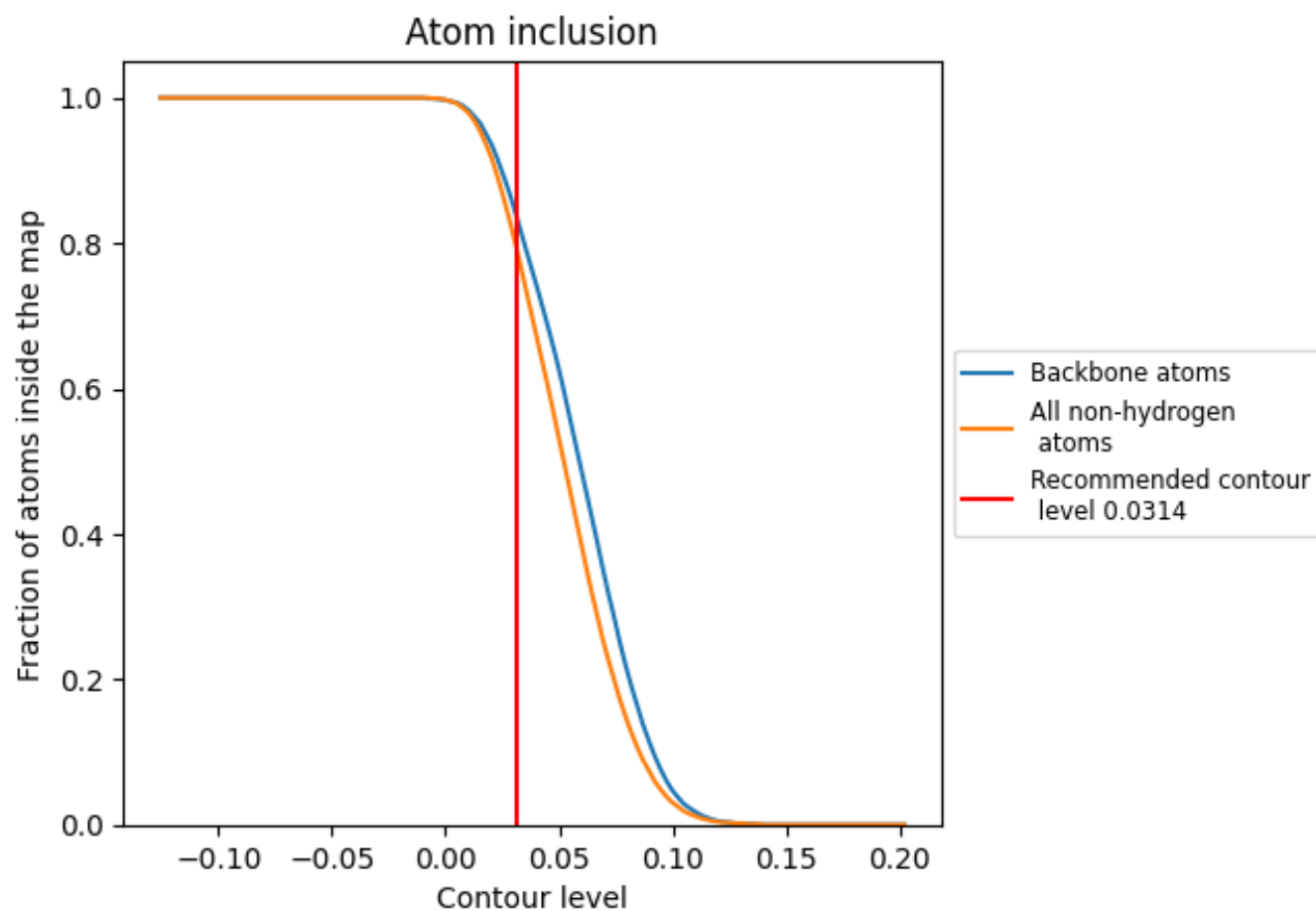
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0314).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.0314) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7920	 0.5870
A	 0.7480	 0.5700
B	 0.9100	 0.6260
C	 0.9160	 0.6280
E	 0.8180	 0.6020
F	 0.6760	 0.5270
G	 0.5540	 0.4910
H	 0.7880	 0.5770
I	 0.7710	 0.5810
J	 0.8310	 0.6050
K	 0.6530	 0.5380
L	 0.8380	 0.6060
M	 0.8250	 0.5980
N	 0.8450	 0.6150
O	 0.7090	 0.5560
P	 0.9150	 0.6330
Q	 0.8880	 0.6250
S	 0.8530	 0.6060
T	 0.8270	 0.6040
U	 0.7270	 0.5630
V	 0.6920	 0.5670
W	 0.7870	 0.5800
X	 0.6890	 0.5640
Y	 0.6030	 0.4920
Z	 0.5780	 0.4910
a	 0.8140	 0.5940
b	 0.6550	 0.5370
c	 0.7600	 0.5830
d	 0.7350	 0.5630
e	 0.7130	 0.5560
f	 0.5840	 0.5040
g	 0.8100	 0.5950
h	 0.7770	 0.5810
i	 0.8800	 0.6170
j	 0.7610	 0.5920



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Chain	Atom inclusion	Q-score
k	 0.8190	 0.6040
l	 0.7940	 0.5910
m	 0.7360	 0.5650
n	 0.6280	 0.5270
o	 0.7620	 0.5850
p	 0.7670	 0.5850
r	 0.8530	 0.6090
s	 0.8550	 0.6090
u	 0.7860	 0.5880
v	 0.5990	 0.5010
w	 0.7490	 0.5630