



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:46 PM UTC

PDB ID : 7VBL / pdb_00007vbl
EMDB ID : EMD-31881
Title : Membrane arm of active state CI from DQ-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-08-31
Resolution : 2.60 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:

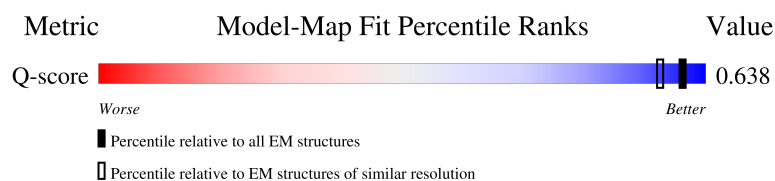
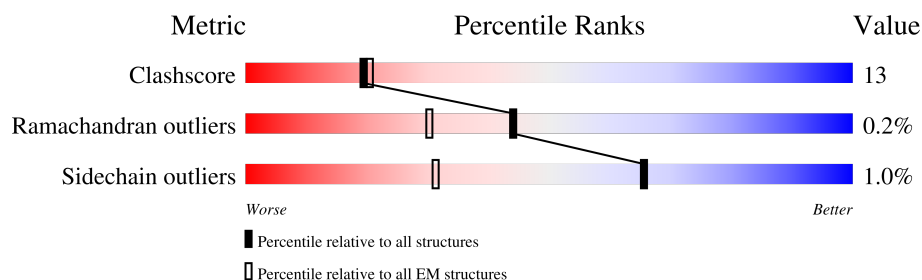
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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

Mol	Chain	Length	Quality of chain
1	Q	44	11% 86% 14%
2	S	70	89% 11%
3	U	83	10% 94% 6%
4	V	140	6% 94% 6%

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Mol	Chain	Length	Quality of chain
5	W	113	
6	X	88	
7	Y	67	
8	Z	80	
9	a	138	
10	b	126	
11	c	156	
12	d	175	
13	e	104	
14	f	49	
15	g	122	
16	h	105	
17	i	347	
18	j	115	
19	k	98	
20	l	606	
21	m	175	
22	n	56	
23	o	128	
24	p	178	
25	r	459	
26	s	318	
27	u	171	
28	v	125	
29	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
30	PEE	l	704	-	-	X	-
31	CDL	l	702	-	-	X	-
31	CDL	r	505	-	-	X	-
33	PLX	r	503	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 40142 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] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Q	44	Total	C	N	O	S	0	0
			363	236	60	66	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S	70	Total	C	N	O	S	0	0
			566	364	103	94	5		

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

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

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	V	140	Total	C	N	O	S	0	0
			1021	651	174	190	6		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	113	Total	C	N	O	S	0	0
			949	614	160	167	8		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	88	Total	C	N	O	S	0	0
			691	445	103	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	67	Total	C	N	O	S	0	0
			584	385	95	103	1		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	80	Total	C	N	O	S	0	0
			611	397	107	106	1		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	98	Total	C	N	O	S	0	0
			819	537	144	137	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	104	Total	C	N	O	S	0	0
			867	553	142	168	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	49	Total	C	N	O	0	0
			377	246	65	66		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	122	Total	C	N	O	S	0	0
			1005	653	174	172	6		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 17 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	j	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	l	606	Total	C	N	O	S	0	0
			4797	3181	743	822	51		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	175	Total	C	N	O	S	0	0
			1273	847	187	226	13		

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

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	p	178	Total	C	N	O	S	0	0
			1534	982	279	265	8		

- Molecule 25 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

- Molecule 26 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	124	Total	C	N	O	S	0	0
			1028	642	195	182	9		

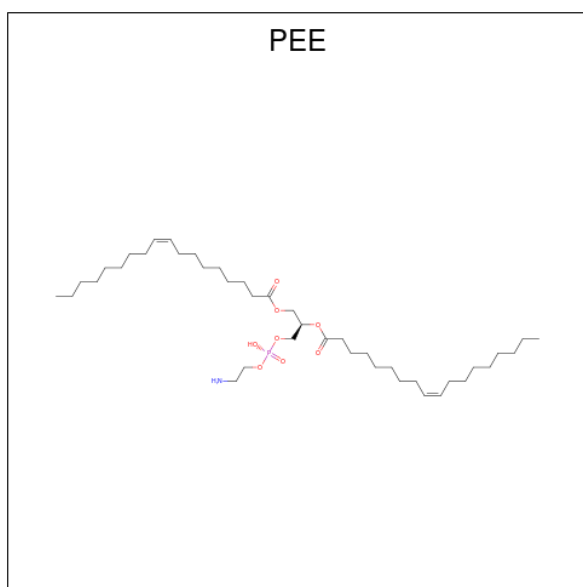
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

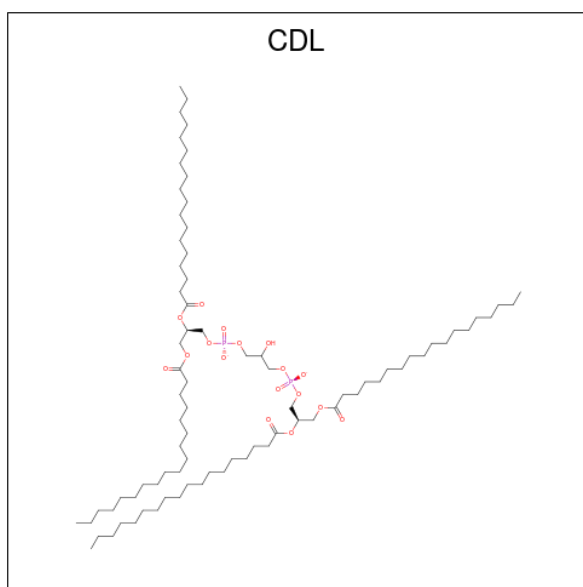
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 30 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: C₄₁H₇₈NO₈P) (labeled as "Ligand of Interest" by depositor).



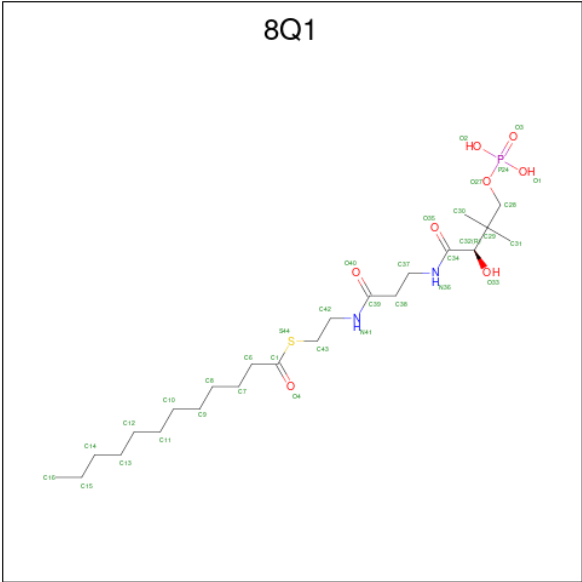
Mol	Chain	Residues	Atoms					AltConf
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	W	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	j	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	l	1	Total	C	N	O	P	0
			40	30	1	8	1	
30	l	1	Total	C	N	O	P	0
			51	41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

- Molecule 31 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



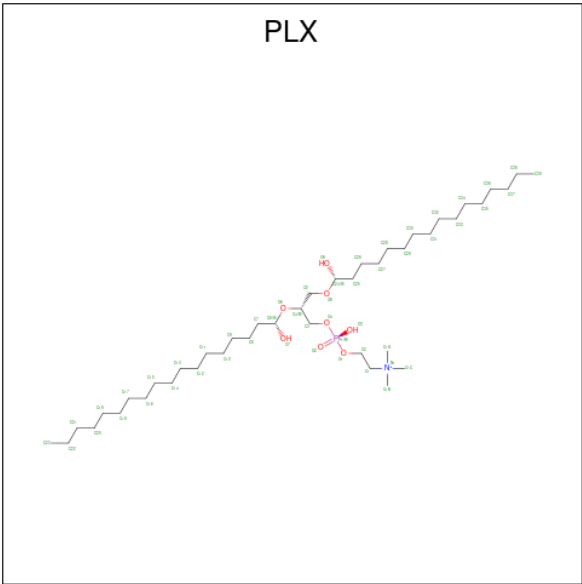
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			94	75	17	2	
31	V	1	Total	C	O	P	0
			100	81	17	2	
31	a	1	Total	C	O	P	0
			100	81	17	2	
31	i	1	Total	C	O	P	0
			87	68	17	2	
31	l	1	Total	C	O	P	0
			94	75	17	2	
31	m	1	Total	C	O	P	0
			100	81	17	2	
31	r	1	Total	C	O	P	0
			99	80	17	2	
31	r	1	Total	C	O	P	0
			100	81	17	2	
31	s	1	Total	C	O	P	0
			89	70	17	2	
31	u	1	Total	C	O	P	0
			55	36	17	2	

- Molecule 32 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 33 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-TRIOX (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



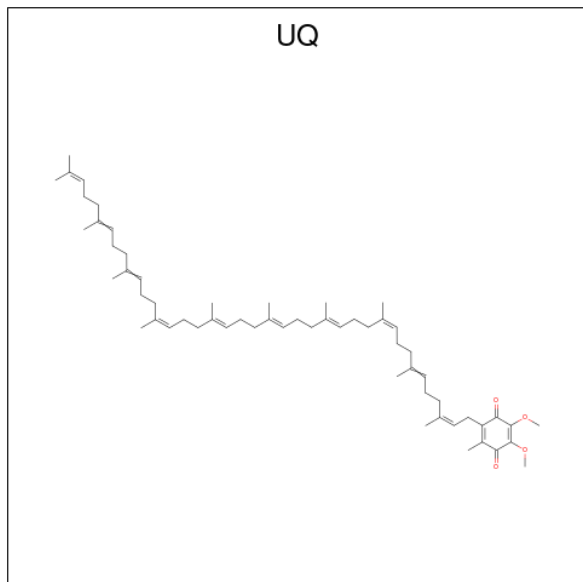
Mol	Chain	Residues	Atoms					AltConf
33	a	1	Total	C	N	O	P	0
			52	42	1	8	1	

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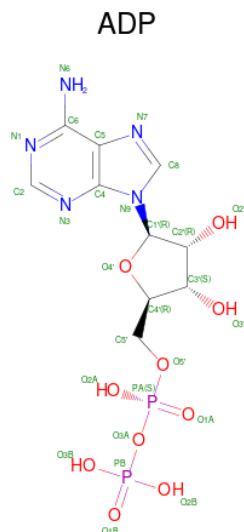
Mol	Chain	Residues	Atoms					AltConf
33	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 34 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
34	s	1	Total	C	O	0
			38	34	4	

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	Q	5	Total O 5 5	0
36	S	4	Total O 4 4	0
36	U	2	Total O 2 2	0
36	W	1	Total O 1 1	0
36	a	1	Total O 1 1	0
36	b	1	Total O 1 1	0
36	c	3	Total O 3 3	0
36	d	3	Total O 3 3	0
36	e	1	Total O 1 1	0
36	h	3	Total O 3 3	0
36	i	74	Total O 74 74	0

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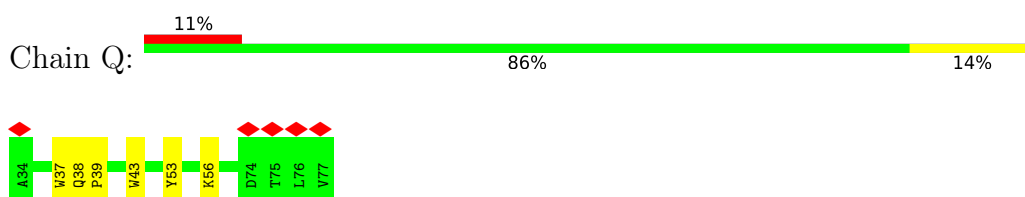
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Mol	Chain	Residues	Atoms		AltConf
36	j	33	Total 33	O 33	0
36	k	35	Total 35	O 35	0
36	l	60	Total 60	O 60	0
36	m	16	Total 16	O 16	0
36	n	2	Total 2	O 2	0
36	p	2	Total 2	O 2	0
36	r	91	Total 91	O 91	0
36	s	92	Total 92	O 92	0
36	w	2	Total 2	O 2	0

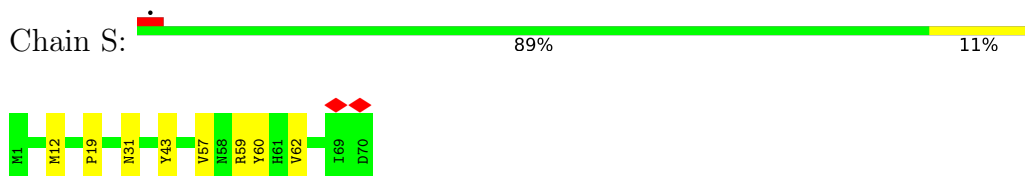
3 Residue-property plots [i](#)

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

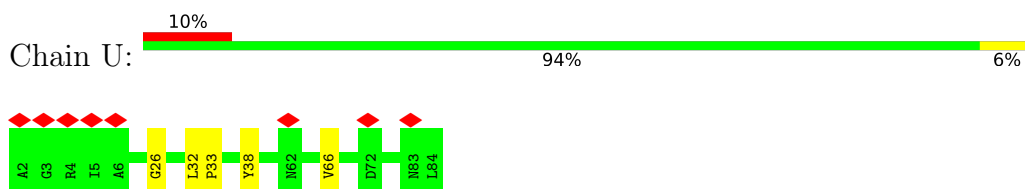
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



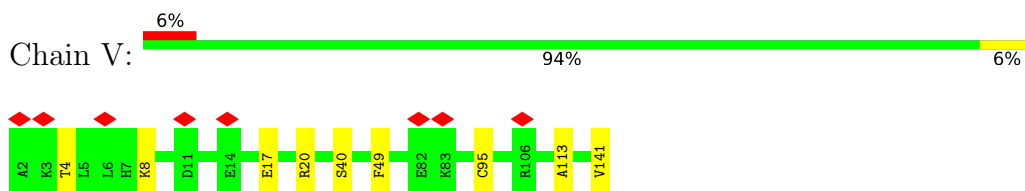
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



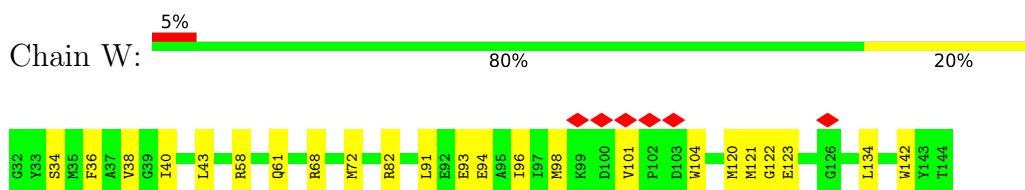
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



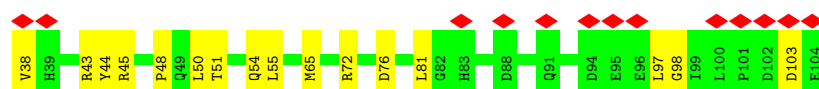
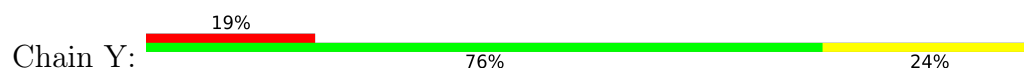
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



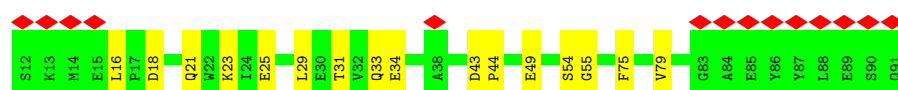
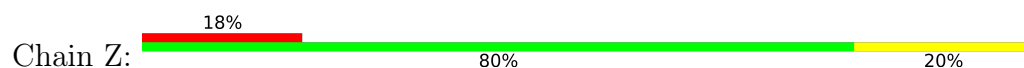
- Molecule 6: Acyl carrier protein, mitochondrial



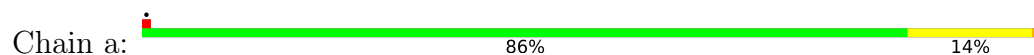
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



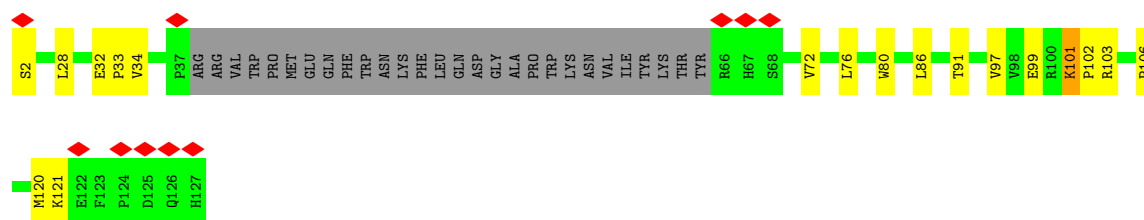
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



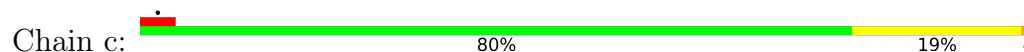
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



E185
I186

- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d:  6% 83% 16%



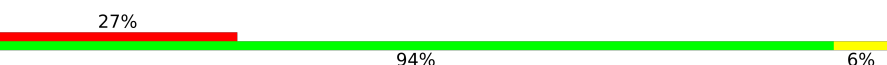
A174
A175
A176

- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:  8% 81% 18%



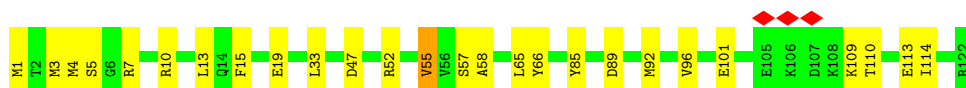
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:  27% 94% 6%



- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:  79% 20%



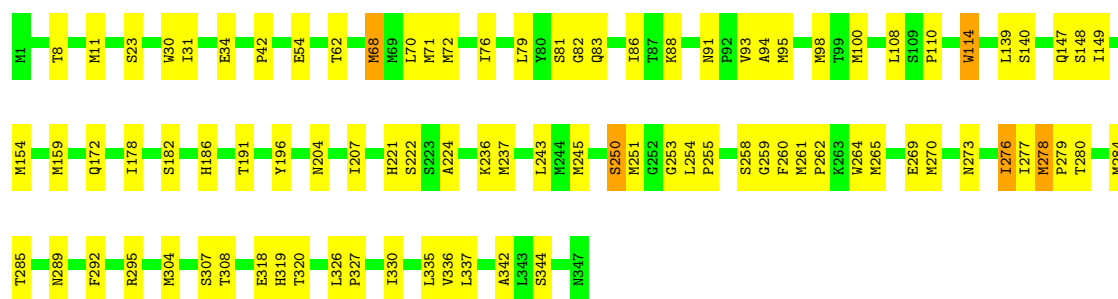
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:  10% 85% 15%

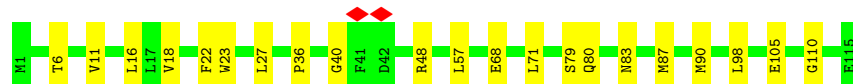
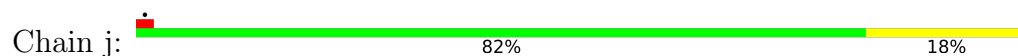


- Molecule 17: NADH-ubiquinone oxidoreductase chain 2

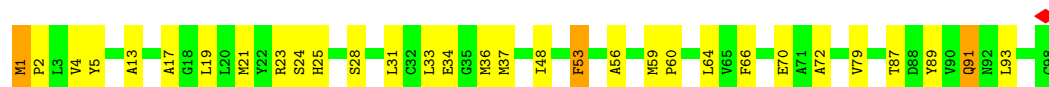
Chain i:  74% 24%



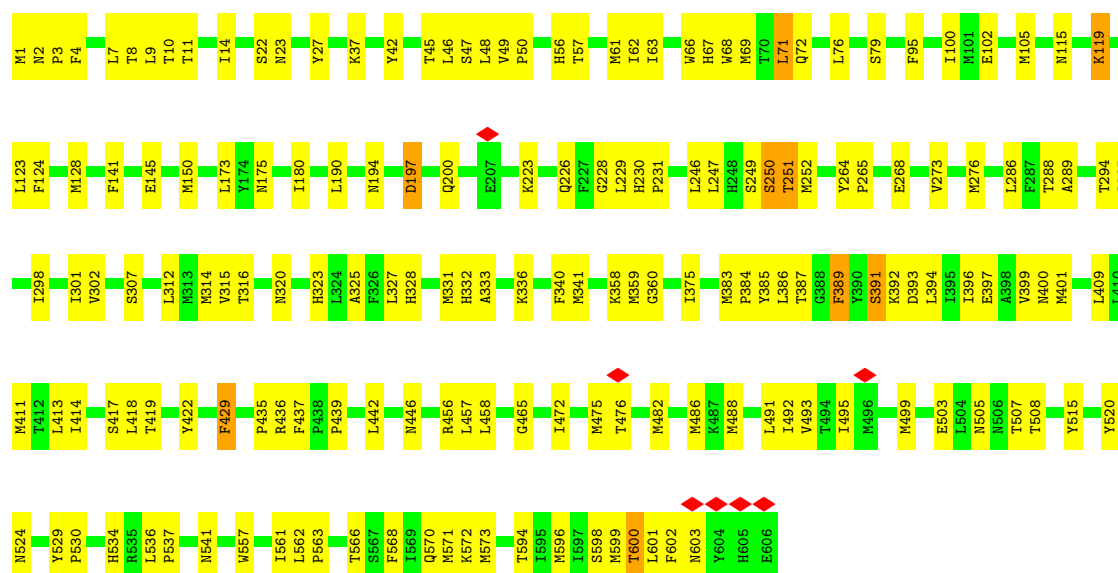
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3



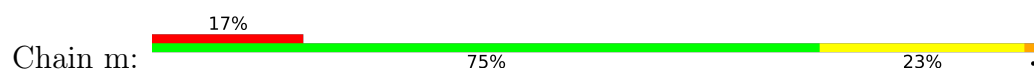
• Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

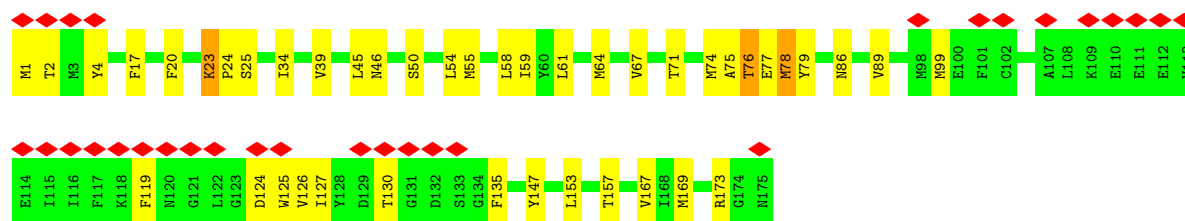


• Molecule 20: NADH-ubiquinone oxidoreductase chain 5

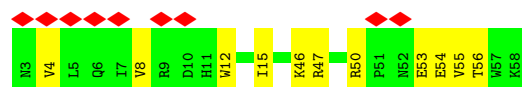
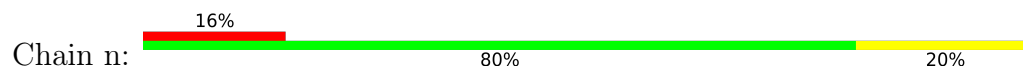


• Molecule 21: NADH-ubiquinone oxidoreductase chain 6

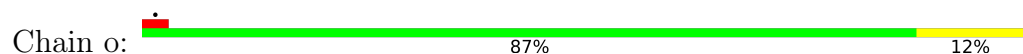




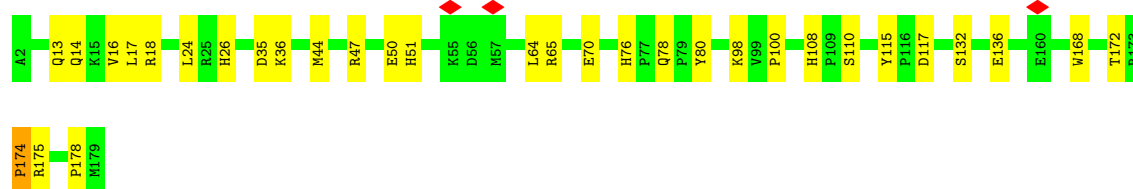
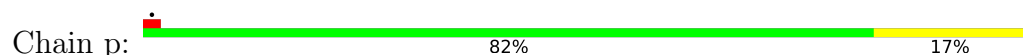
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



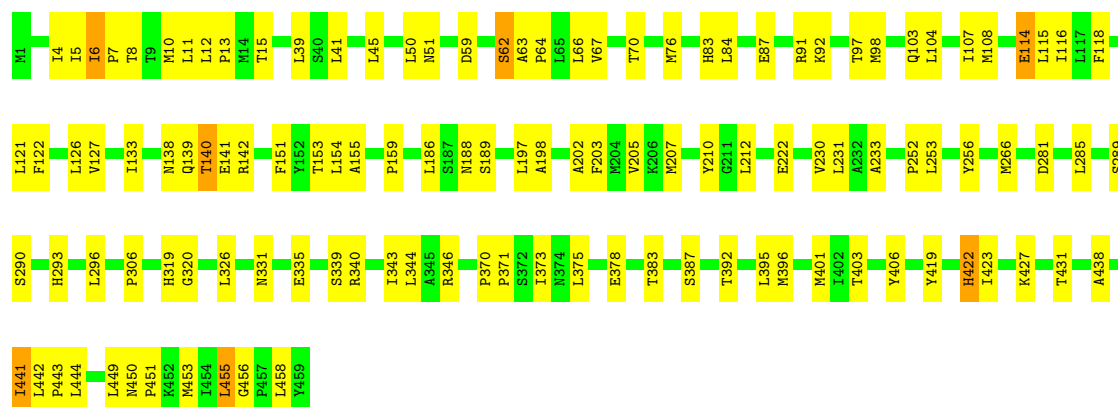
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



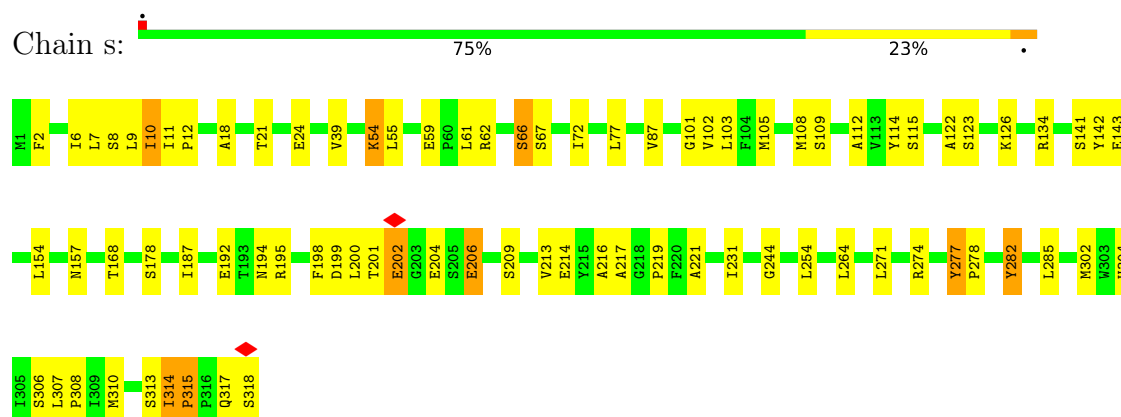
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



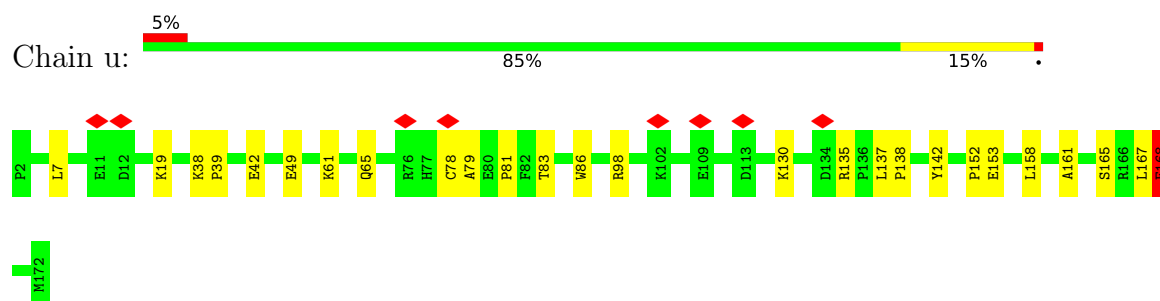
- Molecule 25: NADH-ubiquinone oxidoreductase chain 4



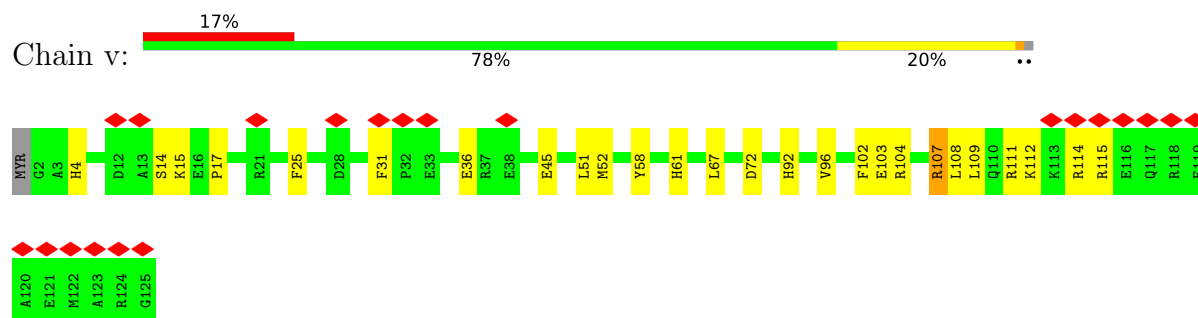
- Molecule 26: NADH-ubiquinone oxidoreductase chain 1



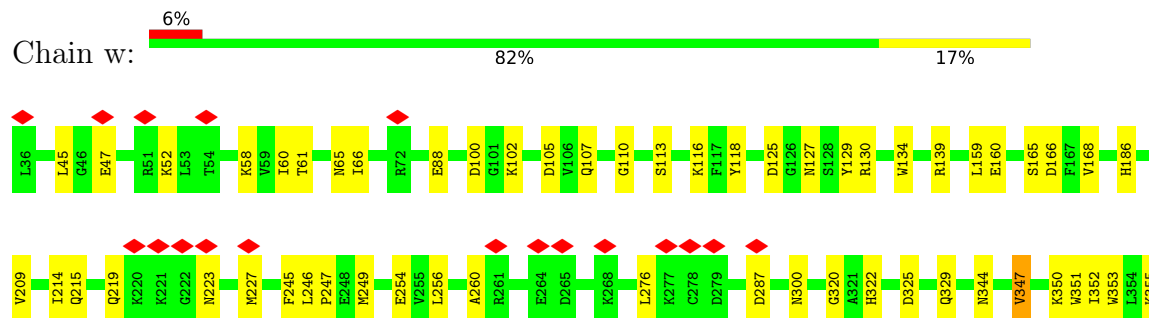
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 29: 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	462013	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	0.076	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0123	Depositor
Map size (Å)	257.808, 257.808, 257.808	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5371, 0.5371, 0.5371	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, PEE, 8Q1, ADP, PLX, UQ

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	Q	0.30	0/380	0.45	0/525
2	S	0.31	0/581	0.57	0/781
3	U	0.26	0/664	0.38	0/912
4	V	0.25	0/1042	0.41	0/1411
5	W	0.31	0/973	0.45	0/1312
6	X	0.29	0/701	0.82	2/948 (0.2%)
7	Y	0.24	0/610	0.45	0/836
8	Z	0.24	0/628	0.50	0/850
9	a	0.33	0/1184	0.50	0/1603
10	b	0.28	0/844	0.60	2/1149 (0.2%)
11	c	0.28	0/1371	0.54	3/1875 (0.2%)
12	d	0.28	0/1494	0.51	2/2015 (0.1%)
13	e	0.29	0/891	0.48	0/1210
14	f	0.23	0/385	0.43	0/522
15	g	0.30	0/1036	0.65	2/1401 (0.1%)
16	h	0.33	0/889	0.59	1/1190 (0.1%)
17	i	0.36	0/2773	0.66	5/3768 (0.1%)
18	j	0.32	0/938	0.52	0/1281
19	k	0.38	0/759	0.80	3/1029 (0.3%)
20	l	0.32	0/4926	0.60	10/6700 (0.1%)
21	m	0.33	0/1304	0.66	5/1773 (0.3%)
22	n	0.24	0/491	0.39	0/663
23	o	0.29	0/1092	0.55	3/1481 (0.2%)
24	p	0.28	0/1590	0.43	0/2155
25	r	0.37	0/3723	0.72	15/5078 (0.3%)
26	s	0.40	0/2581	0.87	17/3529 (0.5%)
27	u	0.30	0/1436	0.53	2/1938 (0.1%)
28	v	0.25	0/1052	0.51	0/1411
29	w	0.27	0/2650	0.47	0/3588
All	All	0.32	0/38988	0.60	72/52934 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
10	b	0	1

There are no bond length outliers.

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	s	10	ILE	N-CA-C	12.06	122.90	110.72
25	r	441	ILE	N-CA-C	10.53	121.36	110.62
25	r	5	ILE	N-CA-C	10.38	121.20	110.72
6	X	71	ALA	CA-C-N	9.81	126.72	119.66
6	X	71	ALA	C-N-CA	9.81	126.72	119.66
17	i	277	ILE	N-CA-C	9.25	120.06	110.62
26	s	315	PRO	CA-C-N	9.18	129.61	120.52
26	s	315	PRO	C-N-CA	9.18	129.61	120.52
25	r	450	ASN	CA-C-N	8.72	128.74	119.05
25	r	450	ASN	C-N-CA	8.72	128.74	119.05
26	s	206	GLU	N-CA-C	8.58	120.41	111.14
15	g	55	VAL	N-CA-C	8.42	119.20	110.62
15	g	3	MET	N-CA-C	8.41	120.44	111.28
10	b	101	LYS	CA-C-N	8.00	128.00	119.76
10	b	101	LYS	C-N-CA	8.00	128.00	119.76
21	m	23	LYS	CA-C-N	7.90	129.71	119.84
21	m	23	LYS	C-N-CA	7.90	129.71	119.84
11	c	75	TYR	CA-C-N	7.76	127.52	119.76
11	c	75	TYR	C-N-CA	7.76	127.52	119.76
26	s	39	VAL	N-CA-C	7.59	118.33	111.81
26	s	277	TYR	CA-C-N	7.49	127.65	120.31
26	s	277	TYR	C-N-CA	7.49	127.65	120.31
25	r	456	GLY	CA-C-N	7.44	127.31	119.05
25	r	456	GLY	C-N-CA	7.44	127.31	119.05
17	i	278	MET	CA-C-N	7.41	127.28	119.05
17	i	278	MET	C-N-CA	7.41	127.28	119.05
19	k	53	PHE	N-CA-C	-7.02	97.78	108.67
25	r	62	SER	N-CA-C	6.73	118.70	111.36
26	s	314	ILE	CA-C-N	6.70	127.28	120.38
26	s	314	ILE	C-N-CA	6.70	127.28	120.38
25	r	422	HIS	N-CA-C	6.69	118.57	111.28
20	l	391	SER	N-CA-C	6.65	118.61	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	o	53	ASP	CA-C-N	6.53	125.97	118.85
23	o	53	ASP	C-N-CA	6.53	125.97	118.85
26	s	67	SER	N-CA-C	-6.51	98.61	108.96
19	k	1	MET	CA-C-N	6.14	126.05	119.85
19	k	1	MET	C-N-CA	6.14	126.05	119.85
25	r	6	ILE	CA-C-N	6.08	125.80	119.05
25	r	6	ILE	C-N-CA	6.08	125.80	119.05
26	s	143	GLU	N-CA-C	6.07	117.57	111.07
25	r	212	LEU	N-CA-C	-5.97	104.64	112.41
21	m	25	SER	CA-C-N	5.89	125.76	119.28
21	m	25	SER	C-N-CA	5.89	125.76	119.28
25	r	138	ASN	N-CA-C	5.85	117.74	111.36
20	l	247	LEU	N-CA-C	5.84	117.72	111.36
20	l	429	PHE	N-CA-C	5.81	117.69	111.36
25	r	455	LEU	N-CA-C	5.76	117.56	111.28
25	r	115	LEU	N-CA-C	5.74	117.54	111.28
20	l	251	THR	N-CA-C	5.70	119.76	112.12
26	s	282	TYR	N-CA-C	5.65	117.44	111.28
20	l	389	PHE	N-CA-C	5.59	117.38	111.28
26	s	66	SER	N-CA-C	5.58	117.89	110.53
26	s	178	SER	N-CA-C	5.54	117.54	110.61
12	d	142	ARG	N-CA-C	5.53	117.38	111.36
26	s	141	SER	N-CA-C	5.48	117.33	111.36
26	s	217	ALA	N-CA-C	5.45	117.29	108.08
20	l	250	SER	N-CA-C	5.44	121.33	114.31
25	r	151	PHE	N-CA-C	5.44	117.21	111.28
26	s	217	ALA	CB-CA-C	-5.31	110.47	116.63
27	u	98	ARG	N-CA-C	5.27	117.03	111.28
21	m	76	THR	N-CA-C	5.20	117.83	110.50
12	d	143	TYR	N-CA-C	5.20	121.34	114.12
27	u	168	PHE	N-CA-C	5.19	121.85	110.80
16	h	70	GLN	N-CA-C	5.18	116.93	111.28
20	l	472	ILE	CA-C-N	5.17	123.38	119.66
20	l	472	ILE	C-N-CA	5.17	123.38	119.66
17	i	114	TRP	N-CA-C	5.15	117.63	111.71
11	c	74	ASP	N-CA-C	5.15	116.89	111.28
20	l	515	TYR	CA-C-N	5.13	125.04	119.76
20	l	515	TYR	C-N-CA	5.13	125.04	119.76
17	i	276	ILE	N-CA-C	5.13	115.90	110.72
23	o	127	ILE	N-CA-C	5.01	115.78	110.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	b	121	LYS	Peptide

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	Q	363	0	332	6	0
2	S	566	0	561	6	0
3	U	643	0	642	6	0
4	V	1021	0	1025	13	0
5	W	949	0	935	23	0
6	X	691	0	665	25	0
7	Y	584	0	529	27	0
8	Z	611	0	580	13	0
9	a	1151	0	1164	29	0
10	b	819	0	835	19	0
11	c	1315	0	1208	25	0
12	d	1461	0	1429	40	0
13	e	867	0	817	27	0
14	f	377	0	353	4	0
15	g	1005	0	999	30	0
16	h	867	0	871	16	0
17	i	2710	0	2874	103	0
18	j	914	0	951	21	0
19	k	748	0	799	44	0
20	l	4797	0	4935	180	0
21	m	1273	0	1234	54	0
22	n	479	0	486	8	0
23	o	1062	0	1072	22	0
24	p	1534	0	1470	23	0
25	r	3631	0	3839	120	0
26	s	2508	0	2607	76	0
27	u	1398	0	1374	19	0
28	v	1028	0	982	47	0
29	w	2590	0	2553	49	0
30	U	102	0	164	9	0
30	W	41	0	59	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	i	47	0	71	11	0
30	j	41	0	59	11	0
30	l	137	0	205	40	0
30	r	51	0	82	16	0
31	V	194	0	294	10	0
31	a	100	0	156	15	0
31	i	87	0	124	4	0
31	l	94	0	141	21	0
31	m	100	0	156	10	0
31	r	199	0	307	53	0
31	s	89	0	125	6	0
31	u	55	0	54	5	0
32	X	35	0	0	1	0
33	a	52	0	88	0	0
33	g	52	0	88	4	0
33	j	104	0	176	9	0
33	r	104	0	176	25	0
34	s	38	0	47	1	0
35	w	27	0	11	6	0
36	Q	5	0	0	0	0
36	S	4	0	0	0	0
36	U	2	0	0	0	0
36	W	1	0	0	0	0
36	a	1	0	0	0	0
36	b	1	0	0	0	0
36	c	3	0	0	0	0
36	d	3	0	0	0	0
36	e	1	0	0	2	0
36	h	3	0	0	1	0
36	i	74	0	0	7	0
36	j	33	0	0	5	0
36	k	35	0	0	11	0
36	l	60	0	0	16	0
36	m	16	0	0	2	0
36	n	2	0	0	0	0
36	p	2	0	0	0	0
36	r	91	0	0	10	0
36	s	92	0	0	11	0
36	w	2	0	0	0	0
All	All	40142	0	40704	1011	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 13.

All (1011) 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)
25:r:104:LEU:CD2	31:r:505:CDL:H861	1.45	1.43
9:a:97:GLU:OE1	12:d:60:ARG:CD	1.71	1.39
25:r:104:LEU:CD2	31:r:505:CDL:C86	2.02	1.37
7:Y:97:LEU:CD2	28:v:107:ARG:HH11	1.36	1.37
9:a:97:GLU:OE1	12:d:60:ARG:HD2	1.08	1.21
17:i:95:MET:CE	17:i:149:ILE:HG22	1.70	1.20
20:l:400:ASN:HB3	20:l:486:MET:CE	1.72	1.20
20:l:2:ASN:ND2	20:l:3:PRO:HD2	1.55	1.19
25:r:104:LEU:HD21	31:r:505:CDL:C86	1.69	1.17
20:l:400:ASN:HB3	20:l:486:MET:HE3	1.22	1.15
29:w:139:ARG:HH12	35:w:401:ADP:N6	1.46	1.14
30:r:501:PEE:H33	30:r:501:PEE:H71	1.16	1.14
28:v:111:ARG:HH12	28:v:115:ARG:NH1	1.45	1.13
20:l:2:ASN:HD22	20:l:3:PRO:CD	1.63	1.12
25:r:104:LEU:HD23	31:r:505:CDL:H861	1.18	1.10
25:r:104:LEU:HD21	31:r:505:CDL:H862	1.12	1.10
23:o:59:VAL:HG22	25:r:423:ILE:HG12	1.24	1.09
20:l:596:MET:SD	31:m:201:CDL:H631	1.92	1.09
30:i:402:PEE:H34	30:i:402:PEE:H42	1.16	1.08
19:k:21:MET:O	21:m:23:LYS:HE3	1.52	1.07
31:a:201:CDL:H191	31:a:201:CDL:H732	1.36	1.07
29:w:139:ARG:NH1	35:w:401:ADP:HN61	1.54	1.06
5:W:121:MET:HE3	21:m:130:THR:HB	1.31	1.04
20:l:228:GLY:HA3	30:l:703:PEE:H38	1.39	1.04
30:W:201:PEE:H42	30:W:201:PEE:H33	1.38	1.02
7:Y:97:LEU:CD2	28:v:107:ARG:NH1	2.22	1.02
7:Y:97:LEU:HD23	28:v:107:ARG:HH11	1.24	1.00
17:i:68:MET:HE2	17:i:68:MET:HA	1.42	1.00
20:l:596:MET:SD	31:m:201:CDL:C63	2.50	0.99
17:i:154:MET:HE1	36:i:573:HOH:O	1.62	0.98
20:l:541:ASN:HD22	30:l:703:PEE:H61	1.28	0.98
7:Y:97:LEU:HD22	28:v:107:ARG:HH11	1.25	0.98
31:l:702:CDL:H371	31:l:702:CDL:C60	1.92	0.98
31:l:702:CDL:H371	31:l:702:CDL:H601	0.99	0.98
31:l:702:CDL:H601	31:l:702:CDL:C37	1.93	0.98
31:l:702:CDL:H521	31:l:702:CDL:HB61	1.44	0.97
26:s:204:GLU:HG2	36:s:509:HOH:O	1.64	0.97
15:g:4:MET:CE	15:g:7:ARG:HD2	1.95	0.96
6:X:71:ALA:HB2	20:l:442:LEU:HD21	1.45	0.95
20:l:2:ASN:HD22	20:l:3:PRO:HD2	0.79	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:97:LEU:CD2	28:v:107:ARG:HD2	1.97	0.95
20:l:286:LEU:HD13	20:l:411:MET:SD	2.08	0.93
17:i:237:MET:SD	17:i:319:HIS:HE1	1.92	0.93
28:v:14:SER:O	28:v:109:LEU:HD21	1.68	0.93
31:a:201:CDL:H111	30:l:704:PEE:H63	1.48	0.93
31:r:505:CDL:C21	31:r:505:CDL:H473	1.99	0.91
7:Y:97:LEU:HD21	28:v:107:ARG:HD2	1.51	0.91
30:r:501:PEE:H79	30:r:501:PEE:H40	1.51	0.91
9:a:97:GLU:O	12:d:62:TYR:HB3	1.70	0.90
23:o:59:VAL:HG22	25:r:423:ILE:CG1	2.01	0.90
26:s:200:LEU:HD13	26:s:282:TYR:CB	2.01	0.90
21:m:76:THR:HG22	36:s:573:HOH:O	1.70	0.89
28:v:111:ARG:NH1	28:v:115:ARG:HD3	1.86	0.89
31:r:505:CDL:H473	31:r:505:CDL:H211	1.54	0.89
20:l:27:TYR:O	20:l:115:ASN:ND2	2.05	0.89
31:l:702:CDL:H841	31:l:702:CDL:H182	1.55	0.89
30:l:704:PEE:H51	30:l:704:PEE:H13	1.54	0.89
28:v:111:ARG:NH1	28:v:115:ARG:HH11	1.70	0.88
9:a:97:GLU:HG3	12:d:62:TYR:HD2	1.38	0.88
17:i:95:MET:HE2	17:i:149:ILE:HG22	1.54	0.88
17:i:335:LEU:HD21	31:r:505:CDL:H391	1.56	0.87
19:k:19:LEU:CD2	19:k:36:MET:HE1	2.04	0.86
5:W:121:MET:CE	21:m:130:THR:HB	2.06	0.86
30:r:501:PEE:H33	30:r:501:PEE:C42	2.05	0.85
28:v:111:ARG:HH12	28:v:115:ARG:HH11	0.86	0.85
31:u:201:CDL:H581	31:u:201:CDL:H541	1.57	0.85
25:r:104:LEU:HD22	31:r:505:CDL:H861	1.55	0.85
30:l:704:PEE:C1	33:r:503:PLX:H21	2.06	0.84
4:V:141:VAL:H	17:i:273:ASN:ND2	1.73	0.84
19:k:21:MET:O	21:m:23:LYS:CE	2.25	0.84
17:i:278:MET:HB3	17:i:279:PRO:HD3	1.60	0.84
25:r:104:LEU:HD23	31:r:505:CDL:C86	1.86	0.84
9:a:97:GLU:OE1	12:d:60:ARG:NE	2.12	0.83
20:l:400:ASN:CB	20:l:486:MET:HE3	2.06	0.83
31:l:702:CDL:H802	31:l:702:CDL:H172	1.59	0.83
25:r:387:SER:HB3	36:r:632:HOH:O	1.78	0.83
17:i:88:LYS:CG	17:i:148:SER:HB3	2.09	0.82
5:W:120:MET:HB3	5:W:123:GLU:HG3	1.61	0.82
20:l:400:ASN:HB3	20:l:486:MET:HE2	1.59	0.82
7:Y:97:LEU:HD22	28:v:107:ARG:NH1	1.91	0.82
17:i:68:MET:HE1	19:k:37:MET:HE2	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:107:GLN:HE22	20:l:194:ASN:HD22	1.25	0.82
25:r:98:MET:HE1	31:r:505:CDL:H211	1.61	0.82
25:r:306:PRO:HB3	25:r:458:LEU:HD12	1.61	0.81
20:l:230:HIS:HE1	36:l:852:HOH:O	1.62	0.81
31:r:505:CDL:H452	31:r:505:CDL:H412	1.61	0.81
30:W:201:PEE:H33	30:W:201:PEE:C25	2.11	0.81
17:i:320:THR:OG1	29:w:300:ASN:HA	1.79	0.80
23:o:59:VAL:CG2	25:r:423:ILE:HG12	2.10	0.80
30:i:402:PEE:H36	30:i:402:PEE:H28	1.62	0.79
30:i:402:PEE:H34	30:i:402:PEE:C25	2.06	0.79
21:m:77:GLU:OE2	36:m:301:HOH:O	2.00	0.79
25:r:326:LEU:HD13	36:r:690:HOH:O	1.82	0.79
20:l:360:GLY:HA3	20:l:435:PRO:HA	1.63	0.79
7:Y:97:LEU:HD23	28:v:107:ARG:CD	2.13	0.78
28:v:111:ARG:NH1	28:v:115:ARG:NH1	2.27	0.78
30:l:704:PEE:C2	33:r:503:PLX:H21	2.14	0.78
12:d:127:LYS:HB2	12:d:127:LYS:NZ	1.96	0.78
31:r:505:CDL:H473	31:r:505:CDL:C20	2.14	0.78
25:r:155:ALA:HB3	30:r:501:PEE:H47	1.63	0.78
31:r:505:CDL:H473	31:r:505:CDL:H202	1.66	0.78
25:r:45:LEU:HD11	25:r:50:LEU:HD23	1.64	0.77
25:r:281:ASP:OD2	25:r:340:ARG:NH2	2.18	0.77
33:r:503:PLX:H151	31:r:504:CDL:H802	1.65	0.77
31:r:505:CDL:H202	31:r:505:CDL:C47	2.14	0.77
9:a:97:GLU:HG3	12:d:62:TYR:CD2	2.20	0.76
18:j:23:TRP:CE2	30:j:201:PEE:H55	2.20	0.76
29:w:125:ASP:O	29:w:130:ARG:NH2	2.18	0.76
6:X:119:ILE:HD12	6:X:135:ALA:HB1	1.68	0.76
15:g:89:ASP:OD2	27:u:161:ALA:HB1	1.85	0.75
17:i:95:MET:HE1	17:i:149:ILE:HG22	1.64	0.75
17:i:276:ILE:HG21	30:r:501:PEE:H14	1.66	0.75
31:a:201:CDL:H111	30:l:704:PEE:C38	2.16	0.75
19:k:19:LEU:HD23	19:k:36:MET:HE1	1.66	0.75
20:l:400:ASN:C	20:l:486:MET:CE	2.60	0.75
30:r:501:PEE:H40	30:r:501:PEE:C46	2.16	0.75
15:g:4:MET:HE1	15:g:7:ARG:HD2	1.67	0.75
20:l:288:THR:HG21	20:l:307:SER:HB3	1.66	0.75
9:a:97:GLU:CD	12:d:60:ARG:HD2	2.10	0.75
31:l:702:CDL:H201	31:l:702:CDL:H861	1.68	0.75
30:l:704:PEE:H1	33:r:503:PLX:H21	1.68	0.75
12:d:127:LYS:HB2	12:d:127:LYS:HZ3	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:r:503:PLX:H181	31:r:504:CDL:H801	1.68	0.75
12:d:107:GLN:HE22	20:l:194:ASN:ND2	1.84	0.74
17:i:236:LYS:HG3	17:i:237:MET:HG3	1.68	0.74
31:l:702:CDL:HB61	31:l:702:CDL:C52	2.18	0.74
29:w:215:GLN:O	29:w:219:GLN:NE2	2.21	0.74
20:l:400:ASN:CB	20:l:486:MET:CE	2.62	0.73
25:r:427:LYS:HE3	36:r:625:HOH:O	1.88	0.73
11:c:116:ARG:HG2	30:l:703:PEE:H49	1.68	0.73
30:W:201:PEE:C1	30:W:201:PEE:H10	2.19	0.73
20:l:541:ASN:ND2	30:l:703:PEE:H61	2.04	0.73
5:W:94:GLU:OE2	5:W:104:TRP:NE1	2.20	0.72
17:i:88:LYS:HG3	17:i:148:SER:HB3	1.69	0.72
25:r:346:ARG:O	25:r:419:TYR:HA	1.90	0.72
30:l:704:PEE:H51	30:l:704:PEE:C11	2.19	0.72
31:r:505:CDL:H382	31:r:505:CDL:H781	1.71	0.72
30:W:201:PEE:H10	30:W:201:PEE:H2	1.72	0.72
36:j:324:HOH:O	21:m:59:ILE:CD1	2.37	0.72
19:k:19:LEU:HD22	19:k:36:MET:HE1	1.70	0.72
28:v:112:LYS:HD2	28:v:112:LYS:C	2.15	0.72
28:v:103:GLU:O	28:v:107:ARG:HG2	1.90	0.72
17:i:91:ASN:HD22	17:i:94:ALA:H	1.35	0.71
17:i:237:MET:SD	17:i:319:HIS:CE1	2.80	0.71
20:l:383:MET:SD	20:l:384:PRO:HD2	2.31	0.71
12:d:107:GLN:NE2	20:l:194:ASN:HD22	1.88	0.71
17:i:269:GLU:OE2	36:i:501:HOH:O	2.07	0.71
25:r:153:THR:OG1	36:r:601:HOH:O	2.09	0.71
30:i:402:PEE:H28	30:i:402:PEE:C22	2.21	0.71
30:i:402:PEE:H42	30:i:402:PEE:C21	2.06	0.71
17:i:88:LYS:HG2	17:i:148:SER:HB3	1.72	0.70
20:l:331:MET:HE2	20:l:331:MET:HA	1.71	0.70
12:d:107:GLN:HE21	20:l:200:GLN:HE22	1.40	0.70
26:s:18:ALA:O	26:s:21:THR:OG1	2.10	0.70
6:X:135:ALA:O	6:X:137:LYS:N	2.25	0.69
10:b:103:ARG:NH1	28:v:67:LEU:HD13	2.06	0.69
18:j:36:PRO:O	36:j:301:HOH:O	2.08	0.69
21:m:78:MET:HG2	21:m:79:TYR:CE2	2.27	0.69
20:l:598:SER:O	20:l:602:PHE:HB2	1.92	0.69
20:l:397:GLU:HB3	36:l:801:HOH:O	1.92	0.69
31:l:702:CDL:H112	31:l:702:CDL:H322	1.73	0.69
11:c:54:LYS:NZ	11:c:74:ASP:OD2	2.25	0.69
22:n:47:ARG:NH1	22:n:53:GLU:OE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:r:501:PEE:H71	30:r:501:PEE:C21	2.10	0.69
30:l:701:PEE:O2P	30:l:701:PEE:H8	1.92	0.69
17:i:23:SER:O	36:i:502:HOH:O	2.09	0.69
9:a:94:GLY:O	12:d:61:TYR:OH	2.10	0.69
31:a:201:CDL:H732	31:a:201:CDL:C19	2.19	0.69
17:i:95:MET:HE2	17:i:149:ILE:CG2	2.22	0.69
18:j:6:THR:HG21	26:s:87:VAL:HG11	1.74	0.69
20:l:328:HIS:HA	20:l:391:SER:OG	1.92	0.69
26:s:8:SER:O	26:s:12:PRO:HG2	1.93	0.69
31:l:702:CDL:H182	31:l:702:CDL:C84	2.22	0.69
36:k:115:HOH:O	21:m:64:MET:CE	2.41	0.69
20:l:383:MET:HB3	20:l:386:LEU:HD12	1.75	0.68
23:o:59:VAL:CG2	25:r:423:ILE:HG23	2.24	0.68
25:r:253:LEU:HD12	25:r:256:TYR:CE1	2.29	0.68
17:i:82:GLY:O	36:i:503:HOH:O	2.12	0.68
17:i:258:SER:OG	17:i:336:VAL:HG12	1.94	0.68
20:l:397:GLU:OE2	36:l:801:HOH:O	2.12	0.68
20:l:341:MET:HE2	20:l:457:LEU:HD12	1.76	0.68
25:r:140:THR:HG22	36:r:641:HOH:O	1.95	0.67
5:W:82:ARG:NH2	16:h:106:PRO:O	2.27	0.67
36:j:324:HOH:O	21:m:59:ILE:HD11	1.93	0.67
19:k:34:GLU:OE2	36:k:101:HOH:O	2.12	0.67
20:l:488:MET:O	20:l:492:ILE:HG13	1.94	0.67
29:w:113:SER:H	29:w:127:ASN:HD21	1.43	0.67
21:m:173:ARG:NH2	36:m:302:HOH:O	2.27	0.67
30:i:402:PEE:H37	30:i:402:PEE:H60	1.77	0.67
28:v:111:ARG:HH11	28:v:115:ARG:HD3	1.57	0.67
17:i:295:ARG:NH2	30:i:402:PEE:O2P	2.18	0.67
26:s:112:ALA:HB3	36:s:529:HOH:O	1.96	0.67
28:v:31:PHE:HE1	28:v:104:ARG:HE	1.42	0.67
30:l:704:PEE:C1	33:r:503:PLX:C2	2.73	0.66
27:u:38:LYS:NZ	27:u:42:GLU:OE2	2.27	0.66
7:Y:72:ARG:HB3	20:l:385:TYR:CD1	2.30	0.66
18:j:23:TRP:CZ2	30:j:201:PEE:H51	2.30	0.66
20:l:320:ASN:OD1	36:l:802:HOH:O	2.12	0.66
23:o:20:PRO:HB3	24:p:65:ARG:HH12	1.59	0.66
11:c:168:LEU:HA	11:c:172:GLY:HA2	1.77	0.66
20:l:327:LEU:O	20:l:331:MET:HG2	1.94	0.66
19:k:23:ARG:HG3	21:m:23:LYS:HE2	1.77	0.66
20:l:249:SER:HB3	20:l:340:PHE:CE2	2.31	0.66
7:Y:97:LEU:CD2	28:v:107:ARG:CD	2.70	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:a:201:CDL:H362	10:b:80:TRP:HB3	1.77	0.66
20:l:66:TRP:CZ3	30:l:704:PEE:H32	2.30	0.66
7:Y:72:ARG:HB3	20:l:385:TYR:CG	2.31	0.66
23:o:59:VAL:HG22	25:r:423:ILE:HG23	1.77	0.66
19:k:79:VAL:HG22	21:m:74:MET:HE1	1.77	0.66
7:Y:51:THR:H	7:Y:54:GLN:HE21	1.42	0.66
7:Y:72:ARG:HG3	20:l:385:TYR:HB3	1.78	0.65
25:r:97:THR:HG21	31:r:505:CDL:H241	1.77	0.65
26:s:304:HIS:ND1	36:s:505:HOH:O	2.29	0.65
20:l:288:THR:HG21	20:l:307:SER:CB	2.25	0.65
20:l:328:HIS:CD2	20:l:391:SER:OG	2.49	0.65
7:Y:97:LEU:HD23	28:v:107:ARG:NH1	2.01	0.65
29:w:47:GLU:OE2	29:w:52:LYS:NZ	2.30	0.65
3:U:26:GLY:HA3	30:U:101:PEE:H37	1.79	0.65
19:k:1:MET:HB3	19:k:2:PRO:HD2	1.79	0.65
17:i:68:MET:HA	17:i:68:MET:CE	2.22	0.65
30:j:201:PEE:C37	33:j:202:PLX:H132	2.27	0.64
20:l:331:MET:HE2	20:l:331:MET:CA	2.27	0.64
26:s:134:ARG:NH1	26:s:206:GLU:OE1	2.29	0.64
20:l:394:LEU:HD11	36:l:858:HOH:O	1.95	0.64
26:s:206:GLU:OE2	36:s:501:HOH:O	2.14	0.64
10:b:103:ARG:HH12	28:v:67:LEU:HD13	1.61	0.64
20:l:401:MET:HG3	20:l:486:MET:HE2	1.79	0.64
26:s:7:LEU:HD23	26:s:10:ILE:HD11	1.78	0.64
26:s:200:LEU:HD13	26:s:282:TYR:HB2	1.78	0.64
20:l:2:ASN:ND2	20:l:3:PRO:CD	2.39	0.64
19:k:1:MET:HB3	19:k:2:PRO:CD	2.28	0.64
26:s:134:ARG:NH2	26:s:206:GLU:OE1	2.30	0.64
13:e:112:TYR:O	25:r:45:LEU:O	2.15	0.64
12:d:106:ILE:HD11	13:e:136:LEU:HD21	1.79	0.64
17:i:276:ILE:N	17:i:276:ILE:HD12	2.13	0.64
20:l:69:MET:HE3	20:l:76:LEU:HD12	1.81	0.63
25:r:140:THR:HG23	25:r:141:GLU:OE2	1.97	0.63
33:r:503:PLX:C18	31:r:504:CDL:H801	2.28	0.63
26:s:72:ILE:HD12	31:s:401:CDL:H122	1.79	0.63
29:w:344:ASN:O	29:w:347:VAL:HG23	1.98	0.63
19:k:1:MET:O	21:m:119:PHE:CB	2.46	0.63
12:d:167:ARG:NE	13:e:153:GLU:OE2	2.25	0.63
17:i:70:LEU:CD1	17:i:98:MET:SD	2.87	0.63
31:l:702:CDL:H841	31:l:702:CDL:C18	2.27	0.63
17:i:250:SER:O	17:i:259:GLY:HA3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:v:51:LEU:O	28:v:52:MET:HG3	1.99	0.62
17:i:95:MET:CE	17:i:149:ILE:CG2	2.62	0.62
20:l:331:MET:HG3	20:l:391:SER:HB2	1.81	0.62
25:r:371:PRO:HD2	31:r:504:CDL:H391	1.80	0.62
19:k:23:ARG:HD3	21:m:23:LYS:O	1.98	0.62
20:l:249:SER:CB	20:l:340:PHE:CE2	2.82	0.62
17:i:42:PRO:HG3	21:m:167:VAL:HG13	1.80	0.62
17:i:265:MET:HA	17:i:265:MET:HE2	1.82	0.62
30:l:704:PEE:H3	33:r:503:PLX:C2	2.29	0.62
25:r:403:THR:HA	25:r:406:TYR:CE2	2.35	0.62
20:l:562:LEU:HB3	20:l:563:PRO:HD3	1.82	0.62
25:r:188:ASN:OD1	25:r:256:TYR:OH	2.16	0.62
5:W:93:GLU:OE2	16:h:92:TYR:OH	2.16	0.62
20:l:67:HIS:HD1	30:l:704:PEE:H12	1.65	0.62
20:l:359:MET:O	20:l:436:ARG:NH2	2.33	0.61
24:p:47:ARG:NH2	24:p:70:GLU:OE2	2.33	0.61
26:s:200:LEU:HD13	26:s:282:TYR:HB3	1.80	0.61
26:s:102:VAL:HG11	26:s:154:LEU:HD11	1.82	0.61
4:V:113:ALA:CB	30:l:701:PEE:H53	2.30	0.61
23:o:59:VAL:HG22	25:r:423:ILE:CG2	2.30	0.61
2:S:31:ASN:ND2	2:S:60:TYR:OH	2.33	0.61
6:X:139:MET:HE3	10:b:2:SER:HB3	1.81	0.61
17:i:91:ASN:HD21	17:i:93:VAL:HB	1.65	0.61
20:l:273:VAL:HA	20:l:276:MET:HE3	1.83	0.61
26:s:209:SER:HB3	26:s:213:VAL:HB	1.83	0.61
19:k:64:LEU:HD23	36:k:126:HOH:O	2.00	0.61
30:r:501:PEE:O1P	30:r:501:PEE:H12	2.01	0.61
26:s:195:ARG:HD3	26:s:231:ILE:HD11	1.83	0.61
20:l:600:THR:HG22	20:l:601:LEU:HD23	1.83	0.60
21:m:61:LEU:O	26:s:114:TYR:OH	2.15	0.60
4:V:40:SER:HA	31:V:201:CDL:HB61	1.83	0.60
26:s:11:ILE:HB	26:s:12:PRO:HD3	1.83	0.60
21:m:45:LEU:HD23	21:m:50:SER:HA	1.83	0.60
12:d:78:GLU:HA	15:g:110:THR:HA	1.82	0.60
17:i:68:MET:CE	19:k:37:MET:HE2	2.29	0.60
7:Y:44:TYR:CD2	8:Z:16:LEU:HD22	2.36	0.60
17:i:11:MET:HG2	31:i:401:CDL:H581	1.84	0.60
17:i:270:MET:HE1	17:i:278:MET:HG2	1.84	0.60
9:a:161:ARG:NH1	15:g:1:MET:H1	1.99	0.60
31:a:201:CDL:HB21	30:l:704:PEE:H49	1.83	0.60
36:e:201:HOH:O	25:r:453:MET:CE	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:400:ASN:O	20:l:486:MET:HE1	2.02	0.60
28:v:103:GLU:OE2	28:v:103:GLU:HA	2.00	0.60
20:l:100:ILE:HD12	20:l:246:LEU:HB2	1.84	0.59
20:l:230:HIS:CE1	36:l:852:HOH:O	2.44	0.59
25:r:370:PRO:HG3	25:r:375:LEU:HD13	1.82	0.59
13:e:55:LEU:HD23	13:e:57:GLU:HB2	1.84	0.59
20:l:401:MET:SD	20:l:482:MET:HE2	2.42	0.59
26:s:54:LYS:HD2	26:s:54:LYS:C	2.28	0.59
17:i:30:TRP:CH2	19:k:37:MET:HE1	2.38	0.59
6:X:91:ASP:HB2	8:Z:44:PRO:CA	2.33	0.58
20:l:197:ASP:OD1	36:l:803:HOH:O	2.17	0.58
31:s:401:CDL:H182	31:s:401:CDL:H362	1.85	0.58
29:w:139:ARG:HH12	35:w:401:ADP:HN61	0.71	0.58
25:r:392:THR:O	25:r:396:MET:HG2	2.04	0.58
22:n:54:GLU:HG2	22:n:55:VAL:HG22	1.85	0.58
17:i:276:ILE:CG2	30:r:501:PEE:H14	2.33	0.58
30:l:701:PEE:H8	30:l:701:PEE:P	2.43	0.58
26:s:61:LEU:HD12	26:s:61:LEU:O	2.03	0.58
17:i:278:MET:CB	17:i:279:PRO:HD3	2.32	0.58
20:l:495:ILE:HG22	20:l:499:MET:HE2	1.85	0.58
21:m:23:LYS:N	21:m:24:PRO:HD3	2.19	0.58
6:X:135:ALA:C	6:X:137:LYS:H	2.12	0.58
15:g:58:ALA:O	29:w:353:TRP:O	2.22	0.58
23:o:59:VAL:HG13	25:r:422:HIS:HE1	1.68	0.58
31:r:504:CDL:H511	31:r:504:CDL:HA31	1.86	0.58
31:r:505:CDL:HB32	31:r:505:CDL:OB7	2.02	0.58
7:Y:76:ASP:O	20:l:385:TYR:OH	2.22	0.58
18:j:68:GLU:HG3	18:j:98:LEU:HD13	1.86	0.58
20:l:596:MET:SD	31:m:201:CDL:C64	2.92	0.58
25:r:116:ILE:HG13	27:u:168:PHE:CD2	2.39	0.58
27:u:49:GLU:OE1	27:u:135:ARG:NH1	2.34	0.58
28:v:111:ARG:HH12	28:v:115:ARG:HD3	1.66	0.58
17:i:95:MET:HE3	17:i:149:ILE:HG22	1.76	0.57
31:V:202:CDL:HB4	23:o:82:PRO:HB2	1.87	0.57
20:l:331:MET:HE2	20:l:331:MET:N	2.19	0.57
33:r:503:PLX:O1	33:r:503:PLX:H1A2	2.04	0.57
3:U:26:GLY:HA3	30:U:101:PEE:C23	2.34	0.57
12:d:159:GLN:HE22	13:e:142:PHE:H	1.50	0.57
20:l:386:LEU:HB2	36:l:817:HOH:O	2.04	0.57
4:V:141:VAL:H	17:i:273:ASN:HD21	1.52	0.57
31:r:504:CDL:H312	31:r:504:CDL:H742	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:198:PHE:CD1	26:s:285:LEU:HD13	2.39	0.57
20:l:273:VAL:HA	20:l:276:MET:CE	2.34	0.57
31:l:702:CDL:H112	31:l:702:CDL:C32	2.34	0.57
25:r:373:ILE:HD11	25:r:444:LEU:HD23	1.85	0.57
31:a:201:CDL:HB21	30:l:704:PEE:C31	2.34	0.57
10:b:72:VAL:HG23	10:b:76:LEU:HD23	1.86	0.57
11:c:85:GLU:OE2	11:c:119:THR:OG1	2.15	0.57
30:j:201:PEE:C37	33:j:202:PLX:C13	2.83	0.57
19:k:48:ILE:HD13	19:k:56:ALA:O	2.03	0.57
20:l:23:ASN:HB2	33:r:503:PLX:H222	1.87	0.57
26:s:200:LEU:HD13	26:s:282:TYR:CA	2.34	0.57
31:a:201:CDL:H111	30:l:704:PEE:C37	2.34	0.56
11:c:39:GLY:H	11:c:74:ASP:CB	2.17	0.56
25:r:104:LEU:HD23	31:r:505:CDL:C87	2.35	0.56
26:s:62:ARG:HG3	26:s:62:ARG:O	2.05	0.56
28:v:111:ARG:HD2	28:v:111:ARG:O	2.04	0.56
36:j:324:HOH:O	21:m:59:ILE:HD13	2.02	0.56
36:k:115:HOH:O	21:m:64:MET:HE3	2.02	0.56
25:r:84:LEU:HD22	25:r:87:GLU:HG3	1.87	0.56
4:V:141:VAL:HG22	4:V:141:VAL:O	2.05	0.56
36:k:115:HOH:O	21:m:64:MET:HE2	2.05	0.56
26:s:216:ALA:O	26:s:219:PRO:HD2	2.05	0.56
8:Z:33:GLN:CD	8:Z:43:ASP:OD1	2.48	0.56
20:l:491:LEU:O	20:l:491:LEU:HD12	2.06	0.56
31:l:702:CDL:OA7	31:l:702:CDL:HA61	2.04	0.56
23:o:59:VAL:HG13	25:r:422:HIS:CE1	2.41	0.56
25:r:189:SER:HA	33:r:502:PLX:H1B3	1.87	0.56
12:d:167:ARG:HH21	13:e:153:GLU:HG3	1.71	0.56
16:h:2:PRO:HA	17:i:140:SER:HB2	1.88	0.56
25:r:45:LEU:CD1	25:r:50:LEU:HD23	2.35	0.56
19:k:17:ALA:HB2	31:m:201:CDL:H812	1.88	0.56
25:r:70:THR:HA	25:r:103:GLN:NE2	2.21	0.56
19:k:19:LEU:HD22	19:k:36:MET:CE	2.36	0.56
25:r:6:ILE:HB	25:r:7:PRO:HD3	1.88	0.56
25:r:198:ALA:HB2	30:r:501:PEE:H22	1.88	0.56
20:l:95:PHE:CZ	20:l:456:ARG:HG2	2.41	0.56
27:u:61:LYS:O	27:u:65:GLN:NE2	2.39	0.56
14:f:39:PRO:HD3	29:w:351:TRP:CD1	2.41	0.55
19:k:33:LEU:HA	19:k:36:MET:HE3	1.86	0.55
19:k:87:THR:HG22	19:k:89:TYR:H	1.71	0.55
20:l:102:GLU:HA	20:l:105:MET:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:343:ILE:O	25:r:346:ARG:NH1	2.36	0.55
4:V:141:VAL:H	17:i:273:ASN:HD22	1.53	0.55
13:e:103:SER:OG	33:r:503:PLX:H282	2.07	0.55
30:l:701:PEE:P	30:l:701:PEE:C3	2.94	0.55
28:v:15:LYS:HA	28:v:109:LEU:CD2	2.36	0.55
4:V:141:VAL:CG2	9:a:157:ARG:HB3	2.36	0.55
25:r:104:LEU:CD2	31:r:505:CDL:H862	1.88	0.55
25:r:449:LEU:HB3	33:r:503:PLX:H4	1.89	0.55
15:g:15:PHE:HB2	33:g:201:PLX:H6	1.89	0.55
20:l:145:GLU:OE1	36:l:804:HOH:O	2.18	0.55
20:l:250:SER:HB2	20:l:333:ALA:HA	1.89	0.55
27:u:78:CYS:HB2	27:u:81:PRO:HD2	1.88	0.55
31:u:201:CDL:H581	31:u:201:CDL:C54	2.30	0.55
9:a:53:ARG:HB3	10:b:28:LEU:HD12	1.89	0.55
17:i:8:THR:HG23	31:i:401:CDL:H791	1.88	0.55
24:p:50:GLU:OE2	24:p:51:HIS:NE2	2.39	0.55
16:h:21:GLN:HB3	16:h:37:GLU:OE2	2.07	0.55
20:l:400:ASN:O	20:l:486:MET:CE	2.54	0.55
16:h:18:MET:HE3	19:k:56:ALA:HA	1.88	0.55
17:i:86:ILE:O	17:i:86:ILE:HG23	2.06	0.55
17:i:245:MET:CE	31:r:505:CDL:H182	2.37	0.55
31:r:505:CDL:H382	31:r:505:CDL:C78	2.36	0.55
7:Y:72:ARG:CB	20:l:385:TYR:CG	2.90	0.55
17:i:100:MET:SD	20:l:598:SER:OG	2.57	0.55
20:l:328:HIS:CA	20:l:391:SER:OG	2.54	0.55
28:v:111:ARG:HD2	28:v:111:ARG:C	2.32	0.55
29:w:344:ASN:HB2	29:w:347:VAL:CG2	2.37	0.55
4:V:49:PHE:HA	31:m:201:CDL:HA61	1.89	0.55
25:r:59:ASP:H	25:r:62:SER:HB2	1.70	0.55
11:c:39:GLY:C	11:c:74:ASP:HB2	2.32	0.54
20:l:27:TYR:OH	20:l:119:LYS:NZ	2.40	0.54
29:w:65:ASN:OD1	29:w:66:ILE:N	2.28	0.54
24:p:35:ASP:OD1	24:p:36:LYS:N	2.40	0.54
29:w:129:TYR:OH	29:w:186:HIS:HD2	1.90	0.54
30:U:102:PEE:H56	26:s:187:ILE:HD12	1.89	0.54
26:s:204:GLU:CG	36:s:509:HOH:O	2.36	0.54
19:k:72:ALA:HB3	36:k:120:HOH:O	2.08	0.54
26:s:142:TYR:CD1	26:s:142:TYR:C	2.86	0.54
9:a:96:ALA:HB1	12:d:62:TYR:HA	1.90	0.54
26:s:200:LEU:HD13	26:s:282:TYR:HA	1.90	0.54
5:W:61:GLN:HE22	26:s:317:GLN:H	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:328:HIS:CB	20:l:391:SER:OG	2.56	0.54
18:j:11:VAL:HG22	30:j:201:PEE:H42	1.90	0.54
31:l:702:CDL:C52	31:l:702:CDL:CB6	2.86	0.54
21:m:54:LEU:HB3	26:s:103:LEU:HD22	1.89	0.54
15:g:58:ALA:O	29:w:353:TRP:C	2.51	0.54
15:g:109:LYS:HB3	15:g:113:GLU:HG3	1.90	0.54
20:l:419:THR:HA	20:l:422:TYR:CE2	2.43	0.54
29:w:113:SER:HB3	29:w:116:LYS:HG2	1.89	0.54
21:m:1:MET:HB2	21:m:125:TRP:HE1	1.73	0.54
6:X:115:GLN:O	6:X:119:ILE:HG12	2.09	0.53
9:a:78:THR:HG21	13:e:96:SER:O	2.08	0.53
17:i:258:SER:CB	17:i:336:VAL:HG12	2.39	0.53
9:a:132:ASN:OD1	25:r:45:LEU:CD1	2.56	0.53
26:s:307:LEU:HA	26:s:310:MET:HE2	1.90	0.53
36:h:203:HOH:O	21:m:127:ILE:HB	2.09	0.53
20:l:328:HIS:HD2	20:l:391:SER:OG	1.91	0.53
20:l:573:MET:SD	30:l:701:PEE:H18	2.48	0.53
13:e:103:SER:OG	33:r:503:PLX:C28	2.56	0.53
15:g:4:MET:HE2	15:g:7:ARG:HD2	1.88	0.53
25:r:114:GLU:OE2	27:u:168:PHE:O	2.25	0.53
28:v:111:ARG:HG2	28:v:114:ARG:HH12	1.74	0.53
11:c:39:GLY:O	11:c:74:ASP:HB2	2.09	0.53
16:h:21:GLN:NE2	16:h:33:CYS:H	2.07	0.53
21:m:86:ASN:HD22	21:m:89:VAL:HG23	1.74	0.53
31:V:202:CDL:H742	31:V:202:CDL:H601	1.91	0.53
10:b:106:PRO:HG3	28:v:45:GLU:HG2	1.91	0.53
16:h:21:GLN:HE22	16:h:33:CYS:H	1.57	0.53
11:c:166:LEU:HB3	11:c:169:GLU:HB2	1.89	0.53
15:g:89:ASP:OD2	27:u:161:ALA:CB	2.54	0.53
25:r:83:HIS:HE1	36:r:618:HOH:O	1.92	0.53
9:a:97:GLU:CG	12:d:62:TYR:CD2	2.92	0.52
31:m:201:CDL:H592	31:m:201:CDL:H782	1.90	0.52
24:p:26:HIS:HD2	24:p:76:HIS:H	1.57	0.52
29:w:61:THR:HG22	29:w:159:LEU:HB2	1.91	0.52
32:X:201:8Q1:C8	24:p:47:ARG:HE	2.21	0.52
17:i:251:MET:HE3	36:i:559:HOH:O	2.09	0.52
25:r:451:PRO:HG2	36:r:667:HOH:O	2.09	0.52
17:i:147:GLN:OE1	17:i:147:GLN:N	2.31	0.52
20:l:375:ILE:HD12	20:l:458:LEU:HD11	1.92	0.52
25:r:10:MET:O	25:r:13:PRO:HD2	2.09	0.52
26:s:282:TYR:OH	36:s:502:HOH:O	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:11:ILE:N	26:s:12:PRO:CD	2.71	0.52
11:c:101:TRP:CE3	23:o:47:TYR:HB2	2.44	0.52
19:k:59:MET:HG3	19:k:60:PRO:HD3	1.91	0.52
20:l:417:SER:HB3	20:l:493:VAL:HG13	1.92	0.52
20:l:417:SER:OG	31:l:702:CDL:H581	2.09	0.52
25:r:449:LEU:HD13	33:r:503:PLX:H92	1.92	0.52
33:r:503:PLX:C15	31:r:504:CDL:H802	2.39	0.52
1:Q:38:GLN:NE2	17:i:304:MET:H	2.07	0.52
5:W:96:ILE:HG21	16:h:92:TYR:HE1	1.73	0.52
25:r:87:GLU:O	25:r:92:LYS:HE2	2.09	0.52
20:l:226:GLN:NE2	20:l:314:MET:HG3	2.25	0.52
24:p:98:LYS:HG2	24:p:178:PRO:HG3	1.91	0.52
7:Y:43:ARG:HD3	7:Y:48:PRO:HA	1.90	0.52
25:r:104:LEU:HG	25:r:108:MET:HE2	1.91	0.52
31:r:504:CDL:H311	31:r:504:CDL:H561	1.91	0.52
5:W:91:LEU:HD22	27:u:7:LEU:HD12	1.91	0.52
19:k:91:GLN:CD	19:k:91:GLN:H	2.18	0.52
20:l:4:PHE:O	20:l:8:THR:HG23	2.10	0.52
20:l:520:TYR:HE1	31:l:702:CDL:OB4	1.92	0.52
25:r:97:THR:HG21	31:r:505:CDL:C24	2.40	0.52
7:Y:97:LEU:HD23	28:v:107:ARG:HD3	1.90	0.52
9:a:132:ASN:OD1	25:r:45:LEU:HD11	2.10	0.52
21:m:23:LYS:N	21:m:24:PRO:CD	2.73	0.52
5:W:61:GLN:NE2	26:s:317:GLN:H	2.07	0.51
8:Z:54:SER:OG	8:Z:55:GLY:N	2.42	0.51
25:r:159:PRO:HB3	30:r:501:PEE:H25	1.93	0.51
31:r:504:CDL:H591	31:r:504:CDL:H332	1.91	0.51
26:s:200:LEU:CD1	26:s:282:TYR:HA	2.40	0.51
8:Z:33:GLN:OE1	8:Z:43:ASP:OD1	2.27	0.51
20:l:175:ASN:ND2	36:l:812:HOH:O	2.41	0.51
20:l:400:ASN:C	20:l:486:MET:HE1	2.36	0.51
27:u:38:LYS:HB3	27:u:39:PRO:HD3	1.92	0.51
29:w:88:GLU:N	29:w:160:GLU:HG3	2.26	0.51
11:c:75:TYR:CG	11:c:76:PRO:HD2	2.45	0.51
19:k:70:GLU:OE1	36:k:104:HOH:O	2.19	0.51
21:m:71:THR:HG23	21:m:75:ALA:HB3	1.92	0.51
22:n:4:VAL:HG22	22:n:8:VAL:HG23	1.92	0.51
31:r:505:CDL:H452	31:r:505:CDL:C41	2.36	0.51
6:X:135:ALA:C	6:X:137:LYS:N	2.66	0.51
15:g:47:ASP:OD2	15:g:66:TYR:OH	2.22	0.51
15:g:52:ARG:NH1	17:i:318:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:91:ASP:HB2	8:Z:44:PRO:CB	2.41	0.51
20:l:536:LEU:HB3	20:l:537:PRO:HD3	1.93	0.51
25:r:127:VAL:HG11	31:r:505:CDL:H451	1.91	0.51
6:X:132:ASP:OD2	24:p:18:ARG:HG2	2.10	0.51
31:a:201:CDL:OB3	33:r:503:PLX:H11	2.11	0.51
17:i:91:ASN:ND2	17:i:93:VAL:HB	2.24	0.51
20:l:68:TRP:CZ3	20:l:69:MET:HE2	2.46	0.51
20:l:530:PRO:O	20:l:534:HIS:HB2	2.10	0.51
29:w:58:LYS:O	29:w:60:ILE:HG13	2.10	0.51
11:c:36:MET:HA	11:c:36:MET:HE2	1.93	0.51
12:d:107:GLN:NE2	20:l:200:GLN:HE22	2.05	0.51
17:i:34:GLU:OE2	36:i:504:HOH:O	2.19	0.51
9:a:184:LYS:O	9:a:185:THR:HG22	2.10	0.51
15:g:19:GLU:HG2	27:u:158:LEU:HD22	1.92	0.51
17:i:276:ILE:N	17:i:276:ILE:CD1	2.73	0.51
31:i:401:CDL:H141	31:i:401:CDL:H341	1.93	0.51
16:h:21:GLN:HE21	16:h:31:GLY:HA3	1.76	0.51
20:l:22:SER:OG	20:l:119:LYS:HE3	2.10	0.51
20:l:141:PHE:HE2	25:r:375:LEU:HD11	1.76	0.51
31:u:201:CDL:H741	31:u:201:CDL:C53	2.40	0.51
30:U:102:PEE:H36	5:W:43:LEU:CD1	2.41	0.50
30:i:402:PEE:C22	30:i:402:PEE:C18	2.85	0.50
25:r:266:MET:HB3	25:r:395:LEU:HD13	1.93	0.50
11:c:75:TYR:OH	11:c:105:ILE:O	2.25	0.50
17:i:222:SER:O	17:i:224:ALA:N	2.44	0.50
20:l:71:LEU:N	20:l:71:LEU:HD22	2.25	0.50
20:l:316:THR:HG23	20:l:325:ALA:HB2	1.92	0.50
20:l:505:ASN:O	20:l:508:THR:HG22	2.10	0.50
29:w:139:ARG:NH1	35:w:401:ADP:N6	2.30	0.50
20:l:394:LEU:CD1	36:l:858:HOH:O	2.56	0.50
20:l:268:GLU:HB3	36:l:802:HOH:O	2.11	0.50
3:U:38:TYR:HB2	26:s:310:MET:O	2.11	0.50
6:X:120:MET:HE1	24:p:24:LEU:HB3	1.93	0.50
33:g:201:PLX:H332	17:i:342:ALA:HB3	1.93	0.50
17:i:30:TRP:CG	17:i:71:MET:HE2	2.47	0.50
31:r:505:CDL:H402	31:r:505:CDL:H811	1.94	0.50
31:u:201:CDL:H741	31:u:201:CDL:H531	1.94	0.50
13:e:55:LEU:CD2	13:e:57:GLU:HB2	2.41	0.50
17:i:62:THR:HG21	17:i:114:TRP:CD1	2.47	0.50
26:s:61:LEU:HD12	26:s:61:LEU:C	2.37	0.50
29:w:353:TRP:H	29:w:353:TRP:CD1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:98:MET:HE3	5:W:101:VAL:HG21	1.92	0.50
19:k:31:LEU:HD21	21:m:67:VAL:HG11	1.93	0.50
31:l:702:CDL:H241	31:l:702:CDL:C20	2.41	0.50
26:s:109:SER:OG	26:s:192:GLU:OE1	2.30	0.50
25:r:87:GLU:OE2	25:r:91:ARG:HB2	2.12	0.50
29:w:110:GLY:HA2	29:w:134:TRP:CE2	2.47	0.50
12:d:69:ARG:NH2	22:n:46:LYS:O	2.37	0.50
20:l:596:MET:SD	31:m:201:CDL:H632	2.47	0.50
17:i:81:SER:O	17:i:83:GLN:N	2.40	0.49
18:j:27:LEU:HD23	26:s:59:GLU:HG3	1.92	0.49
19:k:24:SER:HB3	36:k:118:HOH:O	2.11	0.49
6:X:84:LEU:O	6:X:88:LYS:HG3	2.11	0.49
31:a:201:CDL:H111	30:l:704:PEE:H60	1.94	0.49
17:i:159:MET:HB2	17:i:278:MET:HE1	1.93	0.49
30:j:201:PEE:H31	31:s:401:CDL:H222	1.93	0.49
19:k:25:HIS:O	36:k:102:HOH:O	2.18	0.49
10:b:99:GLU:HG2	20:l:61:MET:HG3	1.95	0.49
17:i:221:HIS:O	17:i:319:HIS:NE2	2.45	0.49
25:r:203:PHE:O	25:r:207:MET:HG2	2.13	0.49
13:e:55:LEU:HD21	29:w:320:GLY:HA3	1.94	0.49
20:l:100:ILE:CD1	20:l:246:LEU:HB2	2.42	0.49
6:X:91:ASP:HB2	8:Z:44:PRO:HA	1.93	0.49
15:g:58:ALA:O	29:w:353:TRP:HA	2.13	0.49
21:m:55:MET:HE1	21:m:58:LEU:HD23	1.95	0.49
24:p:108:HIS:HD2	24:p:110:SER:HB3	1.78	0.49
3:U:66:VAL:O	27:u:130:LYS:HE3	2.12	0.49
11:c:68:ASP:CG	11:c:70:MET:HG2	2.38	0.49
20:l:491:LEU:HD12	20:l:495:ILE:HG12	1.95	0.49
1:Q:39:PRO:HB3	1:Q:43:TRP:CD1	2.47	0.49
26:s:200:LEU:HD12	36:s:546:HOH:O	2.11	0.49
6:X:80:LYS:HA	6:X:83:VAL:HG23	1.94	0.49
18:j:48:ARG:O	21:m:76:THR:HB	2.13	0.49
19:k:4:VAL:HG21	21:m:124:ASP:OD2	2.12	0.49
31:m:201:CDL:H332	31:m:201:CDL:H222	1.94	0.49
20:l:298:ILE:O	20:l:302:VAL:HG23	2.13	0.49
20:l:400:ASN:CB	20:l:486:MET:HE2	2.36	0.49
12:d:160:LYS:HE2	13:e:147:ILE:HG23	1.95	0.48
19:k:21:MET:O	21:m:23:LYS:NZ	2.46	0.48
20:l:429:PHE:O	20:l:436:ARG:NH2	2.45	0.48
1:Q:53:TYR:OH	17:i:295:ARG:NH2	2.46	0.48
30:W:201:PEE:C1	30:W:201:PEE:C4	2.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:95:MET:HE2	17:i:149:ILE:CA	2.43	0.48
25:r:438:ALA:HA	25:r:441:ILE:HG22	1.95	0.48
36:e:201:HOH:O	25:r:453:MET:HE3	2.12	0.48
20:l:566:THR:O	20:l:570:GLN:HG2	2.14	0.48
26:s:209:SER:HB3	26:s:213:VAL:CB	2.43	0.48
29:w:350:LYS:O	29:w:355:LYS:HE3	2.13	0.48
17:i:68:MET:HE1	19:k:37:MET:CE	2.39	0.48
20:l:264:TYR:CD2	20:l:265:PRO:HD3	2.48	0.48
21:m:99:MET:HE1	31:m:201:CDL:H802	1.96	0.48
25:r:198:ALA:HA	30:r:501:PEE:H30	1.95	0.48
26:s:54:LYS:HD2	26:s:54:LYS:O	2.14	0.48
11:c:48:ARG:NH2	11:c:63:GLU:OE1	2.42	0.48
11:c:155:PRO:HD3	28:v:4:HIS:NE2	2.28	0.48
20:l:312:LEU:O	20:l:315:VAL:HG22	2.13	0.48
1:Q:37:TRP:CD2	25:r:140:THR:HB	2.49	0.48
9:a:152:LYS:HD3	15:g:96:VAL:HG21	1.94	0.48
12:d:46:THR:O	12:d:50:GLU:HG3	2.14	0.48
20:l:399:VAL:HG12	20:l:409:LEU:HD13	1.95	0.48
23:o:83:THR:HG22	23:o:85:LYS:H	1.79	0.48
27:u:79:ALA:O	27:u:83:THR:OG1	2.23	0.48
30:W:201:PEE:H32	21:m:39:VAL:HG12	1.95	0.48
31:a:201:CDL:H831	31:a:201:CDL:C87	2.43	0.48
16:h:24:GLU:OE2	16:h:28:LYS:NZ	2.47	0.48
17:i:285:THR:HA	30:i:402:PEE:H67	1.96	0.48
30:l:704:PEE:H3	33:r:503:PLX:H22	1.95	0.48
25:r:4:ILE:CD1	25:r:41:LEU:HD11	2.44	0.48
29:w:287:ASP:OD1	29:w:287:ASP:N	2.42	0.48
4:V:4:THR:O	4:V:8:LYS:HG3	2.14	0.48
7:Y:98:GLY:HA3	28:v:31:PHE:CE1	2.49	0.48
11:c:38:PRO:HG2	23:o:70:TYR:HD2	1.78	0.48
17:i:182:SER:O	17:i:186:HIS:HD2	1.96	0.48
20:l:397:GLU:CB	36:l:801:HOH:O	2.54	0.48
29:w:325:ASP:O	29:w:329:GLN:HG2	2.14	0.48
31:V:201:CDL:H612	31:V:201:CDL:H752	1.95	0.47
5:W:96:ILE:HG21	16:h:92:TYR:CE1	2.49	0.47
15:g:85:TYR:CZ	27:u:165:SER:HB2	2.49	0.47
9:a:132:ASN:HD21	25:r:51:ASN:H	1.62	0.47
20:l:180:ILE:CD1	30:l:703:PEE:H79	2.44	0.47
31:r:504:CDL:H861	31:r:504:CDL:H572	1.96	0.47
5:W:36:PHE:O	5:W:40:ILE:HG12	2.14	0.47
9:a:166:GLY:O	9:a:170:GLN:NE2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:160:GLN:HB3	11:c:183:HIS:CD2	2.49	0.47
30:j:201:PEE:H3	30:j:201:PEE:H10	1.96	0.47
20:l:286:LEU:CD1	20:l:411:MET:SD	2.92	0.47
29:w:165:SER:O	29:w:168:VAL:HG22	2.14	0.47
20:l:401:MET:SD	20:l:482:MET:HB3	2.54	0.47
25:r:87:GLU:OE2	25:r:91:ARG:CB	2.62	0.47
5:W:68:ARG:HD2	21:m:135:PHE:CE2	2.49	0.47
5:W:134:LEU:HG	21:m:2:THR:HB	1.95	0.47
9:a:189:ASN:ND2	27:u:142:TYR:OH	2.35	0.47
18:j:22:PHE:HB3	30:j:201:PEE:H2	1.97	0.47
25:r:289:SER:O	25:r:293:HIS:CD2	2.67	0.47
31:s:401:CDL:H141	31:s:401:CDL:H171	1.54	0.47
31:a:201:CDL:H201	31:a:201:CDL:H752	1.95	0.47
20:l:599:MET:HE3	20:l:599:MET:HB3	1.84	0.47
6:X:125:GLU:OE2	20:l:439:PRO:HG3	2.15	0.47
9:a:66:ARG:HH12	13:e:72:ASP:HB2	1.80	0.47
17:i:72:MET:HE2	17:i:76:ILE:HG13	1.96	0.47
33:j:203:PLX:H372	33:j:203:PLX:H342	1.77	0.47
19:k:13:ALA:HB1	31:m:201:CDL:H821	1.96	0.47
20:l:358:LYS:HG3	24:p:80:TYR:CE1	2.49	0.47
23:o:115:LEU:HG	23:o:120:LYS:O	2.15	0.47
24:p:16:VAL:HG22	24:p:64:LEU:HD13	1.96	0.47
26:s:157:ASN:OD1	26:s:168:THR:OG1	2.29	0.47
29:w:139:ARG:NH1	29:w:166:ASP:OD1	2.45	0.47
8:Z:75:PHE:O	8:Z:79:VAL:HG23	2.15	0.47
18:j:71:LEU:O	21:m:147:TYR:OH	2.20	0.47
23:o:56:ARG:C	23:o:56:ARG:HD2	2.39	0.47
25:r:63:ALA:N	25:r:64:PRO:HD2	2.30	0.47
30:W:201:PEE:H42	30:W:201:PEE:C21	2.18	0.47
11:c:33:THR:OG1	11:c:34:LYS:N	2.44	0.47
26:s:134:ARG:CZ	26:s:206:GLU:OE1	2.63	0.47
17:i:68:MET:HE3	36:k:104:HOH:O	2.14	0.47
17:i:307:SER:OG	17:i:308:THR:N	2.48	0.47
33:j:203:PLX:H311	33:j:203:PLX:H282	1.57	0.47
19:k:2:PRO:HD2	19:k:5:TYR:HD2	1.79	0.47
21:m:78:MET:HG2	21:m:79:TYR:CD2	2.50	0.47
26:s:201:THR:HG23	36:s:525:HOH:O	2.15	0.47
10:b:86:LEU:HD11	20:l:9:LEU:HD12	1.96	0.46
30:i:402:PEE:H37	30:i:402:PEE:C37	2.43	0.46
18:j:80:GLN:HG3	26:s:318:SER:HA	1.97	0.46
25:r:198:ALA:CA	30:r:501:PEE:H30	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:r:505:CDL:H761	31:r:505:CDL:H791	1.59	0.46
31:s:401:CDL:HA61	31:s:401:CDL:H132	1.97	0.46
33:r:502:PLX:H121	33:r:502:PLX:H92	1.52	0.46
26:s:55:LEU:HD13	26:s:221:ALA:HB2	1.96	0.46
7:Y:103:ASP:OD1	7:Y:103:ASP:N	2.45	0.46
20:l:11:THR:HG21	20:l:47:SER:HB3	1.97	0.46
31:l:702:CDL:H241	31:l:702:CDL:H202	1.98	0.46
21:m:78:MET:HG2	21:m:79:TYR:CZ	2.50	0.46
25:r:449:LEU:HD13	33:r:503:PLX:C9	2.45	0.46
31:r:505:CDL:H511	31:r:505:CDL:H542	1.54	0.46
6:X:135:ALA:O	6:X:136:GLU:C	2.57	0.46
4:V:141:VAL:HG23	9:a:157:ARG:HB3	1.96	0.46
12:d:71:VAL:H	12:d:91:GLN:HE22	1.62	0.46
3:U:32:LEU:HB3	26:s:310:MET:SD	2.55	0.46
5:W:96:ILE:CG2	16:h:92:TYR:CE1	2.99	0.46
13:e:73:SER:O	13:e:75:GLY:N	2.48	0.46
13:e:77:ASP:OD1	13:e:78:LYS:N	2.49	0.46
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.51	0.46
22:n:50:ARG:HB2	22:n:53:GLU:HG2	1.97	0.46
31:V:202:CDL:H781	31:V:202:CDL:H812	1.52	0.46
8:Z:23:LYS:HB3	8:Z:25:GLU:OE1	2.14	0.46
31:a:201:CDL:H122	30:l:704:PEE:H67	1.98	0.46
11:c:96:ASP:N	11:c:96:ASP:OD1	2.48	0.46
15:g:5:SER:HA	15:g:10:ARG:NH2	2.30	0.46
15:g:58:ALA:O	29:w:352:ILE:O	2.32	0.46
33:j:203:PLX:H152	33:j:203:PLX:H341	1.97	0.46
20:l:414:ILE:O	20:l:418:LEU:HG	2.16	0.46
30:l:704:PEE:H2	33:r:503:PLX:H21	1.96	0.46
24:p:168:TRP:O	24:p:172:THR:OG1	2.24	0.46
26:s:6:ILE:O	26:s:10:ILE:HG12	2.16	0.46
15:g:57:SER:O	29:w:353:TRP:HA	2.16	0.46
20:l:249:SER:HB2	20:l:340:PHE:CE2	2.49	0.46
20:l:249:SER:HB2	20:l:336:LYS:HG3	1.98	0.46
30:r:501:PEE:H34	30:r:501:PEE:H77	1.98	0.46
20:l:56:HIS:CD2	20:l:57:THR:HG23	2.51	0.45
20:l:503:GLU:O	20:l:507:THR:HG23	2.16	0.45
20:l:599:MET:HA	20:l:603:ASN:CB	2.46	0.45
31:s:401:CDL:H552	31:s:401:CDL:H202	1.97	0.45
20:l:289:ALA:HB1	20:l:418:LEU:CB	2.46	0.45
26:s:7:LEU:HA	26:s:10:ILE:HG12	1.98	0.45
10:b:91:THR:HG21	20:l:1:MET:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:U:102:PEE:H14	30:U:102:PEE:H20	1.82	0.45
17:i:278:MET:N	17:i:279:PRO:CD	2.79	0.45
20:l:66:TRP:HD1	30:l:704:PEE:O1P	1.99	0.45
20:l:175:ASN:ND2	36:l:806:HOH:O	2.31	0.45
31:r:504:CDL:H342	31:r:504:CDL:H372	1.66	0.45
27:u:137:LEU:HD12	27:u:138:PRO:HD2	1.99	0.45
31:V:202:CDL:H792	31:V:202:CDL:H761	1.53	0.45
31:i:401:CDL:H382	31:i:401:CDL:H411	1.76	0.45
20:l:229:LEU:HG	30:l:703:PEE:H37	1.99	0.45
20:l:264:TYR:CG	20:l:265:PRO:HD3	2.51	0.45
25:r:12:LEU:O	25:r:15:THR:HG22	2.16	0.45
31:r:504:CDL:H601	31:r:504:CDL:H772	1.97	0.45
29:w:344:ASN:O	29:w:347:VAL:CG2	2.65	0.45
18:j:87:MET:HG2	21:m:147:TYR:HB3	1.99	0.45
25:r:197:LEU:HB3	30:r:501:PEE:H29	1.99	0.45
26:s:123:SER:HB3	26:s:214:GLU:HG3	1.97	0.45
10:b:32:GLU:OE1	24:p:115:TYR:HA	2.17	0.45
17:i:108:LEU:HD11	17:i:191:THR:HG21	1.98	0.45
20:l:230:HIS:N	20:l:231:PRO:HD3	2.32	0.45
24:p:13:GLN:NE2	24:p:17:LEU:HD11	2.32	0.45
7:Y:50:LEU:HD13	7:Y:55:LEU:HD21	1.99	0.45
12:d:66:ARG:O	13:e:117:TRP:NE1	2.46	0.45
13:e:57:GLU:OE2	29:w:322:HIS:HB2	2.16	0.45
17:i:335:LEU:HD21	31:r:505:CDL:C39	2.37	0.45
33:j:202:PLX:H282	33:j:202:PLX:H251	1.71	0.45
20:l:568:PHE:HE2	30:l:701:PEE:O3	1.99	0.45
25:r:76:MET:SD	25:r:230:VAL:HB	2.57	0.45
26:s:209:SER:HB3	26:s:213:VAL:HA	1.98	0.45
18:j:80:GLN:HG3	26:s:318:SER:CB	2.47	0.45
20:l:229:LEU:HD21	30:l:703:PEE:H36	1.99	0.45
20:l:476:THR:CG2	36:l:833:HOH:O	2.65	0.45
23:o:59:VAL:HG23	25:r:423:ILE:HG23	1.99	0.45
25:r:98:MET:CE	31:r:505:CDL:H211	2.41	0.45
25:r:233:ALA:HA	25:r:320:GLY:HA2	1.98	0.45
20:l:524:ASN:HD21	24:p:78:GLN:HB2	1.82	0.45
2:S:12:MET:HG2	26:s:264:LEU:HD21	1.97	0.44
30:U:101:PEE:H55	30:U:101:PEE:H60	1.76	0.44
7:Y:44:TYR:CE2	8:Z:16:LEU:HD22	2.52	0.44
9:a:171:TYR:HB2	16:h:49:GLY:HA3	1.99	0.44
31:a:201:CDL:H342	31:a:201:CDL:H372	1.85	0.44
18:j:57:LEU:HD21	21:m:169:MET:SD	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:223:LYS:NZ	36:l:813:HOH:O	2.45	0.44
24:p:100:PRO:HD3	25:r:419:TYR:CE2	2.52	0.44
28:v:107:ARG:HE	28:v:107:ARG:HB3	1.53	0.44
28:v:112:LYS:C	28:v:112:LYS:CD	2.86	0.44
7:Y:81:LEU:HD23	20:l:488:MET:HE1	1.98	0.44
19:k:4:VAL:CG2	21:m:124:ASP:OD2	2.65	0.44
33:r:503:PLX:O1	33:r:503:PLX:H1C3	2.14	0.44
3:U:33:PRO:HA	26:s:310:MET:HG2	1.99	0.44
8:Z:18:ASP:O	8:Z:21:GLN:HG2	2.18	0.44
12:d:122:ARG:HA	12:d:122:ARG:HD3	1.83	0.44
13:e:70:ASN:HB3	13:e:73:SER:HB3	2.00	0.44
17:i:207:ILE:HD13	17:i:262:PRO:HD3	1.98	0.44
22:n:12:TRP:O	22:n:15:ILE:HG12	2.17	0.44
29:w:209:VAL:HG22	29:w:260:ALA:HB2	1.97	0.44
2:S:43:TYR:CZ	5:W:68:ARG:HG3	2.52	0.44
8:Z:29:LEU:HD11	8:Z:49:GLU:HB2	1.99	0.44
17:i:254:LEU:HD21	25:r:154:LEU:HD11	2.00	0.44
10:b:32:GLU:OE2	24:p:117:ASP:HB2	2.18	0.44
13:e:57:GLU:OE1	29:w:320:GLY:HA3	2.18	0.44
13:e:136:LEU:HD12	13:e:136:LEU:HA	1.71	0.44
17:i:253:GLY:O	17:i:260:PHE:HB2	2.17	0.44
17:i:264:TRP:CZ2	25:r:116:ILE:HG21	2.53	0.44
21:m:34:ILE:HD11	26:s:114:TYR:CE1	2.52	0.44
25:r:296:LEU:HD21	25:r:378:GLU:HG3	2.00	0.44
29:w:118:TYR:OH	35:w:401:ADP:O2'	2.35	0.44
30:U:101:PEE:H30	30:U:101:PEE:H35	1.45	0.44
31:V:202:CDL:H862	25:r:210:TYR:CE2	2.52	0.44
8:Z:31:THR:O	8:Z:34:GLU:HG3	2.18	0.44
18:j:105:GLU:HG3	18:j:110:GLY:HA3	2.00	0.44
20:l:49:VAL:HB	20:l:50:PRO:HD3	1.98	0.44
23:o:53:ASP:HA	23:o:54:PRO:HD3	1.79	0.44
31:a:201:CDL:H831	31:a:201:CDL:H871	1.98	0.44
10:b:28:LEU:HB3	10:b:32:GLU:HG3	1.99	0.44
17:i:110:PRO:HG2	20:l:594:THR:HG21	1.99	0.44
25:r:133:ILE:HD11	25:r:231:LEU:HD11	2.00	0.44
27:u:19:LYS:HE3	27:u:19:LYS:HB3	1.84	0.44
17:i:261:MET:HB2	17:i:337:LEU:HD12	1.99	0.44
6:X:74:LEU:HB3	6:X:154:VAL:HG21	2.00	0.43
11:c:184:TYR:HA	28:v:36:GLU:HA	2.00	0.43
15:g:1:MET:HA	17:i:196:TYR:O	2.18	0.43
15:g:33:LEU:HD23	15:g:33:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:30:TRP:HH2	19:k:37:MET:HE1	1.82	0.43
31:r:504:CDL:H142	31:r:504:CDL:H331	2.00	0.43
34:s:402:UQ:H152	34:s:402:UQ:H121	1.81	0.43
28:v:31:PHE:HE1	28:v:104:ARG:NE	2.14	0.43
5:W:142:TRP:HE1	21:m:46:ASN:ND2	2.16	0.43
6:X:83:VAL:HG21	6:X:145:VAL:HG22	1.99	0.43
12:d:135:VAL:HG22	13:e:136:LEU:HB3	1.99	0.43
36:j:332:HOH:O	21:m:76:THR:HG21	2.18	0.43
31:l:702:CDL:H352	31:l:702:CDL:H382	1.76	0.43
25:r:108:MET:HE3	25:r:121:LEU:HD22	2.01	0.43
30:r:501:PEE:H62	30:r:501:PEE:H68	1.84	0.43
28:v:92:HIS:O	28:v:96:VAL:HG13	2.18	0.43
28:v:111:ARG:HA	28:v:114:ARG:NH1	2.33	0.43
20:l:124:PHE:CE1	20:l:252:MET:HB2	2.52	0.43
20:l:557:TRP:O	20:l:561:ILE:HG12	2.18	0.43
31:r:505:CDL:C78	31:r:505:CDL:C38	2.96	0.43
31:r:505:CDL:H352	31:r:505:CDL:H381	1.71	0.43
2:S:57:VAL:HB	2:S:59:ARG:NH2	2.34	0.43
17:i:258:SER:HB3	17:i:336:VAL:HG12	2.01	0.43
17:i:284:MET:HE1	25:r:155:ALA:HA	2.00	0.43
20:l:7:LEU:HD22	20:l:46:LEU:HD11	2.01	0.43
10:b:32:GLU:O	10:b:34:VAL:N	2.50	0.43
18:j:16:LEU:HD13	33:j:202:PLX:H212	2.01	0.43
25:r:253:LEU:CD1	25:r:256:TYR:CE1	2.98	0.43
26:s:24:GLU:OE2	26:s:274:ARG:NH1	2.51	0.43
2:S:19:PRO:HB3	26:s:9:LEU:HD12	2.00	0.43
30:W:201:PEE:H59	26:s:108:MET:HE1	1.99	0.43
7:Y:44:TYR:O	7:Y:45:ARG:HB2	2.18	0.43
9:a:133:TYR:OH	12:d:87:GLU:HG2	2.19	0.43
17:i:172:GLN:HB2	17:i:178:ILE:HG13	2.00	0.43
17:i:264:TRP:HZ2	25:r:116:ILE:HG21	1.82	0.43
29:w:223:ASN:O	29:w:227:MET:HG2	2.19	0.43
6:X:94:ASP:HA	6:X:95:PRO:HD3	1.90	0.43
12:d:127:LYS:HA	12:d:130:GLU:HG3	2.01	0.43
20:l:534:HIS:HD2	30:l:703:PEE:O2	2.02	0.43
5:W:58:ARG:HA	5:W:58:ARG:HD3	1.80	0.43
12:d:23:GLN:HB2	28:v:72:ASP:HB3	2.00	0.43
17:i:204:ASN:OD1	36:i:505:HOH:O	2.21	0.43
19:k:28:SER:HB3	21:m:23:LYS:HG2	2.00	0.43
20:l:123:LEU:HB2	20:l:150:MET:HE2	2.01	0.43
20:l:173:LEU:C	20:l:173:LEU:HD23	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:244:GLY:HA2	36:s:549:HOH:O	2.18	0.43
26:s:277:TYR:HA	26:s:278:PRO:HD3	1.81	0.43
20:l:389:PHE:O	20:l:393:ASP:HB2	2.19	0.43
5:W:122:GLY:HA2	21:m:125:TRP:CZ3	2.53	0.43
11:c:67:ASP:O	23:o:81:ARG:NH2	2.52	0.43
25:r:331:ASN:HB3	36:r:631:HOH:O	2.18	0.43
26:s:101:GLY:O	26:s:105:MET:HG2	2.18	0.43
2:S:57:VAL:HG21	2:S:62:VAL:HG21	2.01	0.42
9:a:176:LYS:HD2	16:h:45:HIS:CD2	2.54	0.42
11:c:179:GLU:OE2	11:c:179:GLU:N	2.52	0.42
12:d:160:LYS:NZ	15:g:114:ILE:O	2.51	0.42
20:l:435:PRO:HB3	20:l:437:PHE:CZ	2.53	0.42
25:r:8:THR:O	25:r:11:LEU:HB2	2.19	0.42
31:r:504:CDL:H611	31:r:504:CDL:H581	1.67	0.42
26:s:314:ILE:HA	26:s:315:PRO:HD3	1.70	0.42
31:V:201:CDL:H142	31:V:201:CDL:H112	1.83	0.42
10:b:101:LYS:HA	10:b:102:PRO:HD3	1.67	0.42
17:i:54:GLU:HG3	19:k:93:LEU:HB3	2.00	0.42
31:l:702:CDL:H341	31:l:702:CDL:H311	1.40	0.42
25:r:139:GLN:O	25:r:142:ARG:HG2	2.19	0.42
25:r:455:LEU:HD23	25:r:455:LEU:HA	1.86	0.42
31:r:505:CDL:H412	31:r:505:CDL:H472	2.01	0.42
27:u:83:THR:HA	27:u:86:TRP:CD1	2.54	0.42
4:V:113:ALA:HB1	30:l:701:PEE:H53	1.98	0.42
15:g:52:ARG:HD3	17:i:318:GLU:OE1	2.20	0.42
17:i:42:PRO:CG	21:m:167:VAL:HG13	2.47	0.42
20:l:10:THR:O	20:l:14:ILE:HG23	2.19	0.42
20:l:63:ILE:O	20:l:79:SER:HA	2.19	0.42
20:l:387:THR:HA	20:l:465:GLY:HA3	2.01	0.42
26:s:77:LEU:HD23	26:s:115:SER:HB3	2.01	0.42
29:w:105:ASP:OD2	29:w:107:GLN:HG2	2.19	0.42
31:V:202:CDL:H732	23:o:87:SER:HB3	2.02	0.42
17:i:42:PRO:HG2	21:m:167:VAL:HG22	2.01	0.42
21:m:2:THR:C	21:m:4:TYR:H	2.27	0.42
29:w:246:LEU:HB2	29:w:247:PRO:HD3	2.02	0.42
12:d:135:VAL:HG21	13:e:136:LEU:HD23	2.02	0.42
15:g:13:LEU:HA	33:g:201:PLX:H32	2.02	0.42
25:r:6:ILE:N	25:r:7:PRO:CD	2.83	0.42
25:r:67:VAL:HG12	33:r:503:PLX:H381	2.01	0.42
25:r:290:SER:HA	25:r:319:HIS:HE2	1.84	0.42
25:r:427:LYS:CE	36:r:625:HOH:O	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:442:LEU:N	25:r:443:PRO:CD	2.82	0.42
28:v:61:HIS:CD2	28:v:61:HIS:H	2.36	0.42
12:d:80:LYS:HD3	12:d:80:LYS:HA	1.89	0.42
15:g:55:VAL:HG21	31:r:505:CDL:HB4	2.02	0.42
16:h:20:ILE:HB	16:h:37:GLU:OE1	2.19	0.42
17:i:280:THR:O	17:i:284:MET:HG2	2.20	0.42
20:l:529:TYR:HB3	20:l:530:PRO:HD3	2.00	0.42
28:v:25:PHE:CE2	28:v:108:LEU:HB3	2.55	0.42
30:U:101:PEE:H39	26:s:302:MET:HE1	2.01	0.42
4:V:141:VAL:C	9:a:161:ARG:HH21	2.28	0.42
12:d:62:TYR:CD1	12:d:62:TYR:N	2.85	0.42
14:f:47:THR:HG23	15:g:65:LEU:HD22	2.00	0.42
17:i:254:LEU:HA	17:i:255:PRO:HD3	1.87	0.42
18:j:16:LEU:HD23	18:j:16:LEU:HA	1.93	0.42
20:l:42:TYR:HA	20:l:45:THR:HG22	2.02	0.42
33:r:502:PLX:H22	33:r:502:PLX:H1C3	1.75	0.42
31:V:202:CDL:H872	31:V:202:CDL:H841	1.69	0.42
6:X:105:MET:HE3	6:X:139:MET:HE1	2.01	0.42
17:i:326:LEU:N	17:i:327:PRO:CD	2.83	0.42
25:r:76:MET:HE1	36:r:662:HOH:O	2.20	0.42
31:r:504:CDL:H251	31:r:504:CDL:H222	1.91	0.42
26:s:2:PHE:CE2	26:s:6:ILE:HD11	2.54	0.42
26:s:202:GLU:HB2	36:s:514:HOH:O	2.18	0.42
29:w:110:GLY:HA2	29:w:134:TRP:CD2	2.55	0.42
7:Y:65:MET:SD	20:l:375:ILE:HG12	2.59	0.42
10:b:32:GLU:HB2	10:b:33:PRO:HD3	2.02	0.42
17:i:30:TRP:CZ2	19:k:37:MET:HE1	2.54	0.42
18:j:18:VAL:HG12	30:j:201:PEE:H16	2.01	0.42
24:p:108:HIS:CD2	24:p:110:SER:H	2.37	0.42
26:s:308:PRO:HA	26:s:313:SER:OG	2.19	0.42
17:i:139:LEU:HD23	17:i:139:LEU:HA	1.89	0.42
18:j:79:SER:HA	18:j:87:MET:HE2	2.01	0.42
19:k:33:LEU:HD23	19:k:36:MET:HE3	2.02	0.42
30:l:703:PEE:C11	30:l:703:PEE:H7	2.50	0.42
25:r:118:PHE:O	25:r:122:PHE:HB3	2.20	0.42
25:r:139:GLN:HB2	25:r:222:GLU:OE1	2.20	0.42
27:u:167:LEU:HD12	27:u:167:LEU:HA	1.84	0.42
6:X:119:ILE:HG12	6:X:119:ILE:H	1.46	0.41
12:d:3:ASP:OD1	12:d:3:ASP:N	2.51	0.41
20:l:249:SER:O	20:l:332:HIS:HE1	2.02	0.41
20:l:572:LYS:HD3	20:l:572:LYS:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:285:LEU:C	25:r:285:LEU:HD23	2.45	0.41
31:r:505:CDL:H221	31:r:505:CDL:H401	2.01	0.41
29:w:66:ILE:O	29:w:214:ILE:HD12	2.19	0.41
30:U:101:PEE:H56	30:U:101:PEE:H51	1.88	0.41
10:b:103:ARG:HH12	28:v:67:LEU:CD1	2.30	0.41
11:c:58:ARG:NE	23:o:35:GLU:OE1	2.50	0.41
13:e:74:HIS:HD2	25:r:431:THR:OG1	2.03	0.41
20:l:69:MET:HB3	25:r:451:PRO:HG2	2.02	0.41
30:l:704:PEE:C1	30:l:704:PEE:H9	2.50	0.41
21:m:126:VAL:HG23	21:m:127:ILE:HG23	2.02	0.41
28:v:112:LYS:HD2	28:v:112:LYS:O	2.20	0.41
29:w:100:ASP:C	29:w:102:LYS:H	2.28	0.41
6:X:75:THR:O	6:X:76:LEU:C	2.63	0.41
13:e:92:PHE:O	13:e:96:SER:HB2	2.20	0.41
16:h:36:PHE:CD1	16:h:62:ASP:HB3	2.55	0.41
20:l:294:THR:HG22	31:l:702:CDL:HB62	2.02	0.41
23:o:59:VAL:CG2	25:r:423:ILE:CG2	2.94	0.41
33:r:502:PLX:H101	33:r:502:PLX:H72	1.61	0.41
7:Y:38:VAL:HG11	20:l:446:ASN:HB3	2.01	0.41
17:i:243:LEU:HD22	17:i:330:ILE:HG21	2.02	0.41
20:l:409:LEU:O	20:l:413:LEU:HG	2.19	0.41
31:r:505:CDL:H781	31:r:505:CDL:C38	2.45	0.41
26:s:2:PHE:O	26:s:6:ILE:HG13	2.20	0.41
26:s:194:ASN:O	26:s:199:ASP:HB3	2.20	0.41
5:W:34:SER:O	5:W:38:VAL:HG23	2.21	0.41
12:d:115:GLN:HG2	20:l:62:ILE:HG12	2.02	0.41
13:e:73:SER:C	13:e:75:GLY:H	2.27	0.41
14:f:37:GLY:O	29:w:351:TRP:HD1	2.04	0.41
15:g:85:TYR:CZ	17:i:344:SER:HB3	2.56	0.41
30:i:402:PEE:H14	30:i:402:PEE:H1	1.84	0.41
20:l:295:GLN:HB2	20:l:301:ILE:HG12	2.02	0.41
24:p:174:PRO:O	24:p:175:ARG:HB2	2.20	0.41
25:r:126:LEU:HD21	25:r:153:THR:HG21	2.01	0.41
9:a:184:LYS:C	9:a:186:THR:H	2.29	0.41
22:n:47:ARG:NH1	22:n:56:THR:HG22	2.35	0.41
5:W:68:ARG:O	5:W:72:MET:HG3	2.21	0.41
10:b:97:VAL:HG22	20:l:63:ILE:HG23	2.01	0.41
11:c:56:ASN:OD1	23:o:42:ARG:NH2	2.49	0.41
11:c:183:HIS:HD2	28:v:58:TYR:OH	2.04	0.41
18:j:11:VAL:CG2	30:j:201:PEE:H42	2.50	0.41
20:l:331:MET:SD	20:l:387:THR:HG23	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:116:ILE:HD13	25:r:116:ILE:HA	1.80	0.41
26:s:24:GLU:HG3	26:s:271:LEU:HD22	2.02	0.41
29:w:245:PHE:O	29:w:249:MET:HG2	2.21	0.41
13:e:138:GLU:OE1	13:e:138:GLU:N	2.54	0.41
20:l:48:LEU:HD23	20:l:48:LEU:HA	1.86	0.41
20:l:66:TRP:CE3	30:l:704:PEE:H27	2.55	0.41
20:l:180:ILE:HD12	30:l:703:PEE:H79	2.03	0.41
21:m:153:LEU:O	21:m:157:THR:HG23	2.20	0.41
1:Q:37:TRP:CE3	25:r:140:THR:HA	2.56	0.41
6:X:136:GLU:OE2	24:p:14:GLN:HG2	2.21	0.41
33:j:203:PLX:H132	33:j:203:PLX:H161	1.57	0.41
19:k:87:THR:CG2	19:k:89:TYR:CD1	3.03	0.41
20:l:128:MET:HG2	20:l:251:THR:HG22	2.03	0.41
20:l:392:LYS:O	20:l:396:ILE:HG12	2.20	0.41
20:l:491:LEU:O	20:l:495:ILE:HG12	2.21	0.41
22:n:54:GLU:HG2	22:n:55:VAL:N	2.36	0.41
25:r:186:LEU:O	25:r:252:PRO:HD2	2.20	0.41
25:r:331:ASN:O	25:r:335:GLU:HG3	2.21	0.41
31:r:505:CDL:H412	31:r:505:CDL:C45	2.42	0.41
26:s:200:LEU:CD1	26:s:282:TYR:HB2	2.48	0.41
29:w:45:LEU:O	29:w:45:LEU:HD12	2.20	0.41
4:V:17:GLU:OE2	4:V:20:ARG:NH1	2.47	0.41
6:X:155:TYR:CD1	6:X:155:TYR:N	2.89	0.41
20:l:190:LEU:CD2	25:r:383:THR:HG21	2.51	0.41
20:l:252:MET:HE2	20:l:252:MET:HB3	1.92	0.41
25:r:66:LEU:HD22	25:r:107:ILE:HG23	2.02	0.41
25:r:186:LEU:HD23	25:r:186:LEU:HA	1.89	0.41
26:s:24:GLU:HA	26:s:271:LEU:HD13	2.03	0.41
31:u:201:CDL:C54	31:u:201:CDL:C58	2.99	0.41
29:w:256:LEU:HD11	29:w:276:LEU:HD11	2.01	0.41
15:g:101:GLU:H	15:g:101:GLU:CD	2.29	0.40
17:i:245:MET:HE3	17:i:245:MET:HB3	1.87	0.40
20:l:37:LYS:HE2	20:l:105:MET:HE1	2.03	0.40
30:l:704:PEE:H60	30:l:704:PEE:H55	1.80	0.40
21:m:17:PHE:HA	21:m:20:PHE:CE2	2.55	0.40
25:r:4:ILE:HD12	25:r:41:LEU:HD11	2.02	0.40
25:r:339:SER:HB3	25:r:344:LEU:HD22	2.03	0.40
26:s:66:SER:HB2	26:s:122:ALA:O	2.21	0.40
14:f:39:PRO:HD3	29:w:351:TRP:CG	2.56	0.40
33:g:201:PLX:H71	33:g:201:PLX:H102	1.56	0.40
17:i:31:ILE:HG12	19:k:66:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:98:MET:HE2	17:i:98:MET:HB2	1.94	0.40
18:j:83:ASN:OD1	18:j:83:ASN:N	2.49	0.40
20:l:250:SER:CB	20:l:333:ALA:HA	2.50	0.40
20:l:331:MET:N	20:l:331:MET:CE	2.85	0.40
20:l:600:THR:HG22	20:l:601:LEU:CD2	2.50	0.40
25:r:401:MET:HE2	25:r:401:MET:HB3	1.95	0.40
29:w:254:GLU:OE2	29:w:276:LEU:HB3	2.21	0.40
1:Q:53:TYR:CD1	20:l:571:MET:HE3	2.56	0.40
10:b:120:MET:HE3	28:v:61:HIS:HB2	2.03	0.40
13:e:74:HIS:HB2	13:e:83:ASP:OD2	2.21	0.40
30:j:201:PEE:C37	33:j:202:PLX:H131	2.51	0.40
20:l:323:HIS:NE2	20:l:475:MET:HG2	2.37	0.40
25:r:202:ALA:O	25:r:205:VAL:HG12	2.21	0.40
6:X:76:LEU:N	6:X:156:GLU:O	2.52	0.40
9:a:112:TYR:CD1	12:d:64:TYR:O	2.75	0.40
15:g:92:MET:HE2	15:g:92:MET:HB3	1.91	0.40
17:i:79:LEU:HD21	19:k:1:MET:SD	2.62	0.40
20:l:328:HIS:CG	20:l:391:SER:OG	2.74	0.40
26:s:306:SER:O	26:s:310:MET:HG3	2.21	0.40
12:d:77:CYS:SG	12:d:84:CYS:HB3	2.61	0.40
17:i:70:LEU:HD11	17:i:98:MET:SD	2.62	0.40
17:i:335:LEU:CD2	31:r:505:CDL:H391	2.40	0.40
19:k:53:PHE:HA	36:k:125:HOH:O	2.21	0.40
20:l:66:TRP:HZ3	30:l:704:PEE:H32	1.84	0.40
24:p:44:MET:HB2	24:p:44:MET:HE2	1.65	0.40
24:p:132:SER:O	24:p:136:GLU:HG3	2.22	0.40
28:v:17:PRO:HG2	28:v:102:PHE:CZ	2.56	0.40
29:w:139:ARG:NH2	35:w:401:ADP:N7	2.59	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	Q	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
2	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
3	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
4	V	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
5	W	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
6	X	86/88 (98%)	81 (94%)	4 (5%)	1 (1%)	10	23
7	Y	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
8	Z	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
9	a	136/138 (99%)	132 (97%)	4 (3%)	0	100	100
10	b	94/126 (75%)	86 (92%)	8 (8%)	0	100	100
11	c	154/156 (99%)	144 (94%)	10 (6%)	0	100	100
12	d	173/175 (99%)	169 (98%)	4 (2%)	0	100	100
13	e	102/104 (98%)	98 (96%)	4 (4%)	0	100	100
14	f	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
15	g	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
16	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
17	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
18	j	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	14	30
19	k	96/98 (98%)	95 (99%)	1 (1%)	0	100	100
20	l	604/606 (100%)	578 (96%)	25 (4%)	1 (0%)	43	66
21	m	173/175 (99%)	160 (92%)	13 (8%)	0	100	100
22	n	54/56 (96%)	54 (100%)	0	0	100	100
23	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
24	p	176/178 (99%)	166 (94%)	9 (5%)	1 (1%)	21	42
25	r	457/459 (100%)	452 (99%)	4 (1%)	1 (0%)	43	66
26	s	316/318 (99%)	309 (98%)	7 (2%)	0	100	100
27	u	169/171 (99%)	163 (96%)	3 (2%)	3 (2%)	6	14
28	v	122/125 (98%)	115 (94%)	7 (6%)	0	100	100
29	w	318/320 (99%)	300 (94%)	18 (6%)	0	100	100
All	All	4667/4756 (98%)	4480 (96%)	179 (4%)	8 (0%)	44	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	X	136	GLU
20	l	72	GLN
27	u	168	PHE
18	j	40	GLY
27	u	152	PRO
24	p	174	PRO
25	r	39	LEU
27	u	153	GLU

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	Q	38/38 (100%)	37 (97%)	1 (3%)	40	68
2	S	57/58 (98%)	57 (100%)	0	100	100
3	U	69/69 (100%)	69 (100%)	0	100	100
4	V	101/101 (100%)	100 (99%)	1 (1%)	68	86
5	W	99/99 (100%)	99 (100%)	0	100	100
6	X	74/81 (91%)	58 (78%)	16 (22%)	1	2
7	Y	62/62 (100%)	62 (100%)	0	100	100
8	Z	55/62 (89%)	55 (100%)	0	100	100
9	a	121/121 (100%)	120 (99%)	1 (1%)	73	88
10	b	90/119 (76%)	90 (100%)	0	100	100
11	c	141/141 (100%)	141 (100%)	0	100	100
12	d	155/155 (100%)	152 (98%)	3 (2%)	50	75
13	e	96/96 (100%)	95 (99%)	1 (1%)	68	86
14	f	35/45 (78%)	35 (100%)	0	100	100
15	g	108/109 (99%)	108 (100%)	0	100	100
16	h	93/93 (100%)	93 (100%)	0	100	100
17	i	311/311 (100%)	309 (99%)	2 (1%)	78	91
18	j	100/100 (100%)	99 (99%)	1 (1%)	68	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	k	85/85 (100%)	84 (99%)	1 (1%)	63	83
20	l	536/540 (99%)	532 (99%)	4 (1%)	76	89
21	m	126/141 (89%)	125 (99%)	1 (1%)	73	88
22	n	53/53 (100%)	53 (100%)	0	100	100
23	o	113/113 (100%)	113 (100%)	0	100	100
24	p	159/159 (100%)	159 (100%)	0	100	100
25	r	410/410 (100%)	408 (100%)	2 (0%)	81	92
26	s	275/275 (100%)	271 (98%)	4 (2%)	57	80
27	u	153/153 (100%)	153 (100%)	0	100	100
28	v	104/111 (94%)	103 (99%)	1 (1%)	68	86
29	w	283/283 (100%)	282 (100%)	1 (0%)	84	93
All	All	4102/4183 (98%)	4062 (99%)	40 (1%)	65	86

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	56	LYS
4	V	95	CYS
6	X	76	LEU
6	X	77	GLU
6	X	83	VAL
6	X	86	VAL
6	X	88	LYS
6	X	101	ASN
6	X	106	LYS
6	X	119	ILE
6	X	123	GLU
6	X	124	ASP
6	X	125	GLU
6	X	129	GLU
6	X	136	GLU
6	X	137	LYS
6	X	155	TYR
6	X	156	GLU
9	a	185	THR
12	d	62	TYR
12	d	127	LYS
12	d	134	GLN

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Mol	Chain	Res	Type
13	e	136	LEU
17	i	68	MET
17	i	250	SER
18	j	90	MET
19	k	91	GLN
20	l	71	LEU
20	l	119	LYS
20	l	197	ASP
20	l	600	THR
21	m	78	MET
25	r	114	GLU
25	r	140	THR
26	s	54	LYS
26	s	126	LYS
26	s	202	GLU
26	s	254	LEU
28	v	107	ARG
29	w	347	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	38	GLN
1	Q	46	GLN
2	S	27	HIS
2	S	31	ASN
3	U	40	ASN
4	V	134	GLN
5	W	61	GLN
5	W	76	GLN
5	W	112	HIS
7	Y	49	GLN
7	Y	54	GLN
7	Y	57	GLN
8	Z	21	GLN
10	b	83	HIS
10	b	89	HIS
11	c	84	GLN
11	c	160	GLN
11	c	183	HIS
12	d	56	HIS
12	d	91	GLN

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Mol	Chain	Res	Type
12	d	107	GLN
12	d	134	GLN
12	d	159	GLN
13	e	74	HIS
13	e	86	ASN
13	e	132	ASN
13	e	145	ASN
15	g	63	GLN
15	g	90	HIS
15	g	99	HIS
16	h	21	GLN
16	h	45	HIS
17	i	36	ASN
17	i	47	ASN
17	i	63	GLN
17	i	83	GLN
17	i	91	ASN
17	i	134	GLN
17	i	172	GLN
17	i	174	GLN
17	i	204	ASN
17	i	221	HIS
17	i	232	HIS
17	i	273	ASN
17	i	319	HIS
18	j	26	GLN
18	j	28	ASN
19	k	50	ASN
19	k	92	ASN
20	l	2	ASN
20	l	56	HIS
20	l	59	GLN
20	l	72	GLN
20	l	135	ASN
20	l	165	ASN
20	l	170	GLN
20	l	199	GLN
20	l	226	GLN
20	l	230	HIS
20	l	328	HIS
20	l	354	GLN
20	l	446	ASN

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Mol	Chain	Res	Type
20	l	524	ASN
20	l	534	HIS
20	l	541	ASN
20	l	579	ASN
21	m	46	ASN
21	m	86	ASN
23	o	50	GLN
23	o	79	ASN
24	p	26	HIS
24	p	108	HIS
24	p	139	GLN
24	p	169	HIS
25	r	43	ASN
25	r	51	ASN
25	r	83	HIS
25	r	139	GLN
25	r	251	ASN
25	r	255	ASN
25	r	440	HIS
26	s	5	ASN
26	s	47	GLN
26	s	171	HIS
26	s	194	ASN
26	s	247	HIS
26	s	250	HIS
27	u	16	GLN
27	u	65	GLN
28	v	54	GLN
28	v	61	HIS
28	v	92	HIS
29	w	37	GLN
29	w	107	GLN
29	w	127	ASN
29	w	132	GLN
29	w	186	HIS
29	w	202	HIS
29	w	219	GLN
29	w	235	GLN
29	w	239	ASN
29	w	286	GLN
29	w	292	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	CDL	i	401	-	86,86,99	1.18	8 (9%)	92,98,111	0.91	4 (4%)
30	PEE	i	402	-	46,46,50	1.22	6 (13%)	49,51,55	1.03	2 (4%)
32	8Q1	X	201	-	32,34,34	2.27	7 (21%)	39,43,43	1.66	10 (25%)
34	UQ	s	402	-	38,38,63	3.64	10 (26%)	48,49,79	2.77	17 (35%)
33	PLX	j	203	-	51,51,51	1.18	4 (7%)	53,59,59	0.65	1 (1%)
30	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
30	PEE	U	102	-	50,50,50	1.18	6 (12%)	53,55,55	0.96	2 (3%)
33	PLX	a	202	-	51,51,51	1.18	4 (7%)	53,59,59	0.64	1 (1%)
30	PEE	U	101	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
31	CDL	r	504	-	98,98,99	1.10	9 (9%)	104,110,111	0.95	5 (4%)
33	PLX	r	503	-	51,51,51	0.61	0	53,59,59	0.68	0
31	CDL	V	201	-	93,93,99	1.13	9 (9%)	99,105,111	0.87	4 (4%)
31	CDL	s	401	-	88,88,99	1.11	6 (6%)	94,100,111	1.01	5 (5%)
30	PEE	j	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.02	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PLX	j	202	-	51,51,51	1.19	2 (3%)	53,59,59	0.64	2 (3%)
31	CDL	a	201	-	99,99,99	0.92	4 (4%)	105,111,111	1.08	7 (6%)
33	PLX	r	502	-	51,51,51	1.16	4 (7%)	53,59,59	0.69	1 (1%)
33	PLX	g	201	-	51,51,51	1.19	3 (5%)	53,59,59	0.63	1 (1%)
30	PEE	l	704	-	45,45,50	1.25	6 (13%)	48,50,55	1.02	2 (4%)
30	PEE	l	703	-	50,50,50	1.17	6 (12%)	53,55,55	0.97	2 (3%)
35	ADP	w	401	-	28,29,29	3.16	9 (32%)	43,45,45	1.90	9 (20%)
31	CDL	u	201	-	54,54,99	1.25	4 (7%)	60,66,111	1.23	5 (8%)
30	PEE	W	201	-	40,40,50	1.16	5 (12%)	43,45,55	1.04	2 (4%)
31	CDL	V	202	-	99,99,99	1.09	8 (8%)	105,111,111	0.90	4 (3%)
30	PEE	l	701	-	39,39,50	1.34	6 (15%)	42,44,55	1.10	3 (7%)
31	CDL	m	201	-	99,99,99	1.09	7 (7%)	105,111,111	0.92	6 (5%)
31	CDL	r	505	-	99,99,99	1.11	8 (8%)	105,111,111	0.83	4 (3%)
31	CDL	l	702	-	93,93,99	0.94	4 (4%)	99,105,111	1.15	7 (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
31	CDL	i	401	-	-	47/97/97/110	-
30	PEE	i	402	-	-	15/50/50/54	-
32	8Q1	X	201	-	-	12/41/41/41	-
34	UQ	s	402	-	-	13/33/57/87	0/1/1/1
33	PLX	j	203	-	-	29/55/55/55	-
30	PEE	r	501	-	-	30/54/54/54	-
30	PEE	U	102	-	-	25/54/54/54	-
33	PLX	a	202	-	-	26/55/55/55	-
30	PEE	U	101	-	-	29/54/54/54	-
31	CDL	r	504	-	-	62/109/109/110	-
33	PLX	r	503	-	-	15/55/55/55	-
31	CDL	V	201	-	-	58/104/104/110	-
31	CDL	s	401	-	-	54/99/99/110	-
30	PEE	j	201	-	-	17/44/44/54	-
33	PLX	j	202	-	-	33/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CDL	a	201	-	-	41/110/110/110	-
33	PLX	r	502	-	-	32/55/55/55	-
33	PLX	g	201	-	-	32/55/55/55	-
30	PEE	l	704	-	-	20/49/49/54	-
30	PEE	l	703	-	-	23/54/54/54	-
35	ADP	w	401	-	-	2/16/32/32	0/3/3/3
31	CDL	u	201	-	-	26/65/65/110	-
30	PEE	W	201	-	-	21/44/44/54	-
31	CDL	V	202	-	-	67/110/110/110	-
30	PEE	l	701	-	-	25/43/43/54	-
31	CDL	m	201	-	-	63/110/110/110	-
31	CDL	r	505	-	-	60/110/110/110	-
31	CDL	l	702	-	-	38/104/104/110	-

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	402	UQ	C18-C19	9.99	1.56	1.33
34	s	402	UQ	C13-C14	9.65	1.55	1.33
34	s	402	UQ	C23-C24	9.45	1.54	1.33
34	s	402	UQ	C8-C9	9.32	1.54	1.33
35	w	401	ADP	C3'-C4'	-9.00	1.30	1.53
32	X	201	8Q1	P24-O27	7.80	1.84	1.60
35	w	401	ADP	O4'-C4'	7.65	1.62	1.45
34	s	402	UQ	C28-C29	7.36	1.54	1.32
35	w	401	ADP	PA-O3A	6.42	1.66	1.59
35	w	401	ADP	C6-N6	5.44	1.48	1.34
32	X	201	8Q1	C28-C29	5.41	1.61	1.52
35	w	401	ADP	O4'-C1'	-4.55	1.31	1.42
31	u	201	CDL	OA8-CA7	4.32	1.45	1.33
31	a	201	CDL	OB8-CB7	4.23	1.45	1.33
31	l	702	CDL	OA8-CA7	4.22	1.45	1.33
31	l	702	CDL	OB8-CB7	4.21	1.45	1.33
31	u	201	CDL	OB8-CB7	4.19	1.45	1.33
31	a	201	CDL	OA8-CA7	4.17	1.45	1.33
31	u	201	CDL	OB6-CB5	4.15	1.46	1.34
31	u	201	CDL	OA6-CA5	4.12	1.45	1.34
31	a	201	CDL	OB6-CB5	4.12	1.45	1.34
31	l	702	CDL	OB6-CB5	4.06	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	201	8Q1	C1-S44	4.05	1.85	1.76
31	a	201	CDL	OA6-CA5	4.05	1.45	1.34
31	l	702	CDL	OA6-CA5	3.99	1.45	1.34
30	r	501	PEE	C18-C19	3.85	1.53	1.31
30	l	704	PEE	C18-C19	3.84	1.53	1.31
30	j	201	PEE	C18-C19	3.84	1.53	1.31
30	l	701	PEE	C18-C19	3.83	1.53	1.31
30	l	703	PEE	C18-C19	3.82	1.53	1.31
30	U	101	PEE	C18-C19	3.82	1.53	1.31
30	U	102	PEE	C18-C19	3.82	1.53	1.31
30	W	201	PEE	C18-C19	3.81	1.53	1.31
30	i	402	PEE	C18-C19	3.76	1.53	1.31
30	l	704	PEE	C39-C38	3.75	1.53	1.31
30	U	102	PEE	C39-C38	3.74	1.52	1.31
30	r	501	PEE	C39-C38	3.74	1.52	1.31
30	i	402	PEE	C39-C38	3.73	1.52	1.31
30	l	701	PEE	C39-C38	3.72	1.52	1.31
30	U	101	PEE	C39-C38	3.72	1.52	1.31
30	l	703	PEE	C39-C38	3.70	1.52	1.31
31	i	401	CDL	OA8-CA7	3.51	1.43	1.33
31	V	201	CDL	OA8-CA7	3.49	1.43	1.33
31	r	505	CDL	OA8-CA7	3.40	1.43	1.33
31	V	202	CDL	OA8-CA7	3.36	1.43	1.33
35	w	401	ADP	C8-N9	-3.36	1.31	1.37
31	r	504	CDL	OA8-CA7	3.33	1.43	1.33
32	X	201	8Q1	O27-C28	-3.30	1.33	1.43
31	m	201	CDL	OA8-CA7	3.28	1.42	1.33
31	s	401	CDL	OA8-CA7	3.25	1.42	1.33
32	X	201	8Q1	C34-N36	3.24	1.41	1.33
31	V	201	CDL	OA6-CA5	3.22	1.43	1.34
32	X	201	8Q1	C6-C1	3.20	1.54	1.50
31	m	201	CDL	OA6-CA5	3.16	1.43	1.34
35	w	401	ADP	O2'-C2'	-3.07	1.35	1.43
31	i	401	CDL	OB6-CB5	3.07	1.43	1.34
31	r	505	CDL	OB6-CB5	3.04	1.42	1.34
31	i	401	CDL	OA6-CA5	3.03	1.42	1.34
31	i	401	CDL	OB8-CB7	3.01	1.42	1.33
35	w	401	ADP	O3'-C3'	3.00	1.50	1.43
31	r	505	CDL	OB8-CB7	2.99	1.42	1.33
33	g	201	PLX	O6-C4	-2.98	1.40	1.44
31	V	201	CDL	OB8-CB7	2.96	1.42	1.33
31	V	201	CDL	OB6-CB5	2.95	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	202	CDL	OA6-CA5	2.95	1.42	1.34
31	s	401	CDL	OA6-CA5	2.95	1.42	1.34
31	r	505	CDL	OA6-CA5	2.94	1.42	1.34
31	r	504	CDL	OB6-CB5	2.92	1.42	1.34
33	j	203	PLX	O6-C4	-2.88	1.40	1.44
31	r	504	CDL	OB8-CB7	2.88	1.41	1.33
32	X	201	8Q1	C39-N41	2.85	1.40	1.33
31	V	202	CDL	OB6-CB5	2.83	1.42	1.34
31	s	401	CDL	OB6-CB5	2.82	1.42	1.34
31	m	201	CDL	OB6-CB5	2.78	1.42	1.34
31	m	201	CDL	OB8-CB7	2.76	1.41	1.33
34	s	402	UQ	C6-C1	2.75	1.54	1.46
31	r	504	CDL	OA6-CA5	2.74	1.42	1.34
31	V	202	CDL	OA6-CA4	-2.72	1.40	1.46
31	V	202	CDL	OB8-CB7	2.68	1.41	1.33
31	s	401	CDL	OB8-CB7	2.66	1.41	1.33
33	a	202	PLX	O6-C4	-2.66	1.41	1.44
30	i	402	PEE	O2-C2	-2.64	1.40	1.46
31	r	504	CDL	OA6-CA4	-2.63	1.40	1.46
33	j	202	PLX	O6-C4	-2.61	1.41	1.44
30	W	201	PEE	O2-C2	-2.59	1.40	1.46
30	U	102	PEE	O2-C2	-2.58	1.40	1.46
30	U	101	PEE	O2-C2	-2.56	1.40	1.46
31	r	504	CDL	OB6-CB4	-2.56	1.40	1.46
31	r	505	CDL	OA6-CA4	-2.55	1.40	1.46
30	l	704	PEE	O2-C2	-2.55	1.40	1.46
31	s	401	CDL	OB6-CB4	-2.54	1.40	1.46
31	i	401	CDL	OA6-CA4	-2.53	1.40	1.46
30	l	701	PEE	O2-C2	-2.53	1.40	1.46
30	j	201	PEE	O2-C2	-2.53	1.40	1.46
31	s	401	CDL	OA6-CA4	-2.51	1.40	1.46
31	V	202	CDL	OB6-CB4	-2.51	1.40	1.46
33	r	502	PLX	O6-C4	-2.51	1.41	1.44
30	l	703	PEE	O2-C2	-2.50	1.40	1.46
30	r	501	PEE	O2-C2	-2.50	1.40	1.46
30	j	201	PEE	O3-C30	2.48	1.40	1.33
30	W	201	PEE	O3-C30	2.47	1.40	1.33
31	m	201	CDL	OB6-CB4	-2.46	1.40	1.46
30	l	704	PEE	O3-C30	2.45	1.40	1.33
33	j	202	PLX	C7-C6	2.44	1.55	1.50
30	l	701	PEE	O3-C30	2.43	1.40	1.33
30	U	101	PEE	O3-C30	2.42	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	U	102	PEE	O3-C30	2.42	1.40	1.33
30	i	402	PEE	O3-C30	2.40	1.40	1.33
35	w	401	ADP	C5-N7	-2.38	1.34	1.39
30	l	703	PEE	O3-C30	2.37	1.40	1.33
33	g	201	PLX	C7-C6	2.36	1.55	1.50
31	V	201	CDL	OB6-CB4	-2.36	1.41	1.46
30	r	501	PEE	O3-C30	2.36	1.40	1.33
33	j	203	PLX	C7-C6	2.34	1.55	1.50
34	s	402	UQ	C7-C8	2.34	1.54	1.50
30	l	701	PEE	O2-C10	2.31	1.40	1.34
31	V	201	CDL	PB2-OB2	2.30	1.68	1.59
31	V	202	CDL	PB2-OB2	2.29	1.68	1.59
30	l	704	PEE	O2-C10	2.28	1.40	1.34
30	W	201	PEE	O2-C10	2.28	1.40	1.34
31	i	401	CDL	PB2-OB2	2.28	1.68	1.59
31	i	401	CDL	PB2-OB5	2.26	1.68	1.59
30	l	701	PEE	O3-C3	-2.25	1.40	1.45
30	U	101	PEE	O2-C10	2.25	1.40	1.34
31	r	505	CDL	PB2-OB5	2.25	1.68	1.59
30	j	201	PEE	O2-C10	2.25	1.40	1.34
31	i	401	CDL	OB6-CB4	-2.24	1.41	1.46
30	r	501	PEE	O2-C10	2.24	1.40	1.34
30	i	402	PEE	O2-C10	2.24	1.40	1.34
31	r	505	CDL	PB2-OB2	2.21	1.68	1.59
31	V	201	CDL	PB2-OB5	2.21	1.68	1.59
31	m	201	CDL	OA6-CA4	-2.21	1.41	1.46
30	l	703	PEE	O3-C3	-2.21	1.40	1.45
33	a	202	PLX	C7-C6	2.21	1.55	1.50
30	l	703	PEE	O2-C10	2.20	1.40	1.34
30	U	102	PEE	O2-C10	2.20	1.40	1.34
33	r	502	PLX	C7-C6	2.19	1.55	1.50
30	r	501	PEE	O3-C3	-2.19	1.40	1.45
31	V	201	CDL	OA6-CA4	-2.18	1.41	1.46
31	r	504	CDL	PB2-OB5	2.17	1.67	1.59
31	r	505	CDL	OB6-CB4	-2.17	1.41	1.46
33	r	502	PLX	P1-O4	2.16	1.67	1.59
30	i	402	PEE	O3-C3	-2.16	1.40	1.45
34	s	402	UQ	O4-C4	-2.16	1.18	1.23
30	U	101	PEE	O3-C3	-2.14	1.40	1.45
30	l	704	PEE	O3-C3	-2.14	1.40	1.45
33	j	203	PLX	P1-O1	2.13	1.67	1.59
30	U	102	PEE	O3-C3	-2.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	W	201	PEE	O3-C3	-2.12	1.40	1.45
33	g	201	PLX	P1-O4	2.12	1.67	1.59
30	j	201	PEE	O3-C3	-2.10	1.40	1.45
33	j	203	PLX	P1-O4	2.10	1.67	1.59
34	s	402	UQ	O3-CM3	-2.09	1.40	1.45
33	a	202	PLX	P1-O4	2.08	1.67	1.59
31	V	202	CDL	PB2-OB5	2.08	1.67	1.59
33	r	502	PLX	P1-O1	2.07	1.67	1.59
34	s	402	UQ	C21-C19	2.04	1.55	1.51
31	V	201	CDL	C11-CA5	2.03	1.56	1.50
33	a	202	PLX	P1-O1	2.02	1.67	1.59
31	m	201	CDL	PB2-OB2	2.02	1.67	1.59
31	r	504	CDL	PB2-OB2	2.01	1.67	1.59
31	r	504	CDL	C11-CA5	2.00	1.56	1.50

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	402	UQ	C7-C8-C9	-7.61	113.72	126.83
34	s	402	UQ	C22-C23-C24	-6.25	113.32	127.62
34	s	402	UQ	C12-C13-C14	-6.06	113.76	127.62
34	s	402	UQ	C17-C18-C19	-6.02	113.84	127.62
35	w	401	ADP	C5-C4-N3	-5.42	119.26	126.72
35	w	401	ADP	N3-C2-N1	-4.56	121.68	128.58
31	l	702	CDL	OA6-CA5-C11	4.48	121.18	111.48
31	m	201	CDL	OB6-CB5-C51	4.47	121.16	111.48
34	s	402	UQ	C10-C9-C8	-4.45	112.19	123.63
31	r	504	CDL	OA6-CA5-C11	4.38	120.97	111.48
34	s	402	UQ	C27-C28-C29	-4.30	113.29	127.64
35	w	401	ADP	N3-C4-N9	4.27	134.43	127.17
34	s	402	UQ	C25-C24-C23	-4.24	112.73	123.63
31	a	201	CDL	OB6-CB5-C51	4.24	120.65	111.48
31	s	401	CDL	OA6-CA5-C11	4.19	120.55	111.48
30	j	201	PEE	O2-C10-C11	4.12	120.39	111.48
31	s	401	CDL	OB6-CB5-C51	4.12	120.39	111.48
30	l	701	PEE	O2-C10-C11	4.08	120.31	111.48
30	l	704	PEE	O2-C10-C11	4.05	120.25	111.48
32	X	201	8Q1	C6-C1-S44	4.03	118.20	113.40
30	r	501	PEE	O2-C10-C11	4.02	120.18	111.48
30	W	201	PEE	O2-C10-C11	4.02	120.17	111.48
31	r	504	CDL	OB6-CB5-C51	3.98	120.09	111.48
31	u	201	CDL	OA6-CA5-C11	3.98	120.09	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	i	401	CDL	OB6-CB5-C51	3.93	119.99	111.48
31	V	201	CDL	OB6-CB5-C51	3.93	119.99	111.48
31	i	401	CDL	OA6-CA5-C11	3.92	119.96	111.48
30	U	101	PEE	O2-C10-C11	3.90	119.91	111.48
30	U	102	PEE	O2-C10-C11	3.89	119.90	111.48
34	s	402	UQ	C20-C19-C18	-3.89	113.65	123.63
34	s	402	UQ	C15-C14-C13	-3.88	113.67	123.63
34	s	402	UQ	C21-C19-C18	-3.87	112.47	121.17
31	V	202	CDL	OA6-CA5-C11	3.84	119.79	111.48
31	a	201	CDL	OA6-CA5-C11	3.82	119.75	111.48
31	r	505	CDL	OB6-CB5-C51	3.82	119.75	111.48
31	u	201	CDL	OB6-CB5-C51	3.81	119.72	111.48
32	X	201	8Q1	C43-S44-C1	3.79	113.06	101.84
30	l	703	PEE	O2-C10-C11	3.79	119.69	111.48
34	s	402	UQ	C16-C14-C13	-3.77	112.69	121.17
30	i	402	PEE	O2-C10-C11	3.77	119.64	111.48
34	s	402	UQ	C11-C9-C8	-3.76	112.72	121.17
31	V	202	CDL	OB6-CB5-C51	3.73	119.56	111.48
31	l	702	CDL	OB6-CB5-C51	3.67	119.43	111.48
31	r	505	CDL	OA6-CA5-C11	3.65	119.38	111.48
34	s	402	UQ	C26-C24-C23	-3.55	113.20	121.17
35	w	401	ADP	C2-N3-C4	3.54	120.47	111.83
31	V	201	CDL	OA6-CA5-C11	3.50	119.06	111.48
35	w	401	ADP	N9-C8-N7	-3.47	109.01	113.94
31	m	201	CDL	OA6-CA5-C11	3.30	118.61	111.48
34	s	402	UQ	C30-C29-C28	-3.29	112.79	122.66
31	l	702	CDL	CB4-OB6-CB5	-3.26	109.98	117.80
31	a	201	CDL	OB8-CB7-C71	3.26	121.78	111.83
32	X	201	8Q1	O35-C34-N36	-3.25	116.10	122.98
31	u	201	CDL	OB8-CB7-C71	3.24	121.71	111.83
35	w	401	ADP	C4-N9-C8	3.16	109.06	105.74
35	w	401	ADP	C5-N7-C8	3.16	108.41	103.45
34	s	402	UQ	C31-C29-C28	-3.13	113.26	122.66
31	l	702	CDL	CA4-OA6-CA5	-3.04	110.51	117.80
30	i	402	PEE	O3-C30-C31	3.03	121.06	111.83
31	V	202	CDL	OB8-CB7-C71	3.01	121.01	111.83
31	m	201	CDL	OA8-CA7-C31	2.99	120.95	111.83
31	l	702	CDL	OB8-CB7-C71	2.96	120.86	111.83
35	w	401	ADP	C4-C5-N7	-2.95	107.21	110.58
31	V	201	CDL	OB8-CB7-C71	2.92	120.73	111.83
31	r	504	CDL	OA8-CA7-C31	2.92	120.72	111.83
31	r	504	CDL	OB8-CB7-C71	2.87	120.60	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	l	703	PEE	O3-C30-C31	2.87	120.58	111.83
31	s	401	CDL	OB8-CB7-C71	2.83	120.45	111.83
30	W	201	PEE	O3-C30-C31	2.80	120.37	111.83
30	U	102	PEE	O3-C30-C31	2.79	120.33	111.83
33	r	502	PLX	C1A-N1-C1	2.78	120.96	109.91
31	u	201	CDL	OA8-CA7-C31	2.75	119.51	111.15
32	X	201	8Q1	O2-P24-O27	-2.75	99.51	106.67
31	i	401	CDL	OA8-CA7-C31	2.73	120.16	111.83
30	U	101	PEE	O3-C30-C31	2.71	120.10	111.83
31	i	401	CDL	OB8-CB7-C71	2.70	120.06	111.83
31	s	401	CDL	OA8-CA7-C31	2.69	120.03	111.83
30	j	201	PEE	O3-C30-C31	2.68	120.00	111.83
30	r	501	PEE	O3-C30-C31	2.68	119.99	111.83
32	X	201	8Q1	C32-C34-N36	2.67	121.54	116.48
31	m	201	CDL	OB8-CB7-C71	2.66	119.93	111.83
31	r	505	CDL	OB8-CB7-C71	2.65	119.91	111.83
31	a	201	CDL	OA8-CA7-C31	2.65	119.90	111.83
31	V	202	CDL	OA8-CA7-C31	2.64	119.89	111.83
30	l	704	PEE	O3-C30-C31	2.64	119.88	111.83
31	r	505	CDL	OA8-CA7-C31	2.62	119.81	111.83
31	V	201	CDL	OA8-CA7-C31	2.60	119.75	111.83
33	a	202	PLX	C1A-N1-C1	2.59	120.19	109.91
32	X	201	8Q1	C37-C38-C39	2.56	116.65	112.39
31	l	702	CDL	OA8-CA7-C31	2.53	119.55	111.83
33	g	201	PLX	C1A-N1-C1	2.45	119.65	109.91
33	j	202	PLX	C1A-N1-C1	2.45	119.65	109.91
31	a	201	CDL	CB4-OB6-CB5	-2.38	112.09	117.80
32	X	201	8Q1	O40-C39-N41	-2.37	118.38	123.03
33	j	203	PLX	C1A-N1-C1	2.36	119.31	109.91
30	l	701	PEE	C20-C19-C18	-2.36	112.21	126.42
30	l	701	PEE	O3-C30-C31	2.36	119.03	111.83
34	s	402	UQ	C7-C6-C5	-2.34	120.87	124.89
31	s	401	CDL	CA4-OA6-CA5	-2.30	112.28	117.80
32	X	201	8Q1	O1-P24-O2	2.30	116.44	107.80
31	r	504	CDL	CA4-OA6-CA5	-2.24	112.43	117.80
31	l	702	CDL	OA6-CA5-OA7	-2.23	118.49	123.70
34	s	402	UQ	CM5-C5-C6	-2.22	120.80	124.45
31	u	201	CDL	OB8-CB7-OB9	-2.19	118.15	123.63
33	j	202	PLX	C2-C1-N1	-2.10	109.08	115.82
31	m	201	CDL	CB4-OB6-CB5	-2.05	112.90	117.80
31	a	201	CDL	CA6-CA4-CA3	-2.04	107.03	111.78
31	a	201	CDL	OB8-CB7-OB9	-2.03	118.56	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	w	401	ADP	C4'-O4'-C1'	-2.02	105.00	109.47
31	m	201	CDL	OB6-CB5-OB7	-2.02	118.98	123.70
32	X	201	8Q1	O4-C1-S44	-2.02	120.11	122.68
32	X	201	8Q1	O27-P24-O3	-2.01	101.02	106.44

There are no chirality outliers.

All (915) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	U	101	PEE	C19-C20-C21-C22
30	U	101	PEE	C11-C10-O2-C2
30	U	101	PEE	C1-O3P-P-O1P
30	U	101	PEE	C1-O3P-P-O4P
30	W	201	PEE	C1-O3P-P-O2P
30	W	201	PEE	C1-O3P-P-O1P
30	W	201	PEE	O4P-C4-C5-N
30	i	402	PEE	C11-C10-O2-C2
30	i	402	PEE	O4-C10-O2-C2
30	i	402	PEE	C1-O3P-P-O2P
30	i	402	PEE	C1-O3P-P-O1P
30	i	402	PEE	C1-O3P-P-O4P
30	i	402	PEE	O5-C30-O3-C3
30	i	402	PEE	C31-C30-O3-C3
30	l	701	PEE	C11-C10-O2-C2
30	l	701	PEE	O4-C10-O2-C2
30	l	701	PEE	C1-O3P-P-O2P
30	l	701	PEE	C1-O3P-P-O1P
30	l	701	PEE	C1-O3P-P-O4P
30	l	701	PEE	C4-O4P-P-O3P
30	l	701	PEE	C39-C40-C41-C42
30	l	703	PEE	C11-C10-O2-C2
30	l	704	PEE	C1-O3P-P-O1P
30	l	704	PEE	C4-O4P-P-O3P
30	l	704	PEE	C4-O4P-P-O2P
30	r	501	PEE	C1-O3P-P-O2P
30	r	501	PEE	C4-O4P-P-O3P
30	r	501	PEE	C4-O4P-P-O1P
31	V	201	CDL	CA2-OA2-PA1-OA3
31	V	201	CDL	C1-CB2-OB2-PB2
31	V	201	CDL	CB2-OB2-PB2-OB3
31	V	201	CDL	CB2-OB2-PB2-OB4
31	V	201	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
31	V	201	CDL	CB3-OB5-PB2-OB3
31	V	201	CDL	CB3-OB5-PB2-OB4
31	V	202	CDL	OB5-CB3-CB4-OB6
31	V	202	CDL	C51-CB5-OB6-CB4
31	a	201	CDL	CB2-C1-CA2-OA2
31	a	201	CDL	CA2-OA2-PA1-OA3
31	a	201	CDL	CA2-OA2-PA1-OA5
31	a	201	CDL	CA3-OA5-PA1-OA2
31	a	201	CDL	CA3-OA5-PA1-OA4
31	a	201	CDL	CB2-OB2-PB2-OB3
31	a	201	CDL	CB2-OB2-PB2-OB5
31	a	201	CDL	CB3-OB5-PB2-OB2
31	a	201	CDL	CB3-OB5-PB2-OB3
31	i	401	CDL	CB2-C1-CA2-OA2
31	i	401	CDL	CA2-OA2-PA1-OA3
31	i	401	CDL	CA2-OA2-PA1-OA4
31	i	401	CDL	CA2-OA2-PA1-OA5
31	i	401	CDL	C31-CA7-OA8-CA6
31	i	401	CDL	CB3-OB5-PB2-OB2
31	i	401	CDL	CB3-OB5-PB2-OB3
31	l	702	CDL	CA2-OA2-PA1-OA4
31	l	702	CDL	CA2-OA2-PA1-OA5
31	l	702	CDL	CA3-OA5-PA1-OA2
31	l	702	CDL	CA3-OA5-PA1-OA3
31	l	702	CDL	CA3-OA5-PA1-OA4
31	l	702	CDL	CB2-OB2-PB2-OB4
31	l	702	CDL	CB2-OB2-PB2-OB5
31	l	702	CDL	OB7-CB5-OB6-CB4
31	l	702	CDL	C51-CB5-OB6-CB4
31	m	201	CDL	CA2-OA2-PA1-OA3
31	m	201	CDL	CA3-OA5-PA1-OA2
31	m	201	CDL	CA3-OA5-PA1-OA3
31	m	201	CDL	CA3-OA5-PA1-OA4
31	m	201	CDL	CB2-OB2-PB2-OB3
31	m	201	CDL	CB2-OB2-PB2-OB4
31	m	201	CDL	CB2-OB2-PB2-OB5
31	r	504	CDL	CA2-C1-CB2-OB2
31	r	504	CDL	OA5-CA3-CA4-OA6
31	r	504	CDL	OA9-CA7-OA8-CA6
31	r	504	CDL	C31-CA7-OA8-CA6
31	r	504	CDL	CB3-OB5-PB2-OB2
31	r	504	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
31	r	504	CDL	CB3-OB5-PB2-OB4
31	r	505	CDL	CA3-OA5-PA1-OA2
31	r	505	CDL	CA3-OA5-PA1-OA3
31	r	505	CDL	CB2-OB2-PB2-OB3
31	r	505	CDL	CB2-OB2-PB2-OB4
31	r	505	CDL	CB2-OB2-PB2-OB5
31	r	505	CDL	CB3-OB5-PB2-OB2
31	r	505	CDL	CB3-OB5-PB2-OB3
31	r	505	CDL	CB3-OB5-PB2-OB4
31	s	401	CDL	OA5-CA3-CA4-OA6
31	s	401	CDL	C31-CA7-OA8-CA6
31	s	401	CDL	C51-CB5-OB6-CB4
31	u	201	CDL	CA2-OA2-PA1-OA3
31	u	201	CDL	CA2-OA2-PA1-OA4
31	u	201	CDL	CA2-OA2-PA1-OA5
31	u	201	CDL	CA3-OA5-PA1-OA3
31	u	201	CDL	CB2-OB2-PB2-OB4
31	u	201	CDL	CB2-OB2-PB2-OB5
31	u	201	CDL	CB3-OB5-PB2-OB2
31	u	201	CDL	CB3-OB5-PB2-OB3
31	u	201	CDL	CB3-OB5-PB2-OB4
32	X	201	8Q1	C1-C6-C7-C8
32	X	201	8Q1	O33-C32-C34-N36
32	X	201	8Q1	C42-C43-S44-C1
33	a	202	PLX	C2-O1-P1-O2
33	a	202	PLX	N1-C1-C2-O1
33	a	202	PLX	O9-C24-C25-C26
33	g	201	PLX	C3-O4-P1-O2
33	g	201	PLX	C2-O1-P1-O4
33	g	201	PLX	C2-O1-P1-O2
33	g	201	PLX	C2-O1-P1-O3
33	g	201	PLX	O9-C24-O8-C5
33	j	202	PLX	O7-C6-O6-C4
33	j	202	PLX	C3-C4-O6-C6
33	j	202	PLX	C2-O1-P1-O4
33	j	202	PLX	C2-O1-P1-O2
33	j	202	PLX	C25-C24-O8-C5
33	j	202	PLX	O8-C24-C25-C26
33	j	202	PLX	O9-C24-C25-C26
33	j	203	PLX	O7-C6-C7-C8
33	j	203	PLX	C3-O4-P1-O2
33	j	203	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
33	j	203	PLX	O9-C24-C25-C26
33	r	502	PLX	O7-C6-C7-C8
33	r	502	PLX	C5-C4-O6-C6
33	r	502	PLX	C3-O4-P1-O1
33	r	502	PLX	C2-O1-P1-O2
33	r	502	PLX	O9-C24-C25-C26
34	s	402	UQ	C7-C8-C9-C10
34	s	402	UQ	C7-C8-C9-C11
31	i	401	CDL	OA9-CA7-OA8-CA6
31	s	401	CDL	OA9-CA7-OA8-CA6
30	U	101	PEE	O4-C10-O2-C2
30	j	201	PEE	O4-C10-O2-C2
30	l	703	PEE	O4-C10-O2-C2
31	V	202	CDL	OB7-CB5-OB6-CB4
31	s	401	CDL	OB7-CB5-OB6-CB4
30	j	201	PEE	C11-C10-O2-C2
34	s	402	UQ	C18-C19-C21-C22
31	V	201	CDL	OA9-CA7-OA8-CA6
30	U	101	PEE	C31-C30-O3-C3
31	V	201	CDL	C31-CA7-OA8-CA6
30	l	701	PEE	C17-C18-C19-C20
30	l	704	PEE	C37-C38-C39-C40
34	s	402	UQ	C17-C18-C19-C21
34	s	402	UQ	C22-C23-C24-C26
33	r	502	PLX	C9-C10-C11-C12
31	a	201	CDL	O1-C1-CA2-OA2
31	i	401	CDL	O1-C1-CB2-OB2
31	l	702	CDL	O1-C1-CB2-OB2
31	m	201	CDL	O1-C1-CB2-OB2
35	w	401	ADP	O4'-C4'-C5'-O5'
30	U	101	PEE	O5-C30-O3-C3
31	l	702	CDL	C71-CB7-OB8-CB6
30	U	101	PEE	C17-C18-C19-C20
31	V	201	CDL	C11-C12-C13-C14
33	j	203	PLX	C28-C29-C30-C31
31	V	202	CDL	C11-CA5-OA6-CA4
31	V	201	CDL	CB2-C1-CA2-OA2
31	i	401	CDL	CA2-C1-CB2-OB2
31	r	504	CDL	CB2-C1-CA2-OA2
31	s	401	CDL	CA2-C1-CB2-OB2
31	V	202	CDL	C31-CA7-OA8-CA6
33	j	203	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	V	201	CDL	C58-C59-C60-C61
31	V	202	CDL	C78-C79-C80-C81
31	l	702	CDL	C31-C32-C33-C34
33	j	202	PLX	C25-C26-C27-C28
33	g	201	PLX	C9-C10-C11-C12
33	r	502	PLX	C7-C8-C9-C10
33	g	201	PLX	C7-C8-C9-C10
31	m	201	CDL	C62-C63-C64-C65
30	U	102	PEE	C11-C12-C13-C14
31	V	201	CDL	O1-C1-CA2-OA2
31	s	401	CDL	O1-C1-CA2-OA2
31	s	401	CDL	O1-C1-CB2-OB2
33	r	502	PLX	C11-C12-C13-C14
30	l	704	PEE	C11-C10-O2-C2
31	r	504	CDL	OA6-CA4-CA6-OA8
31	m	201	CDL	CA5-C11-C12-C13
31	r	504	CDL	CB5-C51-C52-C53
34	s	402	UQ	C22-C23-C24-C25
31	r	504	CDL	C16-C17-C18-C19
30	U	102	PEE	C17-C18-C19-C20
31	V	201	CDL	CA7-C31-C32-C33
31	l	702	CDL	C35-C36-C37-C38
31	s	401	CDL	C14-C15-C16-C17
34	s	402	UQ	C27-C28-C29-C31
34	s	402	UQ	C14-C16-C17-C18
31	i	401	CDL	CA7-C31-C32-C33
31	i	401	CDL	CB7-C71-C72-C73
31	m	201	CDL	CA7-C31-C32-C33
31	V	202	CDL	OA9-CA7-OA8-CA6
30	r	501	PEE	C11-C10-O2-C2
31	a	201	CDL	CB5-C51-C52-C53
31	u	201	CDL	CB7-C71-C72-C73
31	r	504	CDL	C58-C59-C60-C61
31	r	505	CDL	C51-C52-C53-C54
31	V	201	CDL	O1-C1-CB2-OB2
31	V	202	CDL	O1-C1-CB2-OB2
31	i	401	CDL	O1-C1-CA2-OA2
31	r	504	CDL	O1-C1-CA2-OA2
31	r	504	CDL	O1-C1-CB2-OB2
31	r	505	CDL	O1-C1-CB2-OB2
31	u	201	CDL	CB5-C51-C52-C53
31	V	202	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
33	g	201	PLX	C31-C32-C33-C34
30	W	201	PEE	C17-C18-C19-C20
31	l	702	CDL	OB9-CB7-OB8-CB6
31	r	505	CDL	CA5-C11-C12-C13
31	V	201	CDL	C62-C63-C64-C65
30	W	201	PEE	C31-C30-O3-C3
31	r	504	CDL	C71-CB7-OB8-CB6
30	U	102	PEE	C34-C35-C36-C37
31	V	202	CDL	C57-C58-C59-C60
31	m	201	CDL	C43-C44-C45-C46
30	l	704	PEE	O4-C10-O2-C2
30	r	501	PEE	O4-C10-O2-C2
31	V	201	CDL	CA2-C1-CB2-OB2
31	V	202	CDL	CA2-C1-CB2-OB2
33	g	201	PLX	C2-C1-N1-C1A
31	V	202	CDL	C76-C77-C78-C79
31	r	504	CDL	C55-C56-C57-C58
31	s	401	CDL	CB7-C71-C72-C73
34	s	402	UQ	C23-C24-C26-C27
33	j	203	PLX	O6-C6-C7-C8
33	j	203	PLX	O8-C24-C25-C26
33	r	502	PLX	O6-C6-C7-C8
31	r	505	CDL	C51-CB5-OB6-CB4
31	r	505	CDL	OB7-CB5-OB6-CB4
31	l	702	CDL	C33-C34-C35-C36
30	U	101	PEE	C30-C31-C32-C33
31	V	201	CDL	C34-C35-C36-C37
31	V	202	CDL	C11-C12-C13-C14
30	j	201	PEE	C31-C30-O3-C3
33	g	201	PLX	C2-C1-N1-C1B
31	r	505	CDL	C76-C77-C78-C79
30	U	101	PEE	C40-C41-C42-C43
31	r	504	CDL	OB9-CB7-OB8-CB6
31	r	505	CDL	C14-C15-C16-C17
33	r	502	PLX	C18-C19-C20-C21
31	r	504	CDL	C35-C36-C37-C38
31	r	504	CDL	C52-C53-C54-C55
31	s	401	CDL	C34-C35-C36-C37
31	s	401	CDL	C52-C53-C54-C55
31	i	401	CDL	CA5-C11-C12-C13
30	l	701	PEE	C37-C38-C39-C40
31	V	201	CDL	C75-C76-C77-C78

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Mol	Chain	Res	Type	Atoms
31	V	202	CDL	C17-C18-C19-C20
31	i	401	CDL	C55-C56-C57-C58
31	m	201	CDL	C56-C57-C58-C59
31	s	401	CDL	C73-C74-C75-C76
33	a	202	PLX	C9-C10-C11-C12
30	W	201	PEE	C12-C13-C14-C15
31	V	201	CDL	C31-C32-C33-C34
31	V	202	CDL	C12-C13-C14-C15
31	i	401	CDL	C14-C15-C16-C17
31	i	401	CDL	C37-C38-C39-C40
31	m	201	CDL	C52-C53-C54-C55
31	m	201	CDL	C76-C77-C78-C79
31	r	504	CDL	C56-C57-C58-C59
31	r	505	CDL	C43-C44-C45-C46
31	r	505	CDL	C75-C76-C77-C78
31	s	401	CDL	C19-C20-C21-C22
31	V	201	CDL	C55-C56-C57-C58
31	r	505	CDL	C59-C60-C61-C62
31	s	401	CDL	C37-C38-C39-C40
31	s	401	CDL	C39-C40-C41-C42
33	j	202	PLX	C18-C19-C20-C21
31	m	201	CDL	C71-C72-C73-C74
33	r	502	PLX	C11-C10-C9-C8
31	V	201	CDL	C11-CA5-OA6-CA4
33	a	202	PLX	C10-C11-C12-C13
33	j	202	PLX	C7-C8-C9-C10
31	u	201	CDL	O1-C1-CB2-OB2
35	w	401	ADP	C3'-C4'-C5'-O5'
33	g	201	PLX	C32-C33-C34-C35
33	j	202	PLX	C11-C12-C13-C14
30	W	201	PEE	O5-C30-O3-C3
31	V	201	CDL	C54-C55-C56-C57
31	i	401	CDL	C59-C60-C61-C62
33	r	502	PLX	C33-C34-C35-C36
30	r	501	PEE	C13-C14-C15-C16
33	a	202	PLX	C13-C14-C15-C16
33	g	201	PLX	C30-C31-C32-C33
31	V	202	CDL	CB7-C71-C72-C73
31	s	401	CDL	C54-C55-C56-C57
33	r	502	PLX	C27-C28-C29-C30
31	V	202	CDL	C54-C55-C56-C57
31	V	201	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
31	r	504	CDL	C51-C52-C53-C54
31	r	504	CDL	C59-C60-C61-C62
31	V	202	CDL	C15-C16-C17-C18
31	V	202	CDL	C73-C74-C75-C76
31	a	201	CDL	C35-C36-C37-C38
31	r	504	CDL	C31-C32-C33-C34
31	r	504	CDL	C62-C63-C64-C65
31	s	401	CDL	C15-C16-C17-C18
31	s	401	CDL	C32-C33-C34-C35
31	s	401	CDL	C71-C72-C73-C74
33	a	202	PLX	C12-C13-C14-C15
33	a	202	PLX	C7-C8-C9-C10
33	j	202	PLX	C32-C33-C34-C35
31	V	202	CDL	C40-C41-C42-C43
31	V	202	CDL	C59-C60-C61-C62
31	m	201	CDL	C35-C36-C37-C38
31	m	201	CDL	C55-C56-C57-C58
31	r	504	CDL	C75-C76-C77-C78
31	r	505	CDL	C74-C75-C76-C77
33	j	202	PLX	C33-C34-C35-C36
33	j	202	PLX	C27-C28-C29-C30
30	i	402	PEE	C34-C35-C36-C37
31	r	504	CDL	C34-C35-C36-C37
31	s	401	CDL	C59-C60-C61-C62
33	g	201	PLX	C2-C1-N1-C1C
31	r	505	CDL	C57-C58-C59-C60
31	r	504	CDL	C18-C19-C20-C21
31	r	504	CDL	C36-C37-C38-C39
31	V	201	CDL	C51-CB5-OB6-CB4
30	l	704	PEE	C34-C35-C36-C37
33	j	203	PLX	C7-C8-C9-C10
33	r	502	PLX	C28-C29-C30-C31
31	r	505	CDL	C53-C54-C55-C56
30	j	201	PEE	O5-C30-O3-C3
31	V	201	CDL	OA7-CA5-OA6-CA4
31	V	201	CDL	OB7-CB5-OB6-CB4
30	l	701	PEE	C32-C33-C34-C35
33	g	201	PLX	C33-C34-C35-C36
31	m	201	CDL	C34-C35-C36-C37
31	s	401	CDL	C82-C83-C84-C85
33	j	202	PLX	C30-C31-C32-C33
30	U	102	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
30	l	703	PEE	C31-C30-O3-C3
31	V	201	CDL	C40-C41-C42-C43
31	i	401	CDL	C76-C77-C78-C79
31	m	201	CDL	C14-C15-C16-C17
31	r	504	CDL	C71-C72-C73-C74
33	a	202	PLX	C14-C15-C16-C17
33	a	202	PLX	C11-C12-C13-C14
30	W	201	PEE	C24-C25-C26-C27
30	U	101	PEE	C34-C35-C36-C37
30	W	201	PEE	C13-C14-C15-C16
30	r	501	PEE	C40-C41-C42-C43
31	m	201	CDL	C51-C52-C53-C54
31	r	505	CDL	C13-C14-C15-C16
33	g	201	PLX	C28-C29-C30-C31
31	V	202	CDL	C60-C61-C62-C63
31	m	201	CDL	C15-C16-C17-C18
31	r	505	CDL	C60-C61-C62-C63
33	j	203	PLX	C29-C30-C31-C32
31	V	201	CDL	C37-C38-C39-C40
31	i	401	CDL	C73-C74-C75-C76
33	r	502	PLX	C12-C13-C14-C15
31	V	201	CDL	C52-C53-C54-C55
33	g	201	PLX	C12-C13-C14-C15
33	j	203	PLX	C12-C13-C14-C15
30	l	701	PEE	C18-C19-C20-C21
31	V	201	CDL	C14-C15-C16-C17
31	V	202	CDL	C75-C76-C77-C78
31	r	504	CDL	C37-C38-C39-C40
30	U	102	PEE	C11-C10-O2-C2
31	l	702	CDL	C11-CA5-OA6-CA4
31	m	201	CDL	C51-CB5-OB6-CB4
31	s	401	CDL	C11-CA5-OA6-CA4
30	l	701	PEE	C30-C31-C32-C33
30	r	501	PEE	C10-C11-C12-C13
31	r	504	CDL	C74-C75-C76-C77
30	l	703	PEE	C15-C16-C17-C18
33	g	201	PLX	C27-C28-C29-C30
33	j	203	PLX	C14-C15-C16-C17
31	m	201	CDL	C33-C34-C35-C36
31	m	201	CDL	C37-C38-C39-C40
31	r	504	CDL	C78-C79-C80-C81
31	s	401	CDL	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
31	s	401	CDL	C56-C57-C58-C59
33	r	502	PLX	C25-C26-C27-C28
31	V	201	CDL	C59-C60-C61-C62
31	r	505	CDL	C34-C35-C36-C37
31	V	202	CDL	C14-C15-C16-C17
31	i	401	CDL	C81-C82-C83-C84
31	l	702	CDL	C15-C16-C17-C18
31	s	401	CDL	C17-C18-C19-C20
30	r	501	PEE	C12-C13-C14-C15
31	V	202	CDL	C79-C80-C81-C82
31	r	505	CDL	CB7-C71-C72-C73
30	l	703	PEE	C31-C32-C33-C34
33	j	203	PLX	C11-C12-C13-C14
31	s	401	CDL	OA7-CA5-OA6-CA4
31	m	201	CDL	OA5-CA3-CA4-OA6
31	r	504	CDL	OB5-CB3-CB4-OB6
31	r	505	CDL	C16-C17-C18-C19
34	s	402	UQ	C27-C28-C29-C30
30	j	201	PEE	C11-C12-C13-C14
30	l	703	PEE	C21-C22-C23-C24
31	m	201	CDL	C78-C79-C80-C81
31	r	505	CDL	C33-C34-C35-C36
31	r	505	CDL	C55-C56-C57-C58
31	i	401	CDL	CB5-C51-C52-C53
30	j	201	PEE	C23-C24-C25-C26
31	i	401	CDL	OB6-CB4-CB6-OB8
33	j	203	PLX	C26-C27-C28-C29
30	U	102	PEE	C13-C14-C15-C16
30	l	701	PEE	C33-C34-C35-C36
30	U	101	PEE	C36-C37-C38-C39
30	U	102	PEE	C38-C39-C40-C41
31	V	202	CDL	C83-C84-C85-C86
30	r	501	PEE	C33-C34-C35-C36
31	V	201	CDL	C71-C72-C73-C74
31	l	702	CDL	C32-C33-C34-C35
31	m	201	CDL	C81-C82-C83-C84
33	g	201	PLX	C11-C12-C13-C14
33	j	202	PLX	C9-C10-C11-C12
33	r	502	PLX	C31-C32-C33-C34
31	r	505	CDL	C35-C36-C37-C38
31	l	702	CDL	OA7-CA5-OA6-CA4
31	V	202	CDL	C74-C75-C76-C77

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Mol	Chain	Res	Type	Atoms
31	s	401	CDL	C12-C13-C14-C15
31	a	201	CDL	C19-C20-C21-C22
31	V	202	CDL	C84-C85-C86-C87
31	s	401	CDL	C83-C84-C85-C86
33	a	202	PLX	C15-C16-C17-C18
30	U	102	PEE	O5-C30-O3-C3
31	V	202	CDL	C42-C43-C44-C45
31	a	201	CDL	C37-C38-C39-C40
33	r	502	PLX	C14-C15-C16-C17
31	m	201	CDL	C39-C40-C41-C42
33	a	202	PLX	C31-C32-C33-C34
30	U	102	PEE	C35-C36-C37-C38
30	j	201	PEE	C19-C20-C21-C22
31	r	504	CDL	C11-C12-C13-C14
31	s	401	CDL	C78-C79-C80-C81
33	j	203	PLX	C25-C26-C27-C28
31	s	401	CDL	OA5-CA3-CA4-CA6
33	j	202	PLX	O4-C3-C4-C5
30	U	102	PEE	O4-C10-O2-C2
31	V	202	CDL	C32-C33-C34-C35
31	V	201	CDL	C76-C77-C78-C79
31	s	401	CDL	C18-C19-C20-C21
30	l	703	PEE	O5-C30-O3-C3
31	l	702	CDL	C31-CA7-OA8-CA6
33	j	202	PLX	C12-C13-C14-C15
31	s	401	CDL	CA7-C31-C32-C33
30	l	703	PEE	C44-C45-C46-C47
30	r	501	PEE	C31-C32-C33-C34
33	j	203	PLX	C33-C34-C35-C36
30	l	704	PEE	C31-C32-C33-C34
31	i	401	CDL	C77-C78-C79-C80
31	i	401	CDL	C34-C35-C36-C37
30	j	201	PEE	C1-C2-C3-O3
30	l	704	PEE	C1-C2-C3-O3
30	r	501	PEE	C1-C2-C3-O3
31	i	401	CDL	CA3-CA4-CA6-OA8
31	r	504	CDL	CA3-CA4-CA6-OA8
31	s	401	CDL	CB3-CB4-CB6-OB8
33	r	503	PLX	C3-C4-C5-O8
31	V	201	CDL	C44-C45-C46-C47
30	l	704	PEE	C14-C15-C16-C17
30	U	102	PEE	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
30	W	201	PEE	C19-C20-C21-C22
30	i	402	PEE	C35-C36-C37-C38
30	l	701	PEE	C35-C36-C37-C38
31	V	201	CDL	C56-C57-C58-C59
31	m	201	CDL	C31-C32-C33-C34
31	a	201	CDL	C57-C58-C59-C60
31	i	401	CDL	C54-C55-C56-C57
33	r	502	PLX	C30-C31-C32-C33
31	a	201	CDL	C34-C35-C36-C37
30	r	501	PEE	C36-C37-C38-C39
31	m	201	CDL	C21-C22-C23-C24
31	i	401	CDL	C75-C76-C77-C78
31	m	201	CDL	C41-C42-C43-C44
31	m	201	CDL	C59-C60-C61-C62
33	a	202	PLX	C16-C17-C18-C19
33	g	201	PLX	C25-C26-C27-C28
33	r	502	PLX	C13-C14-C15-C16
31	V	202	CDL	C23-C24-C25-C26
31	l	702	CDL	OA9-CA7-OA8-CA6
31	r	504	CDL	C14-C15-C16-C17
30	r	501	PEE	C42-C43-C44-C45
31	r	505	CDL	C32-C33-C34-C35
31	V	201	CDL	C51-C52-C53-C54
31	r	504	CDL	CA5-C11-C12-C13
31	r	505	CDL	CA7-C31-C32-C33
31	a	201	CDL	CA2-C1-CB2-OB2
31	a	201	CDL	OA5-CA3-CA4-OA6
31	i	401	CDL	C71-C72-C73-C74
31	m	201	CDL	C77-C78-C79-C80
31	i	401	CDL	C35-C36-C37-C38
31	r	505	CDL	C71-C72-C73-C74
31	V	202	CDL	C63-C64-C65-C66
31	u	201	CDL	C73-C74-C75-C76
33	r	503	PLX	C26-C27-C28-C29
31	l	702	CDL	C21-C22-C23-C24
31	r	505	CDL	C15-C16-C17-C18
32	X	201	8Q1	C11-C12-C13-C14
33	g	201	PLX	C20-C21-C22-C23
31	V	202	CDL	C37-C38-C39-C40
31	V	202	CDL	OB6-CB4-CB6-OB8
33	j	202	PLX	O6-C4-C5-O8
31	s	401	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
33	g	201	PLX	C14-C15-C16-C17
31	a	201	CDL	C83-C84-C85-C86
30	r	501	PEE	C39-C40-C41-C42
31	r	505	CDL	C84-C85-C86-C87
33	g	201	PLX	C36-C37-C38-C39
30	l	704	PEE	C31-C30-O3-C3
31	V	201	CDL	C64-C65-C66-C67
31	r	504	CDL	C82-C83-C84-C85
31	V	202	CDL	C33-C34-C35-C36
33	j	203	PLX	C34-C35-C36-C37
30	r	501	PEE	C17-C18-C19-C20
31	m	201	CDL	C38-C39-C40-C41
30	i	402	PEE	C11-C12-C13-C14
31	m	201	CDL	OB7-CB5-OB6-CB4
31	l	702	CDL	C72-C73-C74-C75
30	l	701	PEE	C2-C1-O3P-P
32	X	201	8Q1	N41-C42-C43-S44
31	r	505	CDL	C62-C63-C64-C65
30	W	201	PEE	C33-C34-C35-C36
31	V	202	CDL	OB5-CB3-CB4-CB6
31	a	201	CDL	OB5-CB3-CB4-CB6
31	m	201	CDL	OA5-CA3-CA4-CA6
31	r	504	CDL	OA5-CA3-CA4-CA6
31	r	504	CDL	OB5-CB3-CB4-CB6
31	m	201	CDL	C52-C51-CB5-OB6
30	U	101	PEE	C38-C39-C40-C41
31	i	401	CDL	C38-C39-C40-C41
31	m	201	CDL	C64-C65-C66-C67
33	g	201	PLX	C13-C14-C15-C16
33	j	202	PLX	C16-C17-C18-C19
30	r	501	PEE	C31-C30-O3-C3
31	m	201	CDL	C22-C23-C24-C25
30	l	703	PEE	C13-C14-C15-C16
33	g	201	PLX	C10-C11-C12-C13
31	m	201	CDL	CB5-C51-C52-C53
31	m	201	CDL	C58-C59-C60-C61
31	m	201	CDL	CA2-C1-CB2-OB2
31	r	504	CDL	C73-C74-C75-C76
30	W	201	PEE	C1-C2-C3-O3
31	V	202	CDL	CB3-CB4-CB6-OB8
31	i	401	CDL	CB3-CB4-CB6-OB8
33	r	502	PLX	C3-C4-C5-O8

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Mol	Chain	Res	Type	Atoms
33	a	202	PLX	C11-C10-C9-C8
33	r	502	PLX	C19-C20-C21-C22
30	l	701	PEE	C31-C30-O3-C3
30	j	201	PEE	C14-C15-C16-C17
31	i	401	CDL	OB5-CB3-CB4-OB6
31	r	505	CDL	OA5-CA3-CA4-OA6
31	V	202	CDL	C77-C78-C79-C80
33	j	202	PLX	C36-C37-C38-C39
31	a	201	CDL	C11-CA5-OA6-CA4
31	V	202	CDL	C1-CB2-OB2-PB2
31	m	201	CDL	C84-C85-C86-C87
30	l	704	PEE	C13-C14-C15-C16
33	r	503	PLX	C18-C19-C20-C21
30	r	501	PEE	C11-C12-C13-C14
30	r	501	PEE	O2-C2-C3-O3
31	s	401	CDL	OB6-CB4-CB6-OB8
31	r	504	CDL	C22-C23-C24-C25
31	V	201	CDL	C72-C73-C74-C75
31	m	201	CDL	C18-C19-C20-C21
33	a	202	PLX	O8-C24-C25-C26
33	r	502	PLX	O8-C24-C25-C26
30	l	701	PEE	C31-C32-C33-C34
32	X	201	8Q1	C10-C11-C12-C13
31	V	202	CDL	C13-C14-C15-C16
31	l	702	CDL	C20-C21-C22-C23
33	j	202	PLX	C13-C14-C15-C16
31	m	201	CDL	C44-C45-C46-C47
31	m	201	CDL	C54-C55-C56-C57
31	r	504	CDL	C32-C33-C34-C35
31	r	504	CDL	CB7-C71-C72-C73
33	j	202	PLX	C20-C21-C22-C23
31	r	505	CDL	C64-C65-C66-C67
31	i	401	CDL	C71-CB7-OB8-CB6
31	i	401	CDL	C39-C40-C41-C42
31	i	401	CDL	C64-C65-C66-C67
31	r	504	CDL	C11-CA5-OA6-CA4
33	a	202	PLX	C34-C35-C36-C37
31	V	201	CDL	C80-C81-C82-C83
30	l	704	PEE	C12-C13-C14-C15
31	a	201	CDL	OA5-CA3-CA4-CA6
31	i	401	CDL	OB5-CB3-CB4-CB6
31	r	505	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
31	i	401	CDL	C52-C53-C54-C55
30	r	501	PEE	C38-C39-C40-C41
30	r	501	PEE	O5-C30-O3-C3
31	i	401	CDL	OB9-CB7-OB8-CB6
31	i	401	CDL	C1-CB2-OB2-PB2
33	j	203	PLX	C27-C28-C29-C30
30	j	201	PEE	C24-C25-C26-C27
31	s	401	CDL	C71-CB7-OB8-CB6
30	l	704	PEE	O5-C30-O3-C3
31	m	201	CDL	C17-C18-C19-C20
30	l	701	PEE	O5-C30-O3-C3
33	j	203	PLX	C30-C31-C32-C33
31	V	201	CDL	CA6-CA4-OA6-CA5
31	m	201	CDL	CA6-CA4-OA6-CA5
32	X	201	8Q1	C13-C14-C15-C16
33	r	503	PLX	C28-C29-C30-C31
30	j	201	PEE	C15-C16-C17-C18
31	V	202	CDL	C61-C62-C63-C64
31	V	201	CDL	C33-C34-C35-C36
33	r	503	PLX	C25-C26-C27-C28
30	U	102	PEE	O3P-C1-C2-O2
31	V	201	CDL	OA5-CA3-CA4-OA6
31	a	201	CDL	OB5-CB3-CB4-OB6
30	l	704	PEE	C16-C17-C18-C19
31	r	504	CDL	C76-C77-C78-C79
31	m	201	CDL	C11-C12-C13-C14
30	W	201	PEE	C5-C4-O4P-P
30	r	501	PEE	C5-C4-O4P-P
30	l	703	PEE	C37-C38-C39-C40
30	W	201	PEE	O2-C2-C3-O3
30	l	703	PEE	O2-C2-C3-O3
30	l	704	PEE	O2-C2-C3-O3
31	V	201	CDL	OA6-CA4-CA6-OA8
31	i	401	CDL	OA6-CA4-CA6-OA8
31	s	401	CDL	OA6-CA4-CA6-OA8
33	r	502	PLX	O6-C4-C5-O8
33	r	503	PLX	O6-C4-C5-O8
30	r	501	PEE	C41-C42-C43-C44
33	j	202	PLX	C31-C32-C33-C34
30	U	101	PEE	C12-C13-C14-C15
33	g	201	PLX	C6-C7-C8-C9
31	V	201	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
31	r	504	CDL	C21-C22-C23-C24
31	a	201	CDL	C21-C22-C23-C24
31	s	401	CDL	OB9-CB7-OB8-CB6
31	s	401	CDL	C75-C76-C77-C78
33	j	202	PLX	N1-C1-C2-O1
31	r	505	CDL	C58-C59-C60-C61
33	j	203	PLX	C32-C33-C34-C35
31	a	201	CDL	OA7-CA5-OA6-CA4
31	a	201	CDL	O1-C1-CB2-OB2
31	r	505	CDL	C82-C83-C84-C85
30	r	501	PEE	C30-C31-C32-C33
31	u	201	CDL	C51-C52-C53-C54
30	U	102	PEE	C23-C24-C25-C26
31	r	504	CDL	C24-C25-C26-C27
33	a	202	PLX	C27-C28-C29-C30
32	X	201	8Q1	O33-C32-C34-O35
33	a	202	PLX	C25-C24-O8-C5
31	V	201	CDL	C32-C31-CA7-OA8
31	V	201	CDL	OA5-CA3-CA4-CA6
32	X	201	8Q1	O27-C28-C29-C31
30	U	101	PEE	C41-C42-C43-C44
31	u	201	CDL	C52-C53-C54-C55
31	m	201	CDL	C73-C74-C75-C76
31	s	401	CDL	C74-C75-C76-C77
31	m	201	CDL	CA4-CA3-OA5-PA1
31	r	504	CDL	OA7-CA5-OA6-CA4
33	j	202	PLX	O4-C3-C4-O6
30	r	501	PEE	C21-C22-C23-C24
31	V	202	CDL	C55-C56-C57-C58
30	U	102	PEE	C21-C22-C23-C24
31	V	202	CDL	C34-C35-C36-C37
31	r	505	CDL	C12-C13-C14-C15
31	V	201	CDL	OB9-CB7-OB8-CB6
30	j	201	PEE	O2-C2-C3-O3
31	u	201	CDL	OA6-CA4-CA6-OA8
31	V	202	CDL	CB2-C1-CA2-OA2
31	l	702	CDL	CA2-C1-CB2-OB2
31	r	504	CDL	C40-C41-C42-C43
31	r	505	CDL	C44-C45-C46-C47
31	V	201	CDL	CA3-CA4-CA6-OA8
33	j	202	PLX	C3-C4-C5-O8
32	X	201	8Q1	O27-C28-C29-C32

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Mol	Chain	Res	Type	Atoms
31	u	201	CDL	C57-C58-C59-C60
31	V	201	CDL	C71-CB7-OB8-CB6
31	u	201	CDL	C72-C73-C74-C75
30	U	101	PEE	C1-O3P-P-O2P
30	W	201	PEE	C1-O3P-P-O4P
30	W	201	PEE	C4-O4P-P-O1P
30	l	701	PEE	C4-O4P-P-O1P
30	r	501	PEE	C1-O3P-P-O1P
30	r	501	PEE	C1-O3P-P-O4P
30	r	501	PEE	C4-O4P-P-O2P
31	V	201	CDL	CB3-OB5-PB2-OB2
31	V	202	CDL	CA3-OA5-PA1-OA2
31	V	202	CDL	CA3-OA5-PA1-OA3
31	V	202	CDL	CA3-OA5-PA1-OA4
31	V	202	CDL	CB2-OB2-PB2-OB3
31	a	201	CDL	CA2-OA2-PA1-OA4
31	a	201	CDL	CB2-OB2-PB2-OB4
31	i	401	CDL	CA3-OA5-PA1-OA3
31	i	401	CDL	CB3-OB5-PB2-OB4
31	l	702	CDL	CB2-OB2-PB2-OB3
31	r	504	CDL	CB2-OB2-PB2-OB3
31	r	504	CDL	CB2-OB2-PB2-OB4
31	r	504	CDL	CB2-OB2-PB2-OB5
31	s	401	CDL	CB2-OB2-PB2-OB3
31	s	401	CDL	CB2-OB2-PB2-OB4
31	s	401	CDL	CB2-OB2-PB2-OB5
31	u	201	CDL	CA3-OA5-PA1-OA2
33	a	202	PLX	C5-C4-O6-C6
33	g	201	PLX	C3-O4-P1-O1
33	g	201	PLX	C3-O4-P1-O3
33	j	202	PLX	C3-O4-P1-O1
33	j	202	PLX	C2-O1-P1-O3
33	j	203	PLX	C3-O4-P1-O1
33	j	203	PLX	C3-O4-P1-O3
33	r	502	PLX	C3-O4-P1-O2
33	r	502	PLX	C3-O4-P1-O3
33	r	502	PLX	C2-O1-P1-O4
33	r	502	PLX	C2-O1-P1-O3
33	r	503	PLX	C5-C4-O6-C6
31	a	201	CDL	CA5-C11-C12-C13
30	U	101	PEE	C21-C22-C23-C24
31	s	401	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
30	r	501	PEE	C14-C15-C16-C17
33	a	202	PLX	C35-C36-C37-C38
30	W	201	PEE	C34-C35-C36-C37
31	V	202	CDL	CA7-C31-C32-C33
33	a	202	PLX	C25-C26-C27-C28
31	l	702	CDL	CA6-CA4-OA6-CA5
31	r	505	CDL	C52-C53-C54-C55
30	U	102	PEE	O3P-C1-C2-C3
31	V	202	CDL	C24-C25-C26-C27
31	m	201	CDL	C61-C62-C63-C64
30	j	201	PEE	C18-C19-C20-C21
31	s	401	CDL	C84-C85-C86-C87
31	r	505	CDL	C61-C62-C63-C64
30	l	703	PEE	O3P-C1-C2-O2
31	V	202	CDL	OA5-CA3-CA4-OA6
31	r	505	CDL	C41-C42-C43-C44
31	r	504	CDL	C54-C55-C56-C57
30	U	101	PEE	C22-C23-C24-C25
31	V	202	CDL	C53-C54-C55-C56
31	V	202	CDL	C71-C72-C73-C74
31	r	505	CDL	OB6-CB4-CB6-OB8
31	r	505	CDL	C72-C71-CB7-OB8
31	V	202	CDL	C16-C17-C18-C19
30	i	402	PEE	C39-C40-C41-C42
30	j	201	PEE	C12-C13-C14-C15
30	U	102	PEE	C44-C45-C46-C47
33	j	202	PLX	C24-C25-C26-C27
33	g	201	PLX	O6-C6-C7-C8
30	j	201	PEE	C31-C32-C33-C34
31	s	401	CDL	CB2-C1-CA2-OA2
30	l	704	PEE	C2-C1-O3P-P
31	a	201	CDL	C73-C74-C75-C76
33	r	502	PLX	C10-C11-C12-C13
31	r	504	CDL	C44-C45-C46-C47
30	U	101	PEE	C44-C45-C46-C47
31	a	201	CDL	C43-C44-C45-C46
33	g	201	PLX	C35-C36-C37-C38
31	s	401	CDL	C51-C52-C53-C54
33	j	203	PLX	C19-C20-C21-C22
31	V	201	CDL	CA5-C11-C12-C13
31	m	201	CDL	C79-C80-C81-C82
31	r	505	CDL	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	V	201	CDL	C36-C37-C38-C39
31	V	202	CDL	C22-C23-C24-C25
30	U	101	PEE	C31-C32-C33-C34
30	l	704	PEE	C11-C12-C13-C14
33	r	503	PLX	C6-C7-C8-C9
30	l	703	PEE	C24-C25-C26-C27
30	l	701	PEE	C3-C2-O2-C10
31	a	201	CDL	CA3-CA4-OA6-CA5
30	i	402	PEE	C24-C25-C26-C27
33	a	202	PLX	C24-C25-C26-C27
31	a	201	CDL	C59-C60-C61-C62
30	i	402	PEE	C18-C19-C20-C21
31	r	505	CDL	C39-C40-C41-C42
31	V	201	CDL	C21-C22-C23-C24
31	r	505	CDL	C73-C74-C75-C76
31	u	201	CDL	OB5-CB3-CB4-OB6
33	j	203	PLX	C10-C11-C12-C13
30	l	701	PEE	C16-C17-C18-C19
30	r	501	PEE	C24-C25-C26-C27
31	i	401	CDL	C16-C17-C18-C19
31	s	401	CDL	C16-C17-C18-C19
33	r	503	PLX	C19-C20-C21-C22
31	l	702	CDL	C36-C37-C38-C39
31	l	702	CDL	C74-C75-C76-C77
31	m	201	CDL	OB6-CB4-CB6-OB8
30	l	703	PEE	C11-C12-C13-C14
33	a	202	PLX	C28-C29-C30-C31
33	r	503	PLX	C11-C10-C9-C8
31	a	201	CDL	C23-C24-C25-C26
30	U	101	PEE	C2-C3-O3-C30
31	r	505	CDL	CA2-C1-CB2-OB2
30	U	102	PEE	C20-C21-C22-C23
33	a	202	PLX	C17-C18-C19-C20
31	l	702	CDL	C16-C17-C18-C19
31	m	201	CDL	C75-C76-C77-C78
31	s	401	CDL	C77-C78-C79-C80
32	X	201	8Q1	C9-C10-C11-C12
31	i	401	CDL	C62-C63-C64-C65
30	U	102	PEE	C12-C13-C14-C15
33	j	202	PLX	C11-C10-C9-C8
30	U	101	PEE	C24-C25-C26-C27
31	l	702	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
30	j	201	PEE	O3-C30-C31-C32
31	u	201	CDL	CA3-CA4-CA6-OA8
31	m	201	CDL	C52-C51-CB5-OB7
30	U	101	PEE	C39-C40-C41-C42
33	j	203	PLX	C36-C37-C38-C39
30	l	703	PEE	C30-C31-C32-C33
34	s	402	UQ	C6-C7-C8-C9
30	l	701	PEE	C38-C39-C40-C41
30	l	703	PEE	C16-C17-C18-C19
31	a	201	CDL	C61-C62-C63-C64
31	u	201	CDL	C54-C55-C56-C57
30	l	704	PEE	C38-C39-C40-C41
31	l	702	CDL	CA4-CA3-OA5-PA1
33	r	502	PLX	C4-C3-O4-P1
31	r	505	CDL	C20-C21-C22-C23
33	j	202	PLX	C10-C11-C12-C13
30	W	201	PEE	C22-C23-C24-C25
31	a	201	CDL	C38-C39-C40-C41
30	l	703	PEE	C42-C43-C44-C45
30	i	402	PEE	C16-C17-C18-C19
30	i	402	PEE	C38-C39-C40-C41
30	l	703	PEE	C36-C37-C38-C39
31	u	201	CDL	C74-C75-C76-C77
30	l	701	PEE	C1-C2-O2-C10
30	U	102	PEE	C18-C19-C20-C21
31	r	504	CDL	C39-C40-C41-C42
31	m	201	CDL	C57-C58-C59-C60
31	r	505	CDL	C37-C38-C39-C40
34	s	402	UQ	C12-C13-C14-C16
33	a	202	PLX	C30-C31-C32-C33
30	U	102	PEE	C16-C17-C18-C19
31	r	505	CDL	C42-C43-C44-C45
31	s	401	CDL	C31-C32-C33-C34
33	r	503	PLX	C13-C14-C15-C16
33	r	503	PLX	O4-C3-C4-O6
31	r	505	CDL	C77-C78-C79-C80
30	l	703	PEE	C1-C2-C3-O3
31	m	201	CDL	OB9-CB7-OB8-CB6
31	u	201	CDL	OA9-CA7-OA8-CA6
33	j	203	PLX	C17-C18-C19-C20
30	W	201	PEE	C18-C19-C20-C21
31	l	702	CDL	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
33	j	203	PLX	C24-C25-C26-C27
31	s	401	CDL	C55-C56-C57-C58
31	l	702	CDL	O1-C1-CA2-OA2
31	u	201	CDL	O1-C1-CA2-OA2
30	U	101	PEE	C16-C17-C18-C19
30	W	201	PEE	C16-C17-C18-C19
31	l	702	CDL	C72-C71-CB7-OB8
30	l	703	PEE	O3P-C1-C2-C3
31	V	202	CDL	OA5-CA3-CA4-CA6
33	j	203	PLX	C7-C6-O6-C4
30	j	201	PEE	C22-C23-C24-C25
33	r	502	PLX	C26-C27-C28-C29
31	V	202	CDL	C32-C31-CA7-OA8
31	r	504	CDL	C51-CB5-OB6-CB4
31	i	401	CDL	C12-C11-CA5-OA6
30	l	703	PEE	C38-C39-C40-C41
31	r	504	CDL	OB7-CB5-OB6-CB4
33	j	203	PLX	C15-C16-C17-C18
31	V	202	CDL	C44-C45-C46-C47
31	i	401	CDL	C51-C52-C53-C54
30	U	101	PEE	O3-C30-C31-C32
31	V	202	CDL	O1-C1-CA2-OA2
31	m	201	CDL	C12-C13-C14-C15
31	a	201	CDL	C60-C61-C62-C63
31	V	202	CDL	C52-C51-CB5-OB6
31	r	505	CDL	C12-C11-CA5-OA6
34	s	402	UQ	C13-C14-C16-C17
33	g	201	PLX	O7-C6-C7-C8
31	V	202	CDL	CA5-C11-C12-C13
31	s	401	CDL	CA3-CA4-CA6-OA8
33	r	503	PLX	C2-C1-N1-C1C
31	V	202	CDL	C82-C83-C84-C85
30	U	102	PEE	C42-C43-C44-C45
30	l	704	PEE	C33-C34-C35-C36
31	V	202	CDL	C72-C73-C74-C75
31	V	201	CDL	OB6-CB4-CB6-OB8
31	r	505	CDL	OA6-CA4-CA6-OA8
31	V	202	CDL	C62-C63-C64-C65
31	r	504	CDL	C81-C82-C83-C84
31	r	504	CDL	C77-C78-C79-C80
31	m	201	CDL	C24-C25-C26-C27
33	r	502	PLX	C36-C37-C38-C39

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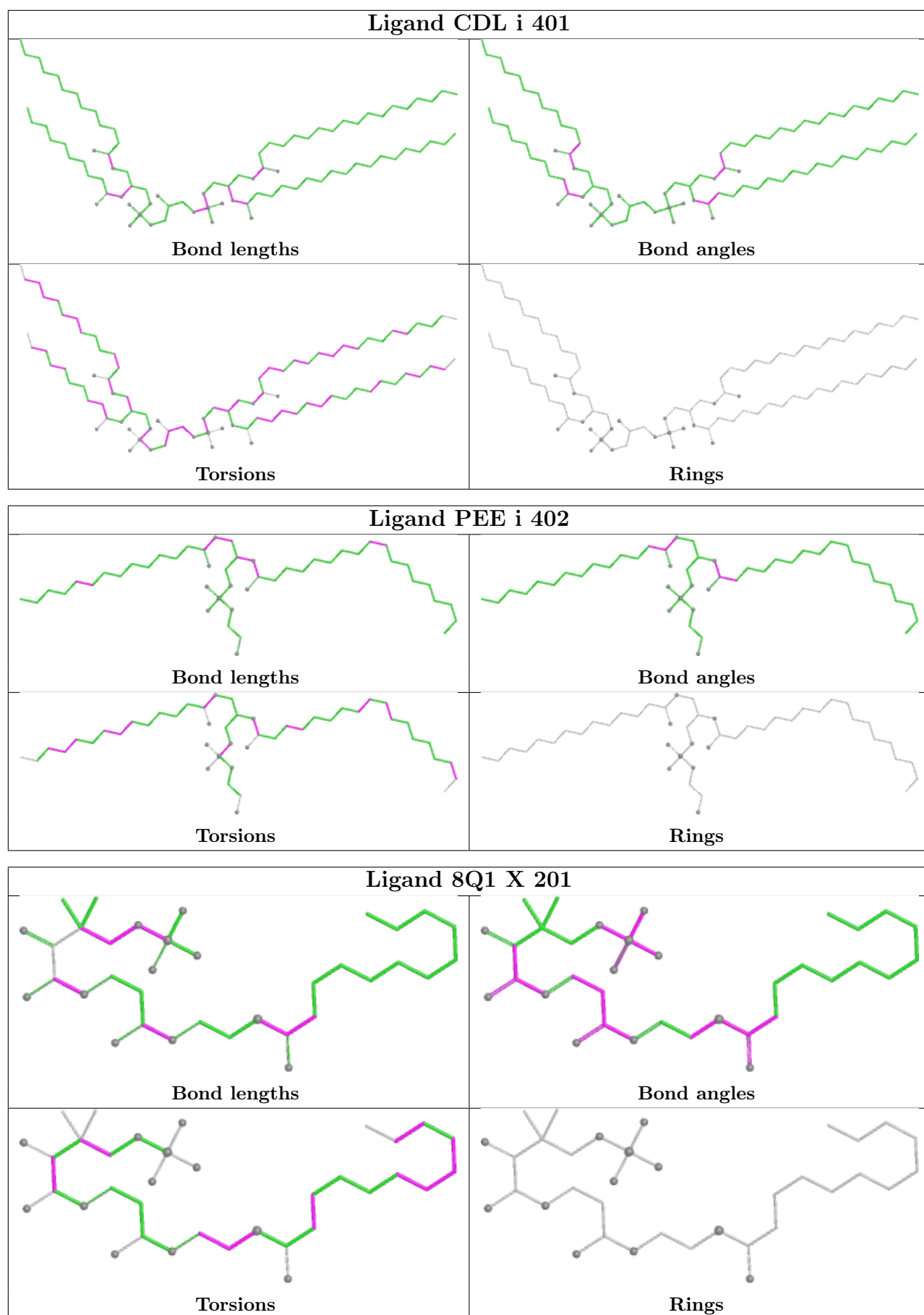
Mol	Chain	Res	Type	Atoms
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32	X	201	8Q1	O27-C28-C29-C30
31	V	201	CDL	C13-C14-C15-C16
31	u	201	CDL	C31-CA7-OA8-CA6
30	l	703	PEE	C3-C2-O2-C10
31	a	201	CDL	CA6-CA4-OA6-CA5
30	l	701	PEE	C11-C12-C13-C14
30	W	201	PEE	O4-C10-O2-C2
31	l	702	CDL	C80-C81-C82-C83
31	a	201	CDL	CA4-CA3-OA5-PA1
31	a	201	CDL	C36-C37-C38-C39
31	r	505	CDL	C78-C79-C80-C81
30	U	101	PEE	O5-C30-C31-C32
33	g	201	PLX	O8-C24-C25-C26
30	l	703	PEE	C33-C34-C35-C36
30	U	101	PEE	C20-C21-C22-C23
33	r	503	PLX	C2-C1-N1-C1B
33	j	202	PLX	C28-C29-C30-C31
30	U	101	PEE	O2-C10-C11-C12
30	U	102	PEE	C31-C32-C33-C34
31	a	201	CDL	C24-C25-C26-C27
33	r	503	PLX	O9-C24-O8-C5
31	l	702	CDL	C72-C71-CB7-OB9
33	g	201	PLX	C4-C5-O8-C24
31	s	401	CDL	C72-C71-CB7-OB8
31	V	202	CDL	C56-C57-C58-C59
31	r	505	CDL	C12-C11-CA5-OA7
31	m	201	CDL	C12-C11-CA5-OA6
31	V	202	CDL	C52-C51-CB5-OB7
31	l	702	CDL	OA5-CA3-CA4-CA6
33	a	202	PLX	O4-C3-C4-C5
31	V	201	CDL	C32-C33-C34-C35
31	V	201	CDL	C32-C31-CA7-OA9
31	r	505	CDL	OB9-CB7-OB8-CB6
30	l	701	PEE	C10-C11-C12-C13
30	U	102	PEE	C37-C38-C39-C40
31	m	201	CDL	C53-C54-C55-C56
30	U	102	PEE	O3-C30-C31-C32
31	V	202	CDL	C36-C37-C38-C39
30	U	101	PEE	O4-C10-C11-C12
31	r	504	CDL	C72-C71-CB7-OB9
30	U	102	PEE	C36-C37-C38-C39

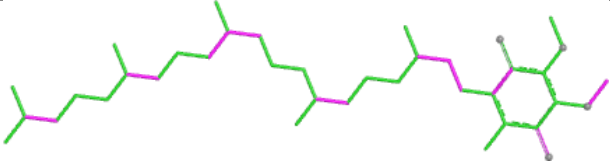
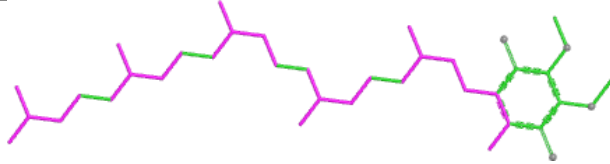
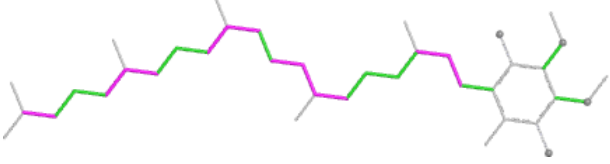
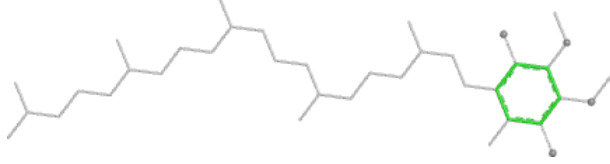
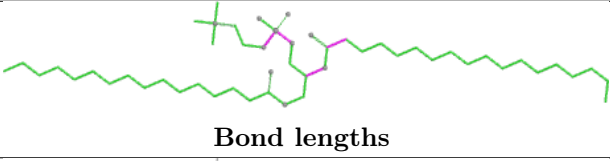
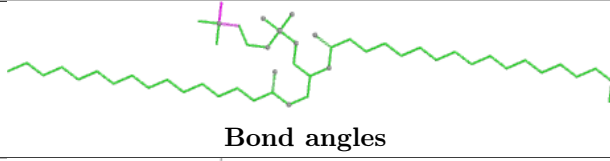
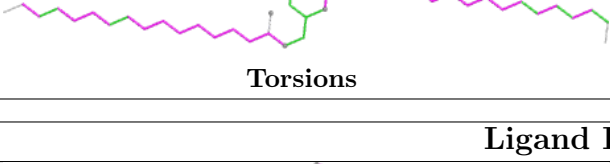
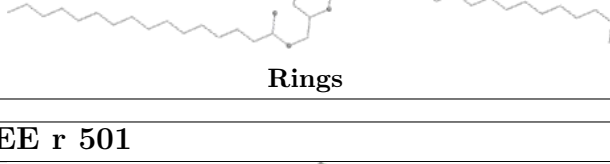
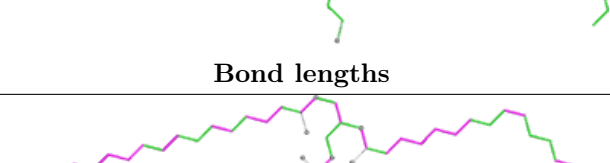
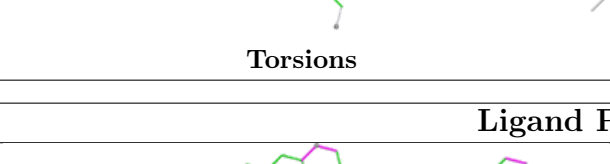
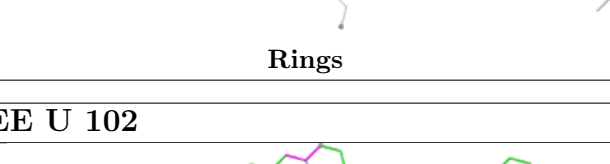
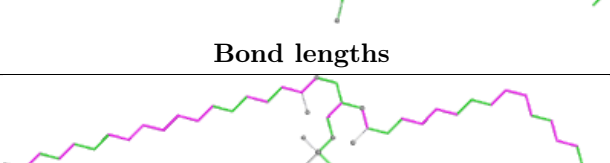
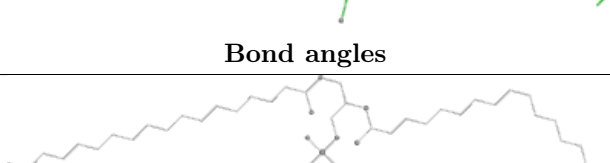
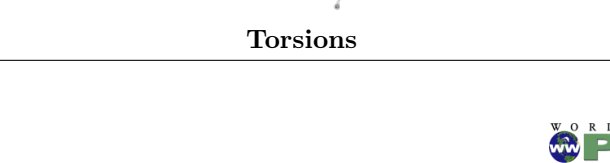
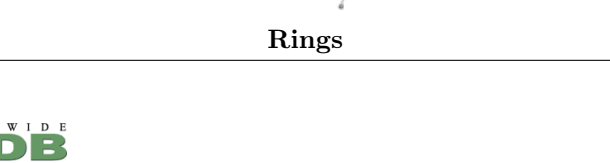
There are no ring outliers.

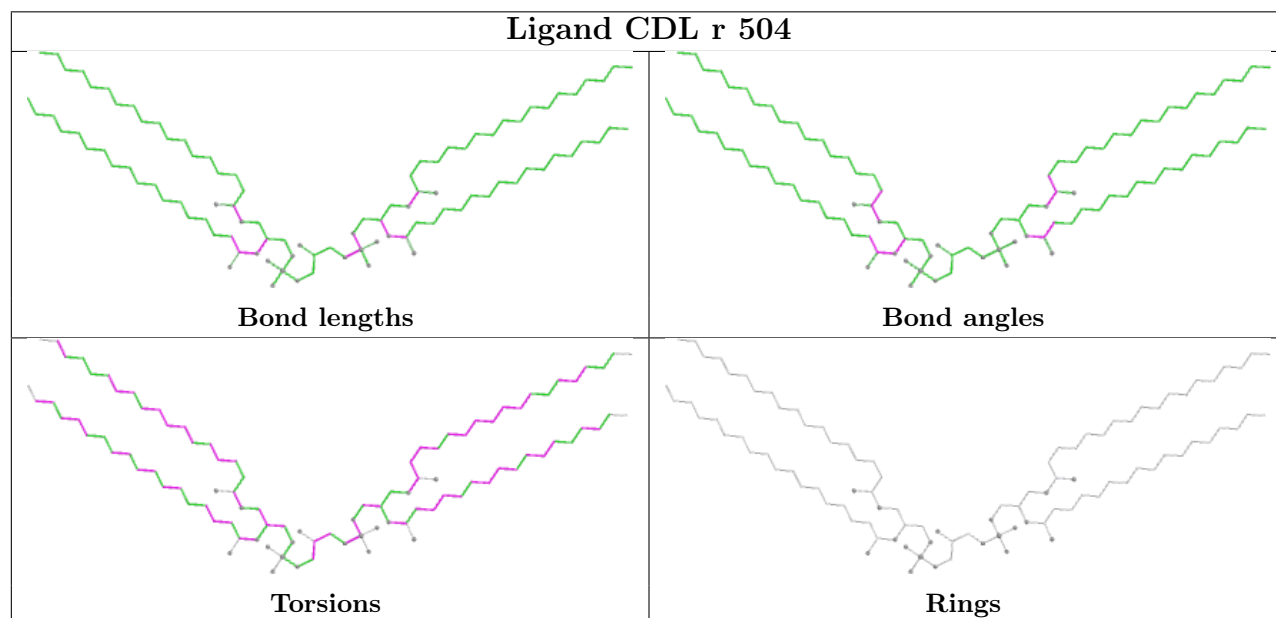
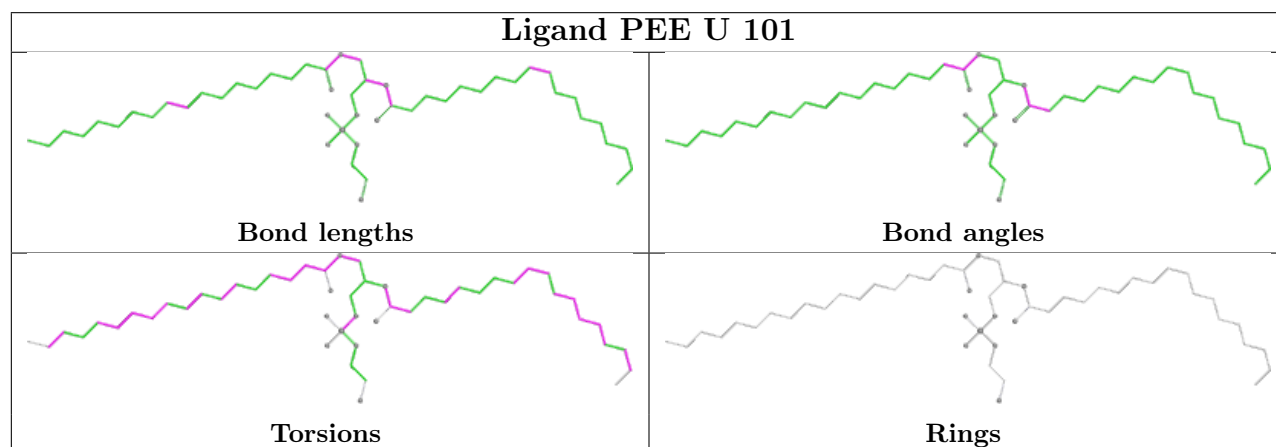
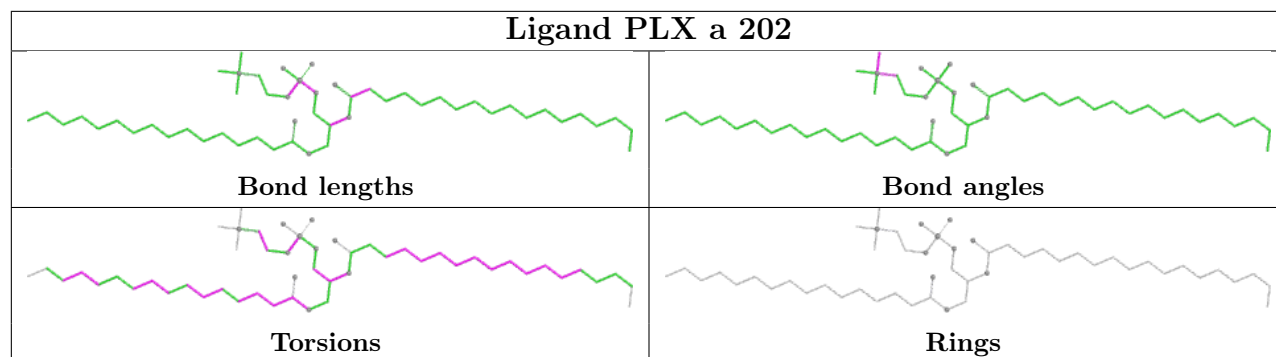
27 monomers are involved in 242 short contacts:

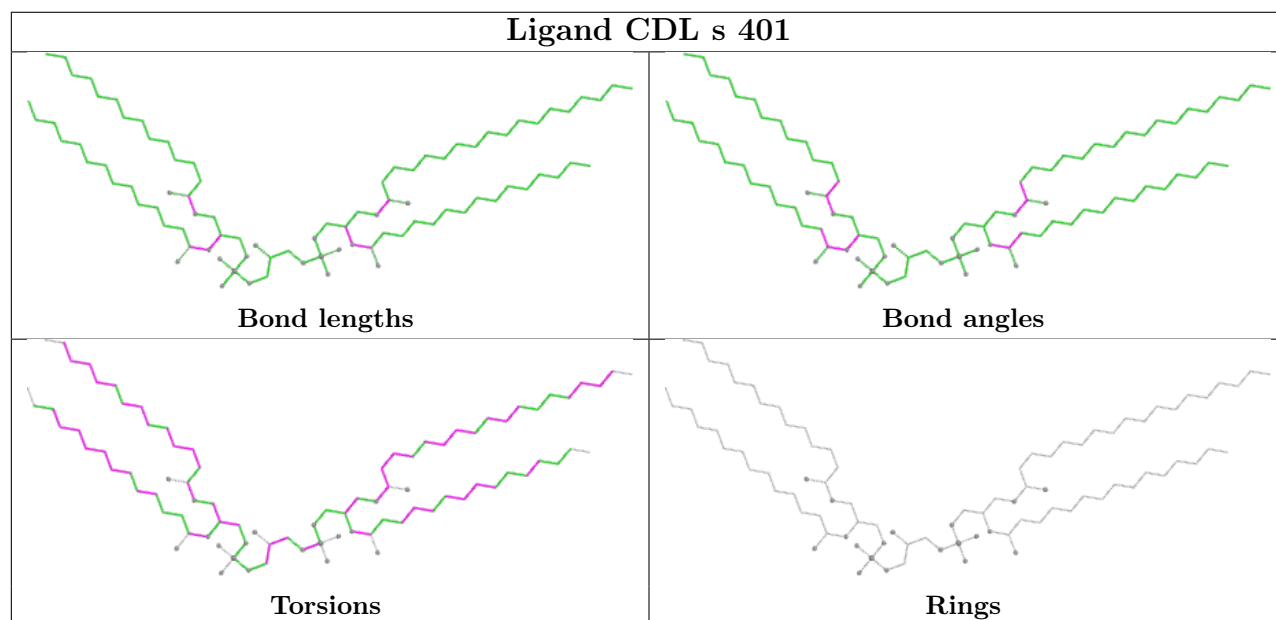
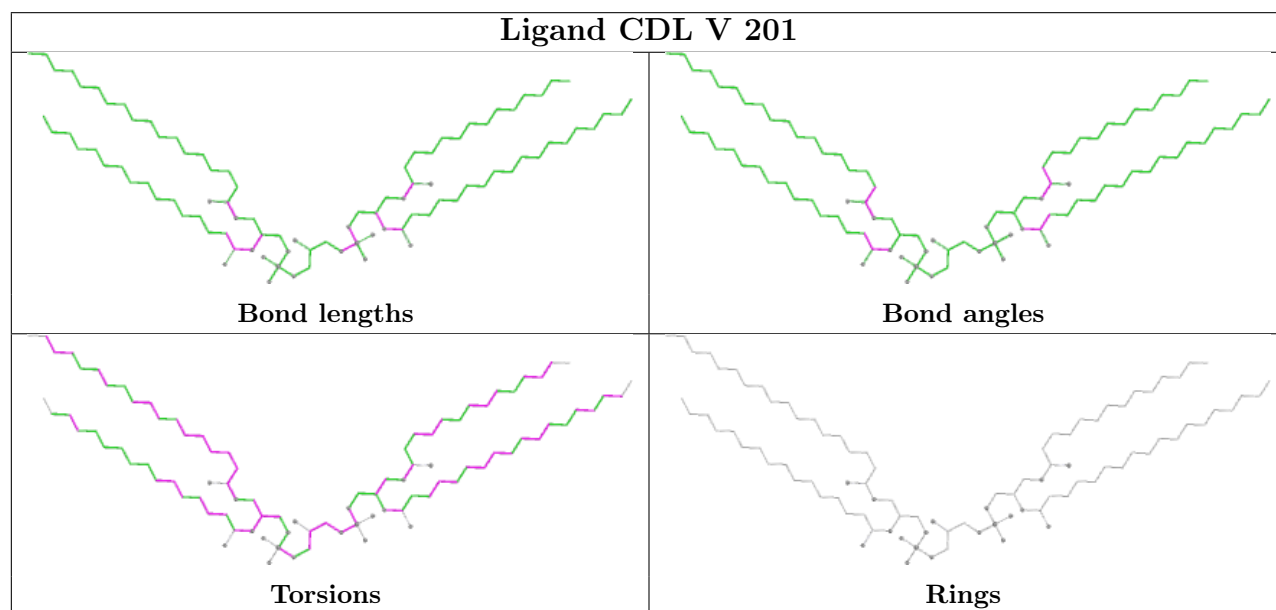
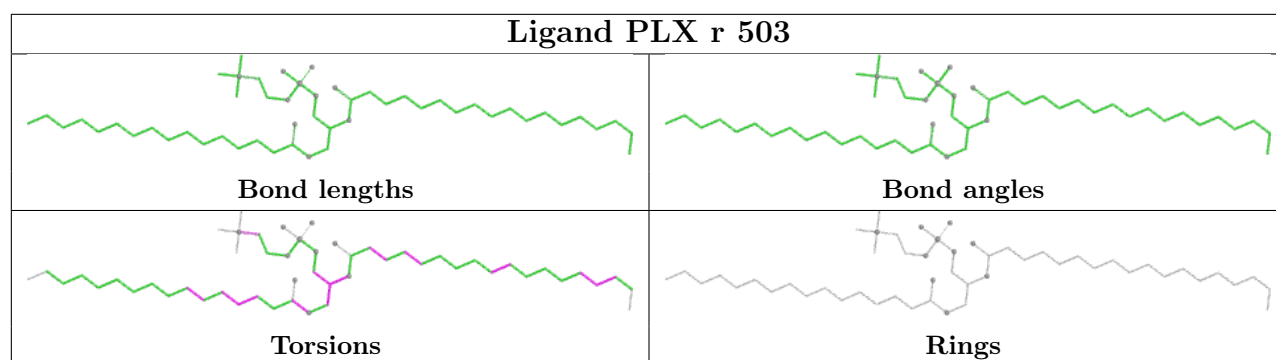
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	i	401	CDL	4	0
30	i	402	PEE	11	0
32	X	201	8Q1	1	0
34	s	402	UQ	1	0
33	j	203	PLX	4	0
30	r	501	PEE	16	0
30	U	102	PEE	3	0
30	U	101	PEE	6	0
31	r	504	CDL	15	0
33	r	503	PLX	21	0
31	V	201	CDL	3	0
31	s	401	CDL	6	0
30	j	201	PEE	11	0
33	j	202	PLX	5	0
31	a	201	CDL	15	0
33	r	502	PLX	4	0
33	g	201	PLX	4	0
30	l	704	PEE	23	0
30	l	703	PEE	10	0
35	w	401	ADP	6	0
31	u	201	CDL	5	0
30	W	201	PEE	8	0
31	V	202	CDL	7	0
30	l	701	PEE	7	0
31	m	201	CDL	10	0
31	r	505	CDL	38	0
31	l	702	CDL	21	0

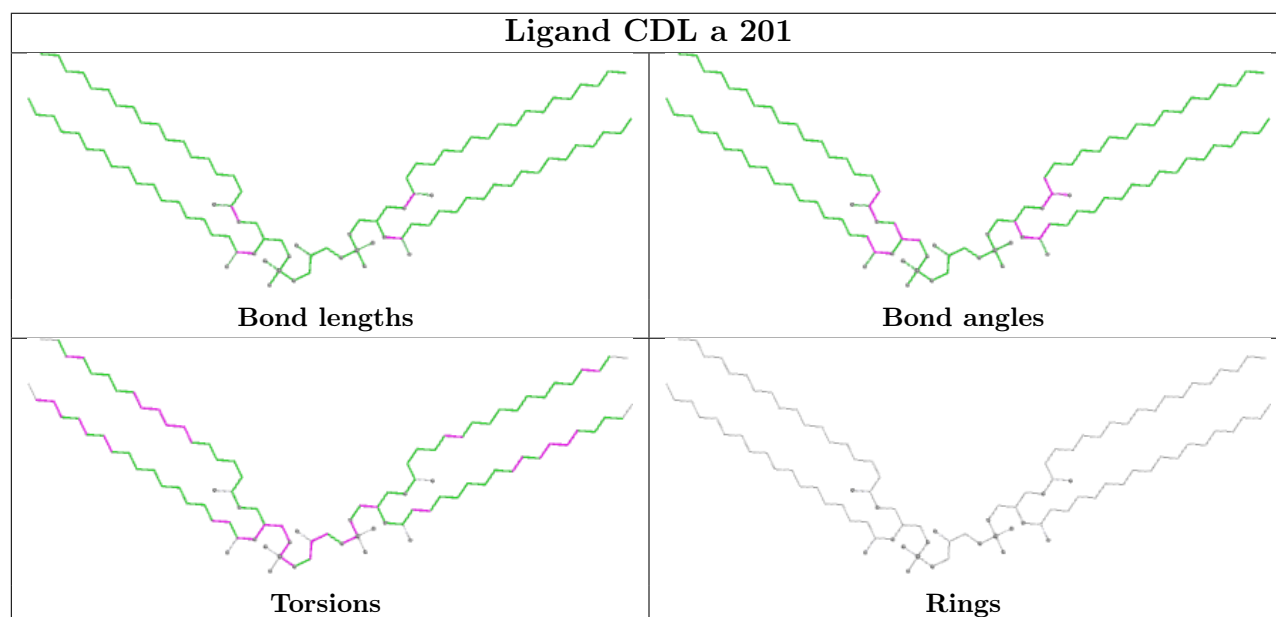
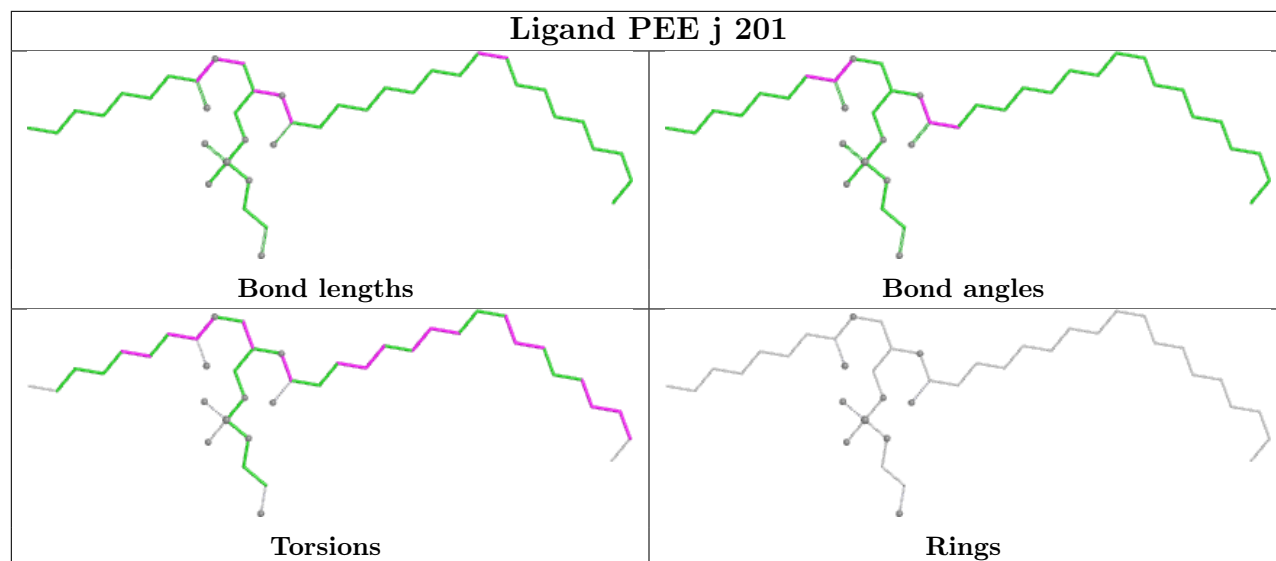
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

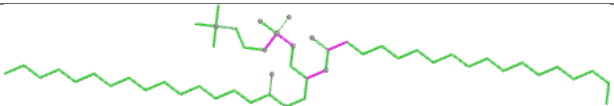
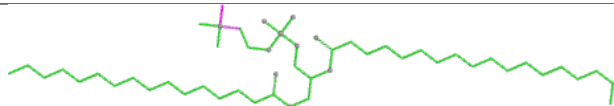
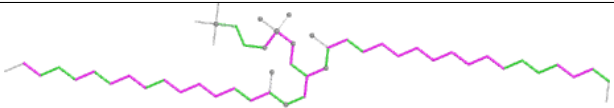
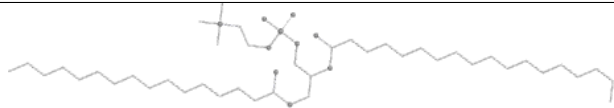


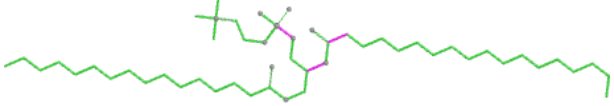
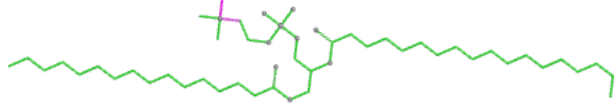
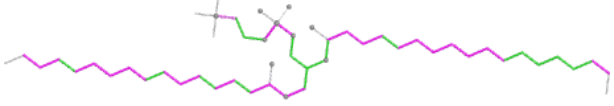
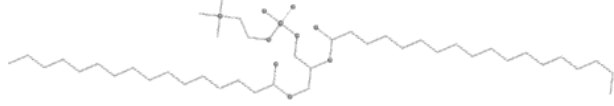
Ligand UQ s 402	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PLX j 203	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEE r 501	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PEE U 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

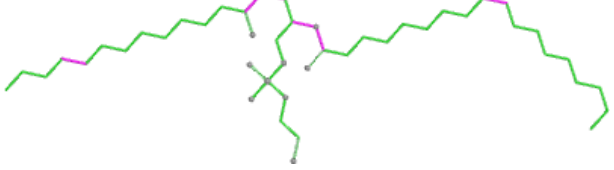
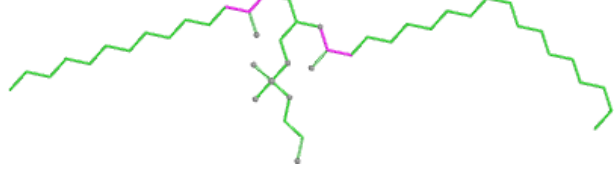
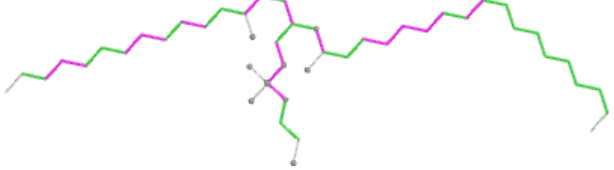
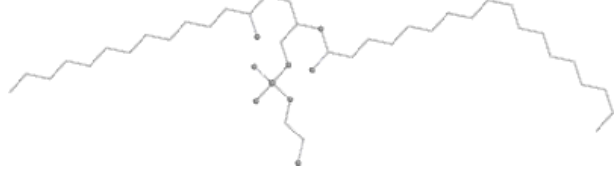


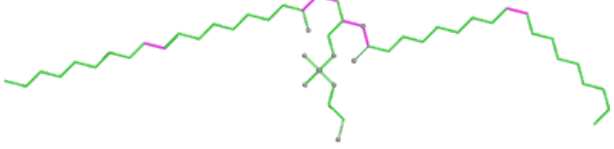
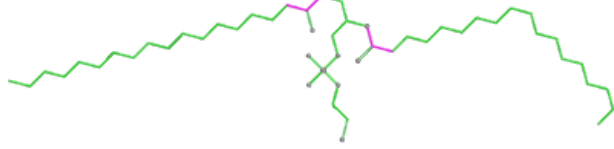
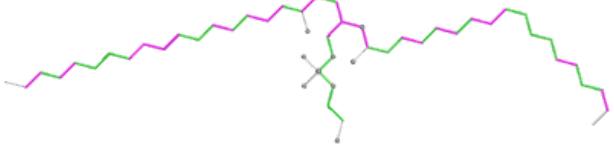
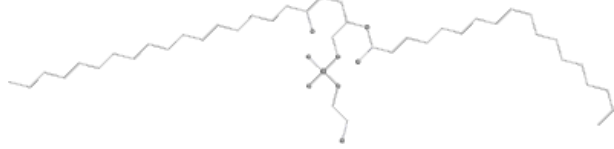


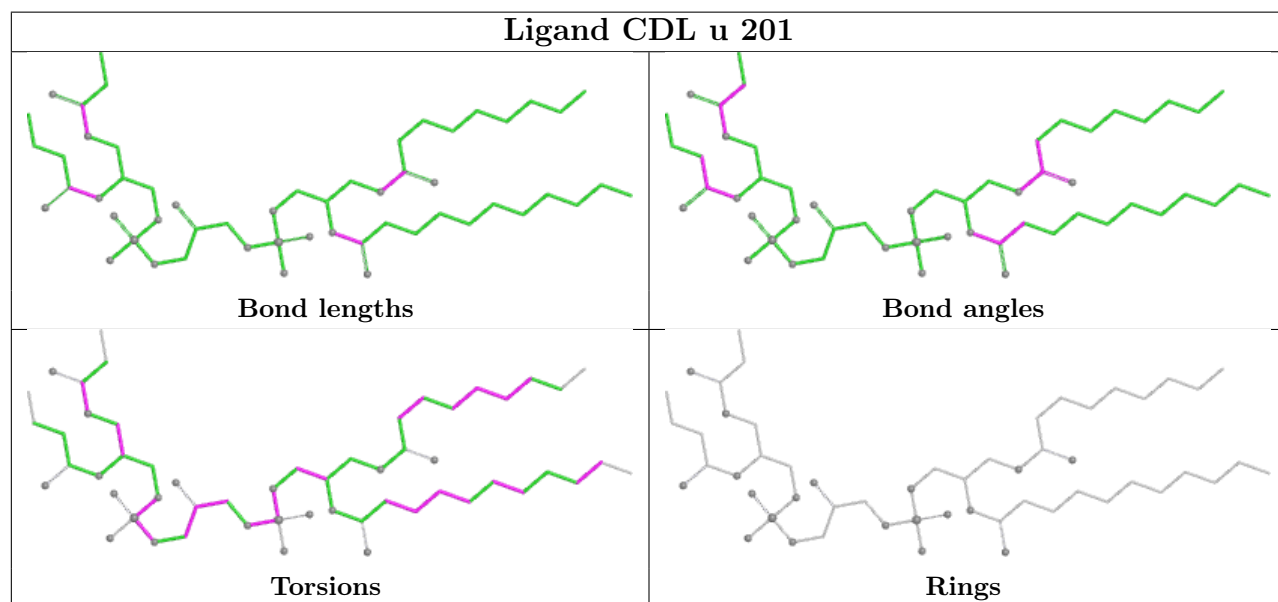
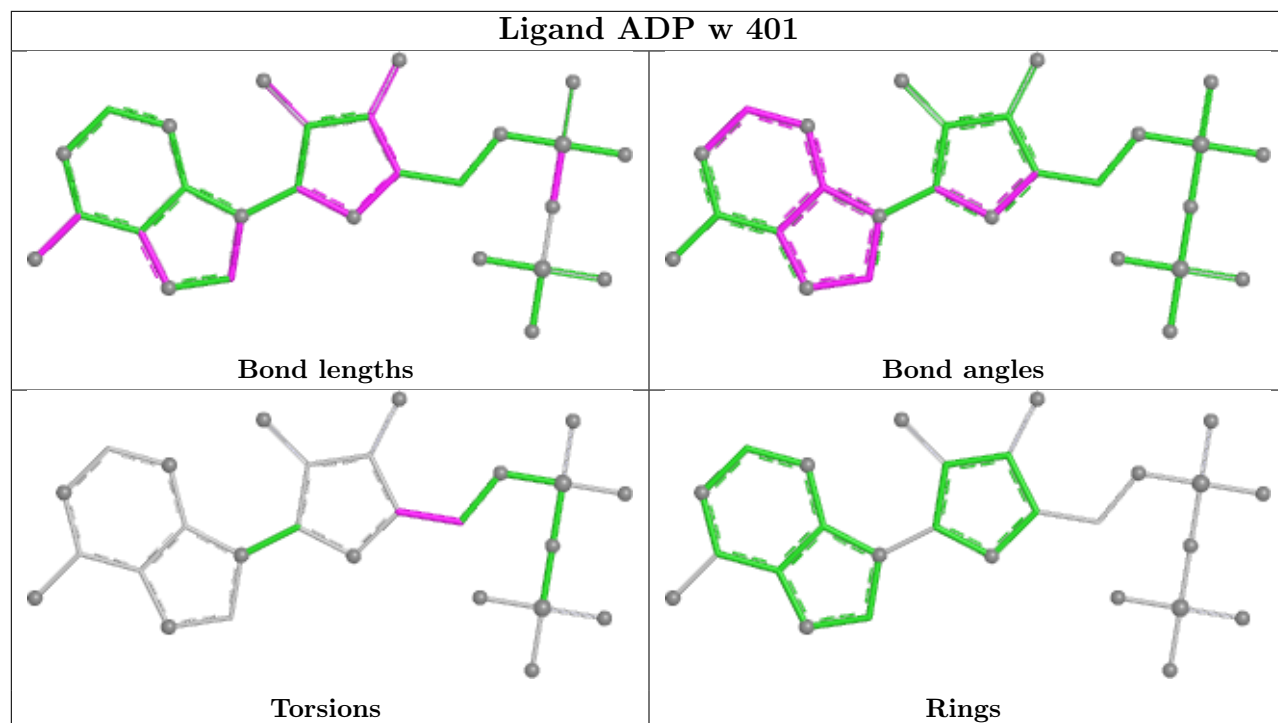


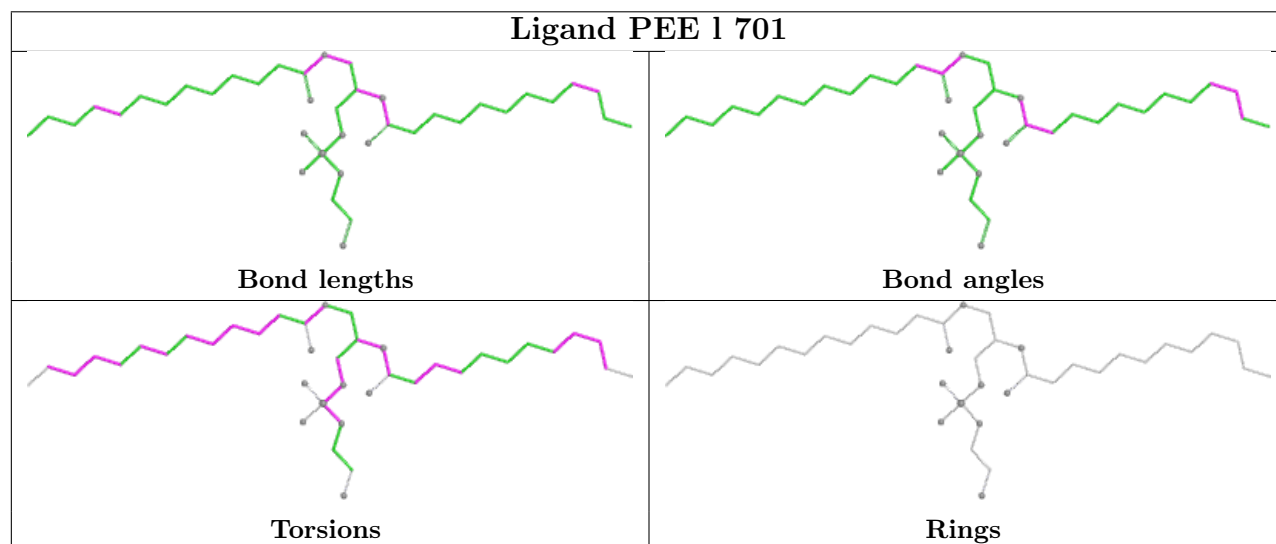
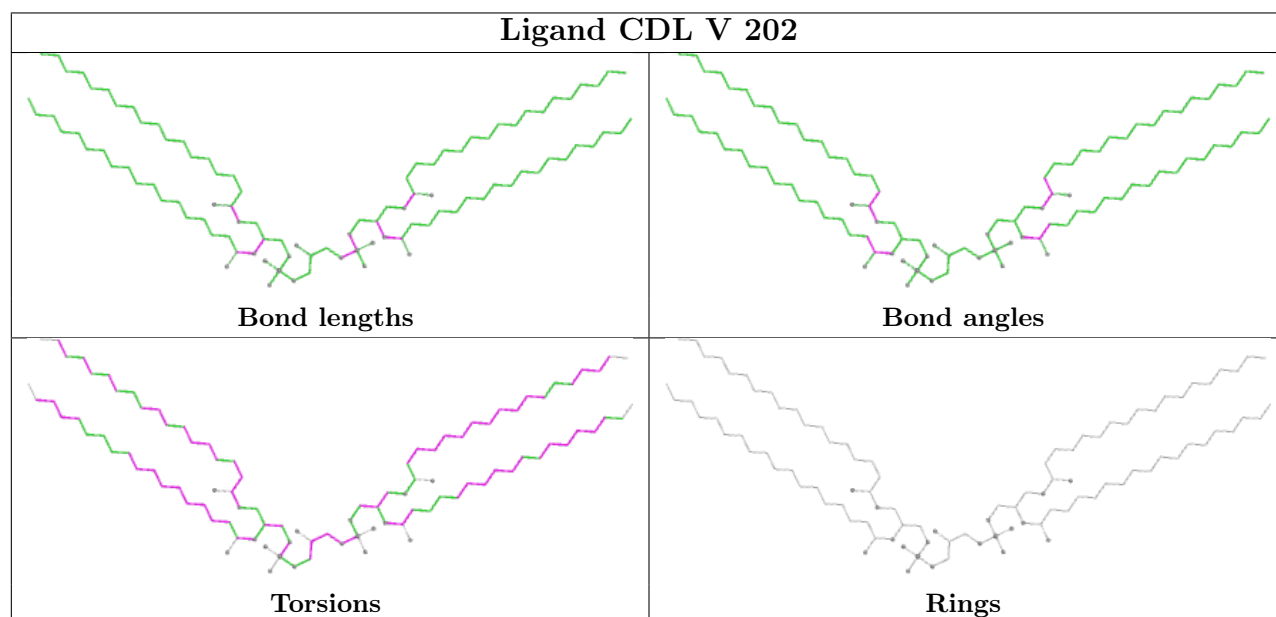
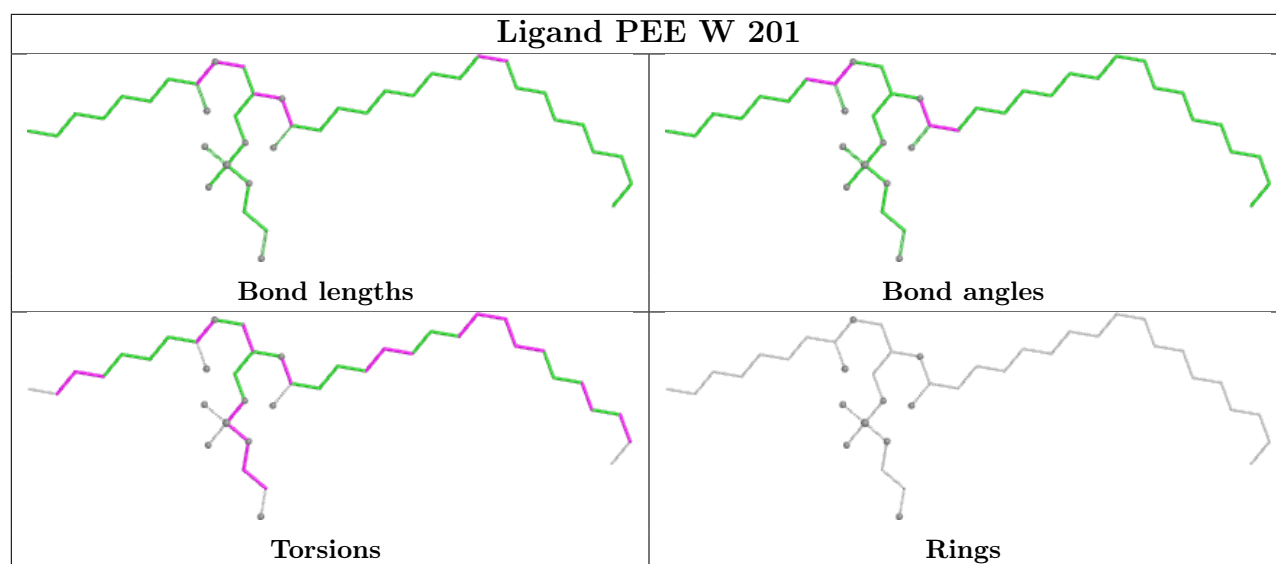
Ligand PLX r 502	
 Bond lengths	 Bond angles
 Torsions	 Rings

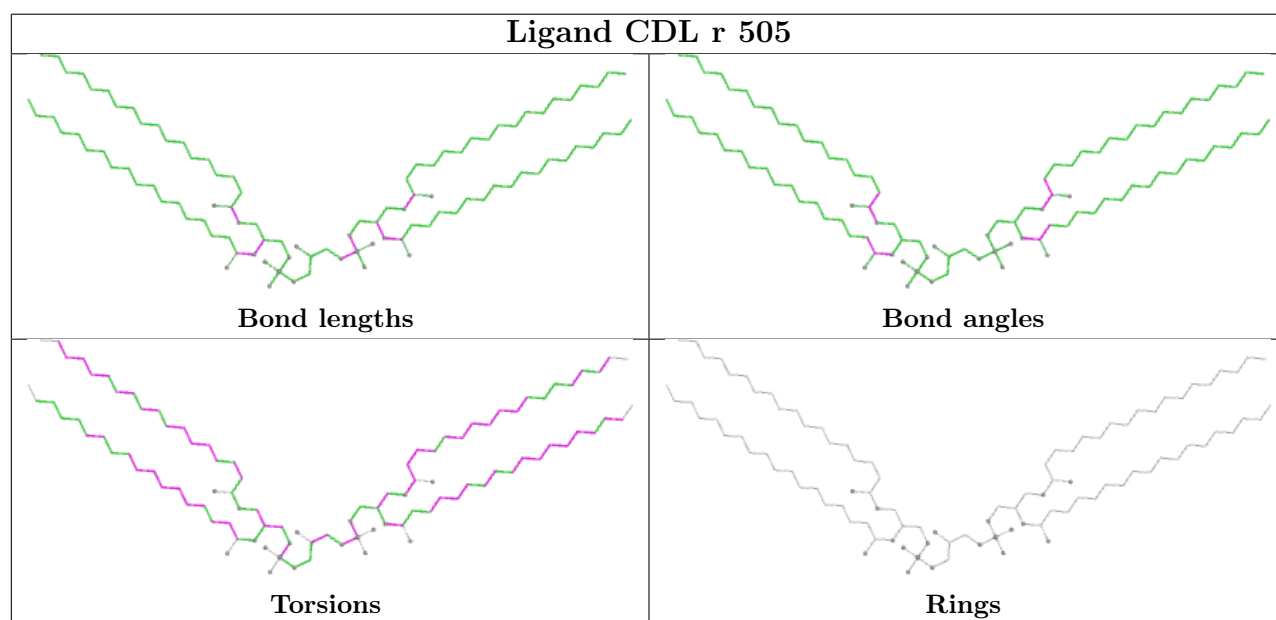
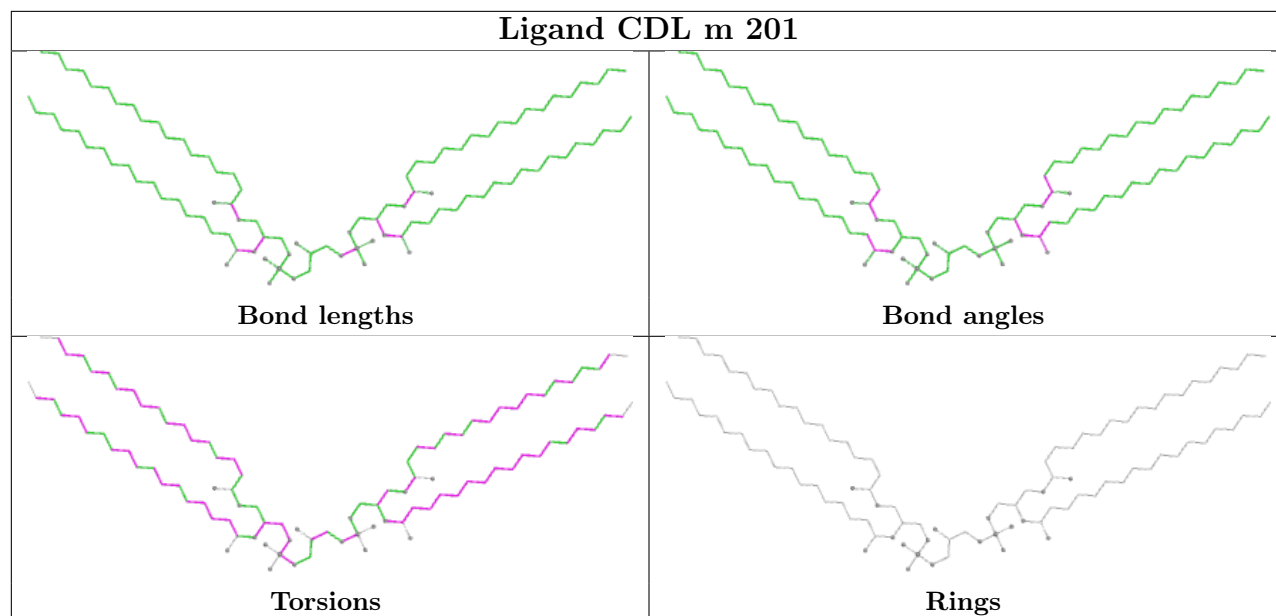
Ligand PLX g 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

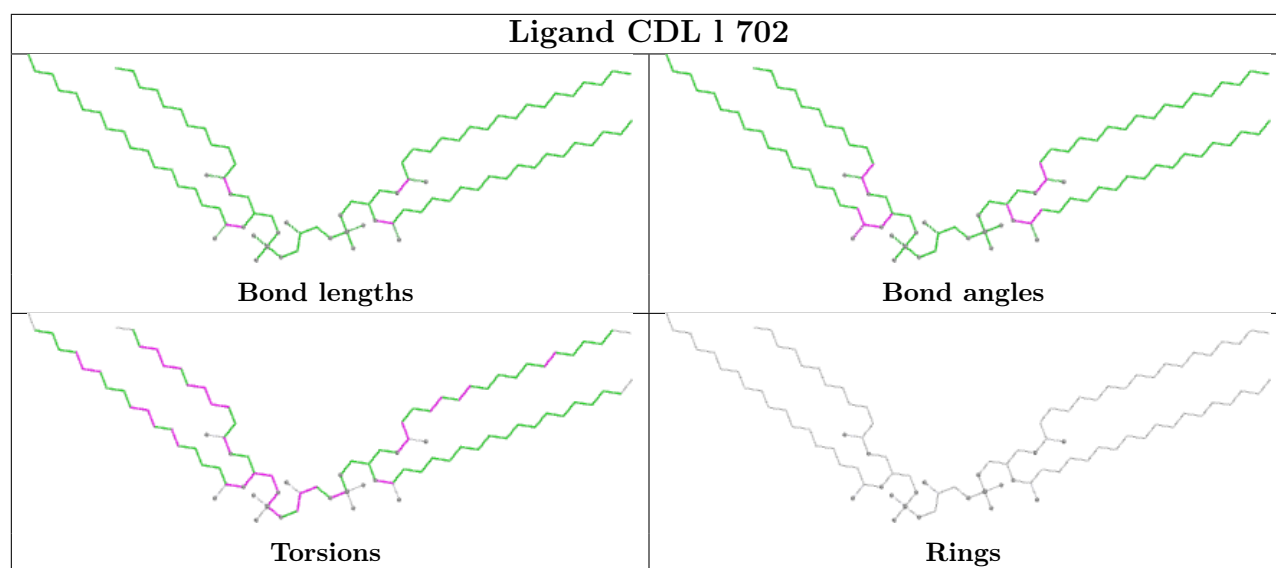
Ligand PEE l 704	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PEE l 703	
 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.

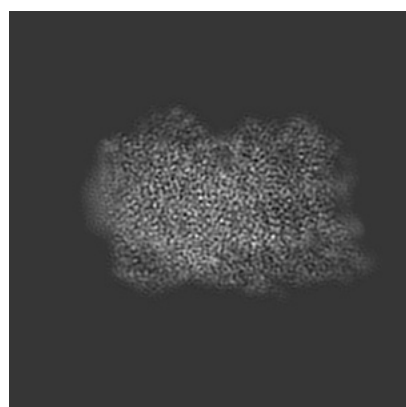
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31881. These allow visual inspection of the internal detail of the map and identification of artifacts.

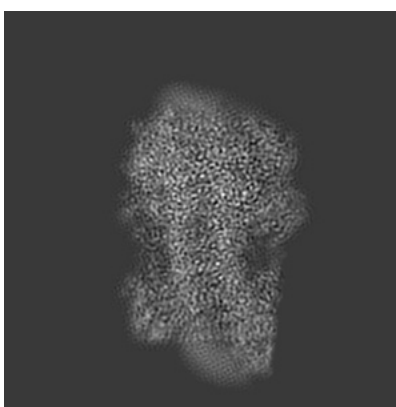
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

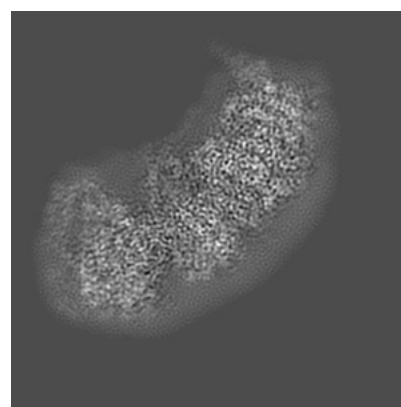
6.1.1 Primary map



X



Y

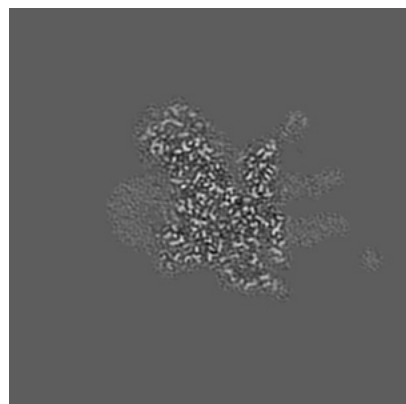


Z

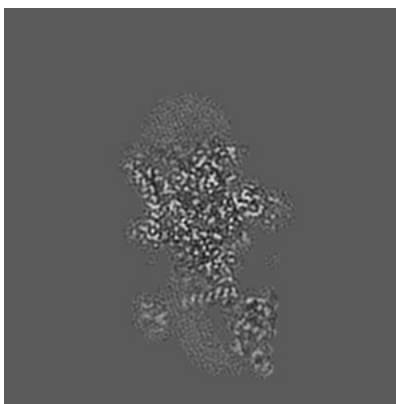
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

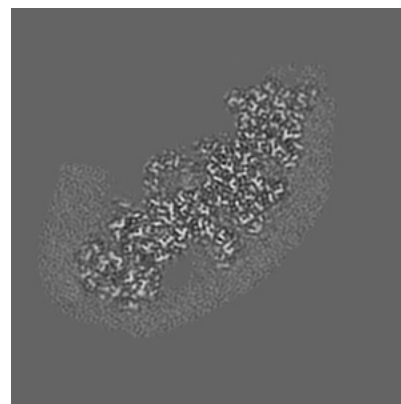
6.2.1 Primary map



X Index: 240



Y Index: 240

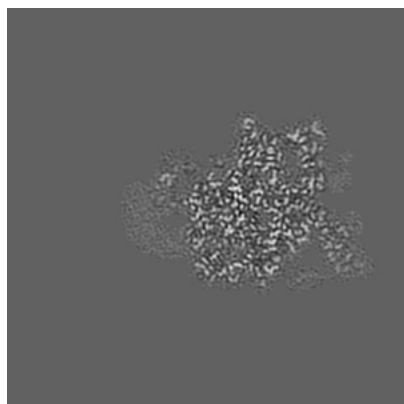


Z Index: 240

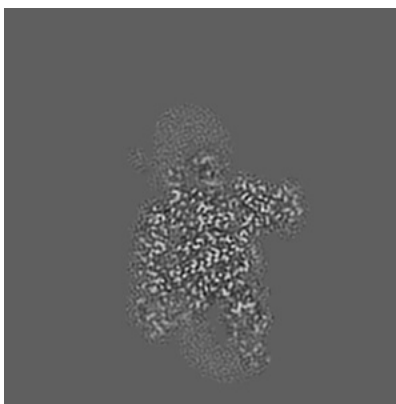
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

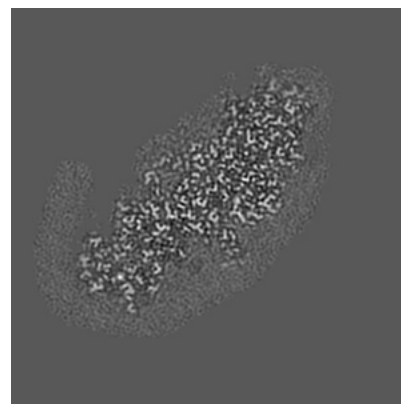
6.3.1 Primary map



X Index: 279



Y Index: 216

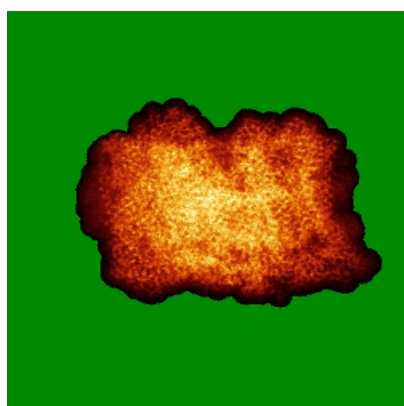


Z Index: 255

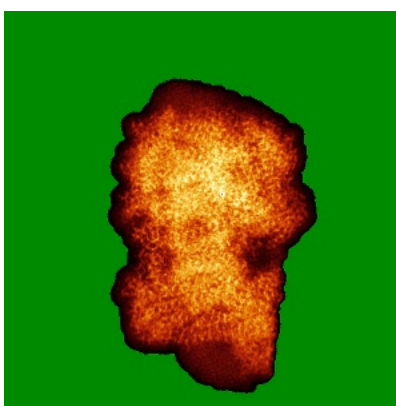
The images above show the largest variance slices of the map in three orthogonal directions.

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

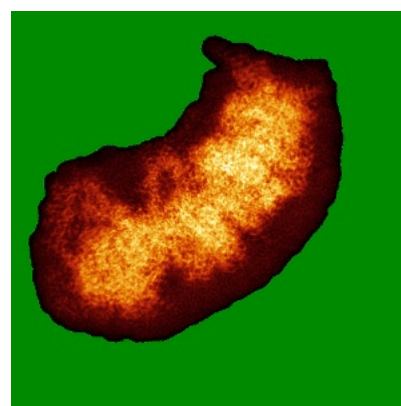
6.4.1 Primary map



X



Y

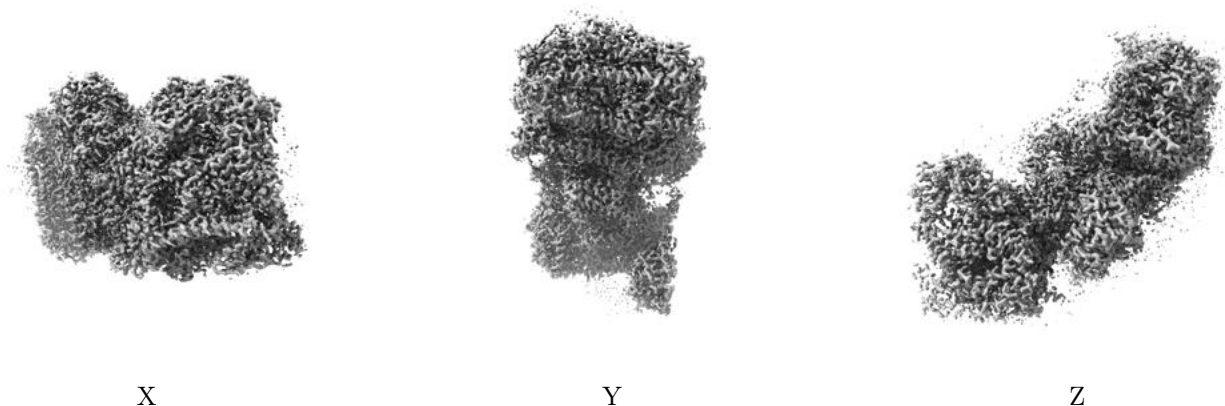


Z

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 0.0123. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

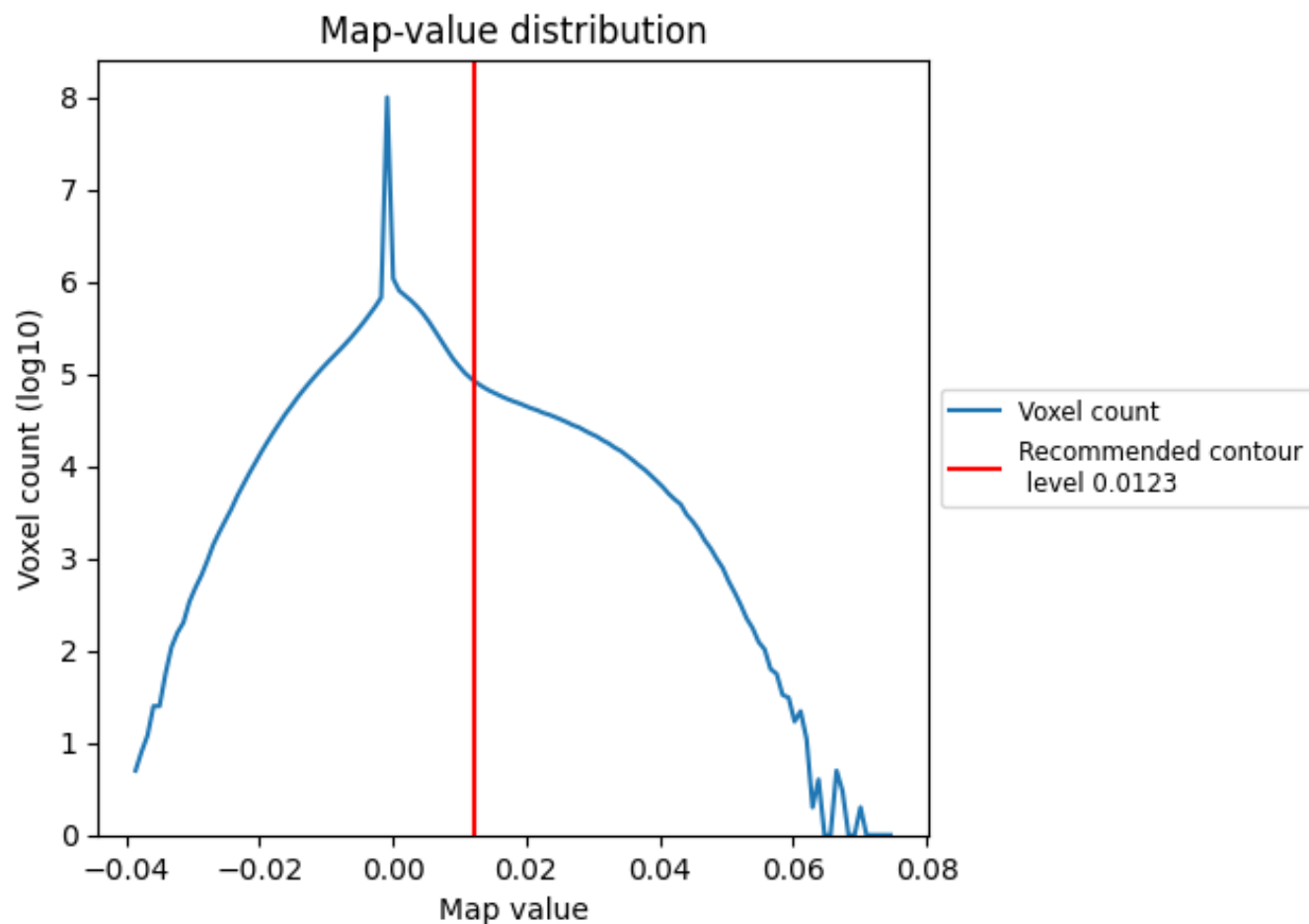
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

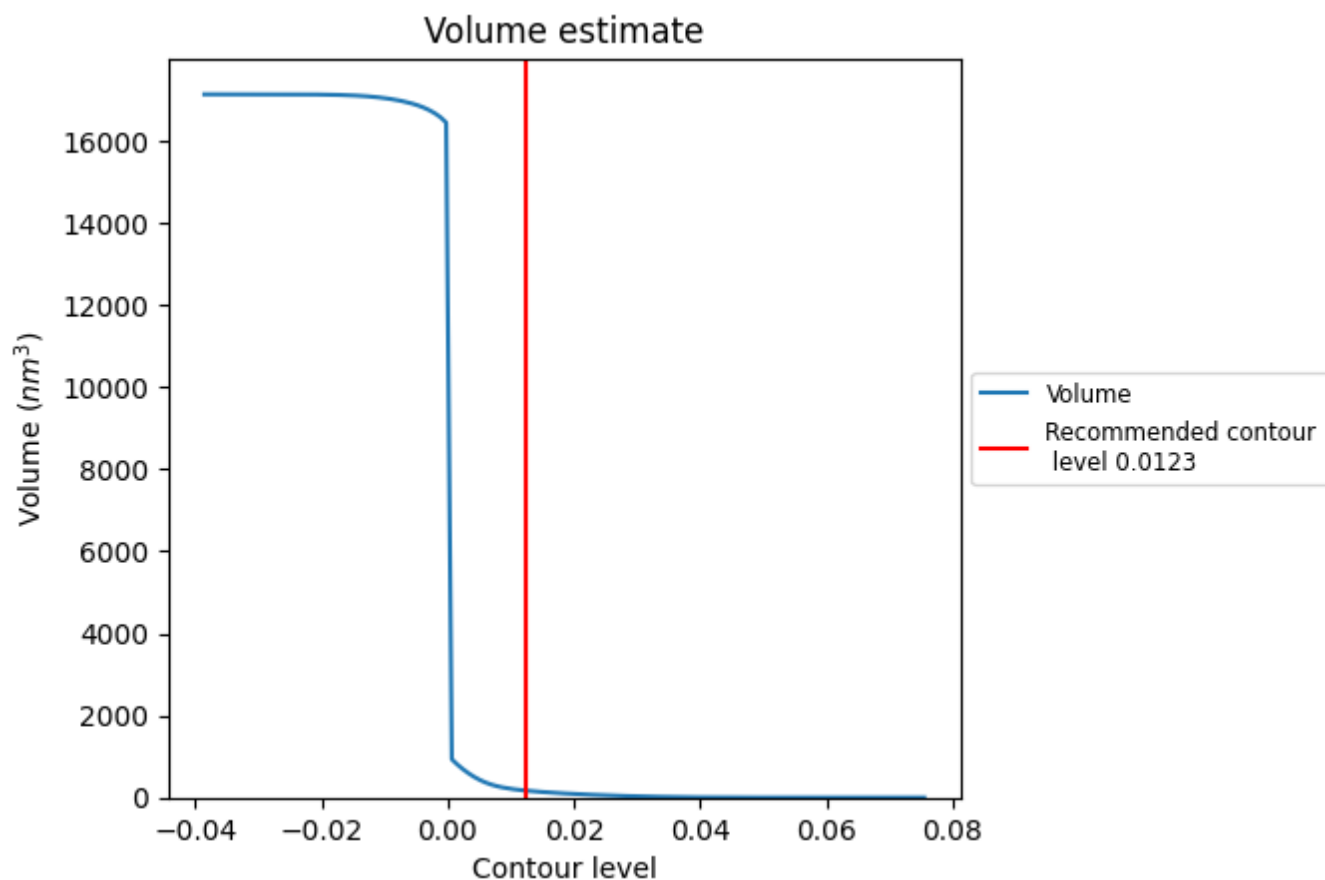
This section contains the results of statistical analysis of the map.

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.

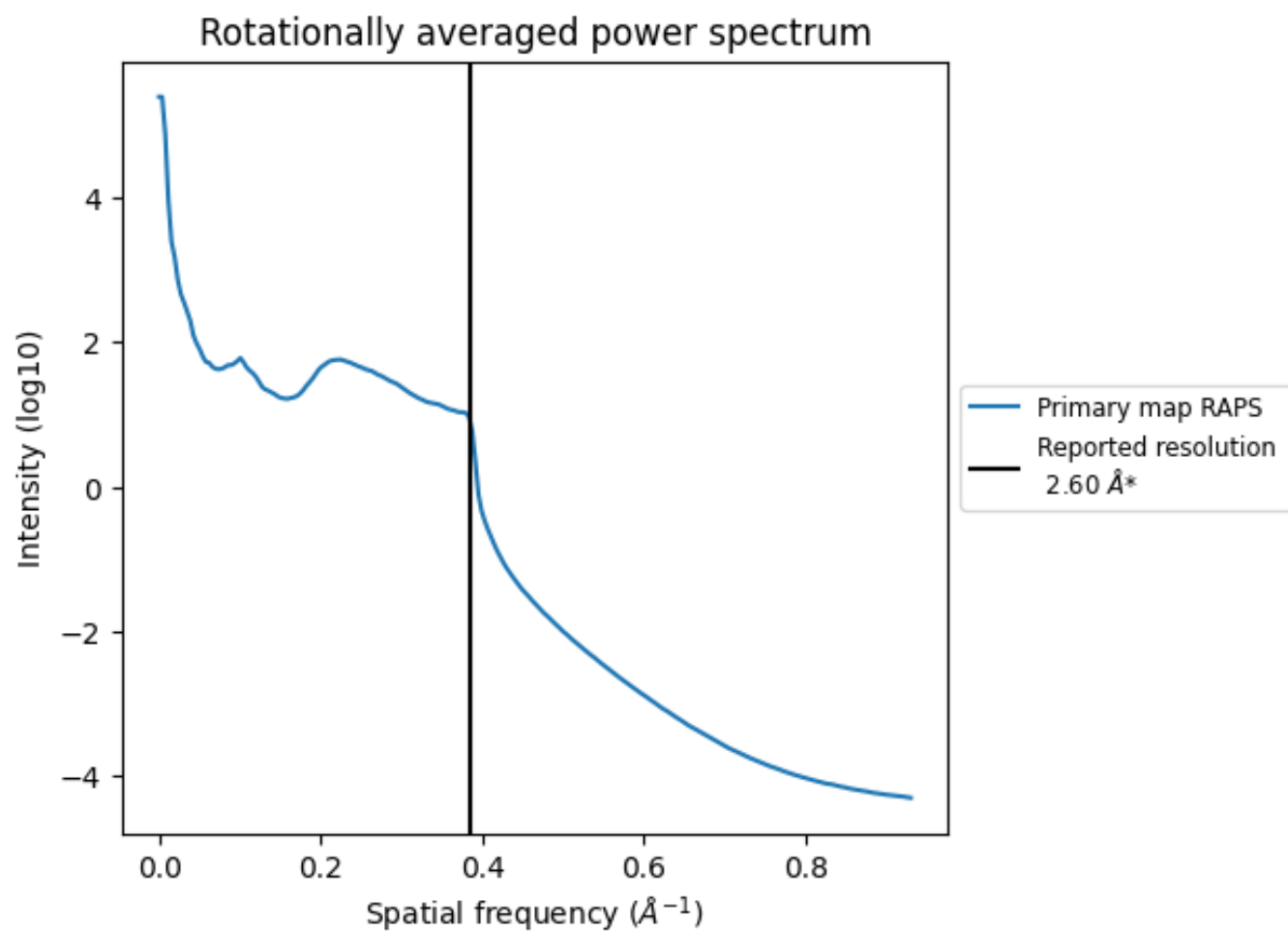
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 171 nm³; this corresponds to an approximate mass of 154 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 0.385 Å⁻¹

8 Fourier-Shell correlation

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

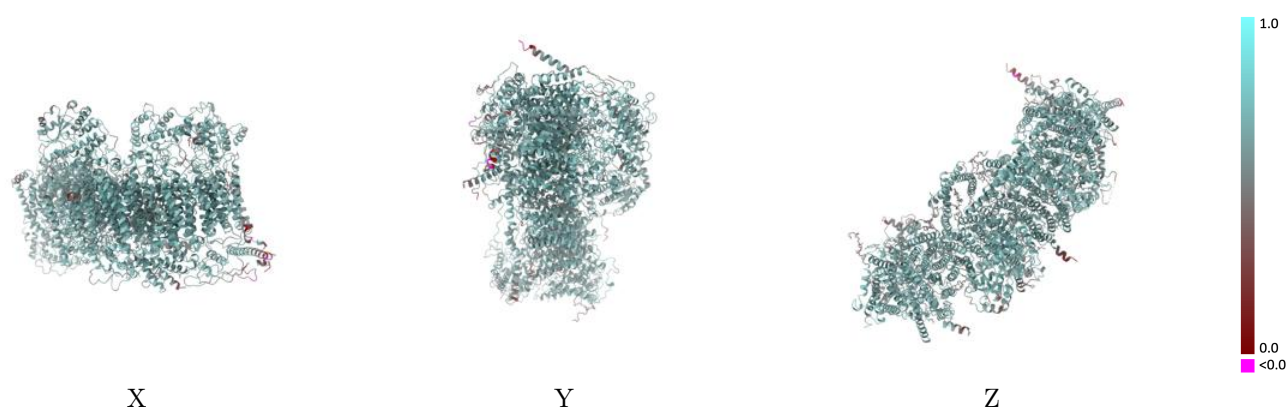
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31881 and PDB model 7VBL. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)

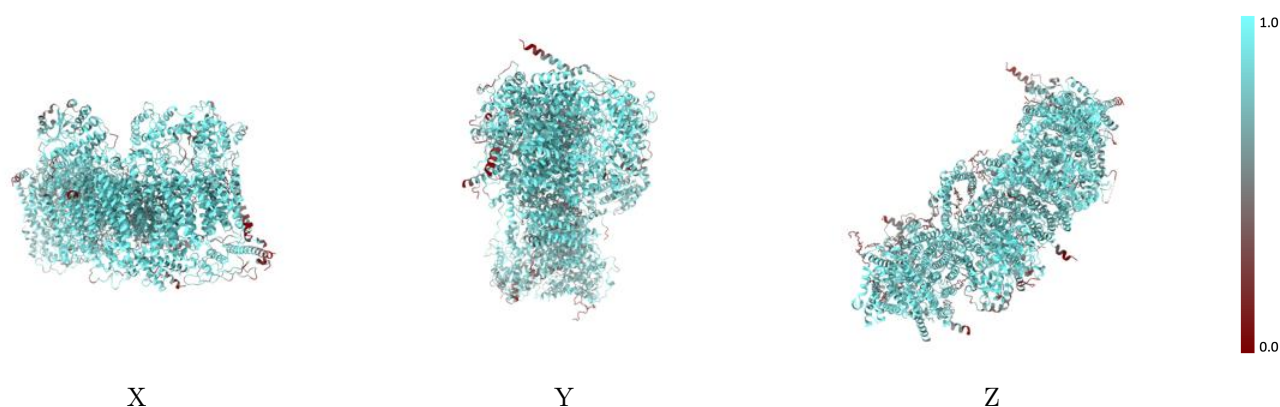
This section was not generated.

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



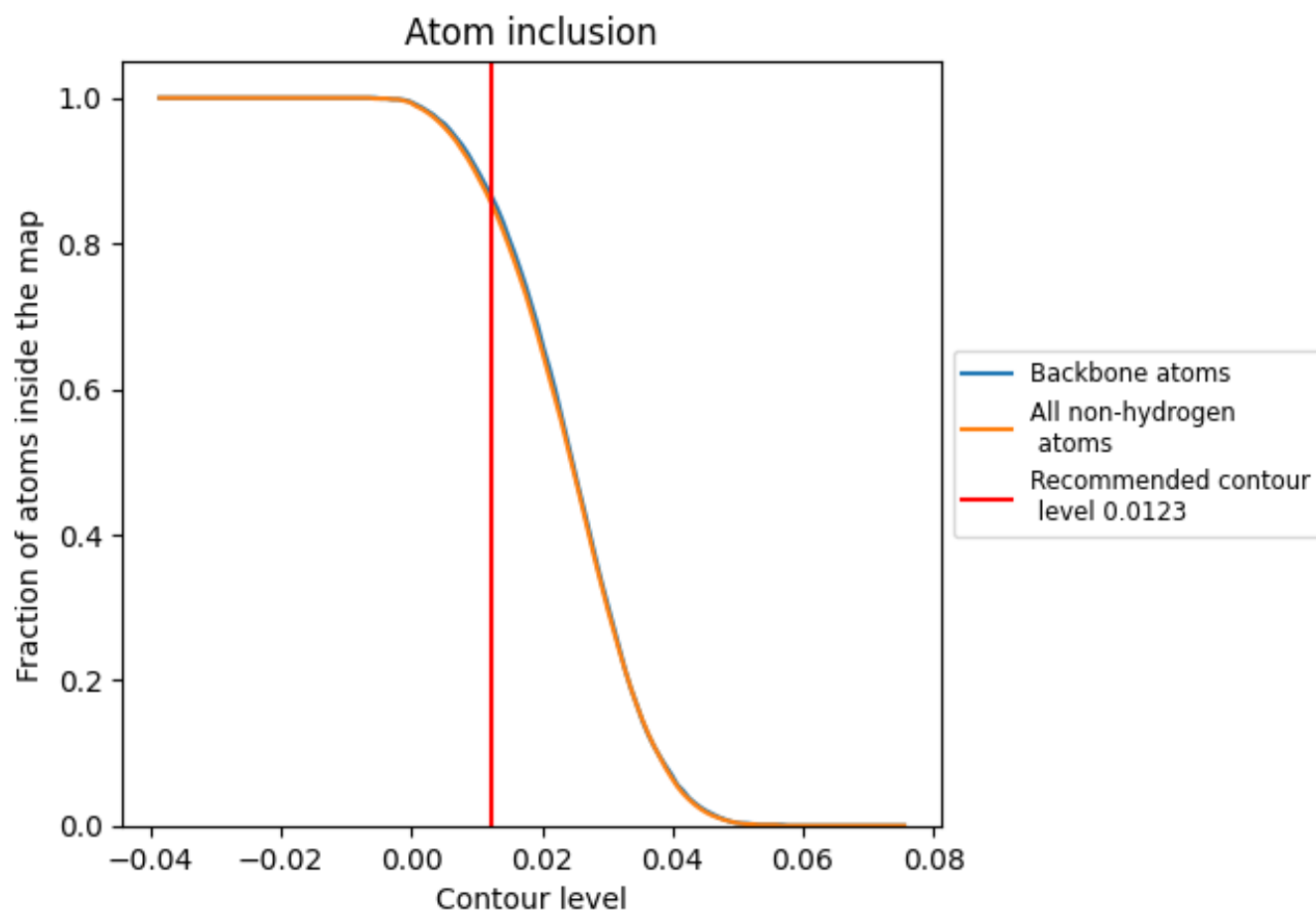
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0123).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.0123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8540	 0.6380
Q	 0.8150	 0.6250
S	 0.8700	 0.6350
U	 0.7620	 0.6040
V	 0.7450	 0.5990
W	 0.8140	 0.6170
X	 0.8380	 0.6110
Y	 0.7070	 0.5640
Z	 0.6990	 0.5660
a	 0.8790	 0.6550
b	 0.8090	 0.5990
c	 0.8660	 0.6440
d	 0.8240	 0.6230
e	 0.8320	 0.6200
f	 0.6860	 0.5760
g	 0.9010	 0.6560
h	 0.8180	 0.6150
i	 0.9430	 0.6820
j	 0.8040	 0.6370
k	 0.9600	 0.6820
l	 0.9060	 0.6620
m	 0.7860	 0.6100
n	 0.7520	 0.5750
o	 0.8780	 0.6460
p	 0.8710	 0.6360
r	 0.9350	 0.6750
s	 0.9010	 0.6600
u	 0.8020	 0.6090
v	 0.7060	 0.5580
w	 0.8430	 0.6320

