



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 10:02 PM UTC

PDB ID : 7VWL / pdb_00007vwl
EMDB ID : EMD-32155
Title : Membrane arm of deactive state CI from rotenone-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-11
Resolution : 2.70 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

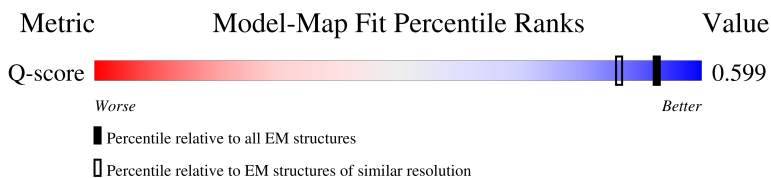
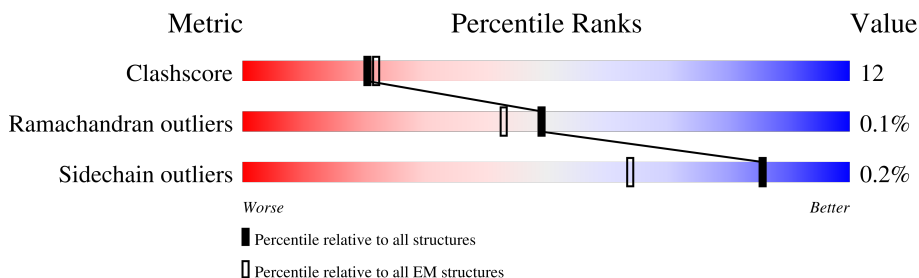
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.



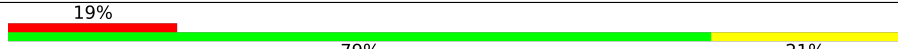
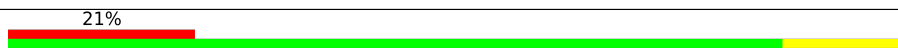
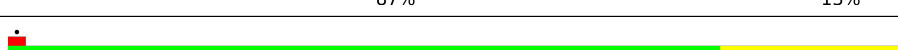
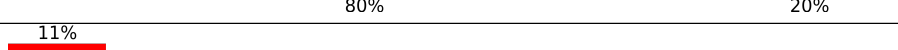
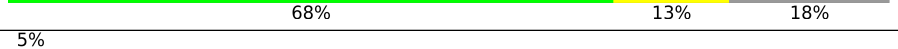
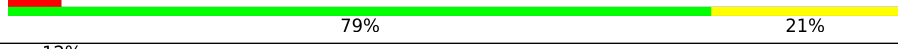
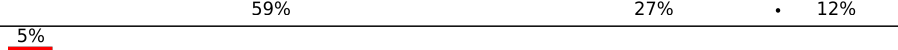
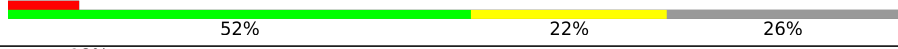
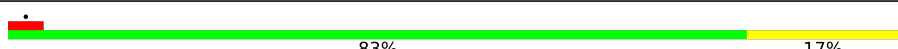
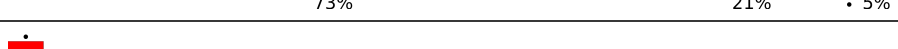
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	40	
2	S	70	
3	U	83	
4	V	140	

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Mol	Chain	Length	Quality of chain
5	W	113	
6	X	88	
7	Y	70	
8	Z	84	
9	a	140	
10	b	126	
11	c	156	
12	d	175	
13	e	107	
14	f	42	
15	g	121	
16	h	105	
17	i	347	
18	j	113	
19	k	98	
20	l	603	
21	m	175	
22	n	56	
23	o	128	
24	p	178	
25	r	459	
26	s	318	
27	u	171	
28	v	131	
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	CDL	a	201	-	-	X	-
30	CDL	i	401	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 39049 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	40	Total	C	N	O	S	0	0
			333	217	56	59	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
			567	364	104	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
			702	452	103	142	5		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	103	Total	C	N	O	S	0	0
			879	573	158	147	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	107	Total	C	N	O	S	0	0
			890	568	145	173	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	f	42	Total	C	N	O	0	0
			343	225	58	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	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	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- 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	603	Total	C	N	O	S	0	0
			4773	3164	740	819	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	m	129	Total	C	N	O	S	0	0
			951	637	138	168	8		

- 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
			448	291	81	75	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	303	Total	C	N	O	S	0	0
			2394	1607	369	397	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
			1032	644	195	184	9		

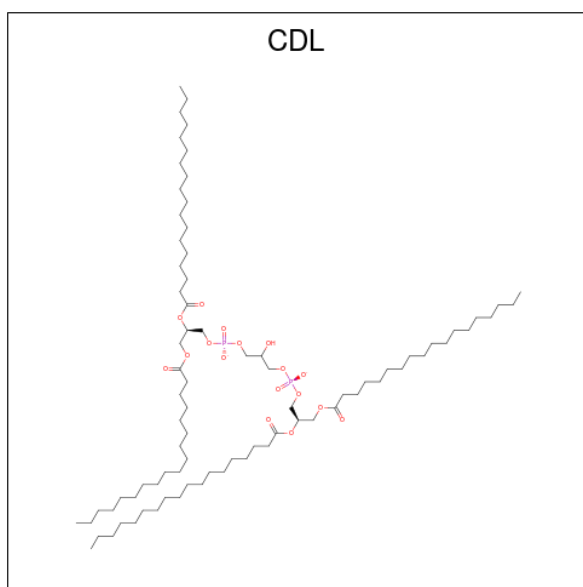
There is a discrepancy between the modelled and reference sequences:

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.

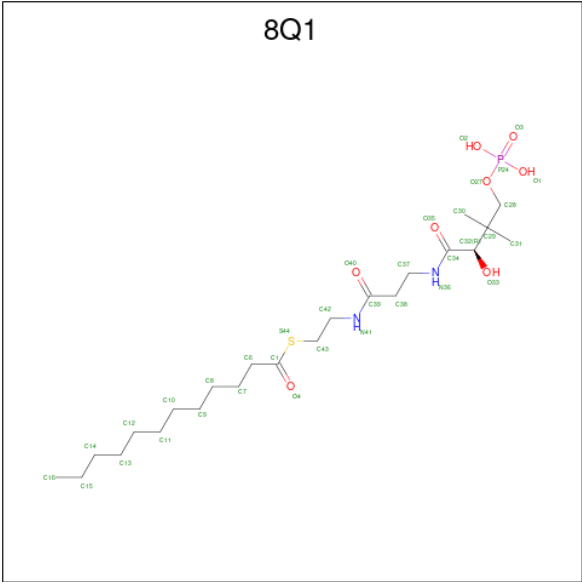
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2576	1640	435	491	10		

- Molecule 30 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



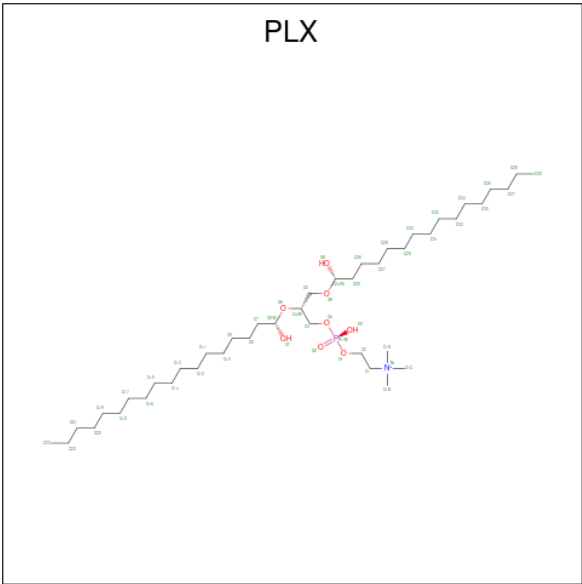
Mol	Chain	Residues	Atoms				AltConf
30	V	1	Total	C	O	P	0
			71	52	17	2	
30	a	1	Total	C	O	P	0
			91	72	17	2	
30	i	1	Total	C	O	P	0
			66	47	17	2	
30	l	1	Total	C	O	P	0
			65	46	17	2	
30	r	1	Total	C	O	P	0
			99	80	17	2	
30	r	1	Total	C	O	P	0
			100	81	17	2	
30	u	1	Total	C	O	P	0
			63	44	17	2	

- Molecule 31 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 32 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).



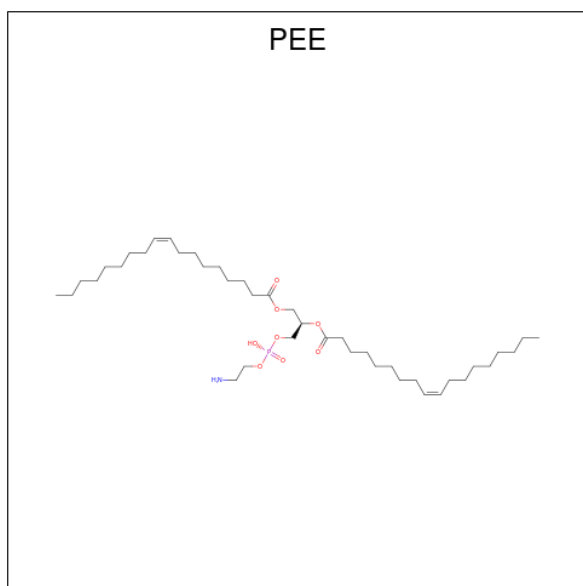
Mol	Chain	Residues	Atoms					AltConf
32	a	1	Total	C	N	O	P	0
			52	42	1	8	1	

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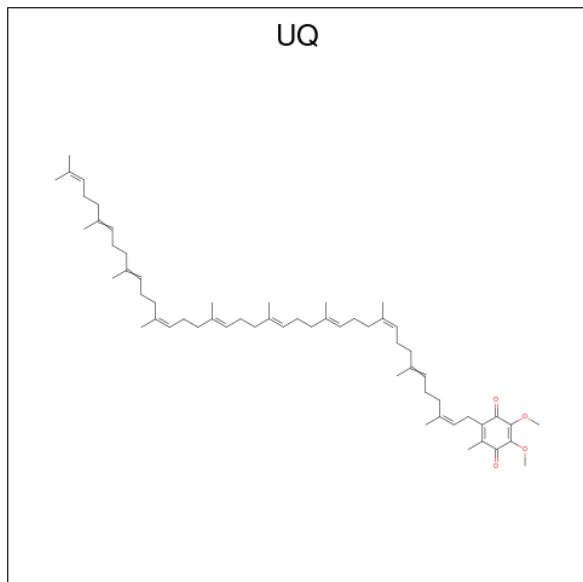
Mol	Chain	Residues	Atoms					AltConf
32	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
32	i	1	Total	C	N	O	P	0
			52	42	1	8	1	
32	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
32	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 33 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



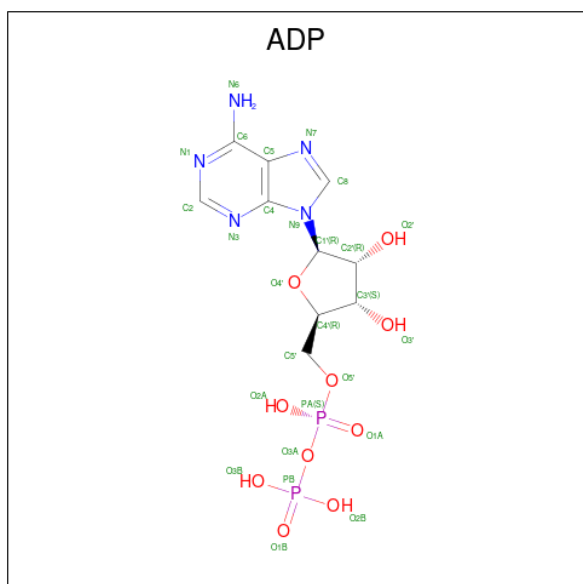
Mol	Chain	Residues	Atoms					AltConf
33	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
33	j	1	Total	C	N	O	P	0
			51	41	1	8	1	
33	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
33	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
33	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
33	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
33	s	1	Total	C	N	O	P	0
			51	41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

- Molecule 34 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (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	

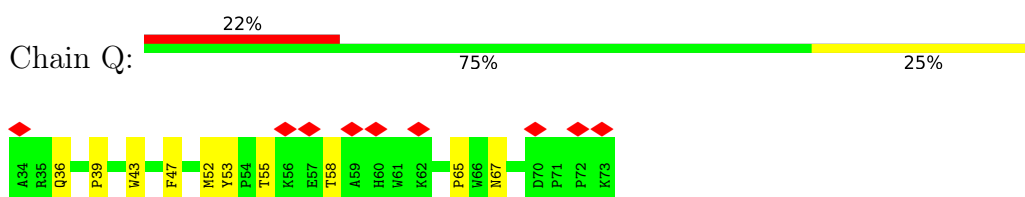
- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	Q	6	Total O 6 6	0
36	S	1	Total O 1 1	0
36	U	3	Total O 3 3	0
36	V	2	Total O 2 2	0
36	a	4	Total O 4 4	0
36	b	1	Total O 1 1	0
36	c	5	Total O 5 5	0
36	d	2	Total O 2 2	0
36	e	2	Total O 2 2	0
36	h	4	Total O 4 4	0
36	i	62	Total O 62 62	0
36	j	14	Total O 14 14	0
36	k	15	Total O 15 15	0
36	l	53	Total O 53 53	0
36	m	14	Total O 14 14	0
36	n	2	Total O 2 2	0
36	p	2	Total O 2 2	0
36	r	84	Total O 84 84	0
36	s	65	Total O 65 65	0
36	u	1	Total O 1 1	0
36	w	3	Total O 3 3	0

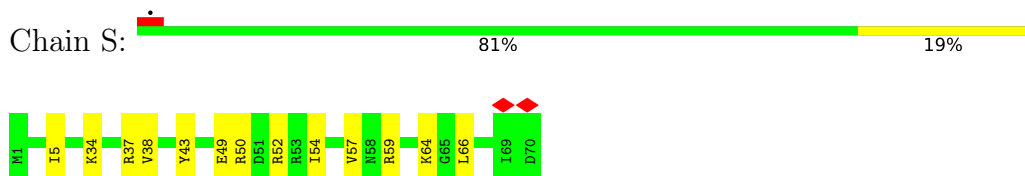
3 Residue-property plots [i](#)

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.

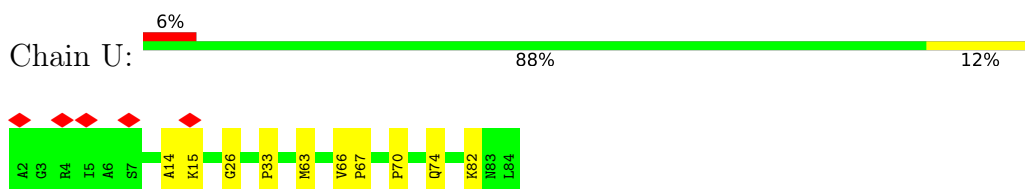
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



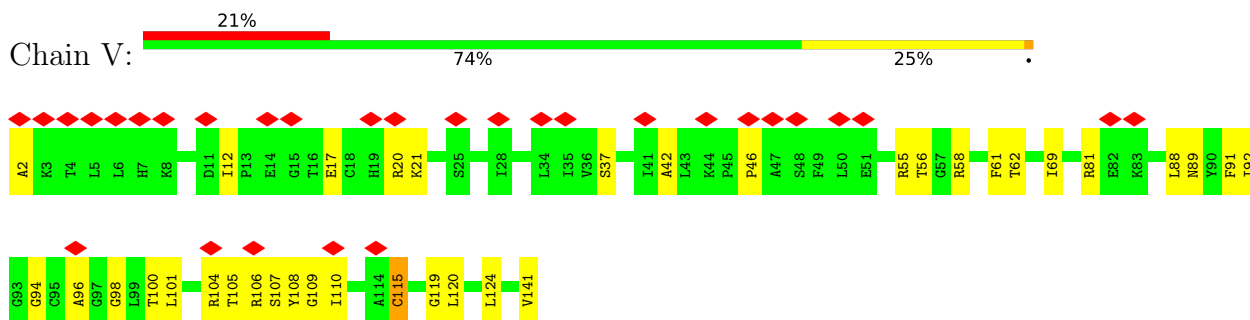
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



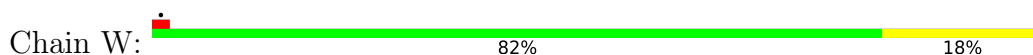
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

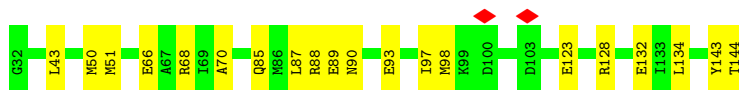


- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

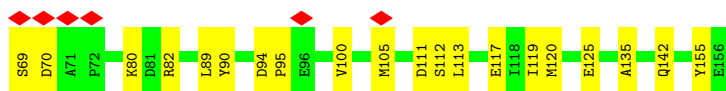
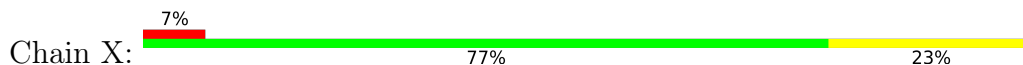


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

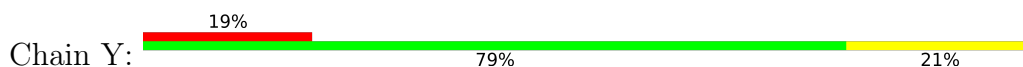




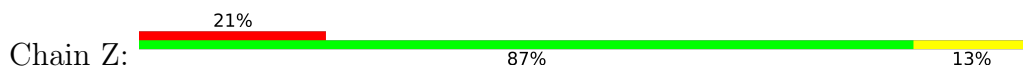
- Molecule 6: Acyl carrier protein, mitochondrial



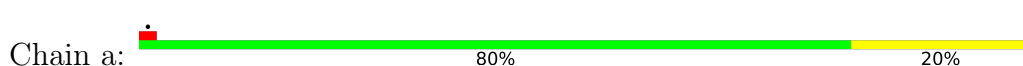
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



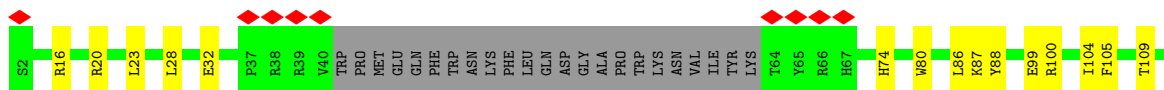
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



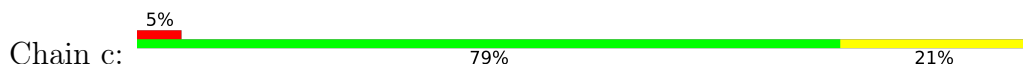
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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

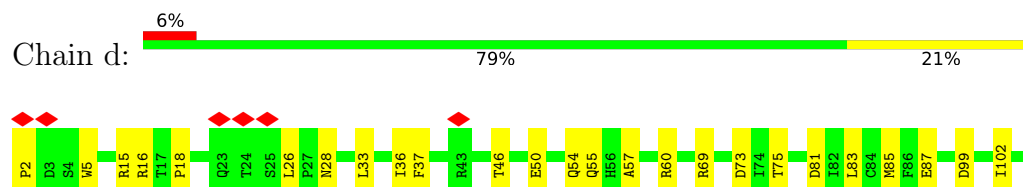


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

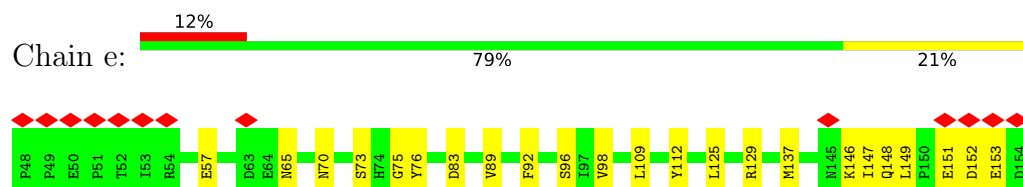




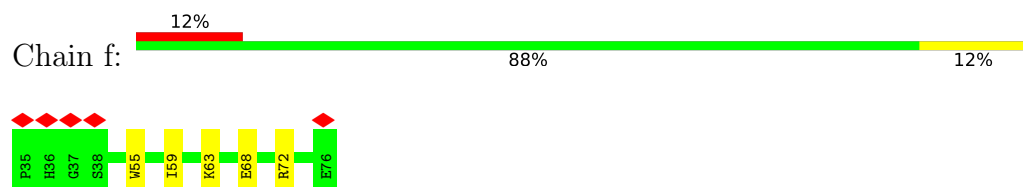
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



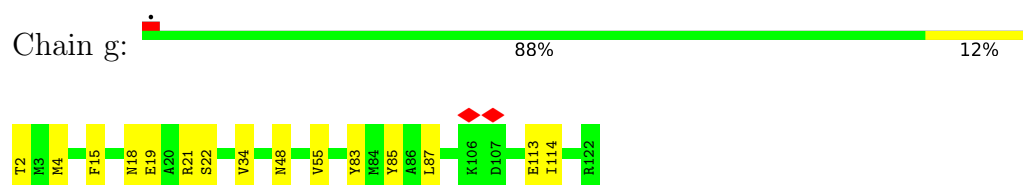
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



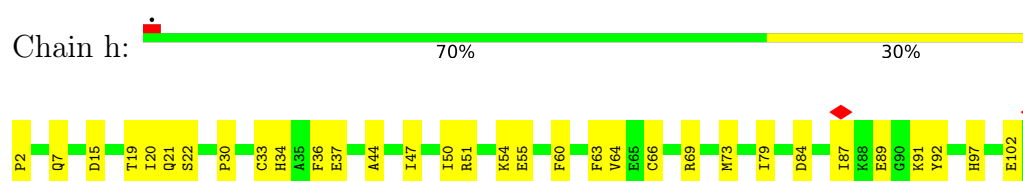
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



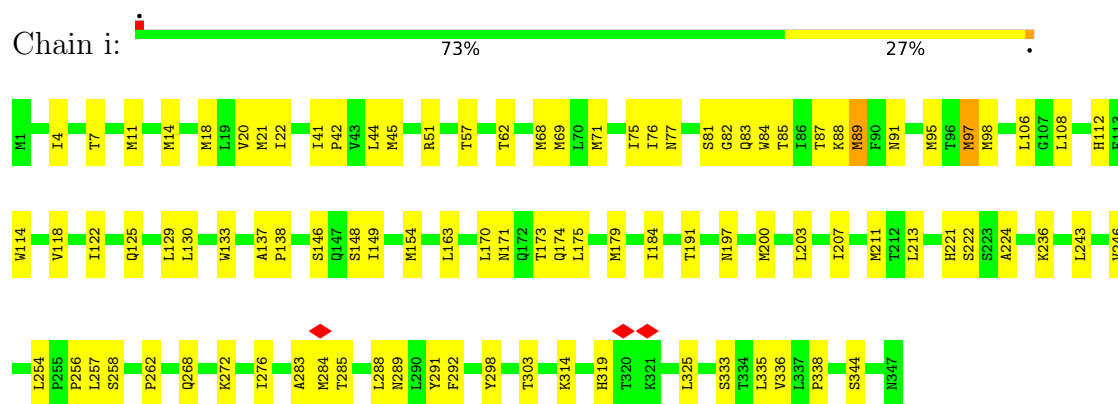
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2



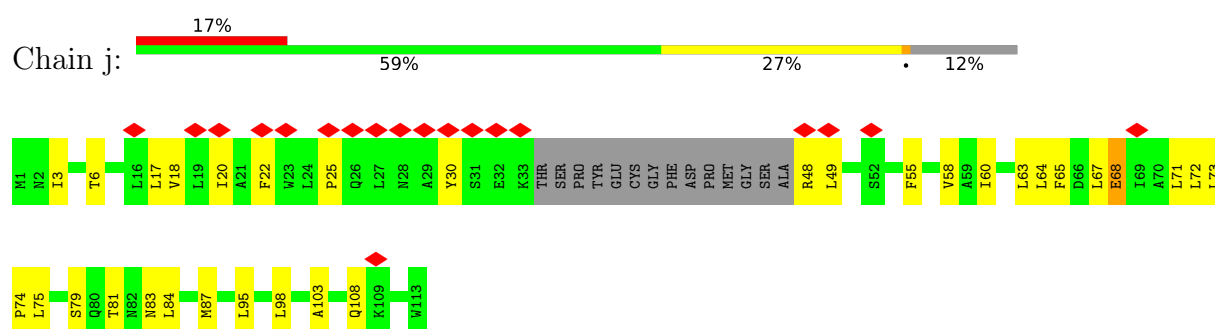
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



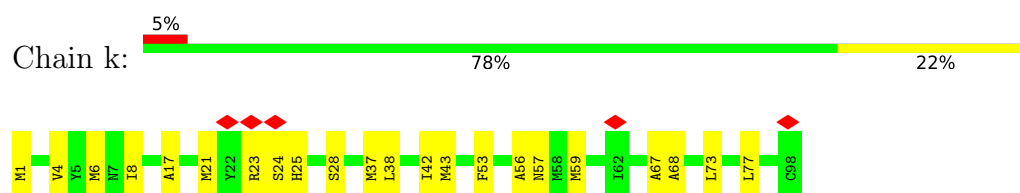
- Molecule 17: NADH-ubiquinone oxidoreductase chain 2



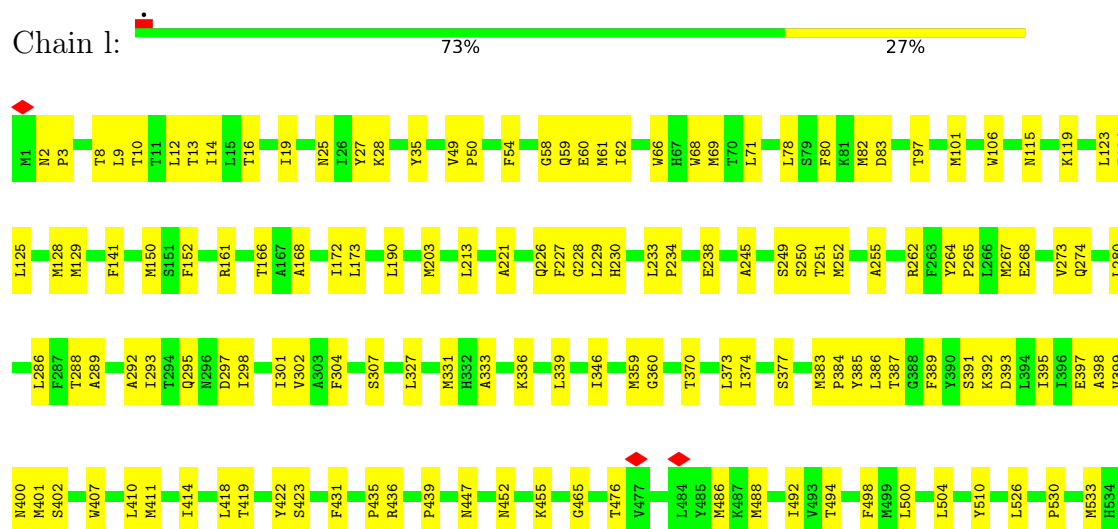
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

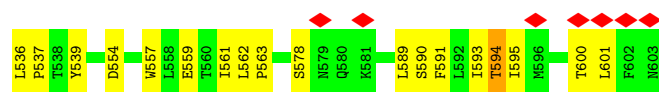


- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

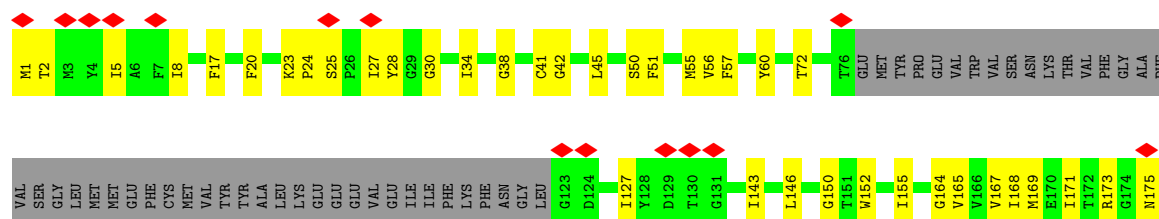


- Molecule 20: NADH-ubiquinone oxidoreductase chain 5

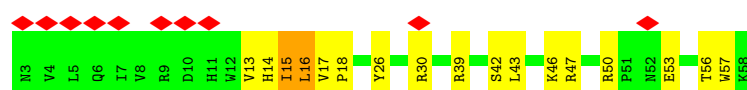




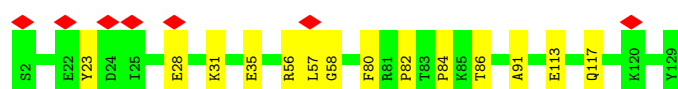
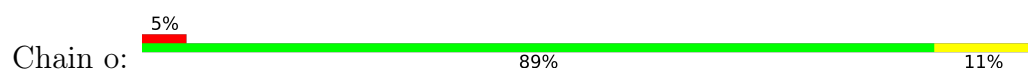
- Molecule 21: NADH-ubiquinone oxidoreductase chain 6



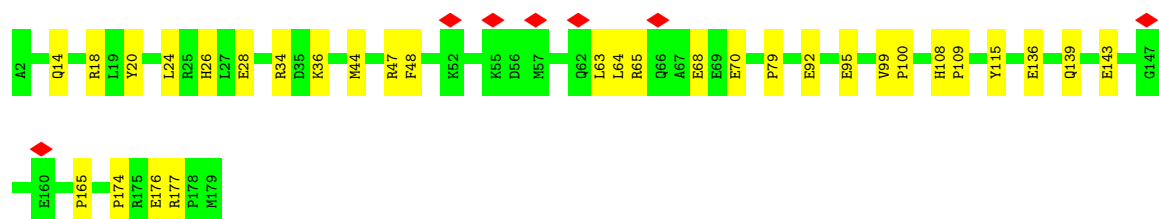
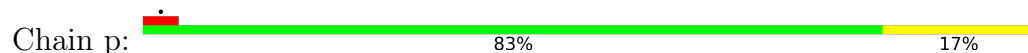
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



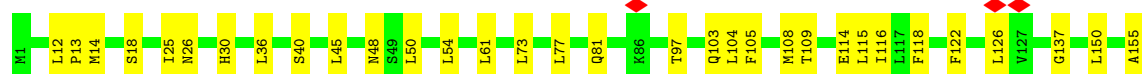
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

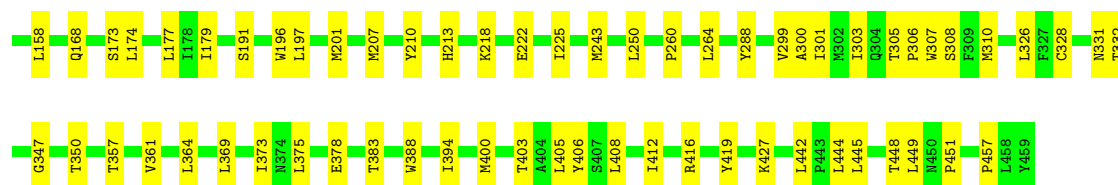


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

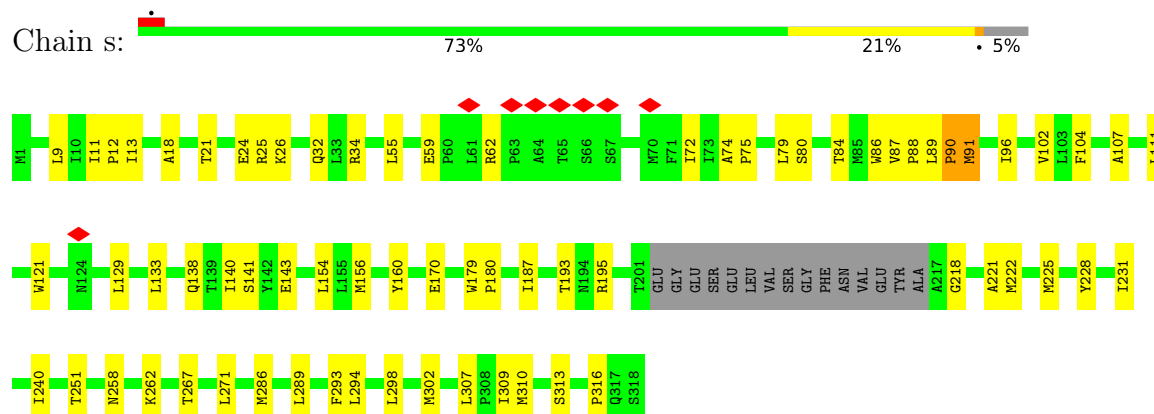


- Molecule 25: NADH-ubiquinone oxidoreductase chain 4

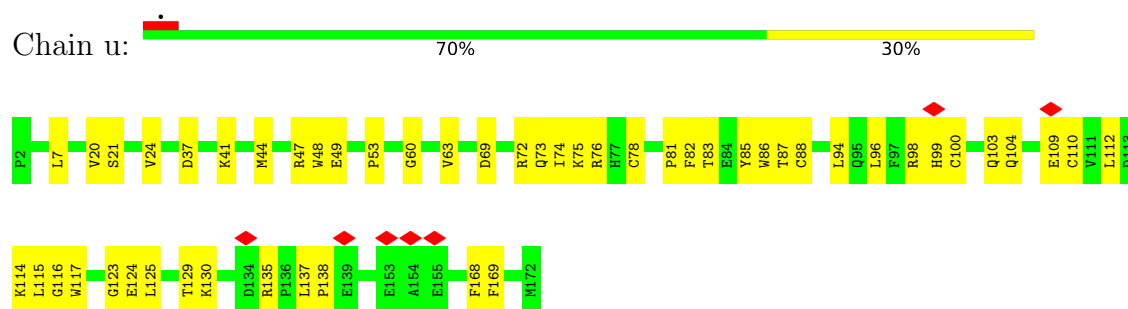




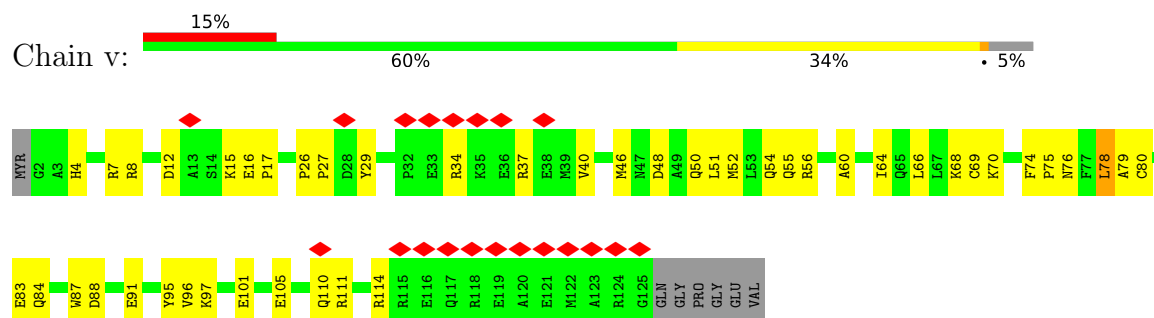
• Molecule 26: NADH-ubiquinone oxidoreductase chain 1



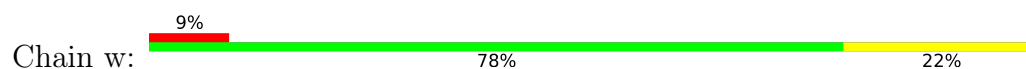
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

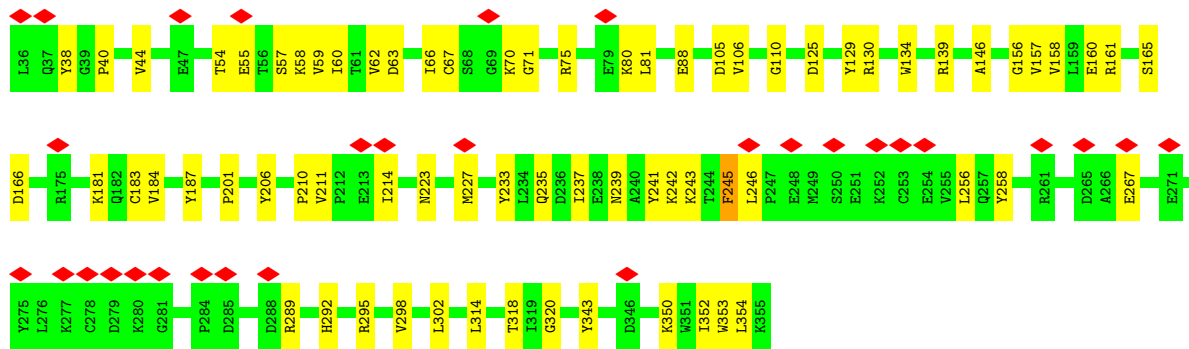


• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



• 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	169835	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	0.070	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	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: PLX, 8Q1, ADP, CDL, UQ, PEE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	Q	0.24	0/350	0.42	0/483
2	S	0.16	0/582	0.37	0/783
3	U	0.13	0/664	0.31	0/912
4	V	0.19	0/1042	0.46	0/1411
5	W	0.16	0/973	0.31	0/1312
6	X	0.14	0/714	0.36	0/967
7	Y	0.14	0/626	0.36	0/857
8	Z	0.12	0/695	0.31	0/939
9	a	0.19	0/1199	0.41	1/1623 (0.1%)
10	b	0.16	0/906	0.37	0/1232
11	c	0.17	0/1371	0.36	0/1875
12	d	0.15	0/1494	0.32	0/2015
13	e	0.16	0/916	0.40	0/1246
14	f	0.17	0/351	0.33	0/474
15	g	0.15	0/1031	0.32	0/1394
16	h	0.18	0/889	0.42	0/1190
17	i	0.18	0/2773	0.39	1/3768 (0.0%)
18	j	0.22	0/819	0.51	0/1117
19	k	0.21	0/759	0.42	0/1029
20	l	0.18	0/4901	0.42	1/6667 (0.0%)
21	m	0.21	0/973	0.50	0/1320
22	n	0.22	0/459	0.62	1/621 (0.2%)
23	o	0.15	0/1092	0.36	0/1481
24	p	0.16	0/1590	0.34	0/2155
25	r	0.18	0/3723	0.38	0/5078
26	s	0.20	0/2464	0.48	0/3369
27	u	0.19	0/1436	0.52	2/1938 (0.1%)
28	v	0.20	0/1056	0.56	1/1416 (0.1%)
29	w	0.17	0/2636	0.44	4/3573 (0.1%)
All	All	0.18	0/38484	0.41	11/52245 (0.0%)

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
26	s	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	89	MET	N-CA-C	7.24	119.17	111.28
9	a	91	VAL	N-CA-C	6.65	116.78	110.53
20	l	600	THR	N-CA-C	6.18	118.09	111.36
29	w	243	LYS	N-CA-C	5.73	117.61	111.36
22	n	16	LEU	N-CA-C	5.64	117.43	111.28
28	v	79	ALA	N-CA-C	5.44	117.21	111.28
27	u	76	ARG	N-CA-C	5.35	117.11	111.28
27	u	87	THR	N-CA-C	-5.15	105.66	111.28
29	w	245	PHE	N-CA-C	5.15	116.89	111.28
29	w	210	PRO	CA-C-N	5.12	123.47	120.24
29	w	210	PRO	C-N-CA	5.12	123.47	120.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	s	91	MET	Peptide

5.2 Too-close contacts

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	333	0	301	9	0
2	S	567	0	565	14	0
3	U	643	0	642	9	0
4	V	1021	0	1027	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	W	949	0	935	19	0
6	X	702	0	683	17	0
7	Y	600	0	539	12	0
8	Z	674	0	643	8	0
9	a	1165	0	1174	27	0
10	b	879	0	899	20	0
11	c	1315	0	1208	24	0
12	d	1461	0	1429	34	0
13	e	890	0	837	22	0
14	f	343	0	344	4	0
15	g	1000	0	994	14	0
16	h	867	0	873	26	0
17	i	2710	0	2874	99	0
18	j	800	0	855	50	0
19	k	748	0	799	23	0
20	l	4773	0	4915	135	0
21	m	951	0	962	51	0
22	n	448	0	426	22	0
23	o	1062	0	1072	12	0
24	p	1534	0	1470	19	0
25	r	3631	0	3839	81	0
26	s	2394	0	2508	72	0
27	u	1398	0	1380	57	0
28	v	1032	0	986	46	0
29	w	2576	0	2520	55	0
30	V	71	0	92	16	0
30	a	91	0	132	35	0
30	i	66	0	76	21	0
30	l	65	0	74	7	0
30	r	199	0	307	19	0
30	u	63	0	70	18	0
31	X	35	0	0	1	0
32	a	52	0	88	10	0
32	e	52	0	88	5	0
32	i	52	0	88	4	0
32	j	52	0	88	6	0
32	r	52	0	88	10	0
33	i	47	0	71	16	0
33	j	51	0	82	9	0
33	l	92	0	138	25	0
33	m	41	0	59	16	0
33	r	51	0	82	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	s	51	0	82	2	0
34	s	28	0	31	7	0
35	w	27	0	11	1	0
36	Q	6	0	0	0	0
36	S	1	0	0	0	0
36	U	3	0	0	0	0
36	V	2	0	0	0	0
36	a	4	0	0	0	0
36	b	1	0	0	0	0
36	c	5	0	0	0	0
36	d	2	0	0	0	0
36	e	2	0	0	0	0
36	h	4	0	0	2	0
36	i	62	0	0	9	0
36	j	14	0	0	1	0
36	k	15	0	0	0	0
36	l	53	0	0	3	0
36	m	14	0	0	2	0
36	n	2	0	0	3	0
36	p	2	0	0	0	0
36	r	84	0	0	5	0
36	s	65	0	0	5	0
36	u	1	0	0	0	0
36	w	3	0	0	0	0
All	All	39049	0	39446	942	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 12.

All (942) 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)
28:v:69:CYS:SG	28:v:80:CYS:HB3	1.56	1.45
27:u:78:CYS:HB3	27:u:110:CYS:SG	1.71	1.30
28:v:69:CYS:SG	28:v:80:CYS:CB	2.30	1.19
29:w:66:ILE:O	29:w:214:ILE:HD11	1.40	1.18
18:j:3:ILE:HG21	33:m:201:PEE:H13	1.23	1.11
22:n:13:VAL:HG12	25:r:14:MET:HG2	1.17	1.09
30:u:201:CDL:H581	30:u:201:CDL:H542	1.33	1.09
26:s:87:VAL:HG23	26:s:88:PRO:HD3	1.36	1.07
17:i:256:PRO:HB2	30:u:201:CDL:H612	1.31	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:84:THR:O	26:s:87:VAL:HG22	1.53	1.06
27:u:78:CYS:CB	27:u:110:CYS:SG	2.42	1.06
18:j:64:LEU:HD13	21:m:165:VAL:HG22	1.32	1.06
33:i:403:PEE:H28	33:i:403:PEE:H36	1.32	1.05
18:j:3:ILE:CG2	33:m:201:PEE:H13	1.91	1.01
4:V:107:SER:HB3	4:V:110:ILE:HG22	1.41	0.99
28:v:69:CYS:HG	28:v:80:CYS:HB3	1.23	0.98
22:n:30:ARG:HD3	30:u:201:CDL:OA4	1.63	0.98
33:i:403:PEE:C20	20:l:562:LEU:HG	1.93	0.98
16:h:33:CYS:HG	16:h:66:CYS:HG	1.01	0.97
30:a:201:CDL:H772	30:a:201:CDL:H201	1.43	0.97
10:b:100:ARG:HB2	20:l:60:GLU:HB2	1.46	0.95
22:n:13:VAL:CG1	25:r:14:MET:HG2	1.96	0.94
11:c:116:ARG:HG2	33:l:702:PEE:H49	1.51	0.92
17:i:95:MET:CE	17:i:149:ILE:HG22	2.00	0.91
30:a:201:CDL:H201	30:a:201:CDL:C77	2.00	0.90
1:Q:47:PHE:HD1	1:Q:52:MET:HE1	1.34	0.90
20:l:590:SER:O	20:l:594:THR:HG22	1.72	0.89
17:i:97:MET:HE2	17:i:97:MET:HA	1.54	0.89
33:i:403:PEE:H32	20:l:562:LEU:HG	1.53	0.88
17:i:18:MET:HE2	17:i:18:MET:HA	1.55	0.88
27:u:103:GLN:N	27:u:103:GLN:OE1	2.08	0.87
9:a:89:VAL:HG13	9:a:93:ILE:HD12	1.56	0.86
29:w:139:ARG:NH2	35:w:401:ADP:N7	2.24	0.86
29:w:70:LYS:NZ	29:w:160:GLU:HG2	1.91	0.86
30:u:201:CDL:H581	30:u:201:CDL:C54	2.06	0.85
18:j:73:LEU:HD13	21:m:55:MET:HE1	1.55	0.85
30:i:401:CDL:HB31	29:w:40:PRO:CB	2.06	0.85
30:a:201:CDL:H251	30:a:201:CDL:H211	1.57	0.85
30:i:401:CDL:HB31	29:w:40:PRO:CG	2.07	0.85
33:i:403:PEE:H36	33:i:403:PEE:C18	2.08	0.84
30:a:201:CDL:H211	30:a:201:CDL:C25	2.08	0.83
20:l:190:LEU:HD23	25:r:383:THR:HG21	1.60	0.83
33:i:403:PEE:H31	20:l:562:LEU:HG	1.59	0.82
27:u:169:PHE:CE1	30:u:201:CDL:H561	2.14	0.82
33:i:403:PEE:H42	33:i:403:PEE:H34	1.58	0.82
32:a:202:PLX:H1A2	32:a:202:PLX:O3	1.80	0.81
26:s:86:TRP:CE3	26:s:91:MET:HE1	2.15	0.81
30:u:201:CDL:H542	30:u:201:CDL:C58	2.10	0.81
11:c:155:PRO:HG3	28:v:4:HIS:CD2	2.14	0.81
26:s:87:VAL:CG2	26:s:88:PRO:HD3	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:5:ILE:HG12	26:s:26:LYS:HG2	1.61	0.80
4:V:107:SER:HB3	4:V:110:ILE:CG2	2.11	0.80
18:j:60:ILE:HG21	21:m:168:ILE:HG21	1.64	0.79
29:w:70:LYS:HZ2	29:w:160:GLU:HG2	1.45	0.79
28:v:15:LYS:HG3	28:v:110:GLN:HE22	1.48	0.79
33:j:201:PEE:H67	33:j:201:PEE:H74	1.64	0.79
18:j:64:LEU:HD13	21:m:165:VAL:CG2	2.12	0.78
17:i:125:GLN:HG2	30:i:401:CDL:OA3	1.83	0.78
28:v:70:LYS:HD2	28:v:80:CYS:SG	2.23	0.78
28:v:78:LEU:HD12	28:v:78:LEU:H	1.47	0.78
4:V:101:LEU:HD23	4:V:101:LEU:O	1.85	0.77
30:V:201:CDL:H873	32:r:502:PLX:H222	1.67	0.77
17:i:154:MET:HE1	36:i:562:HOH:O	1.83	0.77
26:s:86:TRP:HE3	26:s:91:MET:HE1	1.50	0.77
4:V:91:PHE:HE1	4:V:120:LEU:HD22	1.50	0.76
6:X:111:ASP:OD1	6:X:112:SER:N	2.18	0.76
26:s:87:VAL:N	26:s:88:PRO:HD2	2.00	0.76
29:w:88:GLU:OE1	29:w:161:ARG:NH1	2.18	0.76
25:r:197:LEU:HD13	33:r:501:PEE:H73	1.68	0.76
26:s:87:VAL:HG23	26:s:88:PRO:CD	2.14	0.75
12:d:57:ALA:HA	12:d:60:ARG:HD3	1.67	0.75
1:Q:55:THR:HG1	1:Q:58:THR:HG1	1.31	0.75
5:W:134:LEU:HD21	21:m:1:MET:HA	1.68	0.75
30:a:201:CDL:O1	33:l:703:PEE:C32	2.34	0.75
30:a:201:CDL:OB3	32:e:201:PLX:H1B3	1.87	0.74
17:i:95:MET:HE2	17:i:149:ILE:HA	1.66	0.74
18:j:73:LEU:HD12	21:m:55:MET:SD	2.27	0.74
28:v:69:CYS:SG	28:v:80:CYS:HB2	2.27	0.74
30:a:201:CDL:H422	30:a:201:CDL:H381	1.69	0.74
4:V:107:SER:CB	4:V:110:ILE:HG22	2.16	0.74
33:m:201:PEE:H7	33:m:201:PEE:H51	1.69	0.74
27:u:78:CYS:CB	27:u:110:CYS:HG	1.98	0.74
30:a:201:CDL:O1	33:l:703:PEE:H51	1.87	0.73
21:m:42:GLY:HA3	33:m:201:PEE:H28	1.69	0.73
33:i:403:PEE:H31	20:l:562:LEU:CD2	2.19	0.73
20:l:533:MET:HE3	33:l:702:PEE:H24	1.69	0.73
27:u:88:CYS:SG	27:u:103:GLN:HG2	2.29	0.73
18:j:3:ILE:HG21	33:m:201:PEE:C11	2.14	0.73
17:i:256:PRO:CB	30:u:201:CDL:H612	2.15	0.72
33:i:403:PEE:H31	20:l:562:LEU:CG	2.19	0.72
17:i:207:ILE:HG22	17:i:211:MET:HE2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:125:GLN:CG	30:i:401:CDL:OA3	2.37	0.72
30:i:401:CDL:HB31	29:w:40:PRO:HG3	1.70	0.72
18:j:73:LEU:CD1	21:m:55:MET:SD	2.78	0.72
17:i:95:MET:HE2	17:i:149:ILE:CA	2.20	0.71
17:i:108:LEU:HD11	17:i:191:THR:HG21	1.72	0.71
32:a:202:PLX:H1A2	32:a:202:PLX:P1	2.31	0.71
30:V:201:CDL:H721	30:V:201:CDL:H572	1.71	0.71
23:o:23:TYR:OH	24:p:68:GLU:OE1	2.08	0.71
28:v:12:ASP:HB3	28:v:15:LYS:HB2	1.71	0.70
18:j:17:LEU:HG	26:s:222:MET:HE1	1.74	0.70
18:j:64:LEU:CD1	21:m:165:VAL:HG22	2.17	0.70
4:V:2:ALA:HA	20:l:601:LEU:HD12	1.74	0.70
17:i:129:LEU:HD13	30:i:401:CDL:H341	1.75	0.69
25:r:114:GLU:HG2	27:u:169:PHE:HB3	1.75	0.69
26:s:316:PRO:O	36:s:501:HOH:O	2.09	0.69
18:j:73:LEU:HD13	21:m:55:MET:CE	2.22	0.69
17:i:7:THR:HG22	17:i:11:MET:HE2	1.75	0.69
4:V:69:ILE:HG13	4:V:100:THR:HG21	1.74	0.69
29:w:241:TYR:O	29:w:246:LEU:HD23	1.93	0.69
20:l:161:ARG:NH1	20:l:238:GLU:OE1	2.26	0.68
4:V:96:ALA:O	4:V:100:THR:HG23	1.93	0.68
32:a:202:PLX:H111	25:r:40:SER:HB3	1.74	0.68
28:v:70:LYS:CD	28:v:80:CYS:SG	2.81	0.68
25:r:210:TYR:O	25:r:213:HIS:ND1	2.26	0.68
4:V:81:ARG:NH1	4:V:89:ASN:OD1	2.26	0.68
4:V:124:LEU:HD11	33:r:501:PEE:H64	1.74	0.68
1:Q:52:MET:HE2	17:i:173:THR:HG22	1.75	0.67
20:l:227:PHE:O	20:l:230:HIS:ND1	2.25	0.67
17:i:213:LEU:HD13	30:i:401:CDL:H141	1.77	0.67
10:b:105:PHE:HB3	28:v:68:LYS:HD2	1.77	0.67
17:i:268:GLN:HE22	17:i:272:LYS:HE3	1.58	0.67
26:s:193:THR:O	36:s:502:HOH:O	2.11	0.67
17:i:77:ASN:OD1	17:i:89:MET:O	2.13	0.67
24:p:139:GLN:NE2	24:p:143:GLU:OE1	2.28	0.66
26:s:180:PRO:HB3	33:s:401:PEE:H22	1.78	0.66
25:r:191:SER:HB3	33:r:501:PEE:H2	1.76	0.66
29:w:70:LYS:HZ2	29:w:160:GLU:CG	2.09	0.66
4:V:101:LEU:HD23	4:V:101:LEU:C	2.21	0.66
30:a:201:CDL:H111	33:l:703:PEE:H60	1.78	0.66
25:r:260:PRO:HG3	32:r:502:PLX:H132	1.78	0.66
2:S:49:GLU:OE1	2:S:52:ARG:NH2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:213:LEU:CD1	30:i:401:CDL:H141	2.26	0.66
22:n:13:VAL:HG13	25:r:14:MET:HA	1.76	0.65
6:X:89:LEU:HD23	8:Z:48:ASN:HA	1.77	0.65
26:s:26:LYS:NZ	36:s:506:HOH:O	2.30	0.65
26:s:25:ARG:HD2	34:s:402:UQ:HM21	1.78	0.65
1:Q:47:PHE:CD1	1:Q:52:MET:HE1	2.24	0.65
30:a:201:CDL:H191	30:a:201:CDL:H761	1.78	0.65
17:i:11:MET:HE1	30:i:401:CDL:H771	1.78	0.65
29:w:211:VAL:O	29:w:214:ILE:HG22	1.96	0.65
18:j:67:LEU:HD21	19:k:68:ALA:CB	2.27	0.65
33:j:201:PEE:H67	33:j:201:PEE:C44	2.26	0.65
27:u:78:CYS:HB3	27:u:110:CYS:HG	1.56	0.64
8:Z:20:LYS:O	8:Z:23:LYS:NZ	2.31	0.64
20:l:400:ASN:HB3	20:l:486:MET:HE3	1.79	0.64
21:m:57:PHE:CZ	26:s:111:LEU:HD11	2.33	0.64
2:S:38:VAL:HG21	27:u:94:LEU:CD1	2.28	0.64
26:s:156:MET:HE1	36:s:512:HOH:O	1.97	0.64
6:X:69:SER:OG	6:X:70:ASP:N	2.31	0.64
22:n:16:LEU:CD2	30:r:504:CDL:H661	2.28	0.64
20:l:250:SER:HB2	20:l:333:ALA:HA	1.78	0.63
22:n:15:ILE:C	22:n:15:ILE:HD12	2.23	0.63
2:S:38:VAL:HG21	27:u:94:LEU:HD11	1.81	0.63
22:n:30:ARG:CD	30:u:201:CDL:OA4	2.42	0.63
18:j:71:LEU:O	18:j:74:PRO:HD2	1.98	0.63
17:i:18:MET:HE1	17:i:21:MET:SD	2.38	0.63
20:l:66:TRP:CZ3	33:l:703:PEE:H32	2.33	0.63
10:b:99:GLU:OE1	12:d:15:ARG:NH2	2.31	0.63
4:V:108:TYR:HE1	30:V:201:CDL:H112	1.62	0.63
26:s:90:PRO:HD2	26:s:240:ILE:HD13	1.80	0.62
30:a:201:CDL:H532	33:l:703:PEE:H56	1.82	0.62
20:l:346:ILE:HG21	20:l:359:MET:HE3	1.81	0.62
33:r:501:PEE:H35	33:r:501:PEE:H79	1.81	0.62
4:V:91:PHE:CE1	4:V:120:LEU:HD22	2.34	0.62
20:l:510:TYR:O	24:p:36:LYS:NZ	2.30	0.62
33:i:403:PEE:H28	33:i:403:PEE:C22	2.18	0.62
33:l:703:PEE:H8	33:l:703:PEE:O1P	1.99	0.62
4:V:91:PHE:HE1	4:V:120:LEU:CD2	2.13	0.62
23:o:56:ARG:NH1	23:o:58:GLY:O	2.33	0.62
9:a:85:GLY:O	9:a:89:VAL:HG23	2.00	0.62
13:e:112:TYR:HB3	25:r:45:LEU:HD23	1.81	0.61
17:i:262:PRO:HA	36:i:552:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:360:GLY:HA3	20:l:435:PRO:HA	1.82	0.61
33:r:501:PEE:H69	32:r:502:PLX:H381	1.81	0.61
4:V:37:SER:HB3	4:V:56:THR:HG22	1.82	0.61
11:c:160:GLN:OE1	28:v:37:ARG:NH1	2.32	0.61
17:i:171:ASN:ND2	20:l:578:SER:OG	2.30	0.61
9:a:159:LEU:HD22	9:a:163:ARG:HH12	1.65	0.61
30:a:201:CDL:H772	30:a:201:CDL:C20	2.27	0.61
30:a:201:CDL:O1	33:l:703:PEE:H50	2.01	0.61
4:V:2:ALA:HA	20:l:601:LEU:CD1	2.31	0.61
17:i:18:MET:HE2	17:i:18:MET:CA	2.30	0.61
28:v:17:PRO:HB3	28:v:105:GLU:OE1	2.00	0.61
17:i:95:MET:CE	17:i:149:ILE:CG2	2.77	0.61
20:l:66:TRP:HB2	33:l:703:PEE:H19	1.83	0.61
18:j:3:ILE:CG2	33:m:201:PEE:C11	2.74	0.61
10:b:28:LEU:HG	10:b:32:GLU:HG2	1.83	0.60
22:n:14:HIS:CE1	25:r:26:ASN:OD1	2.55	0.60
12:d:163:MET:HE2	13:e:149:LEU:HD11	1.84	0.60
29:w:66:ILE:O	29:w:214:ILE:CD1	2.33	0.60
10:b:100:ARG:HH11	20:l:60:GLU:HG3	1.67	0.60
2:S:50:ARG:NH2	27:u:20:VAL:O	2.36	0.59
12:d:33:LEU:HD21	20:l:49:VAL:HG22	1.84	0.59
30:V:201:CDL:OB9	30:V:201:CDL:H731	2.02	0.59
29:w:165:SER:HB3	29:w:245:PHE:CE1	2.36	0.59
9:a:90:ASN:ND2	30:a:201:CDL:OB4	2.35	0.59
22:n:13:VAL:CG1	25:r:14:MET:HA	2.32	0.59
27:u:96:LEU:HB2	27:u:99:HIS:HD2	1.67	0.59
27:u:169:PHE:HE1	30:u:201:CDL:H561	1.66	0.59
4:V:108:TYR:HE1	30:V:201:CDL:C11	2.15	0.59
5:W:66:GLU:OE1	27:u:123:GLY:N	2.30	0.59
17:i:133:TRP:HE3	30:i:401:CDL:H391	1.66	0.59
36:l:840:HOH:O	25:r:400:MET:HE3	2.00	0.59
19:k:23:ARG:HD3	21:m:23:LYS:HB2	1.84	0.59
25:r:403:THR:HA	25:r:406:TYR:CE2	2.37	0.59
27:u:96:LEU:HD12	27:u:99:HIS:NE2	2.18	0.59
17:i:82:GLY:O	36:i:502:HOH:O	2.17	0.58
3:U:63:MET:O	27:u:130:LYS:NZ	2.33	0.58
21:m:56:VAL:O	21:m:60:TYR:HB3	2.03	0.58
29:w:58:LYS:O	29:w:60:ILE:HG23	2.03	0.58
9:a:141:GLN:NE2	9:a:145:GLU:OE1	2.37	0.58
17:i:14:MET:O	17:i:18:MET:HG2	2.02	0.58
5:W:88:ARG:NH2	27:u:7:LEU:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:391:SER:O	20:l:395:ILE:HG12	2.03	0.58
20:l:591:PHE:O	20:l:595:ILE:HG13	2.03	0.58
21:m:57:PHE:HZ	26:s:111:LEU:HD11	1.67	0.58
29:w:166:ASP:OD2	29:w:187:TYR:OH	2.21	0.58
36:n:101:HOH:O	25:r:14:MET:HG3	2.03	0.58
26:s:87:VAL:CG2	26:s:88:PRO:CD	2.78	0.58
26:s:102:VAL:HG11	26:s:154:LEU:HD11	1.84	0.58
33:m:201:PEE:H59	26:s:104:PHE:HE1	1.67	0.58
4:V:108:TYR:CE1	30:V:201:CDL:H112	2.38	0.58
17:i:283:ALA:HB1	25:r:158:LEU:HD13	1.86	0.58
18:j:6:THR:HG21	26:s:87:VAL:HG11	1.86	0.58
20:l:562:LEU:HB3	20:l:563:PRO:HD3	1.85	0.58
29:w:181:LYS:O	29:w:184:VAL:HG22	2.03	0.58
25:r:451:PRO:HD2	36:r:673:HOH:O	2.03	0.57
13:e:89:VAL:HG21	25:r:25:ILE:HG23	1.85	0.57
30:a:201:CDL:OA7	30:a:201:CDL:HA61	2.04	0.57
29:w:125:ASP:O	29:w:130:ARG:NH2	2.36	0.57
30:V:201:CDL:OB7	30:V:201:CDL:H1	2.05	0.57
20:l:25:ASN:HA	20:l:28:LYS:HE3	1.85	0.57
12:d:50:GLU:O	12:d:54:GLN:HG3	2.04	0.57
4:V:141:VAL:HG11	17:i:272:LYS:HB3	1.86	0.57
10:b:123:PHE:HB3	28:v:40:VAL:HG21	1.85	0.57
19:k:1:MET:HE3	19:k:6:MET:HG3	1.84	0.57
22:n:17:VAL:HB	22:n:18:PRO:HD3	1.86	0.57
27:u:69:ASP:OD1	27:u:72:ARG:NH1	2.33	0.57
28:v:66:LEU:HD13	28:v:83:GLU:HB2	1.87	0.57
18:j:72:LEU:HD22	18:j:75:LEU:HD11	1.87	0.57
27:u:49:GLU:OE1	27:u:135:ARG:NH2	2.38	0.57
6:X:155:TYR:CE1	10:b:23:LEU:HB3	2.40	0.57
4:V:98:GLY:HA3	4:V:115:CYS:HA	1.87	0.57
20:l:526:LEU:HD12	20:l:530:PRO:HG2	1.86	0.57
21:m:17:PHE:HA	21:m:20:PHE:CE2	2.40	0.57
2:S:38:VAL:CG2	27:u:94:LEU:HD13	2.34	0.56
21:m:42:GLY:HA2	33:m:201:PEE:H23	1.86	0.56
26:s:18:ALA:HB2	34:s:402:UQ:H152	1.87	0.56
29:w:62:VAL:HG12	29:w:70:LYS:HB2	1.87	0.56
2:S:38:VAL:CG2	27:u:94:LEU:CD1	2.84	0.56
4:V:61:PHE:HD2	4:V:104:ARG:NH1	2.03	0.56
30:a:201:CDL:H761	30:a:201:CDL:C19	2.36	0.56
18:j:73:LEU:HB2	18:j:74:PRO:HD3	1.87	0.56
20:l:476:THR:HA	28:v:54:GLN:HE22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:m:201:PEE:H52	26:s:104:PHE:CE1	2.40	0.56
25:r:191:SER:HB3	33:r:501:PEE:C1	2.34	0.56
26:s:21:THR:HB	34:s:402:UQ:HM23	1.88	0.56
26:s:55:LEU:HD13	26:s:221:ALA:HB2	1.87	0.56
27:u:85:TYR:HA	27:u:103:GLN:HB3	1.87	0.56
28:v:7:ARG:NE	28:v:16:GLU:OE2	2.34	0.56
28:v:97:LYS:O	28:v:101:GLU:HG2	2.05	0.56
16:h:97:HIS:HA	16:h:102:GLU:HB3	1.87	0.56
32:j:202:PLX:H132	21:m:152:TRP:HZ3	1.68	0.56
4:V:106:ARG:HG3	4:V:106:ARG:O	2.05	0.56
12:d:16:ARG:NH2	28:v:48:ASP:OD2	2.39	0.56
16:h:37:GLU:OE2	36:i:502:HOH:O	2.18	0.56
12:d:26:LEU:HD22	28:v:75:PRO:CB	2.35	0.56
20:l:123:LEU:HD13	30:r:503:CDL:H121	1.88	0.56
20:l:419:THR:HA	20:l:422:TYR:CE2	2.40	0.56
11:c:161:TYR:HB3	11:c:166:LEU:HG	1.88	0.56
30:i:401:CDL:OA7	30:i:401:CDL:HA62	2.04	0.56
22:n:14:HIS:HE1	25:r:26:ASN:OD1	1.89	0.56
29:w:59:VAL:HG13	29:w:201:PRO:HA	1.88	0.56
29:w:80:LYS:NZ	29:w:267:GLU:OE2	2.36	0.55
9:a:126:TYR:O	32:a:202:PLX:H1B2	2.06	0.55
20:l:383:MET:HB3	20:l:386:LEU:HD12	1.88	0.55
21:m:27:ILE:HD13	26:s:121:TRP:CZ3	2.41	0.55
26:s:170:GLU:OE2	27:u:98:ARG:NH1	2.39	0.55
20:l:60:GLU:OE1	20:l:83:ASP:HA	2.07	0.55
23:o:80:PHE:HE1	23:o:86:THR:HG21	1.72	0.55
13:e:125:LEU:HD21	13:e:129:ARG:CZ	2.36	0.55
20:l:173:LEU:HD12	25:r:405:LEU:HD21	1.88	0.55
20:l:559:GLU:O	20:l:563:PRO:HD2	2.07	0.55
30:l:701:CDL:H312	30:l:701:CDL:H522	1.89	0.55
34:s:402:UQ:CM2	36:s:516:HOH:O	2.54	0.55
27:u:114:LYS:HB3	27:u:115:LEU:HD12	1.88	0.55
10:b:86:LEU:HD11	20:l:9:LEU:HD12	1.89	0.55
10:b:104:ILE:HB	28:v:48:ASP:HB3	1.87	0.55
17:i:97:MET:HA	17:i:97:MET:CE	2.32	0.55
4:V:105:THR:O	4:V:105:THR:HG22	2.07	0.55
9:a:133:TYR:OH	12:d:87:GLU:OE2	2.21	0.55
9:a:137:MET:HE2	12:d:83:LEU:HD22	1.88	0.55
11:c:62:TYR:OH	11:c:74:ASP:OD1	2.24	0.55
14:f:72:ARG:NH2	15:g:18:ASN:OD1	2.36	0.55
30:a:201:CDL:H362	10:b:80:TRP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:112:HIS:HB2	17:i:184:ILE:HD13	1.89	0.55
29:w:57:SER:O	29:w:156:GLY:HA3	2.05	0.55
21:m:1:MET:SD	21:m:2:THR:N	2.80	0.55
27:u:96:LEU:HD12	27:u:99:HIS:CD2	2.41	0.55
7:Y:93:THR:OG1	7:Y:96:GLU:OE1	2.23	0.54
30:a:201:CDL:H512	33:l:703:PEE:H52	1.89	0.54
10:b:16:ARG:HD3	10:b:20:ARG:NH2	2.22	0.54
21:m:25:SER:O	21:m:28:TYR:N	2.39	0.54
27:u:85:TYR:CE1	27:u:104:GLN:HB2	2.42	0.54
6:X:120:MET:HE1	24:p:24:LEU:HB3	1.88	0.54
33:j:201:PEE:H72	33:j:201:PEE:H81	1.90	0.54
18:j:68:GLU:OE1	18:j:98:LEU:HD13	2.07	0.54
30:a:201:CDL:H201	30:a:201:CDL:C76	2.36	0.54
32:a:202:PLX:H1A2	32:a:202:PLX:O1	2.06	0.54
17:i:246:VAL:HG21	30:r:504:CDL:H362	1.88	0.54
17:i:268:GLN:NE2	17:i:272:LYS:HE3	2.22	0.54
18:j:22:PHE:HZ	26:s:62:ARG:HD3	1.72	0.54
12:d:102:ILE:HD11	13:e:125:LEU:HD22	1.89	0.54
4:V:12:ILE:HB	4:V:21:LYS:HD3	1.89	0.54
17:i:236:LYS:NZ	17:i:314:LYS:O	2.38	0.54
17:i:243:LEU:HD23	30:r:504:CDL:H361	1.89	0.54
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.43	0.54
6:X:100:VAL:HG12	6:X:142:GLN:HB2	1.88	0.53
12:d:160:LYS:NZ	15:g:114:ILE:O	2.41	0.53
20:l:370:THR:O	20:l:374:ILE:HG12	2.08	0.53
17:i:211:MET:HG2	17:i:333:SER:HB2	1.89	0.53
33:j:201:PEE:H49	33:j:201:PEE:H14	1.89	0.53
25:r:81:GLN:NE2	36:r:608:HOH:O	2.32	0.53
5:W:144:THR:HB	26:s:96:ILE:HG23	1.91	0.53
33:i:403:PEE:H42	33:i:403:PEE:C21	2.33	0.53
17:i:18:MET:HA	17:i:18:MET:CE	2.35	0.53
17:i:76:ILE:HG22	17:i:91:ASN:HD22	1.73	0.53
27:u:169:PHE:CE1	30:u:201:CDL:C56	2.89	0.53
29:w:110:GLY:HA2	29:w:134:TRP:CD2	2.44	0.53
26:s:87:VAL:N	26:s:88:PRO:CD	2.71	0.53
27:u:88:CYS:HB3	27:u:100:CYS:SG	2.48	0.53
9:a:106:VAL:HG23	22:n:50:ARG:HH21	1.74	0.53
26:s:80:SER:O	26:s:84:THR:OG1	2.20	0.53
27:u:24:VAL:HG13	27:u:82:PHE:CE2	2.43	0.53
29:w:211:VAL:HA	29:w:214:ILE:HG22	1.91	0.53
18:j:25:PRO:HG2	36:j:302:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:m:201:PEE:H7	33:m:201:PEE:C32	2.38	0.53
27:u:96:LEU:HB2	27:u:99:HIS:CD2	2.44	0.53
27:u:169:PHE:CZ	30:u:201:CDL:H561	2.44	0.53
32:a:202:PLX:H92	32:a:202:PLX:O6	2.09	0.52
24:p:92:GLU:HB3	24:p:95:GLU:HG3	1.90	0.52
25:r:306:PRO:O	25:r:310:MET:HG3	2.09	0.52
1:Q:53:TYR:HE1	33:i:403:PEE:H2	1.75	0.52
13:e:92:PHE:O	13:e:96:SER:HB2	2.08	0.52
18:j:73:LEU:N	18:j:74:PRO:CD	2.72	0.52
6:X:125:GLU:HG2	20:l:439:PRO:HG2	1.91	0.52
20:l:129:MET:HA	20:l:129:MET:HE2	1.92	0.52
29:w:63:ASP:OD2	29:w:245:PHE:CE2	2.63	0.52
6:X:90:TYR:HE1	8:Z:44:PRO:HB2	1.73	0.52
13:e:57:GLU:OE1	29:w:320:GLY:HA3	2.09	0.52
18:j:17:LEU:HD12	18:j:20:ILE:HD11	1.90	0.52
21:m:45:LEU:HD23	21:m:50:SER:HA	1.92	0.52
5:W:93:GLU:OE1	16:h:92:TYR:OH	2.23	0.52
7:Y:51:THR:HG22	7:Y:53:SER:H	1.74	0.52
15:g:15:PHE:HD1	32:i:402:PLX:H71	1.75	0.52
17:i:174:GLN:OE1	36:i:503:HOH:O	2.19	0.52
21:m:42:GLY:CA	33:m:201:PEE:H28	2.38	0.52
9:a:79:GLY:HA3	30:a:201:CDL:H222	1.92	0.52
9:a:139:ILE:HG23	25:r:54:LEU:HD23	1.91	0.52
12:d:122:ARG:HH22	12:d:129:LEU:HD22	1.75	0.52
33:i:403:PEE:C20	20:l:562:LEU:CG	2.76	0.52
18:j:73:LEU:O	26:s:160:TYR:OH	2.22	0.52
18:j:95:LEU:HD13	26:s:302:MET:HG2	1.92	0.52
25:r:445:LEU:O	25:r:448:THR:HG22	2.10	0.52
4:V:108:TYR:CE1	30:V:201:CDL:C11	2.92	0.52
15:g:34:VAL:HG12	30:u:201:CDL:H771	1.92	0.52
33:i:403:PEE:H31	20:l:562:LEU:HD21	1.92	0.52
21:m:51:PHE:O	21:m:55:MET:HG2	2.10	0.52
24:p:44:MET:HE3	24:p:48:PHE:CE2	2.45	0.52
30:a:201:CDL:OB7	30:a:201:CDL:HB61	2.09	0.51
17:i:95:MET:HE1	17:i:149:ILE:HG22	1.89	0.51
21:m:72:THR:HG22	26:s:121:TRP:HH2	1.74	0.51
25:r:412:ILE:HA	25:r:416:ARG:HG3	1.92	0.51
21:m:41:CYS:SG	21:m:57:PHE:HB2	2.50	0.51
26:s:24:GLU:OE2	26:s:228:TYR:OH	2.23	0.51
11:c:83:GLN:NE2	11:c:97:LEU:O	2.36	0.51
25:r:225:ILE:HD13	25:r:331:ASN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:43:TYR:CZ	5:W:68:ARG:HG3	2.46	0.51
13:e:70:ASN:O	13:e:73:SER:HB2	2.10	0.51
16:h:21:GLN:HA	19:k:53:PHE:CE1	2.46	0.51
1:Q:39:PRO:HB3	1:Q:43:TRP:CD1	2.46	0.51
17:i:95:MET:HE3	17:i:149:ILE:HG22	1.90	0.51
30:l:701:CDL:H331	30:l:701:CDL:H541	1.92	0.51
17:i:276:ILE:HG21	33:r:501:PEE:H14	1.93	0.51
20:l:68:TRP:CH2	20:l:69:MET:HE2	2.45	0.51
26:s:86:TRP:CZ3	26:s:91:MET:HE1	2.45	0.51
27:u:137:LEU:HD12	27:u:138:PRO:HD2	1.92	0.51
16:h:22:SER:CB	16:h:34:HIS:CD2	2.94	0.51
18:j:67:LEU:HD21	19:k:68:ALA:HB3	1.93	0.51
25:r:207:MET:HE1	36:r:655:HOH:O	2.11	0.51
29:w:165:SER:HB3	29:w:245:PHE:CZ	2.46	0.51
7:Y:100:LEU:HB2	28:v:111:ARG:HH12	1.76	0.51
18:j:67:LEU:HD21	19:k:68:ALA:HB1	1.93	0.51
20:l:393:ASP:O	20:l:397:GLU:HG3	2.10	0.51
29:w:54:THR:O	29:w:55:GLU:HG3	2.10	0.51
17:i:89:MET:HE1	17:i:98:MET:CE	2.41	0.51
17:i:125:GLN:HG3	30:i:401:CDL:OA3	2.11	0.51
18:j:63:LEU:CD1	36:m:313:HOH:O	2.59	0.51
20:l:119:LYS:NZ	30:r:503:CDL:OA3	2.44	0.51
21:m:146:LEU:O	21:m:150:GLY:N	2.43	0.51
21:m:164:GLY:O	21:m:168:ILE:HG12	2.11	0.51
29:w:235:GLN:NE2	29:w:239:ASN:OD1	2.44	0.51
30:V:201:CDL:H761	23:o:91:ALA:HB2	1.93	0.50
11:c:127:ASN:O	11:c:131:LYS:HG3	2.11	0.50
9:a:184:LYS:HB3	16:h:30:PRO:HB3	1.93	0.50
30:a:201:CDL:H251	30:a:201:CDL:C21	2.35	0.50
10:b:32:GLU:HG3	24:p:115:TYR:HD1	1.75	0.50
27:u:114:LYS:C	27:u:115:LEU:HD12	2.35	0.50
20:l:359:MET:O	20:l:436:ARG:NH2	2.44	0.50
24:p:100:PRO:HG3	25:r:419:TYR:CE1	2.46	0.50
27:u:83:THR:HA	27:u:86:TRP:CD1	2.46	0.50
29:w:38:TYR:HH	29:w:292:HIS:HD1	1.58	0.50
12:d:75:THR:OG1	13:e:146:LYS:HE3	2.11	0.50
27:u:112:LEU:O	27:u:116:GLY:HA2	2.12	0.50
27:u:169:PHE:HE1	30:u:201:CDL:C56	2.23	0.50
18:j:73:LEU:HD13	21:m:55:MET:SD	2.51	0.50
28:v:84:GLN:O	28:v:88:ASP:OD2	2.30	0.50
29:w:146:ALA:HB1	29:w:157:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:55:ARG:HA	4:V:58:ARG:HG2	1.94	0.50
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.94	0.50
19:k:23:ARG:HG3	19:k:24:SER:H	1.77	0.50
20:l:166:THR:CG2	33:l:702:PEE:H2	2.42	0.50
21:m:25:SER:O	21:m:27:ILE:N	2.44	0.50
25:r:299:VAL:O	25:r:303:ILE:HG12	2.12	0.50
17:i:335:LEU:HD21	30:r:504:CDL:H391	1.94	0.50
22:n:30:ARG:HG3	22:n:30:ARG:HH11	1.77	0.50
28:v:60:ALA:O	28:v:64:ILE:HG12	2.12	0.50
4:V:106:ARG:C	4:V:106:ARG:HE	2.20	0.50
20:l:71:LEU:HD12	25:r:310:MET:HE1	1.93	0.50
8:Z:22:TRP:HB3	8:Z:50:ALA:HB3	1.94	0.49
16:h:22:SER:HB3	16:h:34:HIS:CD2	2.47	0.49
17:i:51:ARG:NH1	36:i:513:HOH:O	2.45	0.49
30:i:401:CDL:CA7	30:i:401:CDL:H342	2.42	0.49
25:r:105:PHE:O	25:r:109:THR:OG1	2.22	0.49
25:r:201:MET:HG3	33:r:501:PEE:H33	1.94	0.49
6:X:80:LYS:HE3	6:X:100:VAL:HG21	1.94	0.49
7:Y:43:ARG:HG3	7:Y:46:GLN:HB2	1.95	0.49
9:a:92:PHE:HD1	12:d:55:GLN:HE21	1.58	0.49
30:a:201:CDL:H381	30:a:201:CDL:C42	2.37	0.49
1:Q:52:MET:O	17:i:171:ASN:OD1	2.31	0.49
22:n:50:ARG:HB2	22:n:53:GLU:HB2	1.94	0.49
30:a:201:CDL:C82	25:r:442:LEU:HD23	2.42	0.49
16:h:50:ILE:HG22	16:h:54:LYS:HE3	1.94	0.49
25:r:218:LYS:O	25:r:222:GLU:HG2	2.12	0.49
4:V:91:PHE:CD1	32:r:502:PLX:H302	2.48	0.49
4:V:101:LEU:C	4:V:101:LEU:CD2	2.86	0.49
30:i:401:CDL:HB31	29:w:40:PRO:HB2	1.89	0.49
20:l:66:TRP:CB	33:l:703:PEE:H19	2.42	0.49
17:i:68:MET:HE2	17:i:68:MET:HA	1.94	0.49
25:r:373:ILE:HD11	25:r:444:LEU:HD23	1.94	0.49
29:w:62:VAL:CG1	29:w:70:LYS:HB2	2.42	0.49
13:e:148:GLN:HB2	15:g:113:GLU:HB3	1.94	0.49
20:l:66:TRP:HZ3	33:l:703:PEE:H38	1.78	0.49
21:m:5:ILE:HA	21:m:8:ILE:HG12	1.95	0.49
3:U:67:PRO:HG2	27:u:129:THR:HG22	1.95	0.49
7:Y:87:PRO:HG3	28:v:96:VAL:HG22	1.95	0.49
9:a:147:ALA:HB2	25:r:173:SER:HB2	1.95	0.49
10:b:74:HIS:NE2	20:l:35:TYR:OH	2.34	0.49
17:i:95:MET:HE2	17:i:149:ILE:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:114:LYS:CB	27:u:115:LEU:HD12	2.43	0.49
9:a:184:LYS:O	16:h:30:PRO:HG3	2.13	0.48
2:S:54:ILE:HD11	27:u:21:SER:HA	1.95	0.48
4:V:62:THR:OG1	4:V:104:ARG:HG2	2.13	0.48
17:i:213:LEU:HD13	30:i:401:CDL:C14	2.43	0.48
33:j:201:PEE:H35	33:j:201:PEE:H30	1.47	0.48
4:V:61:PHE:HD2	4:V:104:ARG:HH12	1.62	0.48
17:i:4:ILE:HD11	29:w:44:VAL:HG13	1.94	0.48
17:i:88:LYS:HG3	17:i:148:SER:OG	2.13	0.48
17:i:203:LEU:HD23	36:i:552:HOH:O	2.13	0.48
20:l:554:ASP:OD2	25:r:288:TYR:OH	2.22	0.48
25:r:197:LEU:HD13	33:r:501:PEE:C43	2.40	0.48
12:d:26:LEU:HD22	28:v:75:PRO:HB2	1.95	0.48
20:l:331:MET:HB3	20:l:387:THR:HG22	1.95	0.48
20:l:407:TRP:CZ2	20:l:411:MET:HE3	2.48	0.48
20:l:536:LEU:HB3	20:l:537:PRO:HD3	1.95	0.48
29:w:314:LEU:O	29:w:318:THR:HG22	2.14	0.48
12:d:73:ASP:OD1	12:d:73:ASP:N	2.45	0.48
20:l:288:THR:HG21	20:l:307:SER:HB3	1.95	0.48
33:l:703:PEE:H28	30:r:503:CDL:H271	1.95	0.48
29:w:181:LYS:O	29:w:184:VAL:N	2.45	0.48
1:Q:65:PRO:HB2	1:Q:67:ASN:O	2.14	0.48
3:U:67:PRO:HA	3:U:74:GLN:HE21	1.79	0.48
12:d:114:GLN:HG3	20:l:203:MET:HG2	1.95	0.48
20:l:13:THR:O	20:l:16:THR:OG1	2.30	0.48
21:m:57:PHE:HD1	26:s:107:ALA:HB1	1.78	0.48
26:s:138:GLN:HA	26:s:286:MET:HE1	1.96	0.48
6:X:82:ARG:NE	6:X:125:GLU:OE2	2.39	0.48
10:b:100:ARG:HE	12:d:118:GLY:HA3	1.78	0.48
11:c:117:VAL:HG21	20:l:539:TYR:HB2	1.95	0.48
13:e:98:VAL:HG22	25:r:36:LEU:HB2	1.94	0.48
19:k:23:ARG:H	21:m:23:LYS:HZ2	1.62	0.48
20:l:59:GLN:HE21	20:l:61:MET:HE3	1.79	0.48
20:l:410:LEU:O	20:l:414:ILE:HG12	2.13	0.48
20:l:452:ASN:HA	20:l:455:LYS:HG2	1.95	0.48
21:m:173:ARG:HD3	29:w:289:ARG:CZ	2.44	0.48
26:s:140:ILE:O	26:s:143:GLU:HG2	2.13	0.48
11:c:55:TYR:OH	11:c:74:ASP:O	2.23	0.48
17:i:325:LEU:CD1	30:i:401:CDL:H132	2.43	0.48
23:o:57:LEU:HD23	23:o:57:LEU:O	2.13	0.48
25:r:12:LEU:HB2	25:r:13:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:v:15:LYS:HG3	28:v:110:GLN:NE2	2.24	0.48
30:V:201:CDL:H511	23:o:84:PRO:HD3	1.95	0.48
9:a:120:TRP:O	9:a:124:THR:HG22	2.14	0.48
12:d:33:LEU:HD12	12:d:36:ILE:HD11	1.96	0.48
28:v:66:LEU:CD1	28:v:83:GLU:HB2	2.44	0.48
9:a:159:LEU:HD22	9:a:163:ARG:NH1	2.29	0.47
18:j:30:TYR:CE2	26:s:59:GLU:HB2	2.48	0.47
20:l:190:LEU:HD21	25:r:307:TRP:CH2	2.48	0.47
21:m:175:ASN:OD1	29:w:289:ARG:NH2	2.39	0.47
33:m:201:PEE:H2	33:m:201:PEE:C4	2.44	0.47
18:j:84:LEU:HD13	26:s:309:ILE:HG23	1.96	0.47
20:l:395:ILE:O	20:l:399:VAL:HG23	2.13	0.47
20:l:504:LEU:HD13	30:l:701:CDL:H511	1.96	0.47
25:r:13:PRO:HB3	30:r:504:CDL:H581	1.97	0.47
32:e:201:PLX:H122	30:r:503:CDL:H631	1.95	0.47
17:i:85:THR:HG22	17:i:87:THR:HG23	1.96	0.47
20:l:295:GLN:HB2	20:l:301:ILE:HG12	1.96	0.47
20:l:298:ILE:O	20:l:302:VAL:HG23	2.14	0.47
29:w:60:ILE:HD11	29:w:158:VAL:HG22	1.96	0.47
7:Y:105:ASP:N	7:Y:105:ASP:OD1	2.47	0.47
16:h:89:GLU:OE1	16:h:91:LYS:NZ	2.46	0.47
25:r:14:MET:O	25:r:18:SER:OG	2.25	0.47
25:r:73:LEU:HD22	25:r:103:GLN:OE1	2.13	0.47
5:W:51:MET:HA	26:s:313:SER:HB2	1.97	0.47
15:g:83:TYR:CZ	15:g:87:LEU:HD11	2.49	0.47
20:l:233:LEU:HB3	20:l:234:PRO:HD3	1.97	0.47
20:l:264:TYR:CD2	20:l:265:PRO:HD3	2.50	0.47
25:r:303:ILE:HG22	25:r:305:THR:HG23	1.97	0.47
27:u:115:LEU:HD12	27:u:115:LEU:N	2.30	0.47
4:V:109:GLY:H	30:V:201:CDL:HB32	1.79	0.47
9:a:75:ILE:HD13	30:a:201:CDL:C82	2.44	0.47
11:c:184:TYR:HA	28:v:34:ARG:HH12	1.78	0.47
14:f:68:GLU:HG2	15:g:21:ARG:HE	1.79	0.47
18:j:72:LEU:C	18:j:74:PRO:HD2	2.40	0.47
20:l:268:GLU:HA	20:l:274:GLN:NE2	2.30	0.47
25:r:196:TRP:CD1	25:r:250:LEU:HB3	2.49	0.47
25:r:357:THR:O	25:r:361:VAL:HG23	2.15	0.47
28:v:76:ASN:C	28:v:76:ASN:HD22	2.22	0.47
17:i:89:MET:HE1	17:i:98:MET:HE2	1.95	0.47
17:i:154:MET:HE2	17:i:191:THR:HB	1.97	0.47
30:a:201:CDL:H322	33:l:703:PEE:H62	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:58:ARG:NE	23:o:35:GLU:OE2	2.44	0.47
20:l:331:MET:SD	20:l:465:GLY:HA2	2.55	0.47
20:l:557:TRP:O	20:l:561:ILE:HG12	2.14	0.47
30:r:503:CDL:H312	30:r:503:CDL:H742	1.97	0.47
12:d:99:ASP:OD2	12:d:142:ARG:NH1	2.48	0.47
17:i:95:MET:HE2	17:i:149:ILE:N	2.29	0.47
36:n:101:HOH:O	25:r:30:HIS:CE1	2.68	0.47
25:r:347:GLY:O	25:r:350:THR:HG22	2.14	0.47
15:g:85:TYR:CZ	17:i:344:SER:HB3	2.49	0.46
30:i:401:CDL:H331	30:i:401:CDL:OA9	2.15	0.46
22:n:39:ARG:HG3	22:n:57:TRP:CE2	2.50	0.46
25:r:126:LEU:HD21	25:r:150:LEU:HD12	1.97	0.46
25:r:300:ALA:O	25:r:308:SER:HB3	2.15	0.46
11:c:81:ARG:HD3	11:c:85:GLU:OE2	2.15	0.46
30:l:701:CDL:H541	30:l:701:CDL:H572	1.57	0.46
24:p:63:LEU:C	24:p:65:ARG:H	2.23	0.46
25:r:118:PHE:O	25:r:122:PHE:HB3	2.16	0.46
12:d:69:ARG:NH1	22:n:43:LEU:O	2.45	0.46
18:j:67:LEU:CD2	19:k:68:ALA:HB3	2.46	0.46
27:u:115:LEU:HD22	27:u:117:TRP:CH2	2.51	0.46
32:e:201:PLX:H1C3	33:l:703:PEE:O2P	2.16	0.46
18:j:108:GLN:HB2	21:m:169:MET:HE1	1.96	0.46
20:l:292:ALA:HB2	20:l:304:PHE:HB3	1.97	0.46
20:l:488:MET:O	20:l:492:ILE:HG12	2.16	0.46
27:u:74:ILE:HD11	27:u:117:TRP:HZ3	1.79	0.46
9:a:168:TRP:CD2	15:g:2:THR:HG23	2.51	0.46
19:k:8:ILE:HG21	19:k:43:MET:HB2	1.97	0.46
20:l:128:MET:HG2	20:l:251:THR:HG22	1.98	0.46
26:s:79:LEU:HD11	26:s:222:MET:SD	2.55	0.46
17:i:291:TYR:CZ	33:i:403:PEE:H49	2.51	0.46
20:l:267:MET:HE1	20:l:273:VAL:HG12	1.98	0.46
20:l:407:TRP:CE2	20:l:411:MET:HE3	2.51	0.46
25:r:61:LEU:HB2	25:r:457:PRO:HD3	1.97	0.46
27:u:37:ASP:OD1	27:u:41:LYS:HG2	2.16	0.46
3:U:33:PRO:HA	26:s:310:MET:HG2	1.96	0.46
9:a:127:ASP:CG	32:a:202:PLX:H12	2.40	0.46
11:c:118:ASP:O	20:l:535:ARG:HD3	2.15	0.46
17:i:118:VAL:O	17:i:122:ILE:HG12	2.16	0.46
19:k:25:HIS:O	19:k:28:SER:N	2.41	0.46
20:l:49:VAL:HB	20:l:50:PRO:HD3	1.96	0.46
20:l:286:LEU:HD22	20:l:411:MET:SD	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:43:LEU:HG	26:s:179:TRP:HE1	1.81	0.46
11:c:176:LYS:HA	11:c:176:LYS:HD2	1.79	0.46
12:d:160:LYS:HE2	13:e:147:ILE:HG23	1.98	0.46
20:l:589:LEU:O	20:l:593:ILE:HG13	2.16	0.46
28:v:70:LYS:HD3	28:v:80:CYS:SG	2.56	0.46
9:a:127:ASP:OD1	32:a:202:PLX:H12	2.16	0.46
10:b:99:GLU:OE2	20:l:2:ASN:ND2	2.49	0.46
20:l:172:ILE:HG21	25:r:408:LEU:HD12	1.97	0.46
29:w:71:GLY:O	29:w:75:ARG:HG3	2.16	0.46
2:S:66:LEU:HD21	27:u:75:LYS:HA	1.98	0.46
33:m:201:PEE:H52	26:s:104:PHE:HE1	1.81	0.46
4:V:17:GLU:OE2	4:V:20:ARG:HD3	2.15	0.45
4:V:120:LEU:HD21	32:r:502:PLX:H332	1.98	0.45
11:c:113:ILE:HG13	11:c:115:ASN:HB2	1.98	0.45
17:i:130:LEU:O	36:i:504:HOH:O	2.21	0.45
20:l:494:THR:HG22	20:l:498:PHE:CE2	2.51	0.45
2:S:64:LYS:HA	2:S:64:LYS:HD3	1.67	0.45
30:a:201:CDL:H422	30:a:201:CDL:C38	2.37	0.45
10:b:87:LYS:HD3	10:b:88:TYR:CZ	2.52	0.45
26:s:24:GLU:HA	26:s:271:LEU:HD13	1.98	0.45
7:Y:105:ASP:O	28:v:29:TYR:OH	2.30	0.45
9:a:89:VAL:O	9:a:93:ILE:HB	2.16	0.45
16:h:7:GLN:NE2	16:h:15:ASP:OD1	2.36	0.45
16:h:21:GLN:HA	19:k:53:PHE:CD1	2.52	0.45
24:p:47:ARG:HH22	24:p:70:GLU:CD	2.24	0.45
8:Z:30:GLU:O	8:Z:34:GLU:HG2	2.15	0.45
13:e:125:LEU:HD21	13:e:129:ARG:NH1	2.31	0.45
17:i:213:LEU:CD1	30:i:401:CDL:C14	2.93	0.45
20:l:54:PHE:O	20:l:58:GLY:N	2.45	0.45
28:v:52:MET:HB2	28:v:55:GLN:HG3	1.97	0.45
11:c:125:SER:O	11:c:129:MET:HG3	2.16	0.45
19:k:4:VAL:O	19:k:8:ILE:HG12	2.16	0.45
25:r:174:LEU:HA	25:r:179:ILE:HD11	1.98	0.45
30:a:201:CDL:H191	30:a:201:CDL:H732	1.99	0.45
16:h:51:ARG:HA	16:h:54:LYS:HG2	1.99	0.45
20:l:280:LEU:CD2	33:l:702:PEE:H47	2.46	0.45
21:m:38:GLY:HA3	33:m:201:PEE:H41	1.99	0.45
26:s:195:ARG:HD3	26:s:231:ILE:HD11	1.99	0.45
16:h:54:LYS:HG3	16:h:55:GLU:HG3	1.98	0.45
17:i:146:SER:O	17:i:149:ILE:HG12	2.17	0.45
21:m:38:GLY:HA3	33:m:201:PEE:H40	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:96:ASP:OD1	11:c:96:ASP:N	2.48	0.45
11:c:113:ILE:C	11:c:115:ASN:H	2.24	0.45
17:i:42:PRO:HG2	21:m:167:VAL:HG22	1.98	0.45
18:j:48:ARG:HB2	18:j:49:LEU:H	1.58	0.45
25:r:77:LEU:O	25:r:81:GLN:HG3	2.16	0.45
33:r:501:PEE:H79	33:r:501:PEE:C22	2.45	0.45
29:w:241:TYR:O	29:w:246:LEU:CD2	2.64	0.45
30:V:201:CDL:HB61	23:o:82:PRO:CB	2.47	0.45
7:Y:71:TRP:CD1	7:Y:72:ARG:HH21	2.35	0.45
10:b:104:ILE:HD13	12:d:18:PRO:HG3	1.99	0.45
15:g:19:GLU:O	15:g:22:SER:OG	2.33	0.45
20:l:80:PHE:HB3	20:l:82:MET:HE2	1.97	0.45
30:V:201:CDL:HB61	23:o:82:PRO:HB2	1.99	0.45
12:d:46:THR:O	12:d:50:GLU:HG3	2.17	0.45
20:l:591:PHE:HA	20:l:594:THR:CG2	2.47	0.45
25:r:104:LEU:HG	25:r:108:MET:HE2	1.99	0.45
9:a:140:LEU:HD21	25:r:177:LEU:HB3	1.99	0.44
9:a:174:ILE:HG21	16:h:20:ILE:HG21	1.99	0.44
2:S:37:ARG:O	5:W:143:TYR:OH	2.26	0.44
3:U:26:GLY:HA3	33:j:201:PEE:H37	1.99	0.44
30:a:201:CDL:H201	30:a:201:CDL:H761	1.98	0.44
10:b:100:ARG:HD3	20:l:60:GLU:HG3	1.98	0.44
16:h:44:ALA:O	16:h:47:ILE:HG22	2.17	0.44
18:j:18:VAL:HG22	26:s:222:MET:HG3	2.00	0.44
22:n:30:ARG:HG3	22:n:30:ARG:NH1	2.32	0.44
30:V:201:CDL:H862	25:r:264:LEU:HD21	1.99	0.44
10:b:109:THR:HB	10:b:116:VAL:HG22	1.98	0.44
16:h:19:THR:HA	17:i:84:TRP:HB2	1.99	0.44
20:l:27:TYR:O	20:l:115:ASN:ND2	2.44	0.44
33:l:703:PEE:H31	25:r:449:LEU:HD23	1.99	0.44
27:u:112:LEU:O	27:u:116:GLY:N	2.50	0.44
29:w:70:LYS:HG3	29:w:71:GLY:N	2.32	0.44
29:w:256:LEU:HB3	29:w:258:TYR:CE2	2.53	0.44
36:h:204:HOH:O	21:m:127:ILE:HG22	2.17	0.44
19:k:23:ARG:HG2	21:m:23:LYS:HZ2	1.83	0.44
20:l:141:PHE:HE2	25:r:375:LEU:HD11	1.81	0.44
23:o:113:GLU:O	23:o:117:GLN:HG2	2.17	0.44
24:p:14:GLN:HB3	24:p:18:ARG:NH1	2.32	0.44
25:r:364:LEU:HD22	25:r:369:LEU:HD22	1.98	0.44
30:a:201:CDL:H211	30:a:201:CDL:H182	1.69	0.44
18:j:72:LEU:O	18:j:75:LEU:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:8:THR:HG21	20:l:82:MET:HG3	1.99	0.44
26:s:9:LEU:O	26:s:13:ILE:HG12	2.18	0.44
18:j:72:LEU:C	18:j:74:PRO:CD	2.90	0.44
33:j:201:PEE:H59	33:j:201:PEE:H64	1.77	0.44
20:l:228:GLY:HA3	33:l:702:PEE:H38	2.00	0.44
20:l:500:LEU:HD23	30:l:701:CDL:H342	2.00	0.44
24:p:26:HIS:CD2	24:p:79:PRO:HB3	2.52	0.44
24:p:108:HIS:CD2	24:p:109:PRO:HD2	2.52	0.44
24:p:136:GLU:HG2	24:p:165:PRO:HA	1.99	0.44
25:r:50:LEU:HD23	25:r:50:LEU:HA	1.90	0.44
27:u:47:ARG:NH2	27:u:53:PRO:HG3	2.32	0.44
29:w:81:LEU:HD23	29:w:81:LEU:HA	1.79	0.44
4:V:91:PHE:CE1	32:r:502:PLX:H302	2.53	0.44
18:j:65:PHE:CD2	18:j:98:LEU:HD11	2.52	0.44
32:j:202:PLX:H342	32:j:202:PLX:H372	1.81	0.44
22:n:26:TYR:OH	22:n:30:ARG:NH2	2.41	0.44
29:w:233:TYR:CE2	29:w:237:ILE:HD11	2.53	0.44
11:c:58:ARG:HD2	23:o:35:GLU:HG3	1.98	0.44
15:g:55:VAL:HG11	30:r:504:CDL:H712	1.99	0.44
16:h:69:ARG:O	16:h:73:MET:HG3	2.18	0.44
18:j:87:MET:HE1	26:s:309:ILE:HD11	1.99	0.44
20:l:19:ILE:HG21	30:r:503:CDL:H852	1.99	0.44
20:l:66:TRP:HB2	33:l:703:PEE:C14	2.46	0.44
26:s:89:LEU:HA	26:s:90:PRO:HD3	1.82	0.44
6:X:113:LEU:O	6:X:117:GLU:HG3	2.17	0.44
19:k:56:ALA:O	19:k:59:MET:HG3	2.17	0.44
20:l:418:LEU:HD23	30:l:701:CDL:H562	2.00	0.44
25:r:243:MET:HB3	25:r:301:ILE:HG21	1.99	0.44
30:r:504:CDL:H332	30:r:504:CDL:H202	2.00	0.44
29:w:63:ASP:O	29:w:206:TYR:HA	2.17	0.44
4:V:109:GLY:N	30:V:201:CDL:HB32	2.33	0.43
7:Y:76:ASP:O	20:l:385:TYR:OH	2.33	0.43
12:d:28:ASN:HA	28:v:75:PRO:HG3	1.99	0.43
26:s:225:MET:SD	34:s:402:UQ:H153	2.58	0.43
5:W:90:ASN:ND2	5:W:123:GLU:O	2.51	0.43
13:e:137:MET:HE3	13:e:137:MET:HB2	1.80	0.43
17:i:41:ILE:HG13	19:k:73:LEU:HD21	2.00	0.43
33:i:403:PEE:C18	33:i:403:PEE:C22	2.85	0.43
19:k:38:LEU:O	19:k:42:ILE:HG12	2.18	0.43
21:m:23:LYS:N	21:m:24:PRO:HD3	2.33	0.43
27:u:88:CYS:HB3	27:u:100:CYS:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:97:ILE:HG22	5:W:98:MET:HE2	2.00	0.43
30:a:201:CDL:C62	20:l:9:LEU:HD22	2.49	0.43
17:i:44:LEU:HD22	17:i:122:ILE:HG21	2.00	0.43
17:i:69:MET:HE3	17:i:97:MET:HE1	1.99	0.43
17:i:81:SER:O	17:i:83:GLN:N	2.48	0.43
20:l:384:PRO:HA	20:l:389:PHE:CD1	2.53	0.43
20:l:401:MET:SD	20:l:486:MET:HE2	2.58	0.43
25:r:155:ALA:HB1	33:r:501:PEE:H43	2.00	0.43
34:s:402:UQ:H101	34:s:402:UQ:H121	1.70	0.43
4:V:69:ILE:CG1	4:V:100:THR:HG21	2.45	0.43
12:d:26:LEU:HD22	28:v:75:PRO:HB3	2.00	0.43
17:i:129:LEU:CD1	30:i:401:CDL:H341	2.47	0.43
17:i:258:SER:OG	17:i:336:VAL:HG22	2.18	0.43
20:l:78:LEU:HD11	30:r:503:CDL:H251	2.00	0.43
20:l:128:MET:HE1	20:l:255:ALA:HB2	2.01	0.43
20:l:398:ALA:O	20:l:402:SER:OG	2.31	0.43
26:s:298:LEU:O	26:s:302:MET:HG3	2.19	0.43
27:u:78:CYS:C	27:u:81:PRO:HD2	2.43	0.43
28:v:87:TRP:O	28:v:91:GLU:HG2	2.19	0.43
28:v:114:ARG:HG3	28:v:114:ARG:HH11	1.83	0.43
29:w:350:LYS:HA	29:w:350:LYS:HD3	1.71	0.43
3:U:82:LYS:HB3	3:U:82:LYS:HE2	1.69	0.43
12:d:81:ASP:O	12:d:85:MET:HG3	2.19	0.43
20:l:119:LYS:HZ1	30:r:503:CDL:H511	1.83	0.43
26:s:307:LEU:HA	26:s:310:MET:HE3	2.01	0.43
30:u:201:CDL:H521	30:u:201:CDL:H551	1.88	0.43
7:Y:78:ASP:OD2	7:Y:83:HIS:ND1	2.27	0.43
20:l:106:TRP:CD1	20:l:447:ASN:HD22	2.37	0.43
20:l:373:LEU:HD13	20:l:431:PHE:HE2	1.84	0.43
26:s:11:ILE:HB	26:s:12:PRO:HD3	2.01	0.43
5:W:50:MET:HE2	26:s:156:MET:HG3	1.99	0.43
16:h:22:SER:HA	16:h:34:HIS:HD2	1.83	0.43
17:i:84:TRP:CH2	19:k:59:MET:HE3	2.54	0.43
18:j:79:SER:HA	18:j:87:MET:HE2	2.00	0.43
25:r:116:ILE:HG13	27:u:168:PHE:CD1	2.54	0.43
25:r:326:LEU:HD13	36:r:663:HOH:O	2.18	0.43
30:u:201:CDL:H752	30:u:201:CDL:H781	1.41	0.43
12:d:119:GLU:HB3	28:v:50:GLN:HB2	2.00	0.43
17:i:57:THR:HA	19:k:77:LEU:HD13	2.00	0.43
21:m:25:SER:HB3	21:m:28:TYR:HD2	1.83	0.43
30:u:201:CDL:H781	30:u:201:CDL:H812	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:a:202:PLX:C11	25:r:40:SER:HB3	2.46	0.43
16:h:2:PRO:HD2	32:i:402:PLX:H1C2	2.00	0.43
17:i:222:SER:O	17:i:224:ALA:N	2.52	0.43
17:i:325:LEU:HD13	30:i:401:CDL:H132	2.01	0.43
25:r:378:GLU:OE2	36:r:601:HOH:O	2.21	0.43
30:r:503:CDL:H551	30:r:503:CDL:H582	1.54	0.43
29:w:295:ARG:HA	29:w:298:VAL:HG22	2.01	0.43
29:w:343:TYR:HA	29:w:352:ILE:HD12	2.01	0.43
17:i:268:GLN:HG3	27:u:168:PHE:CZ	2.54	0.43
20:l:221:ALA:HA	20:l:226:GLN:HG2	2.01	0.43
22:n:17:VAL:HG23	36:n:101:HOH:O	2.18	0.43
24:p:28:GLU:OE1	24:p:34:ARG:NH1	2.49	0.43
25:r:97:THR:HG21	30:r:504:CDL:H242	2.00	0.43
5:W:51:MET:HG3	26:s:313:SER:HB3	2.01	0.42
5:W:128:ARG:HB3	5:W:132:GLU:OE2	2.19	0.42
17:i:298:TYR:O	17:i:303:THR:OG1	2.33	0.42
22:n:17:VAL:N	22:n:18:PRO:CD	2.82	0.42
1:Q:36:GLN:NE2	25:r:137:GLY:O	2.52	0.42
4:V:94:GLY:HA3	4:V:119:GLY:HA2	2.01	0.42
5:W:98:MET:HE3	16:h:79:ILE:HA	2.00	0.42
18:j:63:LEU:HD12	36:m:313:HOH:O	2.19	0.42
25:r:168:GLN:HB2	25:r:174:LEU:HG	2.01	0.42
7:Y:45:ARG:HG2	20:l:439:PRO:HB3	2.01	0.42
9:a:136:THR:HG21	25:r:48:ASN:HD22	1.84	0.42
12:d:33:LEU:HA	12:d:36:ILE:HG12	2.02	0.42
17:i:106:LEU:HG	17:i:138:PRO:HB2	2.01	0.42
26:s:129:LEU:O	26:s:133:LEU:HG	2.19	0.42
28:v:46:MET:HE2	28:v:56:ARG:HB3	2.00	0.42
6:X:90:TYR:CE1	8:Z:44:PRO:HB2	2.53	0.42
12:d:37:PHE:CE1	20:l:3:PRO:HB3	2.54	0.42
32:i:402:PLX:H72	32:i:402:PLX:H101	1.57	0.42
20:l:327:LEU:O	20:l:331:MET:HG2	2.18	0.42
34:s:402:UQ:HM53	34:s:402:UQ:H72	1.73	0.42
28:v:74:PHE:HB3	28:v:75:PRO:HD3	2.01	0.42
2:S:57:VAL:HG23	2:S:59:ARG:HE	1.85	0.42
6:X:82:ARG:NH2	6:X:125:GLU:O	2.53	0.42
31:X:201:8Q1:O40	31:X:201:8Q1:N36	2.52	0.42
30:a:201:CDL:H521	33:l:703:PEE:H14	2.02	0.42
32:a:202:PLX:H111	25:r:40:SER:CB	2.45	0.42
13:e:65:ASN:ND2	25:r:427:LYS:HE2	2.34	0.42
13:e:76:TYR:HB2	13:e:83:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:37:GLU:HB2	16:h:63:PHE:CE1	2.54	0.42
20:l:97:THR:HG21	20:l:125:LEU:HD22	2.01	0.42
20:l:229:LEU:HG	33:l:702:PEE:C23	2.49	0.42
4:V:42:ALA:HA	20:l:589:LEU:HD23	2.02	0.42
17:i:18:MET:CE	17:i:21:MET:SD	3.07	0.42
17:i:213:LEU:HD11	30:i:401:CDL:H141	2.00	0.42
18:j:55:PHE:HA	18:j:58:VAL:HG12	2.01	0.42
3:U:63:MET:HE3	3:U:66:VAL:HG21	2.02	0.42
3:U:70:PRO:HB3	27:u:124:GLU:O	2.20	0.42
30:V:201:CDL:H792	20:l:557:TRP:CD2	2.55	0.42
5:W:70:ALA:HB2	27:u:125:LEU:HD13	2.01	0.42
30:a:201:CDL:H111	33:l:703:PEE:C37	2.49	0.42
12:d:113:CYS:O	12:d:117:GLU:HG2	2.19	0.42
13:e:151:GLU:HG3	13:e:153:GLU:HG3	2.02	0.42
36:h:204:HOH:O	21:m:127:ILE:CG2	2.67	0.42
32:r:502:PLX:H1C3	32:r:502:PLX:H22	1.76	0.42
26:s:267:THR:O	26:s:271:LEU:HG	2.20	0.42
29:w:105:ASP:OD1	29:w:106:VAL:N	2.52	0.42
17:i:254:LEU:O	17:i:257:LEU:HB2	2.19	0.42
18:j:81:THR:C	18:j:83:ASN:H	2.28	0.42
20:l:97:THR:O	20:l:101:MET:HG3	2.19	0.42
32:r:502:PLX:H301	32:r:502:PLX:H331	1.61	0.42
29:w:353:TRP:CZ3	29:w:354:LEU:HG	2.55	0.42
11:c:122:THR:OG1	11:c:124:VAL:O	2.31	0.42
14:f:55:TRP:O	14:f:59:ILE:HG12	2.19	0.42
16:h:60:PHE:O	16:h:64:VAL:HG23	2.20	0.42
33:j:201:PEE:H74	33:j:201:PEE:C40	2.36	0.42
20:l:392:LYS:NZ	36:l:807:HOH:O	2.35	0.42
24:p:176:GLU:HG2	24:p:177:ARG:N	2.35	0.42
28:v:51:LEU:HD21	28:v:64:ILE:HD13	2.00	0.42
5:W:85:GLN:O	5:W:89:GLU:HG3	2.20	0.42
17:i:45:MET:SD	21:m:171:ILE:HD12	2.60	0.42
17:i:338:PRO:HD3	30:u:201:CDL:H621	2.02	0.42
20:l:10:THR:O	20:l:14:ILE:HG12	2.20	0.42
20:l:392:LYS:HE3	36:l:821:HOH:O	2.20	0.42
21:m:146:LEU:HD12	21:m:150:GLY:HA3	2.02	0.42
22:n:42:SER:O	22:n:46:LYS:HG3	2.20	0.42
30:r:504:CDL:H792	30:r:504:CDL:H761	1.70	0.42
29:w:223:ASN:O	29:w:227:MET:HG2	2.20	0.42
32:e:201:PLX:H121	32:e:201:PLX:H152	1.71	0.41
15:g:2:THR:HG22	15:g:4:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:j:202:PLX:H322	32:j:202:PLX:H351	1.54	0.41
19:k:37:MET:HG3	19:k:67:ALA:CB	2.50	0.41
20:l:494:THR:HG22	20:l:498:PHE:HE2	1.85	0.41
25:r:394:ILE:H	25:r:394:ILE:HD12	1.85	0.41
4:V:69:ILE:HG21	4:V:100:THR:CG2	2.50	0.41
8:Z:31:THR:O	8:Z:35:LYS:HG3	2.19	0.41
32:j:202:PLX:H132	21:m:152:TRP:CZ3	2.52	0.41
20:l:152:PHE:CD1	20:l:168:ALA:HB1	2.55	0.41
30:l:701:CDL:H741	30:l:701:CDL:H321	2.02	0.41
21:m:30:GLY:O	21:m:34:ILE:HG13	2.20	0.41
23:o:28:GLU:HA	23:o:31:LYS:HG2	2.02	0.41
32:r:502:PLX:H91	32:r:502:PLX:H121	1.88	0.41
26:s:32:GLN:OE1	26:s:34:ARG:NH2	2.53	0.41
26:s:294:LEU:O	26:s:298:LEU:HG	2.20	0.41
11:c:32:VAL:HA	11:c:36:MET:HE3	2.03	0.41
32:e:201:PLX:C1C	33:l:703:PEE:O2P	2.68	0.41
32:i:402:PLX:H22	32:i:402:PLX:H1C3	1.80	0.41
32:r:502:PLX:H6	32:r:502:PLX:H51	1.39	0.41
8:Z:13:LYS:HD2	8:Z:13:LYS:HA	1.72	0.41
24:p:63:LEU:O	24:p:64:LEU:HB3	2.19	0.41
25:r:115:LEU:HD22	25:r:174:LEU:HD22	2.02	0.41
25:r:303:ILE:HD12	25:r:388:TRP:CG	2.55	0.41
27:u:94:LEU:N	27:u:94:LEU:HD22	2.35	0.41
29:w:241:TYR:C	29:w:246:LEU:HD23	2.44	0.41
30:a:201:CDL:H761	30:a:201:CDL:C20	2.51	0.41
12:d:2:PRO:HD2	12:d:5:TRP:CZ2	2.55	0.41
12:d:115:GLN:CD	20:l:62:ILE:HG12	2.46	0.41
13:e:73:SER:O	13:e:75:GLY:N	2.54	0.41
15:g:34:VAL:CG1	30:u:201:CDL:H771	2.50	0.41
17:i:71:MET:O	17:i:75:ILE:HG12	2.20	0.41
17:i:163:LEU:HA	17:i:285:THR:HG21	2.02	0.41
18:j:17:LEU:HA	18:j:20:ILE:HG12	2.03	0.41
27:u:69:ASP:O	27:u:73:GLN:HG3	2.20	0.41
28:v:74:PHE:N	28:v:75:PRO:CD	2.83	0.41
4:V:88:LEU:O	4:V:92:ILE:HG13	2.20	0.41
11:c:156:VAL:HG11	28:v:95:TYR:CZ	2.56	0.41
12:d:37:PHE:CZ	20:l:3:PRO:HB3	2.55	0.41
18:j:103:ALA:CB	33:j:201:PEE:H19	2.51	0.41
32:j:202:PLX:H311	32:j:202:PLX:H282	1.90	0.41
19:k:17:ALA:O	19:k:21:MET:HG2	2.20	0.41
20:l:331:MET:HG3	20:l:391:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:377:SER:HB3	20:l:423:SER:OG	2.20	0.41
26:s:141:SER:HB3	26:s:289:LEU:HD23	2.02	0.41
26:s:258:ASN:OD1	26:s:262:LYS:HE3	2.20	0.41
29:w:242:LYS:HA	29:w:246:LEU:HD23	2.02	0.41
3:U:14:ALA:O	3:U:15:LYS:HG2	2.20	0.41
4:V:106:ARG:HA	4:V:106:ARG:NE	2.35	0.41
30:a:201:CDL:H211	30:a:201:CDL:H252	1.95	0.41
18:j:18:VAL:HA	26:s:222:MET:HE3	2.02	0.41
19:k:57:ASN:HB3	21:m:143:ILE:HG13	2.02	0.41
30:r:504:CDL:H571	30:r:504:CDL:H602	1.92	0.41
26:s:251:THR:HG23	26:s:251:THR:O	2.21	0.41
26:s:289:LEU:HD12	26:s:293:PHE:HB2	2.03	0.41
6:X:69:SER:HG	6:X:70:ASP:H	1.66	0.41
13:e:73:SER:C	13:e:75:GLY:H	2.28	0.41
17:i:20:VAL:HG11	17:i:137:ALA:HB1	2.03	0.41
17:i:22:ILE:O	36:i:505:HOH:O	2.22	0.41
32:j:202:PLX:H352	21:m:155:ILE:HG23	2.03	0.41
20:l:12:LEU:HD22	20:l:129:MET:HB3	2.02	0.41
26:s:74:ALA:HB3	26:s:75:PRO:HD3	2.01	0.41
7:Y:43:ARG:CG	7:Y:46:GLN:HB2	2.51	0.41
11:c:145:TRP:CZ2	11:c:149:ILE:HD11	2.55	0.41
14:f:59:ILE:HG22	14:f:63:LYS:HE2	2.03	0.41
16:h:36:PHE:HB3	16:h:63:PHE:HA	2.03	0.41
17:i:62:THR:HG21	17:i:114:TRP:CD1	2.56	0.41
17:i:284:MET:O	33:i:403:PEE:H67	2.21	0.41
18:j:3:ILE:HG12	33:m:201:PEE:H53	2.03	0.41
20:l:150:MET:HE3	20:l:150:MET:HA	2.02	0.41
20:l:249:SER:OG	20:l:336:LYS:HG3	2.21	0.41
22:n:47:ARG:HH21	22:n:56:THR:HG22	1.86	0.41
29:w:129:TYR:CD1	29:w:183:CYS:HB3	2.56	0.41
5:W:87:LEU:HD23	5:W:87:LEU:HA	1.94	0.41
6:X:105:MET:HE1	6:X:112:SER:HA	2.02	0.41
9:a:78:THR:OG1	13:e:96:SER:HB3	2.21	0.41
17:i:175:LEU:O	17:i:179:MET:HG2	2.21	0.41
18:j:73:LEU:CB	18:j:74:PRO:HD3	2.48	0.41
20:l:297:ASP:O	20:l:301:ILE:HG13	2.21	0.41
33:r:501:PEE:H22	33:r:501:PEE:H28	1.77	0.41
13:e:109:LEU:HD23	13:e:109:LEU:HA	1.95	0.40
16:h:84:ASP:HA	16:h:87:ILE:HG22	2.02	0.40
20:l:83:ASP:OD2	20:l:262:ARG:NH1	2.54	0.40
20:l:213:LEU:HB3	20:l:273:VAL:HG11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:289:ALA:O	20:l:293:ILE:HG23	2.21	0.40
27:u:60:GLY:HA2	27:u:63:VAL:HG22	2.02	0.40
28:v:26:PRO:HA	28:v:27:PRO:HD3	1.97	0.40
10:b:123:PHE:HD2	28:v:40:VAL:HG11	1.86	0.40
13:e:152:ASP:OD1	13:e:152:ASP:N	2.45	0.40
17:i:42:PRO:HG3	21:m:167:VAL:HG13	2.03	0.40
17:i:170:LEU:HD11	17:i:288:LEU:HD22	2.02	0.40
18:j:73:LEU:CD1	21:m:55:MET:HE1	2.37	0.40
5:W:128:ARG:HD3	5:W:132:GLU:OE2	2.22	0.40
6:X:94:ASP:HA	6:X:95:PRO:HD3	1.95	0.40
9:a:58:LYS:HA	24:p:99:VAL:HG21	2.02	0.40
17:i:197:ASN:HD22	17:i:200:MET:HG2	1.85	0.40
17:i:221:HIS:O	17:i:319:HIS:HE1	2.04	0.40
20:l:339:LEU:HD23	20:l:339:LEU:HA	1.97	0.40
27:u:73:GLN:HB3	27:u:115:LEU:HD21	2.03	0.40
2:S:34:LYS:HB2	2:S:34:LYS:HE3	1.80	0.40
11:c:84:GLN:O	11:c:98:ARG:NH1	2.54	0.40
17:i:84:TRP:HH2	19:k:59:MET:HE3	1.85	0.40
17:i:95:MET:CE	17:i:149:ILE:HA	2.44	0.40
20:l:61:MET:O	20:l:62:ILE:HD13	2.20	0.40
20:l:124:PHE:HE1	20:l:252:MET:HG3	1.86	0.40
26:s:72:ILE:O	26:s:75:PRO:HD2	2.22	0.40
26:s:218:GLY:O	26:s:222:MET:HG2	2.21	0.40
27:u:44:MET:O	27:u:48:TRP:HE3	2.05	0.40
28:v:69:CYS:CB	28:v:83:GLU:HG3	2.51	0.40
15:g:48:ASN:HB3	15:g:55:VAL:HA	2.03	0.40
20:l:245:ALA:O	20:l:249:SER:HB3	2.21	0.40
24:p:20:TYR:HD1	24:p:48:PHE:CE2	2.39	0.40
25:r:328:CYS:O	25:r:332:THR:HG23	2.22	0.40
26:s:187:ILE:HD12	33:s:401:PEE:H56	2.03	0.40
29:w:302:LEU:HD23	29:w:302:LEU:HA	1.97	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	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
2	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
3	U	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
4	V	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	41
5	W	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
8	Z	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
9	a	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	b	99/126 (79%)	92 (93%)	7 (7%)	0	100	100
11	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
12	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
13	e	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
14	f	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
15	g	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
16	h	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
17	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
18	j	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
19	k	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
20	l	601/603 (100%)	573 (95%)	28 (5%)	0	100	100
21	m	125/175 (71%)	111 (89%)	14 (11%)	0	100	100
22	n	54/56 (96%)	54 (100%)	0	0	100	100
23	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
24	p	176/178 (99%)	167 (95%)	8 (4%)	1 (1%)	21	44
25	r	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
26	s	299/318 (94%)	288 (96%)	10 (3%)	1 (0%)	36	60
27	u	169/171 (99%)	163 (96%)	6 (4%)	0	100	100
28	v	122/131 (93%)	115 (94%)	7 (6%)	0	100	100
29	w	318/320 (99%)	303 (95%)	14 (4%)	1 (0%)	36	60
All	All	4586/4757 (96%)	4399 (96%)	183 (4%)	4 (0%)	49	73

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	w	67	CYS
4	V	46	PRO
26	s	90	PRO
24	p	174	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	34/34 (100%)	34 (100%)	0	100	100
2	S	58/58 (100%)	58 (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	10/99 (10%)	10 (100%)	0	100	100
8	Z	16/65 (25%)	16 (100%)	0	100	100
9	a	122/122 (100%)	122 (100%)	0	100	100
10	b	40/119 (34%)	40 (100%)	0	100	100
12	d	2/155 (1%)	2 (100%)	0	100	100
13	e	45/99 (46%)	45 (100%)	0	100	100
14	f	36/38 (95%)	36 (100%)	0	100	100
15	g	108/108 (100%)	108 (100%)	0	100	100
16	h	93/93 (100%)	93 (100%)	0	100	100
17	i	311/311 (100%)	310 (100%)	1 (0%)	86	94
18	j	88/99 (89%)	87 (99%)	1 (1%)	65	85
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	534/537 (99%)	533 (100%)	1 (0%)	87	95
21	m	99/141 (70%)	99 (100%)	0	100	100
22	n	44/53 (83%)	43 (98%)	1 (2%)	44	73
23	o	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	p	159/159 (100%)	159 (100%)	0	100	100
25	r	410/410 (100%)	410 (100%)	0	100	100
26	s	263/275 (96%)	263 (100%)	0	100	100
27	u	153/153 (100%)	152 (99%)	1 (1%)	76	90
28	v	105/115 (91%)	103 (98%)	2 (2%)	50	77
29	w	280/283 (99%)	280 (100%)	0	100	100
All	All	3378/3894 (87%)	3370 (100%)	8 (0%)	85	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	V	115	CYS
17	i	97	MET
18	j	68	GLU
20	l	594	THR
22	n	15	ILE
27	u	109	GLU
28	v	8	ARG
28	v	78	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
4	V	129	GLN
9	a	170	GLN
14	f	62	HIS
15	g	119	HIS
16	h	34	HIS
17	i	83	GLN
17	i	134	GLN
17	i	171	ASN
17	i	268	GLN
17	i	310	ASN
19	k	50	ASN
20	l	175	ASN
20	l	192	HIS
20	l	354	GLN
20	l	518	GLN
22	n	14	HIS

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Mol	Chain	Res	Type
23	o	79	ASN
24	p	75	GLN
24	p	141	GLN
25	r	30	HIS
25	r	175	ASN
25	r	184	HIS
25	r	338	HIS
25	r	390	ASN
26	s	194	ASN
27	u	64	ASN
27	u	77	HIS
27	u	95	GLN
27	u	99	HIS
28	v	4	HIS
28	v	85	HIS
29	w	127	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

22 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
30	CDL	u	201	-	62,62,99	1.14	4 (6%)	68,74,111	1.14	4 (5%)
32	PLX	j	202	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
30	CDL	V	201	-	70,70,99	1.08	4 (5%)	76,82,111	1.11	6 (7%)
33	PEE	l	702	-	45,45,50	1.24	6 (13%)	48,50,55	1.02	2 (4%)
32	PLX	i	402	-	51,51,51	1.21	3 (5%)	53,59,59	0.62	1 (1%)
30	CDL	i	401	-	65,65,99	1.13	4 (6%)	71,77,111	1.23	8 (11%)
30	CDL	l	701	-	64,64,99	1.30	9 (14%)	70,76,111	1.01	4 (5%)
33	PEE	r	501	-	50,50,50	1.17	6 (12%)	53,55,55	0.98	2 (3%)
35	ADP	w	401	-	28,29,29	3.17	9 (32%)	43,45,45	1.90	8 (18%)
34	UQ	s	402	-	28,28,63	3.32	9 (32%)	36,37,79	2.70	12 (33%)
33	PEE	l	703	-	45,45,50	1.24	6 (13%)	48,50,55	1.00	2 (4%)
30	CDL	r	503	-	98,98,99	1.11	9 (9%)	104,110,111	0.90	4 (3%)
33	PEE	i	403	-	46,46,50	1.22	6 (13%)	49,51,55	1.02	2 (4%)
33	PEE	s	401	-	50,50,50	1.18	6 (12%)	53,55,55	1.01	2 (3%)
30	CDL	r	504	-	99,99,99	1.11	8 (8%)	105,111,111	0.86	4 (3%)
32	PLX	e	201	-	51,51,51	1.20	5 (9%)	53,59,59	0.64	1 (1%)
31	8Q1	X	201	-	32,34,34	2.23	7 (21%)	39,43,43	1.83	12 (30%)
32	PLX	r	502	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)
30	CDL	a	201	-	90,90,99	0.96	4 (4%)	96,102,111	1.11	6 (6%)
33	PEE	m	201	-	40,40,50	1.17	5 (12%)	43,45,55	1.01	2 (4%)
32	PLX	a	202	-	51,51,51	0.60	0	53,59,59	0.69	0
33	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.99	2 (3%)

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
30	CDL	u	201	-	-	17/73/73/110	-
32	PLX	j	202	-	-	30/55/55/55	-
30	CDL	V	201	-	-	28/81/81/110	-
33	PEE	l	702	-	-	18/49/49/54	-
32	PLX	i	402	-	-	27/55/55/55	-
30	CDL	i	401	-	-	29/76/76/110	-
30	CDL	l	701	-	-	36/75/75/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PEE	r	501	-	-	22/54/54/54	-
35	ADP	w	401	-	-	4/16/32/32	0/3/3/3
34	UQ	s	402	-	-	9/21/45/87	0/1/1/1
33	PEE	l	703	-	-	24/49/49/54	-
30	CDL	r	503	-	-	56/109/109/110	-
33	PEE	i	403	-	-	19/50/50/54	-
33	PEE	s	401	-	-	26/54/54/54	-
30	CDL	r	504	-	-	66/110/110/110	-
32	PLX	e	201	-	-	33/55/55/55	-
31	8Q1	X	201	-	-	19/41/41/41	-
32	PLX	r	502	-	-	24/55/55/55	-
30	CDL	a	201	-	-	26/101/101/110	-
33	PEE	m	201	-	-	17/44/44/54	-
32	PLX	a	202	-	-	13/55/55/55	-
33	PEE	j	201	-	-	22/54/54/54	-

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	402	UQ	C13-C14	9.67	1.55	1.33
34	s	402	UQ	C8-C9	9.30	1.54	1.33
35	w	401	ADP	C3'-C4'	-8.94	1.30	1.53
34	s	402	UQ	C18-C19	7.90	1.56	1.32
35	w	401	ADP	O4'-C4'	7.76	1.62	1.45
31	X	201	8Q1	P24-O27	7.36	1.83	1.60
35	w	401	ADP	PA-O3A	6.49	1.66	1.59
35	w	401	ADP	C6-N6	5.46	1.48	1.34
31	X	201	8Q1	C28-C29	5.12	1.61	1.52
35	w	401	ADP	O4'-C1'	-4.52	1.31	1.42
30	i	401	CDL	OB8-CB7	4.29	1.45	1.33
30	a	201	CDL	OB8-CB7	4.24	1.45	1.33
30	a	201	CDL	OA8-CA7	4.21	1.45	1.33
30	u	201	CDL	OA8-CA7	4.20	1.45	1.33
30	i	401	CDL	OA8-CA7	4.20	1.45	1.33
30	V	201	CDL	OA6-CA5	4.17	1.46	1.34
30	u	201	CDL	OA6-CA5	4.15	1.46	1.34
30	a	201	CDL	OA6-CA5	4.15	1.46	1.34
30	V	201	CDL	OA8-CA7	4.14	1.45	1.33
30	V	201	CDL	OB8-CB7	4.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	u	201	CDL	OB8-CB7	4.13	1.45	1.33
30	i	401	CDL	OB6-CB5	4.11	1.45	1.34
30	V	201	CDL	OB6-CB5	4.08	1.45	1.34
30	a	201	CDL	OB6-CB5	4.07	1.45	1.34
30	i	401	CDL	OA6-CA5	4.04	1.45	1.34
30	u	201	CDL	OB6-CB5	3.94	1.45	1.34
33	m	201	PEE	C18-C19	3.83	1.53	1.31
33	l	702	PEE	C18-C19	3.83	1.53	1.31
31	X	201	8Q1	C1-S44	3.82	1.85	1.76
33	s	401	PEE	C18-C19	3.82	1.53	1.31
33	l	703	PEE	C18-C19	3.81	1.53	1.31
33	j	201	PEE	C18-C19	3.81	1.53	1.31
33	i	403	PEE	C18-C19	3.80	1.53	1.31
33	r	501	PEE	C18-C19	3.80	1.53	1.31
33	r	501	PEE	C39-C38	3.74	1.53	1.31
33	j	201	PEE	C39-C38	3.73	1.52	1.31
33	l	702	PEE	C39-C38	3.73	1.52	1.31
33	s	401	PEE	C39-C38	3.73	1.52	1.31
33	i	403	PEE	C39-C38	3.72	1.52	1.31
33	l	703	PEE	C39-C38	3.71	1.52	1.31
30	l	701	CDL	OA8-CA7	3.50	1.43	1.33
31	X	201	8Q1	C6-C1	3.44	1.54	1.50
31	X	201	8Q1	O27-C28	-3.43	1.32	1.43
30	r	503	CDL	OA8-CA7	3.42	1.43	1.33
30	r	504	CDL	OA8-CA7	3.37	1.43	1.33
31	X	201	8Q1	C34-N36	3.30	1.41	1.33
35	w	401	ADP	C8-N9	-3.29	1.32	1.37
35	w	401	ADP	O2'-C2'	-3.07	1.35	1.43
30	r	504	CDL	OB6-CB5	3.06	1.42	1.34
35	w	401	ADP	O3'-C3'	3.03	1.50	1.43
30	l	701	CDL	OB6-CB5	3.03	1.42	1.34
30	l	701	CDL	OA6-CA5	3.01	1.42	1.34
30	l	701	CDL	OB8-CB7	3.01	1.42	1.33
30	r	504	CDL	OB8-CB7	2.99	1.42	1.33
32	e	201	PLX	O6-C4	-2.98	1.40	1.44
30	r	503	CDL	OB6-CB5	2.97	1.42	1.34
30	r	503	CDL	OB8-CB7	2.94	1.41	1.33
32	i	402	PLX	O6-C4	-2.94	1.40	1.44
30	r	503	CDL	OA6-CA5	2.93	1.42	1.34
30	r	504	CDL	OA6-CA5	2.89	1.42	1.34
31	X	201	8Q1	C39-N41	2.87	1.40	1.33
32	j	202	PLX	O6-C4	-2.68	1.41	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	s	401	PEE	O2-C2	-2.67	1.40	1.46
34	s	402	UQ	C6-C1	2.64	1.53	1.46
30	r	504	CDL	OA6-CA4	-2.60	1.40	1.46
33	l	702	PEE	O2-C2	-2.56	1.40	1.46
30	r	503	CDL	OA6-CA4	-2.55	1.40	1.46
32	r	502	PLX	C7-C6	2.53	1.56	1.50
33	j	201	PEE	O2-C2	-2.52	1.40	1.46
33	i	403	PEE	O2-C2	-2.52	1.40	1.46
33	l	703	PEE	O2-C2	-2.52	1.40	1.46
33	m	201	PEE	O2-C2	-2.51	1.40	1.46
33	r	501	PEE	O2-C2	-2.51	1.40	1.46
30	l	701	CDL	OA6-CA4	-2.50	1.40	1.46
32	j	202	PLX	C7-C6	2.50	1.56	1.50
33	m	201	PEE	O3-C30	2.46	1.40	1.33
33	j	201	PEE	O3-C30	2.43	1.40	1.33
33	s	401	PEE	O3-C30	2.43	1.40	1.33
33	l	703	PEE	O3-C30	2.42	1.40	1.33
33	i	403	PEE	O3-C30	2.42	1.40	1.33
33	l	702	PEE	O3-C30	2.41	1.40	1.33
35	w	401	ADP	C5-N7	-2.40	1.34	1.39
33	r	501	PEE	O3-C30	2.39	1.40	1.33
32	i	402	PLX	C7-C6	2.35	1.55	1.50
30	l	701	CDL	OB6-CB4	-2.34	1.41	1.46
30	r	503	CDL	OB6-CB4	-2.31	1.41	1.46
32	e	201	PLX	C7-C6	2.31	1.55	1.50
33	j	201	PEE	O2-C10	2.30	1.40	1.34
33	l	703	PEE	O2-C10	2.30	1.40	1.34
33	l	702	PEE	O2-C10	2.28	1.40	1.34
33	m	201	PEE	O2-C10	2.26	1.40	1.34
33	i	403	PEE	O2-C10	2.26	1.40	1.34
30	r	504	CDL	PB2-OB2	2.25	1.68	1.59
30	r	504	CDL	PB2-OB5	2.24	1.68	1.59
30	l	701	CDL	PB2-OB2	2.22	1.68	1.59
30	r	503	CDL	PB2-OB2	2.22	1.68	1.59
33	r	501	PEE	O3-C3	-2.21	1.40	1.45
30	r	504	CDL	OB6-CB4	-2.21	1.41	1.46
30	l	701	CDL	PB2-OB5	2.21	1.68	1.59
32	r	502	PLX	P1-O4	2.21	1.68	1.59
33	s	401	PEE	O2-C10	2.20	1.40	1.34
32	r	502	PLX	O6-C4	-2.19	1.41	1.44
34	s	402	UQ	O4-C4	-2.19	1.18	1.23
33	r	501	PEE	O2-C10	2.19	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	l	703	PEE	O3-C3	-2.19	1.40	1.45
32	j	202	PLX	P1-O4	2.18	1.67	1.59
30	r	503	CDL	PB2-OB5	2.18	1.67	1.59
32	i	402	PLX	P1-O4	2.16	1.67	1.59
34	s	402	UQ	C7-C8	2.16	1.54	1.50
33	j	201	PEE	O3-C3	-2.15	1.40	1.45
33	i	403	PEE	O3-C3	-2.14	1.40	1.45
33	s	401	PEE	O3-C3	-2.14	1.40	1.45
32	j	202	PLX	P1-O1	2.13	1.67	1.59
33	m	201	PEE	O3-C3	-2.13	1.40	1.45
33	l	702	PEE	O3-C3	-2.13	1.40	1.45
32	e	201	PLX	P1-O4	2.13	1.67	1.59
32	r	502	PLX	P1-O1	2.10	1.67	1.59
30	r	503	CDL	C11-CA5	2.09	1.56	1.50
34	s	402	UQ	O3-CM3	-2.08	1.40	1.45
30	l	701	CDL	C11-CA5	2.03	1.56	1.50
34	s	402	UQ	O2-CM2	-2.02	1.40	1.45
34	s	402	UQ	O1-C1	-2.01	1.18	1.23
32	e	201	PLX	P1-O1	2.00	1.67	1.59
32	e	201	PLX	C1-C2	2.00	1.57	1.51

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	402	UQ	C7-C8-C9	-8.91	111.49	126.83
34	s	402	UQ	C12-C13-C14	-6.04	113.80	127.62
31	X	201	8Q1	C6-C1-S44	5.59	120.07	113.40
35	w	401	ADP	C5-C4-N3	-5.46	119.20	126.72
35	w	401	ADP	N3-C2-N1	-4.54	121.70	128.58
30	i	401	CDL	OA6-CA5-C11	4.51	121.24	111.48
35	w	401	ADP	N3-C4-N9	4.29	134.46	127.17
34	s	402	UQ	C10-C9-C8	-4.28	112.64	123.63
34	s	402	UQ	C17-C18-C19	-4.17	113.75	127.64
30	a	201	CDL	OB6-CB5-C51	4.15	120.45	111.48
33	s	401	PEE	O2-C10-C11	4.15	120.45	111.48
30	r	503	CDL	OA6-CA5-C11	4.07	120.30	111.48
34	s	402	UQ	C11-C9-C8	-4.07	112.03	121.17
33	i	403	PEE	O2-C10-C11	4.07	120.28	111.48
30	l	701	CDL	OA6-CA5-C11	4.06	120.25	111.48
30	r	503	CDL	OB6-CB5-C51	3.99	120.11	111.48
33	l	702	PEE	O2-C10-C11	3.99	120.11	111.48
30	r	504	CDL	OB6-CB5-C51	3.98	120.09	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	V	201	CDL	OB6-CB5-C51	3.96	120.06	111.48
33	m	201	PEE	O2-C10-C11	3.94	120.00	111.48
33	r	501	PEE	O2-C10-C11	3.94	120.00	111.48
30	i	401	CDL	OB6-CB5-C51	3.93	119.99	111.48
30	a	201	CDL	OA6-CA5-C11	3.92	119.97	111.48
33	j	201	PEE	O2-C10-C11	3.88	119.88	111.48
34	s	402	UQ	C16-C14-C13	-3.87	112.48	121.17
30	r	504	CDL	OA6-CA5-C11	3.86	119.84	111.48
30	u	201	CDL	OB6-CB5-C51	3.85	119.80	111.48
30	l	701	CDL	OB6-CB5-C51	3.83	119.76	111.48
34	s	402	UQ	C15-C14-C13	-3.82	113.81	123.63
33	l	703	PEE	O2-C10-C11	3.80	119.69	111.48
35	w	401	ADP	C2-N3-C4	3.55	120.49	111.83
35	w	401	ADP	N9-C8-N7	-3.48	109.00	113.94
34	s	402	UQ	C7-C6-C5	-3.31	119.22	124.89
34	s	402	UQ	C21-C19-C18	-3.25	112.90	122.66
31	X	201	8Q1	O35-C34-N36	-3.24	116.11	122.98
31	X	201	8Q1	C43-S44-C1	3.23	111.38	101.84
35	w	401	ADP	C5-N7-C8	3.18	108.45	103.45
35	w	401	ADP	C4-N9-C8	3.12	109.01	105.74
31	X	201	8Q1	O4-C1-S44	-3.09	118.76	122.68
34	s	402	UQ	CM5-C5-C6	-3.03	119.47	124.45
30	a	201	CDL	OB8-CB7-C71	3.01	121.00	111.83
35	w	401	ADP	C4-C5-N7	-2.96	107.20	110.58
34	s	402	UQ	C20-C19-C18	-2.95	113.80	122.66
30	i	401	CDL	CA4-OA6-CA5	-2.94	110.77	117.80
31	X	201	8Q1	O2-P24-O27	-2.90	99.10	106.67
33	l	702	PEE	O3-C30-C31	2.88	120.62	111.83
30	u	201	CDL	OA8-CA7-C31	2.86	120.57	111.83
33	m	201	PEE	O3-C30-C31	2.84	120.50	111.83
30	r	503	CDL	OB8-CB7-C71	2.84	120.49	111.83
30	i	401	CDL	OA8-CA7-C31	2.83	120.47	111.83
30	u	201	CDL	OA6-CA5-C11	2.83	121.31	110.93
33	s	401	PEE	O3-C30-C31	2.79	120.34	111.83
30	a	201	CDL	CB4-OB6-CB5	-2.76	111.19	117.80
30	V	201	CDL	OB8-CB7-C71	2.75	120.22	111.83
33	r	501	PEE	O3-C30-C31	2.74	120.20	111.83
30	a	201	CDL	OA8-CA7-C31	2.73	120.15	111.83
32	e	201	PLX	C1A-N1-C1	2.71	120.68	109.91
33	i	403	PEE	O3-C30-C31	2.70	120.06	111.83
33	j	201	PEE	O3-C30-C31	2.69	120.04	111.83
30	r	504	CDL	OA8-CA7-C31	2.67	119.97	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	r	504	CDL	OB8-CB7-C71	2.67	119.96	111.83
33	l	703	PEE	O3-C30-C31	2.67	119.96	111.83
30	u	201	CDL	OB8-CB7-C71	2.66	119.95	111.83
32	i	402	PLX	C1A-N1-C1	2.65	120.43	109.91
30	l	701	CDL	OA8-CA7-C31	2.64	119.88	111.83
31	X	201	8Q1	C32-C34-N36	2.63	121.47	116.48
30	l	701	CDL	OB8-CB7-C71	2.60	119.76	111.83
30	V	201	CDL	OA8-CA7-C31	2.59	119.73	111.83
30	r	503	CDL	OA8-CA7-C31	2.59	119.72	111.83
30	i	401	CDL	OB8-CB7-C71	2.53	119.56	111.83
32	r	502	PLX	C1A-N1-C1	2.47	119.74	109.91
30	V	201	CDL	OA6-CA5-C11	2.47	120.01	110.93
30	V	201	CDL	CB4-OB6-CB5	-2.44	111.96	117.80
31	X	201	8Q1	O4-C1-C6	-2.43	121.17	123.98
32	j	202	PLX	C1A-N1-C1	2.42	119.53	109.91
31	X	201	8Q1	O1-P24-O2	2.39	116.75	107.80
31	X	201	8Q1	O40-C39-N41	-2.37	118.38	123.03
34	s	402	UQ	C7-C6-C1	2.28	121.16	118.52
30	i	401	CDL	OA6-CA5-OA7	-2.17	118.62	123.70
30	i	401	CDL	CB4-OB6-CB5	-2.11	112.75	117.80
31	X	201	8Q1	C37-C38-C39	2.05	115.80	112.39
30	V	201	CDL	OB6-CB5-OB7	-2.04	118.94	123.70
31	X	201	8Q1	O27-P24-O3	-2.03	100.94	106.44
31	X	201	8Q1	C7-C6-C1	2.03	116.75	112.27
30	a	201	CDL	OB6-CB5-OB7	-2.02	118.98	123.70
30	i	401	CDL	OA8-CA7-OA9	-2.01	118.60	123.63

There are no chirality outliers.

All (565) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	V	201	CDL	CA2-OA2-PA1-OA4
30	V	201	CDL	CA2-OA2-PA1-OA5
30	V	201	CDL	CB2-OB2-PB2-OB4
30	V	201	CDL	CB2-OB2-PB2-OB5
30	V	201	CDL	CB3-OB5-PB2-OB2
30	V	201	CDL	CB3-OB5-PB2-OB4
30	a	201	CDL	CA2-OA2-PA1-OA3
30	a	201	CDL	CA2-OA2-PA1-OA5
30	a	201	CDL	CB2-OB2-PB2-OB5
30	i	401	CDL	CA3-OA5-PA1-OA2
30	i	401	CDL	CA3-OA5-PA1-OA4

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Mol	Chain	Res	Type	Atoms
30	i	401	CDL	CB2-OB2-PB2-OB4
30	i	401	CDL	CB2-OB2-PB2-OB5
30	i	401	CDL	CB3-OB5-PB2-OB2
30	i	401	CDL	CB3-OB5-PB2-OB4
30	l	701	CDL	O1-C1-CA2-OA2
30	l	701	CDL	O1-C1-CB2-OB2
30	l	701	CDL	CA2-C1-CB2-OB2
30	l	701	CDL	CA2-OA2-PA1-OA5
30	l	701	CDL	CB2-OB2-PB2-OB3
30	l	701	CDL	CB2-OB2-PB2-OB4
30	l	701	CDL	CB2-OB2-PB2-OB5
30	l	701	CDL	OB6-CB4-CB6-OB8
30	r	503	CDL	CA2-OA2-PA1-OA3
30	r	503	CDL	CA2-OA2-PA1-OA4
30	r	503	CDL	CA2-OA2-PA1-OA5
30	r	503	CDL	CB2-OB2-PB2-OB3
30	r	503	CDL	CB2-OB2-PB2-OB4
30	r	503	CDL	CB2-OB2-PB2-OB5
30	r	503	CDL	CB3-OB5-PB2-OB2
30	r	503	CDL	CB3-OB5-PB2-OB3
30	r	503	CDL	CB3-OB5-PB2-OB4
30	r	504	CDL	O1-C1-CB2-OB2
30	r	504	CDL	CA2-C1-CB2-OB2
30	r	504	CDL	CA3-OA5-PA1-OA2
30	r	504	CDL	CB2-OB2-PB2-OB3
30	r	504	CDL	CB3-OB5-PB2-OB2
30	r	504	CDL	CB3-OB5-PB2-OB4
30	u	201	CDL	CB2-C1-CA2-OA2
30	u	201	CDL	CA3-OA5-PA1-OA2
30	u	201	CDL	CA3-OA5-PA1-OA3
30	u	201	CDL	CA3-OA5-PA1-OA4
30	u	201	CDL	CB2-OB2-PB2-OB4
30	u	201	CDL	CB2-OB2-PB2-OB5
31	X	201	8Q1	C1-C6-C7-C8
31	X	201	8Q1	O4-C1-S44-C43
31	X	201	8Q1	C6-C1-S44-C43
31	X	201	8Q1	C28-C29-C32-C34
31	X	201	8Q1	C28-C29-C32-O33
31	X	201	8Q1	C30-C29-C32-C34
31	X	201	8Q1	C30-C29-C32-O33
31	X	201	8Q1	C31-C29-C32-C34
31	X	201	8Q1	C31-C29-C32-O33

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Mol	Chain	Res	Type	Atoms
31	X	201	8Q1	N36-C37-C38-C39
31	X	201	8Q1	C42-C43-S44-C1
32	a	202	PLX	O7-C6-O6-C4
32	a	202	PLX	C3-O4-P1-O1
32	e	201	PLX	O7-C6-O6-C4
32	e	201	PLX	C3-O4-P1-O1
32	e	201	PLX	C3-O4-P1-O3
32	e	201	PLX	C2-O1-P1-O4
32	e	201	PLX	C2-O1-P1-O2
32	e	201	PLX	C2-O1-P1-O3
32	e	201	PLX	C25-C24-O8-C5
32	i	402	PLX	O7-C6-O6-C4
32	i	402	PLX	C3-O4-P1-O1
32	i	402	PLX	C3-O4-P1-O2
32	i	402	PLX	C25-C24-O8-C5
32	j	202	PLX	O7-C6-C7-C8
32	j	202	PLX	C3-O4-P1-O2
32	j	202	PLX	O9-C24-O8-C5
32	j	202	PLX	O9-C24-C25-C26
32	r	502	PLX	O7-C6-O6-C4
32	r	502	PLX	C5-C4-O6-C6
32	r	502	PLX	O9-C24-C25-C26
33	i	403	PEE	C1-O3P-P-O2P
33	i	403	PEE	C1-O3P-P-O1P
33	i	403	PEE	C1-O3P-P-O4P
33	j	201	PEE	C19-C20-C21-C22
33	l	702	PEE	C11-C10-O2-C2
33	l	702	PEE	C4-O4P-P-O3P
33	l	702	PEE	C4-O4P-P-O2P
33	l	702	PEE	C4-O4P-P-O1P
33	m	201	PEE	C11-C10-O2-C2
33	m	201	PEE	C4-O4P-P-O3P
33	m	201	PEE	C4-O4P-P-O1P
33	r	501	PEE	C4-O4P-P-O3P
33	r	501	PEE	C4-O4P-P-O2P
33	r	501	PEE	C4-O4P-P-O1P
33	s	401	PEE	C4-O4P-P-O2P
34	s	402	UQ	C7-C8-C9-C10
34	s	402	UQ	C7-C8-C9-C11
35	w	401	ADP	C5'-O5'-PA-O1A
35	w	401	ADP	C5'-O5'-PA-O2A
33	m	201	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
34	s	402	UQ	C17-C18-C19-C21
33	m	201	PEE	C31-C30-O3-C3
30	r	503	CDL	OA9-CA7-OA8-CA6
33	l	702	PEE	O4-C10-O2-C2
33	m	201	PEE	O4-C10-O2-C2
30	r	503	CDL	C31-CA7-OA8-CA6
30	r	504	CDL	C71-CB7-OB8-CB6
30	i	401	CDL	O1-C1-CA2-OA2
30	r	503	CDL	O1-C1-CB2-OB2
30	u	201	CDL	O1-C1-CA2-OA2
30	l	701	CDL	C71-CB7-OB8-CB6
30	r	504	CDL	C51-CB5-OB6-CB4
33	i	403	PEE	C11-C10-O2-C2
30	l	701	CDL	OB9-CB7-OB8-CB6
30	r	504	CDL	OB9-CB7-OB8-CB6
34	s	402	UQ	C12-C11-C9-C8
33	l	703	PEE	C31-C30-O3-C3
32	r	502	PLX	C9-C10-C11-C12
33	j	201	PEE	C17-C18-C19-C20
33	l	703	PEE	C37-C38-C39-C40
33	s	401	PEE	C37-C38-C39-C40
33	l	703	PEE	O5-C30-O3-C3
30	r	504	CDL	OB7-CB5-OB6-CB4
33	i	403	PEE	O4-C10-O2-C2
30	i	401	CDL	CB2-C1-CA2-OA2
30	r	503	CDL	CA2-C1-CB2-OB2
30	i	401	CDL	C31-CA7-OA8-CA6
30	r	503	CDL	C71-CB7-OB8-CB6
33	j	201	PEE	C31-C30-O3-C3
32	i	402	PLX	C7-C8-C9-C10
30	r	503	CDL	C55-C56-C57-C58
32	j	202	PLX	C28-C29-C30-C31
32	r	502	PLX	C30-C31-C32-C33
30	r	503	CDL	OB9-CB7-OB8-CB6
33	j	201	PEE	O5-C30-O3-C3
30	l	701	CDL	CB5-C51-C52-C53
30	r	504	CDL	OA6-CA4-CA6-OA8
33	l	703	PEE	C10-C11-C12-C13
30	l	701	CDL	C54-C55-C56-C57
30	r	504	CDL	C76-C77-C78-C79
33	r	501	PEE	C17-C18-C19-C20
30	i	401	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
33	j	201	PEE	C40-C41-C42-C43
32	e	201	PLX	C2-C1-N1-C1A
30	l	701	CDL	CB7-C71-C72-C73
30	r	503	CDL	CB7-C71-C72-C73
33	s	401	PEE	C10-C11-C12-C13
30	V	201	CDL	C31-CA7-OA8-CA6
30	r	503	CDL	CB5-C51-C52-C53
33	r	501	PEE	C10-C11-C12-C13
30	i	401	CDL	OA9-CA7-OA8-CA6
30	l	701	CDL	C71-C72-C73-C74
32	j	202	PLX	C32-C33-C34-C35
33	r	501	PEE	C41-C42-C43-C44
30	l	701	CDL	C11-C12-C13-C14
30	r	504	CDL	CA7-C31-C32-C33
33	r	501	PEE	C15-C16-C17-C18
30	a	201	CDL	CA7-C31-C32-C33
33	i	403	PEE	C10-C11-C12-C13
33	j	201	PEE	C11-C10-O2-C2
33	r	501	PEE	C11-C10-O2-C2
33	r	501	PEE	O4-C10-O2-C2
30	u	201	CDL	C75-C76-C77-C78
32	e	201	PLX	C2-C1-N1-C1C
33	j	201	PEE	C30-C31-C32-C33
32	i	402	PLX	O8-C24-C25-C26
32	j	202	PLX	O8-C24-C25-C26
33	j	201	PEE	C34-C35-C36-C37
33	j	201	PEE	O4-C10-O2-C2
30	r	504	CDL	C74-C75-C76-C77
30	i	401	CDL	OB9-CB7-OB8-CB6
32	r	502	PLX	C11-C12-C13-C14
30	V	201	CDL	OA9-CA7-OA8-CA6
30	V	201	CDL	C60-C61-C62-C63
30	u	201	CDL	C11-CA5-OA6-CA4
33	m	201	PEE	C31-C32-C33-C34
33	r	501	PEE	C22-C23-C24-C25
30	r	504	CDL	C32-C33-C34-C35
30	r	504	CDL	C41-C42-C43-C44
33	l	703	PEE	C31-C32-C33-C34
33	r	501	PEE	C12-C13-C14-C15
30	r	503	CDL	C20-C21-C22-C23
32	e	201	PLX	C11-C12-C13-C14
33	l	703	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	r	504	CDL	C17-C18-C19-C20
31	X	201	8Q1	C7-C8-C9-C10
32	e	201	PLX	C10-C11-C12-C13
32	i	402	PLX	C10-C11-C12-C13
32	a	202	PLX	O9-C24-C25-C26
32	e	201	PLX	O9-C24-C25-C26
32	i	402	PLX	O9-C24-C25-C26
30	l	701	CDL	C56-C57-C58-C59
30	r	503	CDL	C74-C75-C76-C77
30	r	504	CDL	C72-C73-C74-C75
32	r	502	PLX	C28-C29-C30-C31
30	l	701	CDL	C55-C56-C57-C58
33	m	201	PEE	C13-C14-C15-C16
32	e	201	PLX	C29-C30-C31-C32
30	V	201	CDL	C51-CB5-OB6-CB4
32	e	201	PLX	C33-C34-C35-C36
30	r	503	CDL	C52-C53-C54-C55
30	r	504	CDL	CB5-C51-C52-C53
30	r	503	CDL	C62-C63-C64-C65
30	u	201	CDL	OA7-CA5-OA6-CA4
30	l	701	CDL	C73-C74-C75-C76
30	l	701	CDL	CB2-C1-CA2-OA2
30	r	503	CDL	C14-C15-C16-C17
30	r	503	CDL	C73-C74-C75-C76
32	e	201	PLX	C28-C29-C30-C31
32	j	202	PLX	C7-C8-C9-C10
32	i	402	PLX	C27-C28-C29-C30
33	l	702	PEE	C31-C32-C33-C34
30	r	504	CDL	C55-C56-C57-C58
32	i	402	PLX	C28-C29-C30-C31
32	j	202	PLX	C15-C16-C17-C18
33	j	201	PEE	C22-C23-C24-C25
32	r	502	PLX	C12-C13-C14-C15
33	s	401	PEE	C23-C24-C25-C26
32	e	201	PLX	C2-C1-N1-C1B
34	s	402	UQ	C12-C13-C14-C15
30	r	503	CDL	C75-C76-C77-C78
30	r	504	CDL	C43-C44-C45-C46
30	r	504	CDL	C71-C72-C73-C74
32	j	202	PLX	C27-C28-C29-C30
30	r	503	CDL	C56-C57-C58-C59
30	r	504	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	i	402	PLX	C12-C13-C14-C15
32	r	502	PLX	C16-C17-C18-C19
33	s	401	PEE	C30-C31-C32-C33
30	V	201	CDL	OB7-CB5-OB6-CB4
30	i	401	CDL	C36-C37-C38-C39
30	l	701	CDL	C72-C73-C74-C75
32	i	402	PLX	C35-C36-C37-C38
32	j	202	PLX	C14-C15-C16-C17
30	r	504	CDL	C31-CA7-OA8-CA6
33	l	702	PEE	C31-C30-O3-C3
30	r	504	CDL	C56-C57-C58-C59
33	r	501	PEE	C13-C14-C15-C16
30	r	503	CDL	C71-C72-C73-C74
32	e	201	PLX	C12-C13-C14-C15
32	j	202	PLX	C10-C11-C12-C13
33	l	703	PEE	C33-C34-C35-C36
31	X	201	8Q1	C11-C12-C13-C14
32	e	201	PLX	C9-C10-C11-C12
30	r	503	CDL	O1-C1-CA2-OA2
32	e	201	PLX	C25-C26-C27-C28
32	i	402	PLX	C11-C10-C9-C8
30	r	503	CDL	C35-C36-C37-C38
32	e	201	PLX	C14-C15-C16-C17
30	a	201	CDL	C51-CB5-OB6-CB4
30	i	401	CDL	C11-CA5-OA6-CA4
33	s	401	PEE	C11-C10-O2-C2
33	s	401	PEE	O4-C10-O2-C2
30	a	201	CDL	C39-C40-C41-C42
30	i	401	CDL	C11-C12-C13-C14
32	j	202	PLX	C12-C13-C14-C15
32	j	202	PLX	C34-C35-C36-C37
32	r	502	PLX	C15-C16-C17-C18
33	s	401	PEE	C31-C30-O3-C3
30	r	504	CDL	C62-C63-C64-C65
32	r	502	PLX	C27-C28-C29-C30
32	i	402	PLX	C18-C19-C20-C21
30	r	503	CDL	C81-C82-C83-C84
30	r	504	CDL	C75-C76-C77-C78
32	j	202	PLX	C25-C26-C27-C28
30	V	201	CDL	OB6-CB4-CB6-OB8
30	i	401	CDL	OB6-CB4-CB6-OB8
30	l	701	CDL	OA6-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
33	j	201	PEE	C36-C37-C38-C39
33	s	401	PEE	C33-C34-C35-C36
33	s	401	PEE	C13-C14-C15-C16
33	s	401	PEE	C34-C35-C36-C37
33	s	401	PEE	C40-C41-C42-C43
32	r	502	PLX	C13-C14-C15-C16
33	l	702	PEE	O5-C30-O3-C3
30	r	504	CDL	C73-C74-C75-C76
30	i	401	CDL	OA7-CA5-OA6-CA4
30	r	504	CDL	OA9-CA7-OA8-CA6
30	r	503	CDL	C59-C60-C61-C62
32	i	402	PLX	C25-C26-C27-C28
30	r	503	CDL	C54-C55-C56-C57
32	i	402	PLX	C13-C14-C15-C16
32	r	502	PLX	C7-C8-C9-C10
33	m	201	PEE	C11-C12-C13-C14
33	l	703	PEE	C11-C10-O2-C2
32	j	202	PLX	C9-C10-C11-C12
33	r	501	PEE	C36-C37-C38-C39
33	s	401	PEE	C17-C18-C19-C20
30	V	201	CDL	CA3-CA4-CA6-OA8
30	r	503	CDL	CB3-CB4-CB6-OB8
30	r	504	CDL	CA3-CA4-CA6-OA8
30	u	201	CDL	CA3-CA4-CA6-OA8
33	r	501	PEE	C1-C2-C3-O3
34	s	402	UQ	C14-C16-C17-C18
30	r	503	CDL	C40-C41-C42-C43
33	s	401	PEE	C15-C16-C17-C18
33	i	403	PEE	C31-C30-O3-C3
33	s	401	PEE	O5-C30-O3-C3
30	i	401	CDL	C31-C32-C33-C34
30	i	401	CDL	C33-C34-C35-C36
30	l	701	CDL	C32-C33-C34-C35
31	X	201	8Q1	C10-C11-C12-C13
30	r	504	CDL	C52-C53-C54-C55
30	u	201	CDL	CA6-CA4-OA6-CA5
32	r	502	PLX	C33-C34-C35-C36
30	r	504	CDL	C37-C38-C39-C40
33	j	201	PEE	C11-C12-C13-C14
30	r	503	CDL	C82-C83-C84-C85
32	i	402	PLX	C32-C33-C34-C35
33	j	201	PEE	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
30	V	201	CDL	C64-C65-C66-C67
30	V	201	CDL	C71-CB7-OB8-CB6
32	e	201	PLX	C16-C17-C18-C19
30	r	504	CDL	C59-C60-C61-C62
33	s	401	PEE	C20-C21-C22-C23
30	r	504	CDL	C11-C12-C13-C14
33	s	401	PEE	C21-C22-C23-C24
30	r	503	CDL	C32-C33-C34-C35
32	e	201	PLX	C30-C31-C32-C33
30	r	503	CDL	OB6-CB4-CB6-OB8
30	r	504	CDL	OB6-CB4-CB6-OB8
32	j	202	PLX	O6-C4-C5-O8
30	l	701	CDL	C57-C58-C59-C60
33	j	201	PEE	C38-C39-C40-C41
33	i	403	PEE	C35-C36-C37-C38
32	r	502	PLX	C31-C32-C33-C34
30	l	701	CDL	C33-C34-C35-C36
33	l	702	PEE	C21-C22-C23-C24
32	e	201	PLX	C26-C27-C28-C29
30	a	201	CDL	C31-C32-C33-C34
30	a	201	CDL	C71-CB7-OB8-CB6
32	r	502	PLX	C29-C30-C31-C32
30	a	201	CDL	OB7-CB5-OB6-CB4
33	l	702	PEE	C22-C23-C24-C25
30	a	201	CDL	OB5-CB3-CB4-CB6
30	i	401	CDL	OA5-CA3-CA4-CA6
32	i	402	PLX	C9-C10-C11-C12
30	i	401	CDL	C35-C36-C37-C38
33	i	403	PEE	O5-C30-O3-C3
32	a	202	PLX	C34-C35-C36-C37
30	i	401	CDL	CA7-C31-C32-C33
32	j	202	PLX	C26-C27-C28-C29
32	j	202	PLX	C31-C32-C33-C34
30	V	201	CDL	CB3-CB4-CB6-OB8
30	l	701	CDL	CA3-CA4-CA6-OA8
30	l	701	CDL	CB3-CB4-CB6-OB8
30	r	504	CDL	CB3-CB4-CB6-OB8
31	X	201	8Q1	O33-C32-C34-N36
33	i	403	PEE	C1-C2-C3-O3
33	l	703	PEE	C1-C2-C3-O3
32	i	402	PLX	C36-C37-C38-C39
30	r	504	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
30	u	201	CDL	C57-C58-C59-C60
32	a	202	PLX	C14-C15-C16-C17
34	s	402	UQ	C12-C11-C9-C10
32	i	402	PLX	C30-C31-C32-C33
32	j	202	PLX	O4-C3-C4-O6
31	X	201	8Q1	C6-C7-C8-C9
30	r	503	CDL	C36-C37-C38-C39
30	r	504	CDL	C12-C13-C14-C15
30	r	504	CDL	C39-C40-C41-C42
32	r	502	PLX	C14-C15-C16-C17
33	s	401	PEE	C32-C33-C34-C35
30	V	201	CDL	OA6-CA4-CA6-OA8
33	i	403	PEE	O2-C2-C3-O3
30	a	201	CDL	C38-C39-C40-C41
33	l	703	PEE	O4-C10-O2-C2
31	X	201	8Q1	O4-C1-C6-C7
31	X	201	8Q1	S44-C1-C6-C7
32	j	202	PLX	O6-C6-C7-C8
30	r	504	CDL	C60-C61-C62-C63
33	l	702	PEE	C15-C16-C17-C18
30	u	201	CDL	C53-C54-C55-C56
33	j	201	PEE	C12-C13-C14-C15
32	i	402	PLX	C33-C34-C35-C36
30	r	504	CDL	C34-C35-C36-C37
32	a	202	PLX	C16-C17-C18-C19
33	r	501	PEE	C31-C30-O3-C3
32	j	202	PLX	O4-C3-C4-C5
33	i	403	PEE	C18-C19-C20-C21
30	a	201	CDL	OB9-CB7-OB8-CB6
32	e	201	PLX	C31-C32-C33-C34
30	V	201	CDL	OB9-CB7-OB8-CB6
30	r	503	CDL	C51-CB5-OB6-CB4
30	i	401	CDL	C71-C72-C73-C74
30	r	503	CDL	C37-C38-C39-C40
33	m	201	PEE	C3-C2-O2-C10
30	r	504	CDL	C20-C21-C22-C23
33	l	702	PEE	C13-C14-C15-C16
30	i	401	CDL	OA5-CA3-CA4-OA6
33	s	401	PEE	O3P-C1-C2-O2
30	i	401	CDL	CB3-CB4-CB6-OB8
32	e	201	PLX	C3-C4-C5-O8
32	j	202	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
33	j	201	PEE	C43-C44-C45-C46
32	r	502	PLX	O6-C4-C5-O8
33	l	702	PEE	C32-C33-C34-C35
30	r	503	CDL	C11-CA5-OA6-CA4
33	r	501	PEE	O5-C30-O3-C3
32	r	502	PLX	C25-C24-O8-C5
30	V	201	CDL	C78-C79-C80-C81
33	r	501	PEE	C20-C21-C22-C23
30	l	701	CDL	OA5-CA3-CA4-CA6
33	s	401	PEE	O3P-C1-C2-C3
30	r	504	CDL	C57-C58-C59-C60
30	r	504	CDL	C82-C83-C84-C85
30	r	503	CDL	OB7-CB5-OB6-CB4
30	V	201	CDL	C74-C75-C76-C77
30	a	201	CDL	C18-C19-C20-C21
33	l	703	PEE	C13-C14-C15-C16
30	V	201	CDL	CB4-CB3-OB5-PB2
30	a	201	CDL	OA5-CA3-CA4-OA6
30	a	201	CDL	OB5-CB3-CB4-OB6
30	l	701	CDL	OA5-CA3-CA4-OA6
30	l	701	CDL	C52-C53-C54-C55
30	u	201	CDL	OA6-CA4-CA6-OA8
32	e	201	PLX	O6-C4-C5-O8
33	l	703	PEE	O2-C2-C3-O3
33	r	501	PEE	O2-C2-C3-O3
32	e	201	PLX	C11-C10-C9-C8
32	j	202	PLX	C3-C4-C5-O8
30	r	503	CDL	C53-C54-C55-C56
30	r	503	CDL	C42-C43-C44-C45
30	r	504	CDL	C44-C45-C46-C47
30	r	504	CDL	C36-C37-C38-C39
30	r	503	CDL	OA7-CA5-OA6-CA4
30	a	201	CDL	CA2-OA2-PA1-OA4
30	a	201	CDL	CB2-OB2-PB2-OB3
30	a	201	CDL	CB3-OB5-PB2-OB3
30	i	401	CDL	CA2-OA2-PA1-OA3
30	i	401	CDL	CB2-OB2-PB2-OB3
30	l	701	CDL	CA2-OA2-PA1-OA3
30	l	701	CDL	CB3-OB5-PB2-OB3
30	r	504	CDL	CA2-OA2-PA1-OA3
30	r	504	CDL	CA2-OA2-PA1-OA5
30	r	504	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
30	r	504	CDL	CB3-OB5-PB2-OB3
32	a	202	PLX	C3-O4-P1-O2
32	a	202	PLX	C2-O1-P1-O2
32	e	201	PLX	C3-O4-P1-O2
32	i	402	PLX	C2-O1-P1-O2
32	j	202	PLX	C3-O4-P1-O1
32	j	202	PLX	C3-O4-P1-O3
32	j	202	PLX	C2-O1-P1-O3
33	l	703	PEE	C4-O4P-P-O3P
33	s	401	PEE	C1-O3P-P-O2P
33	s	401	PEE	C1-O3P-P-O4P
33	s	401	PEE	C4-O4P-P-O3P
33	s	401	PEE	C4-O4P-P-O1P
35	w	401	ADP	C5'-O5'-PA-O3A
31	X	201	8Q1	C9-C10-C11-C12
32	r	502	PLX	C32-C33-C34-C35
33	m	201	PEE	C19-C20-C21-C22
30	r	504	CDL	CB4-CB3-OB5-PB2
33	i	403	PEE	C2-C1-O3P-P
30	r	503	CDL	C44-C45-C46-C47
33	l	703	PEE	C39-C40-C41-C42
33	l	702	PEE	C38-C39-C40-C41
33	l	703	PEE	C18-C19-C20-C21
30	V	201	CDL	C51-C52-C53-C54
30	i	401	CDL	CA6-CA4-OA6-CA5
30	V	201	CDL	C58-C59-C60-C61
30	u	201	CDL	C76-C77-C78-C79
33	i	403	PEE	C21-C22-C23-C24
30	V	201	CDL	C63-C64-C65-C66
33	j	201	PEE	O2-C2-C3-O3
32	i	402	PLX	C14-C15-C16-C17
32	r	502	PLX	C3-C4-C5-O8
33	i	403	PEE	C36-C37-C38-C39
30	i	401	CDL	C37-C38-C39-C40
30	r	503	CDL	C60-C61-C62-C63
33	l	703	PEE	C2-C1-O3P-P
30	r	503	CDL	OB5-CB3-CB4-OB6
33	l	702	PEE	C36-C37-C38-C39
33	m	201	PEE	C16-C17-C18-C19
33	s	401	PEE	C38-C39-C40-C41
30	r	503	CDL	C23-C24-C25-C26
32	j	202	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
33	i	403	PEE	C24-C25-C26-C27
33	r	501	PEE	C38-C39-C40-C41
30	r	504	CDL	C64-C65-C66-C67
30	r	504	CDL	C31-C32-C33-C34
32	i	402	PLX	C29-C30-C31-C32
33	l	703	PEE	C16-C17-C18-C19
30	V	201	CDL	C61-C62-C63-C64
30	r	504	CDL	C13-C14-C15-C16
32	e	201	PLX	C13-C14-C15-C16
30	V	201	CDL	CA6-CA4-OA6-CA5
30	a	201	CDL	CA3-CA4-OA6-CA5
33	l	703	PEE	C15-C16-C17-C18
32	e	201	PLX	C24-C25-C26-C27
30	r	504	CDL	C80-C81-C82-C83
30	l	701	CDL	C51-C52-C53-C54
32	i	402	PLX	C16-C17-C18-C19
30	a	201	CDL	C71-C72-C73-C74
33	l	702	PEE	O2-C2-C3-O3
33	s	401	PEE	C14-C15-C16-C17
30	r	503	CDL	C39-C40-C41-C42
34	s	402	UQ	C13-C14-C16-C17
30	a	201	CDL	C73-C74-C75-C76
30	a	201	CDL	C54-C55-C56-C57
30	a	201	CDL	CB5-C51-C52-C53
33	l	703	PEE	C30-C31-C32-C33
33	r	501	PEE	C30-C31-C32-C33
32	a	202	PLX	C30-C31-C32-C33
30	r	504	CDL	C33-C34-C35-C36
32	i	402	PLX	O6-C4-C5-O8
33	j	201	PEE	C41-C42-C43-C44
33	r	501	PEE	C23-C24-C25-C26
30	a	201	CDL	O1-C1-CA2-OA2
30	a	201	CDL	C34-C35-C36-C37
30	u	201	CDL	C77-C78-C79-C80
33	l	703	PEE	C12-C13-C14-C15
32	r	502	PLX	C4-C5-O8-C24
33	i	403	PEE	C38-C39-C40-C41
30	a	201	CDL	CA6-CA4-OA6-CA5
33	m	201	PEE	C12-C13-C14-C15
33	i	403	PEE	C34-C35-C36-C37
30	r	503	CDL	OA5-CA3-CA4-OA6
33	j	201	PEE	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	l	702	PEE	C1-C2-C3-O3
30	r	503	CDL	C76-C77-C78-C79
33	l	702	PEE	C16-C17-C18-C19
33	l	703	PEE	C38-C39-C40-C41
33	j	201	PEE	C16-C17-C18-C19
33	m	201	PEE	C18-C19-C20-C21
33	l	703	PEE	C23-C24-C25-C26
32	i	402	PLX	C7-C6-O6-C4
32	j	202	PLX	C7-C6-O6-C4
30	r	504	CDL	C63-C64-C65-C66
32	a	202	PLX	C25-C26-C27-C28
30	r	504	CDL	C79-C80-C81-C82
30	r	503	CDL	C72-C71-CB7-OB8
33	j	201	PEE	O3-C30-C31-C32
30	V	201	CDL	C55-C56-C57-C58
30	r	504	CDL	C52-C51-CB5-OB6
30	l	701	CDL	C32-C31-CA7-OA8
33	i	403	PEE	C23-C24-C25-C26
30	l	701	CDL	C58-C59-C60-C61
33	r	501	PEE	C24-C25-C26-C27
30	r	504	CDL	CA4-CA3-OA5-PA1
32	j	202	PLX	C25-C24-O8-C5
30	r	504	CDL	C84-C85-C86-C87
30	r	504	CDL	C15-C16-C17-C18
33	m	201	PEE	C23-C24-C25-C26
32	a	202	PLX	C18-C19-C20-C21
32	e	201	PLX	C36-C37-C38-C39
30	r	504	CDL	C42-C43-C44-C45
30	V	201	CDL	CA3-CA4-OA6-CA5
32	a	202	PLX	C32-C33-C34-C35
33	l	703	PEE	O2-C10-C11-C12
30	r	504	CDL	C52-C51-CB5-OB7
34	s	402	UQ	C9-C11-C12-C13
30	r	503	CDL	C72-C71-CB7-OB9
32	e	201	PLX	O8-C24-C25-C26
32	r	502	PLX	O8-C24-C25-C26
30	r	504	CDL	OB5-CB3-CB4-OB6
32	a	202	PLX	O9-C24-O8-C5
32	e	201	PLX	O9-C24-O8-C5
32	r	502	PLX	O9-C24-O8-C5
33	j	201	PEE	O5-C30-C31-C32
33	m	201	PEE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
30	l	701	CDL	C32-C31-CA7-OA9
33	m	201	PEE	O3-C30-C31-C32
30	r	504	CDL	C61-C62-C63-C64
33	l	703	PEE	C2-C3-O3-C30
30	r	503	CDL	C12-C11-CA5-OA6
35	w	401	ADP	PB-O3A-PA-O2A
30	r	503	CDL	C12-C11-CA5-OA7
30	l	701	CDL	C12-C11-CA5-OA6

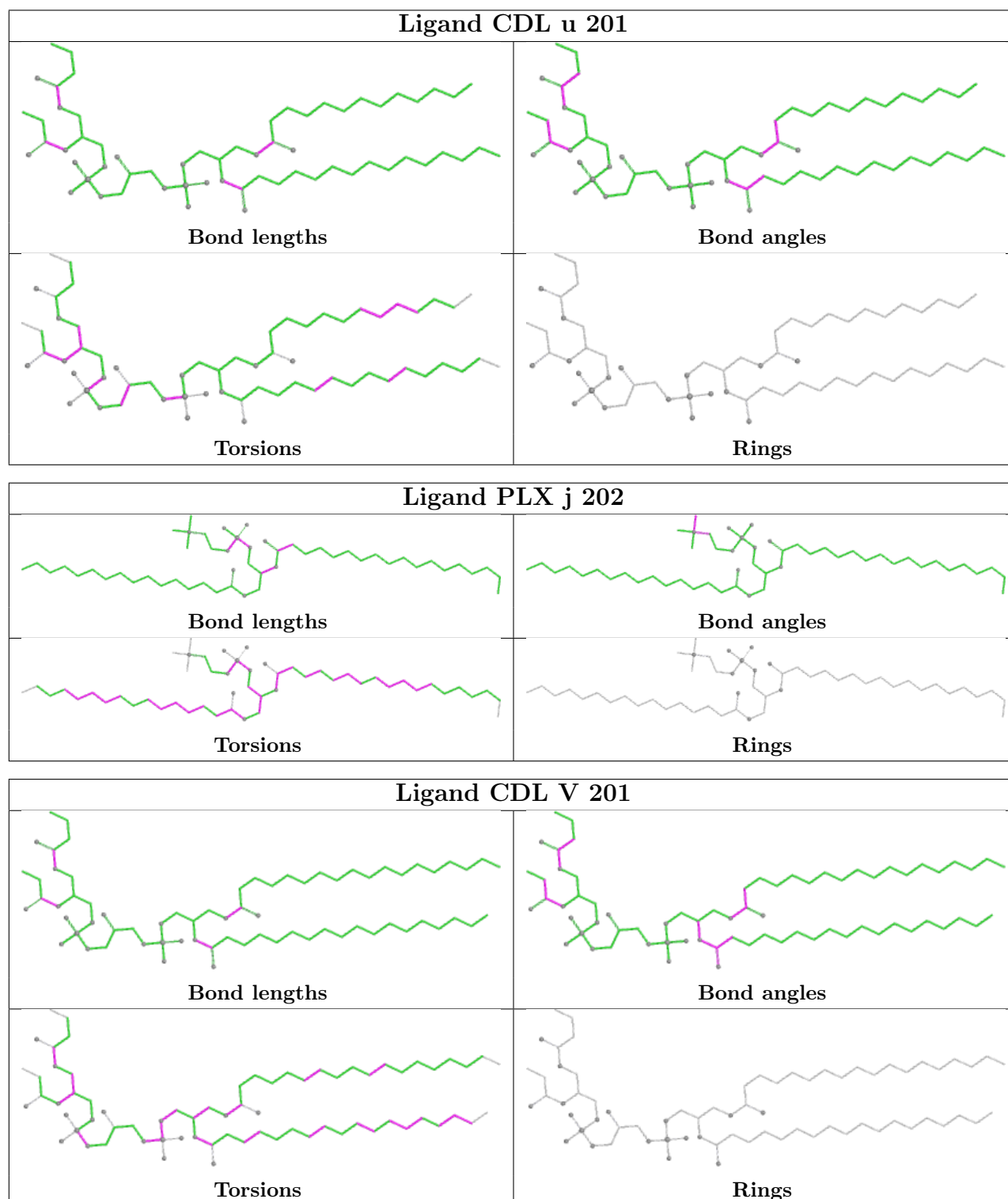
There are no ring outliers.

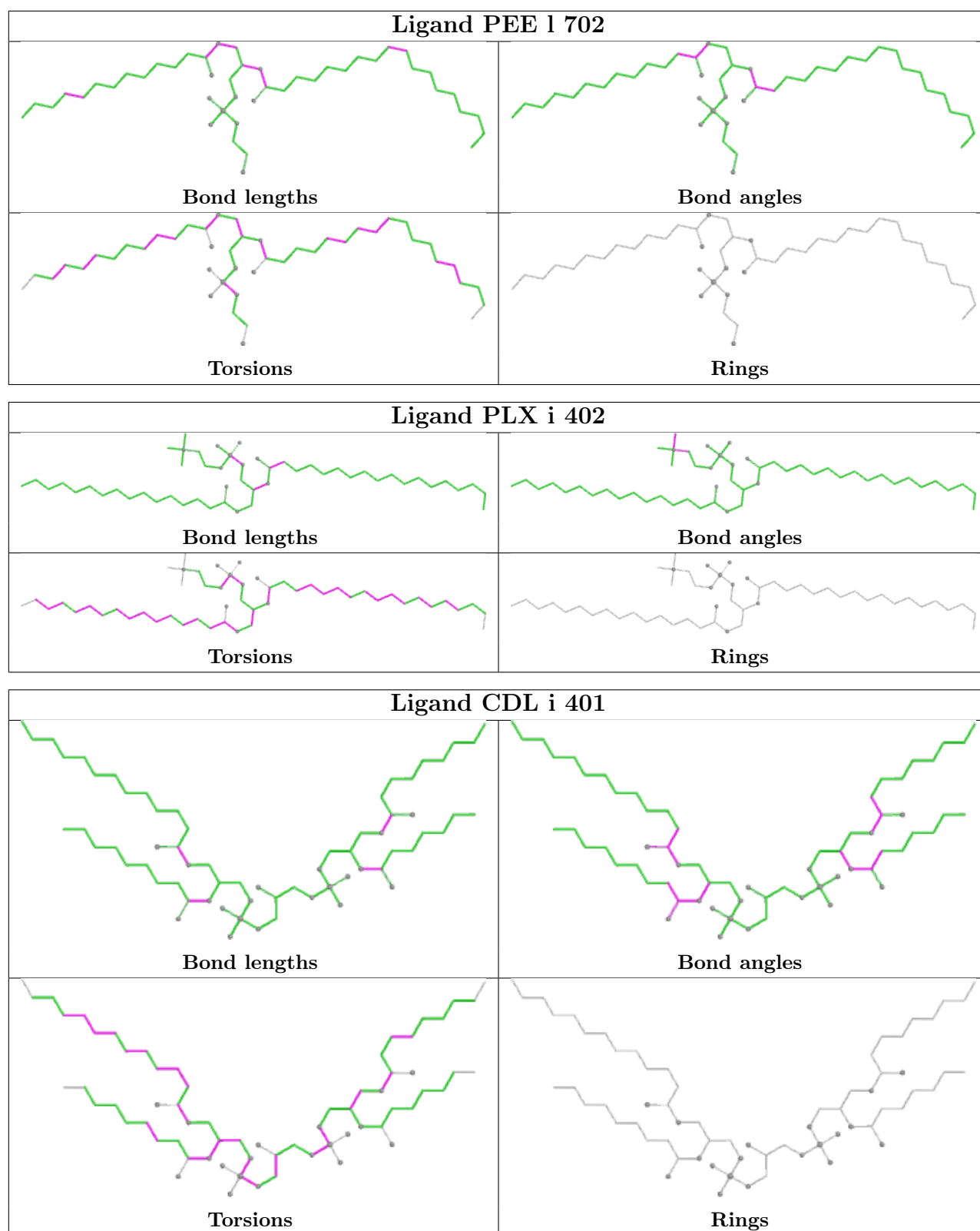
22 monomers are involved in 224 short contacts:

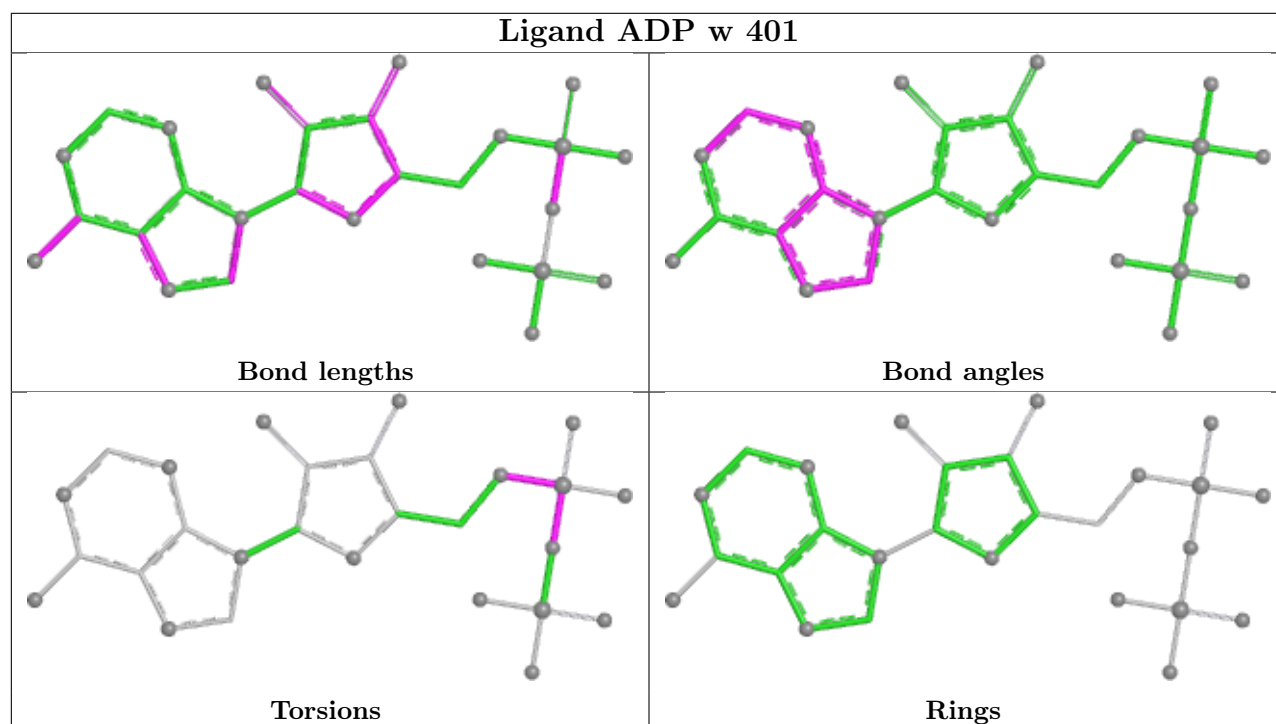
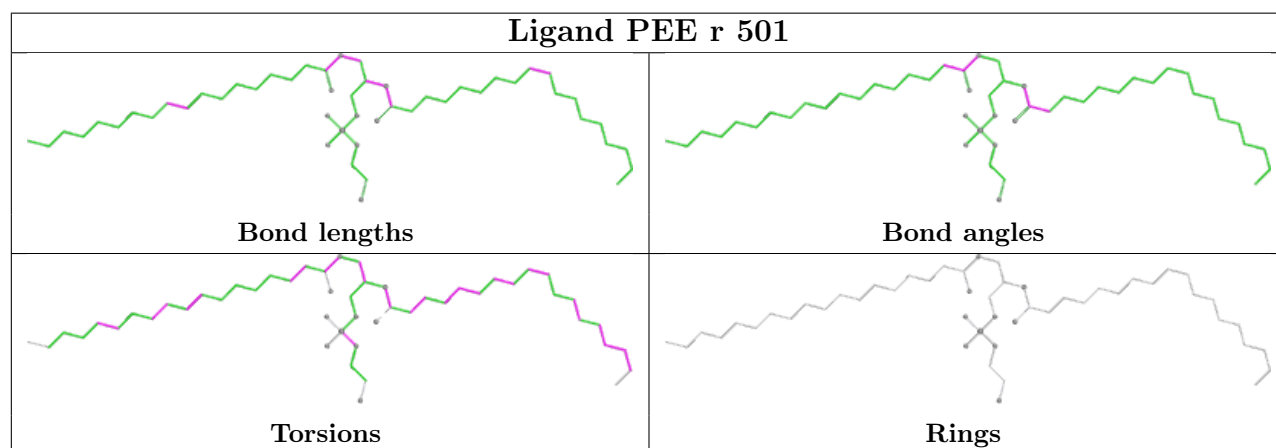
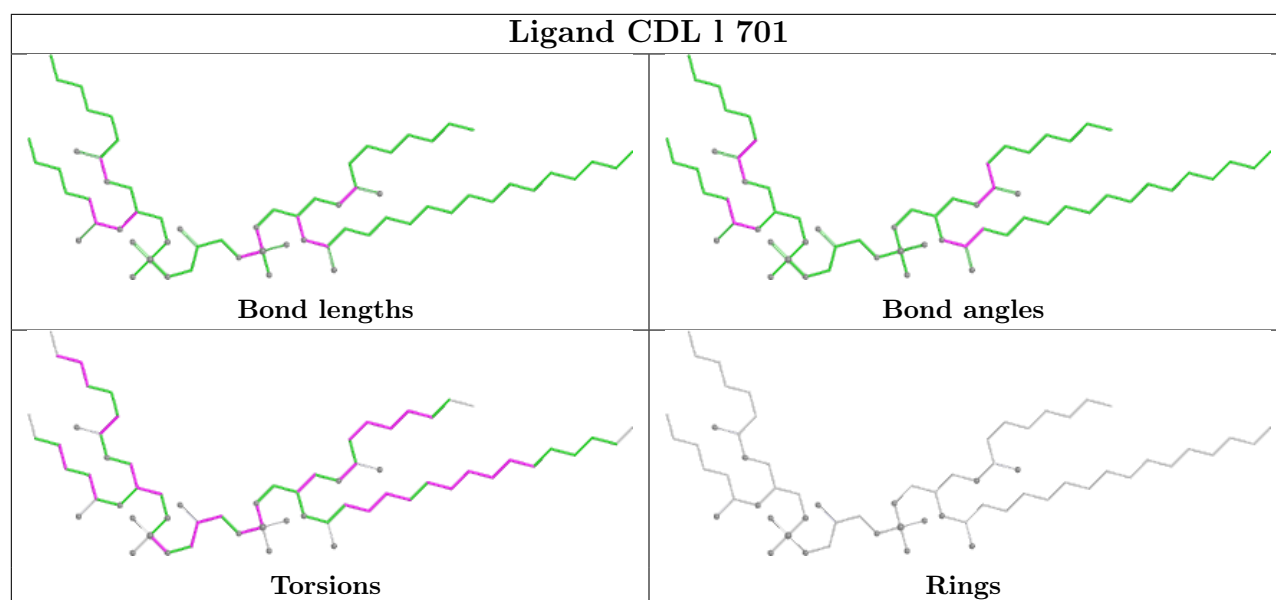
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	u	201	CDL	18	0
32	j	202	PLX	6	0
30	V	201	CDL	16	0
33	l	702	PEE	6	0
32	i	402	PLX	4	0
30	i	401	CDL	21	0
30	l	701	CDL	7	0
33	r	501	PEE	12	0
35	w	401	ADP	1	0
34	s	402	UQ	7	0
33	l	703	PEE	19	0
30	r	503	CDL	9	0
33	i	403	PEE	16	0
33	s	401	PEE	2	0
30	r	504	CDL	10	0
32	e	201	PLX	5	0
31	X	201	8Q1	1	0
32	r	502	PLX	10	0
30	a	201	CDL	35	0
33	m	201	PEE	16	0
32	a	202	PLX	10	0
33	j	201	PEE	9	0

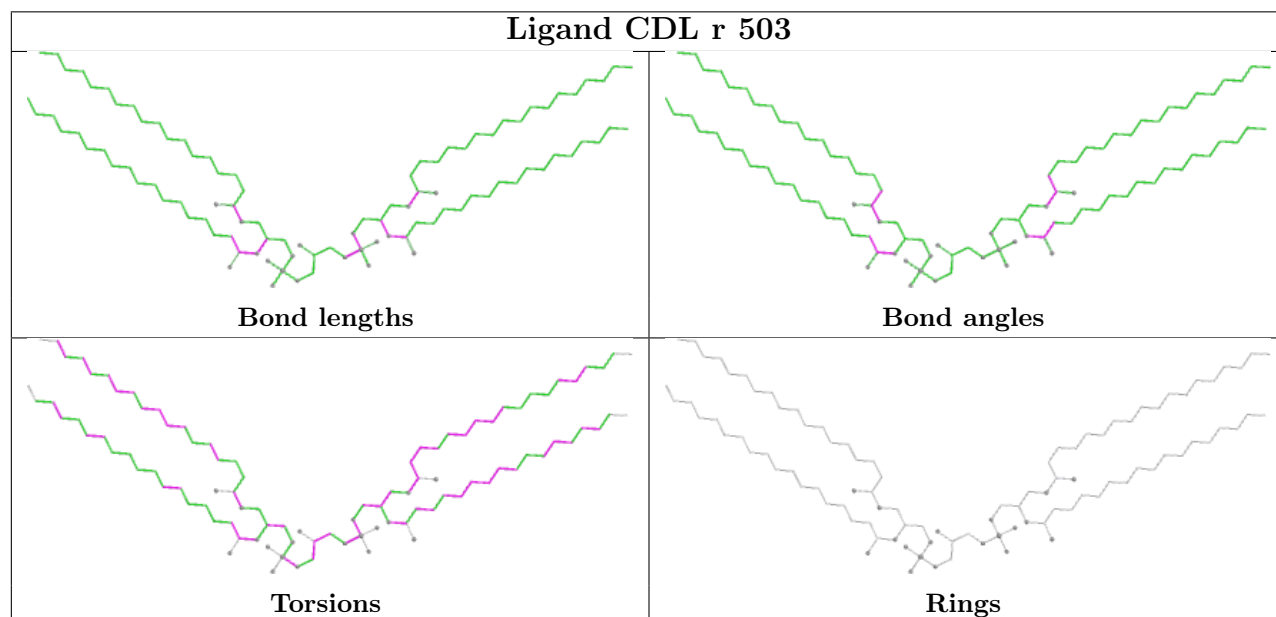
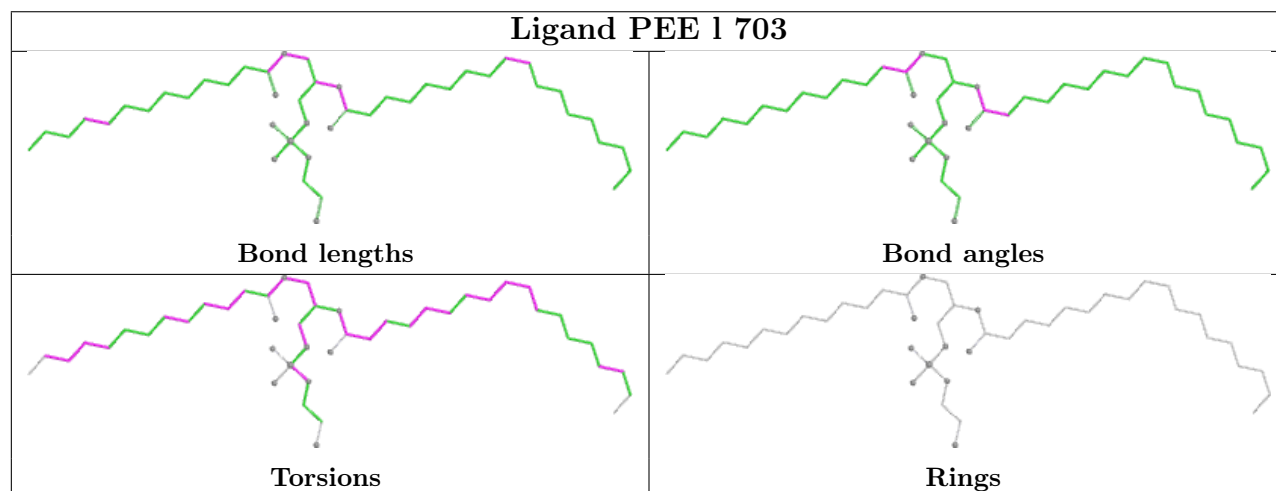
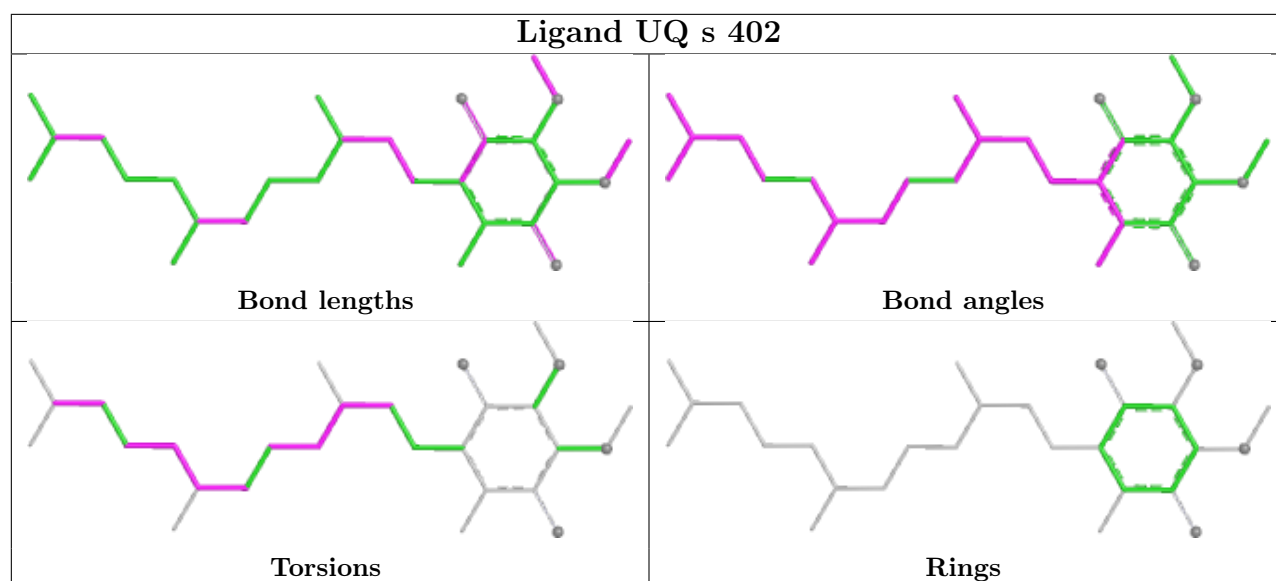
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

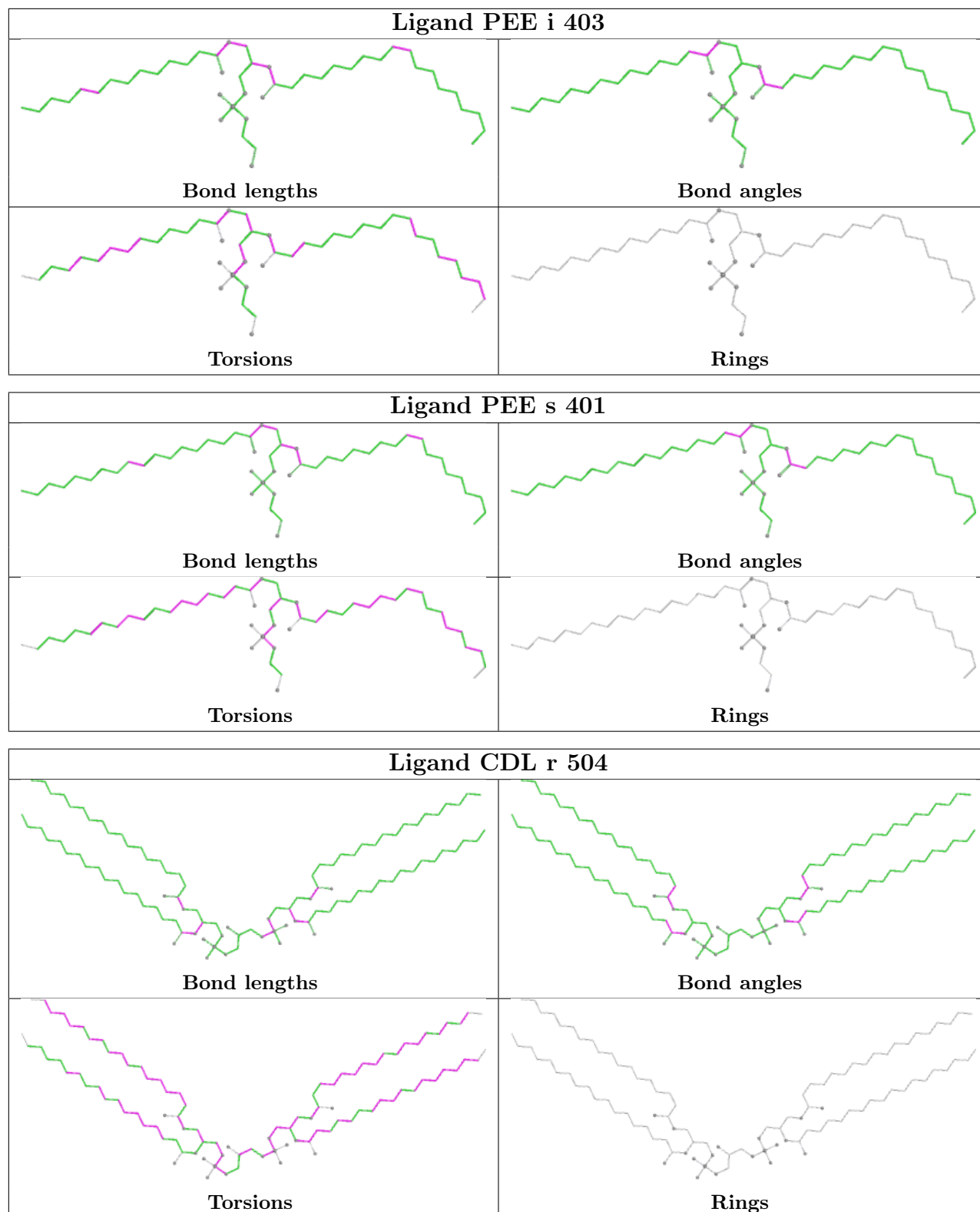
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

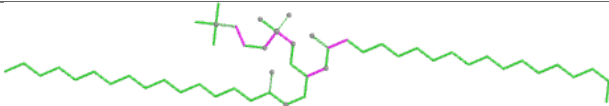
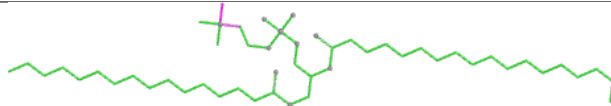
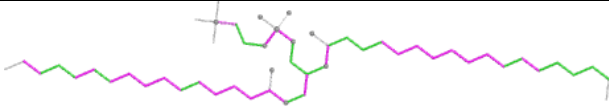
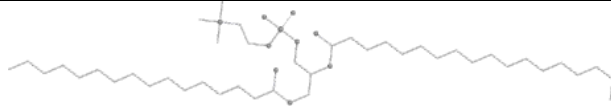


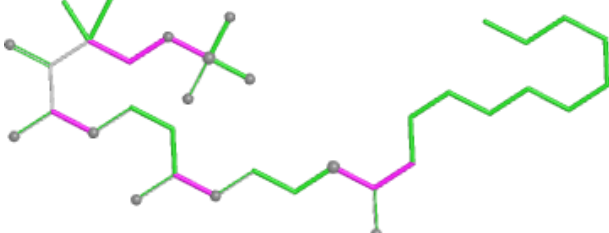
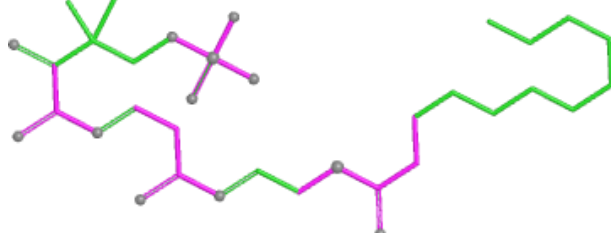
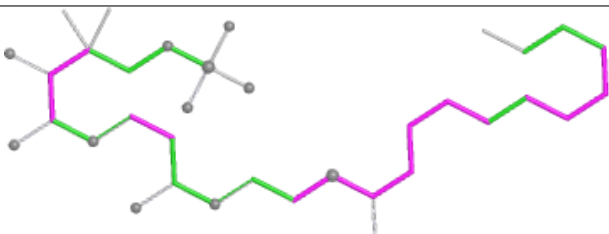
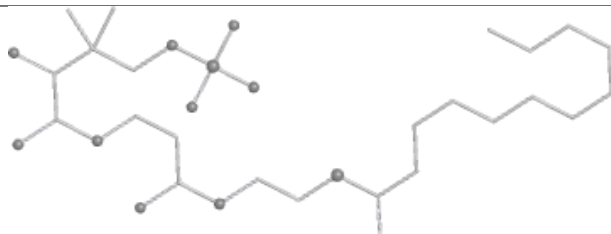


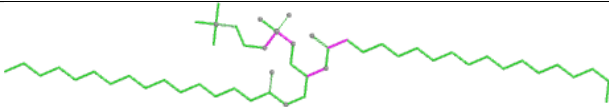
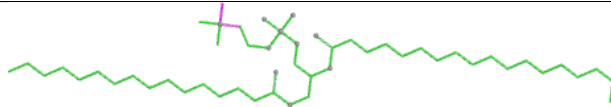
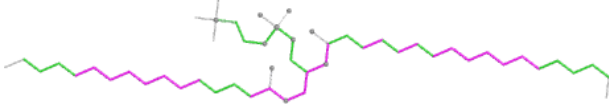
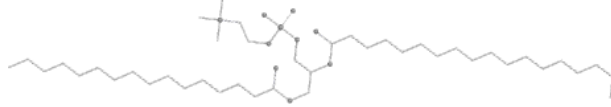


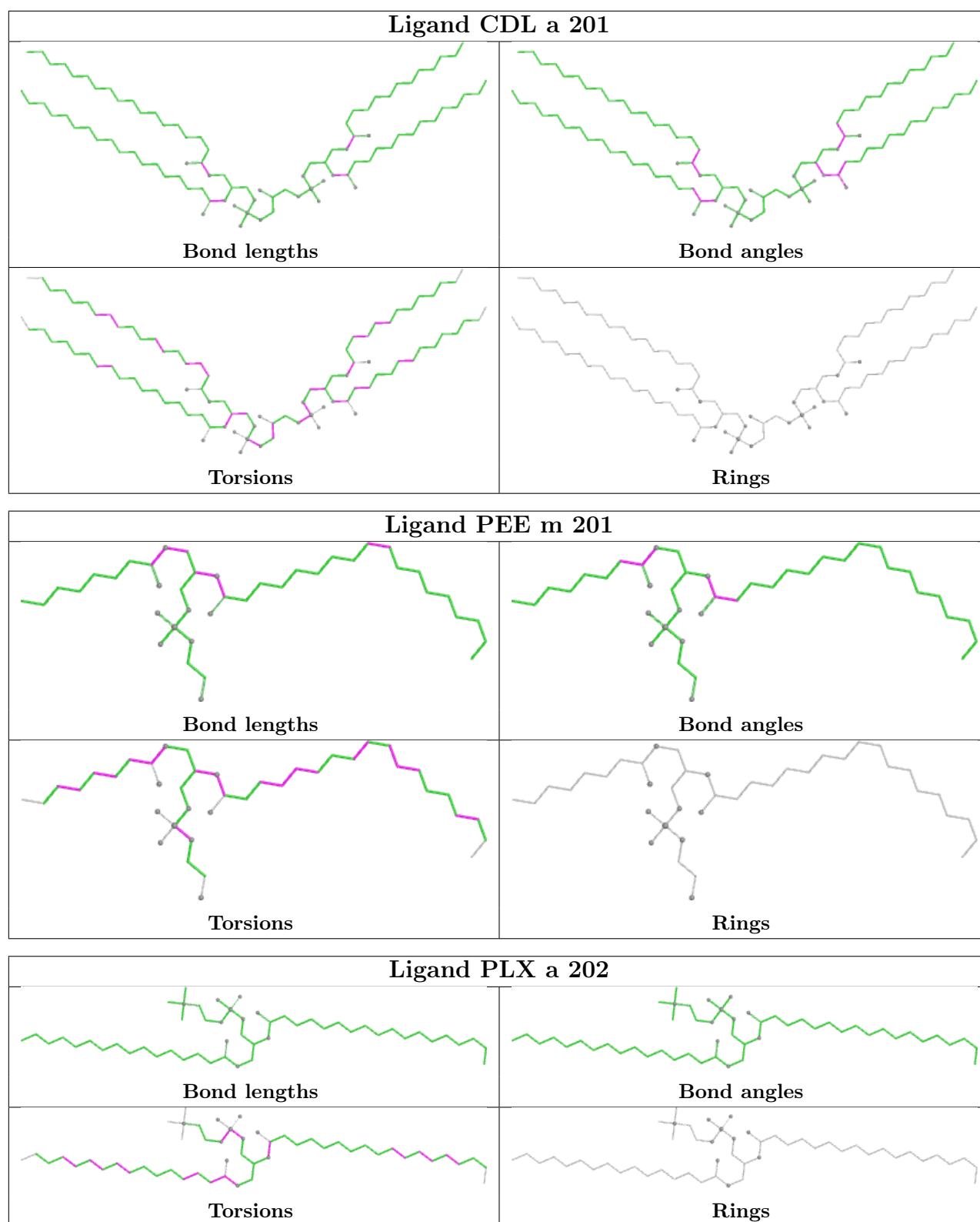


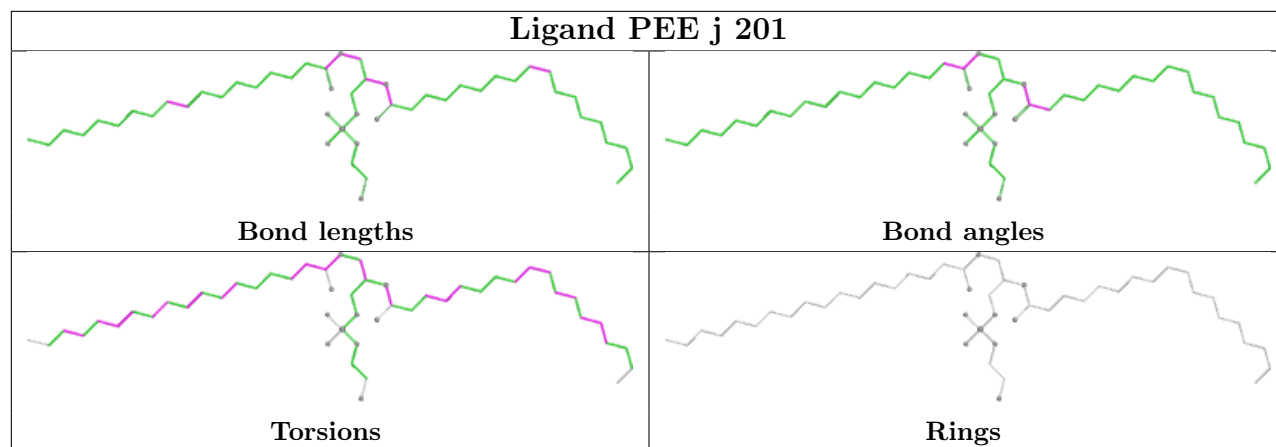


Ligand PLX e 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand 8Q1 X 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PLX r 502	
	
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.

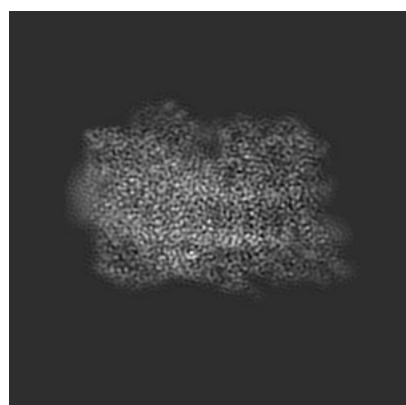
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32155. These allow visual inspection of the internal detail of the map and identification of artifacts.

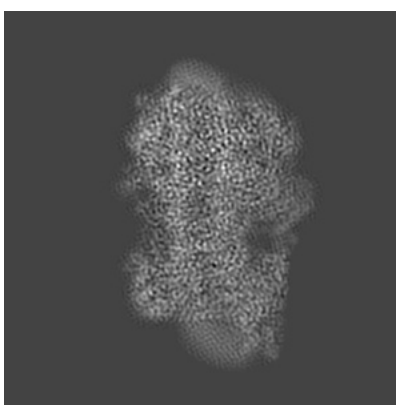
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

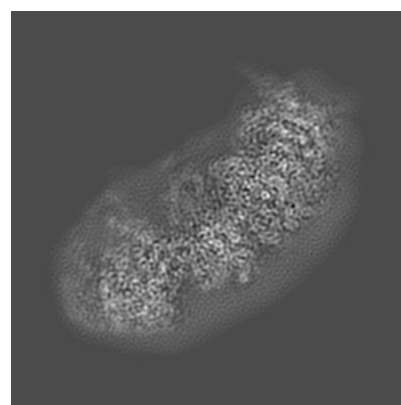
6.1.1 Primary map



X



Y

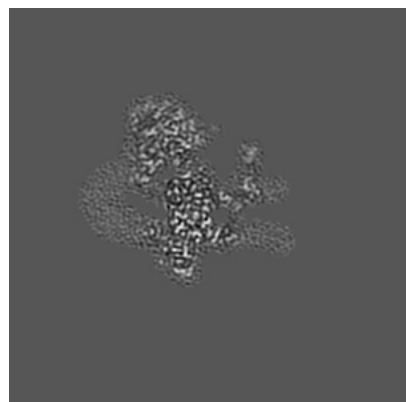


Z

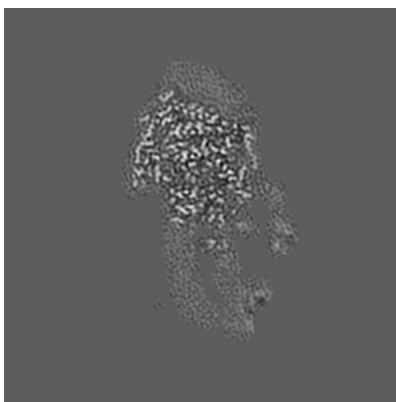
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

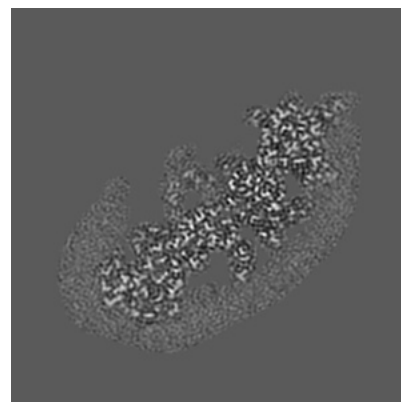
6.2.1 Primary map



X Index: 240



Y Index: 240

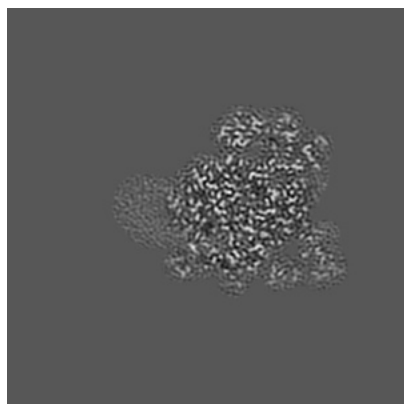


Z Index: 240

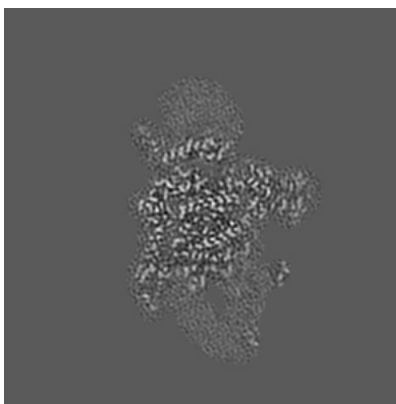
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

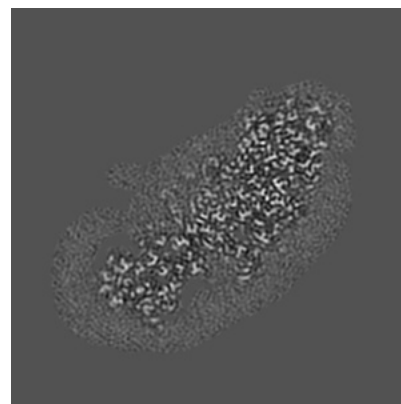
6.3.1 Primary map



X Index: 321



Y Index: 202

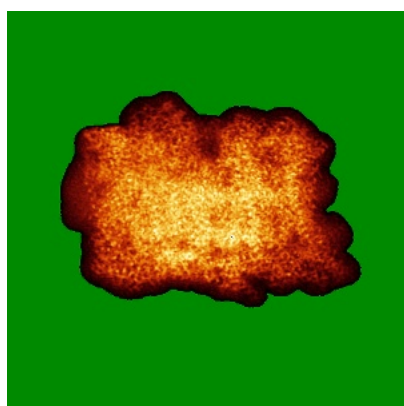


Z Index: 258

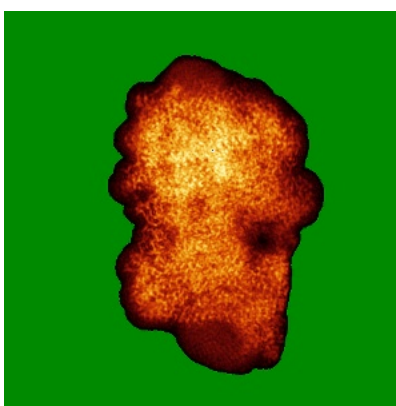
The images above show the largest variance slices of the map in three orthogonal directions.

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

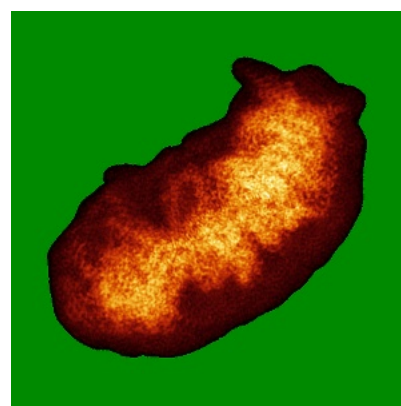
6.4.1 Primary map



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

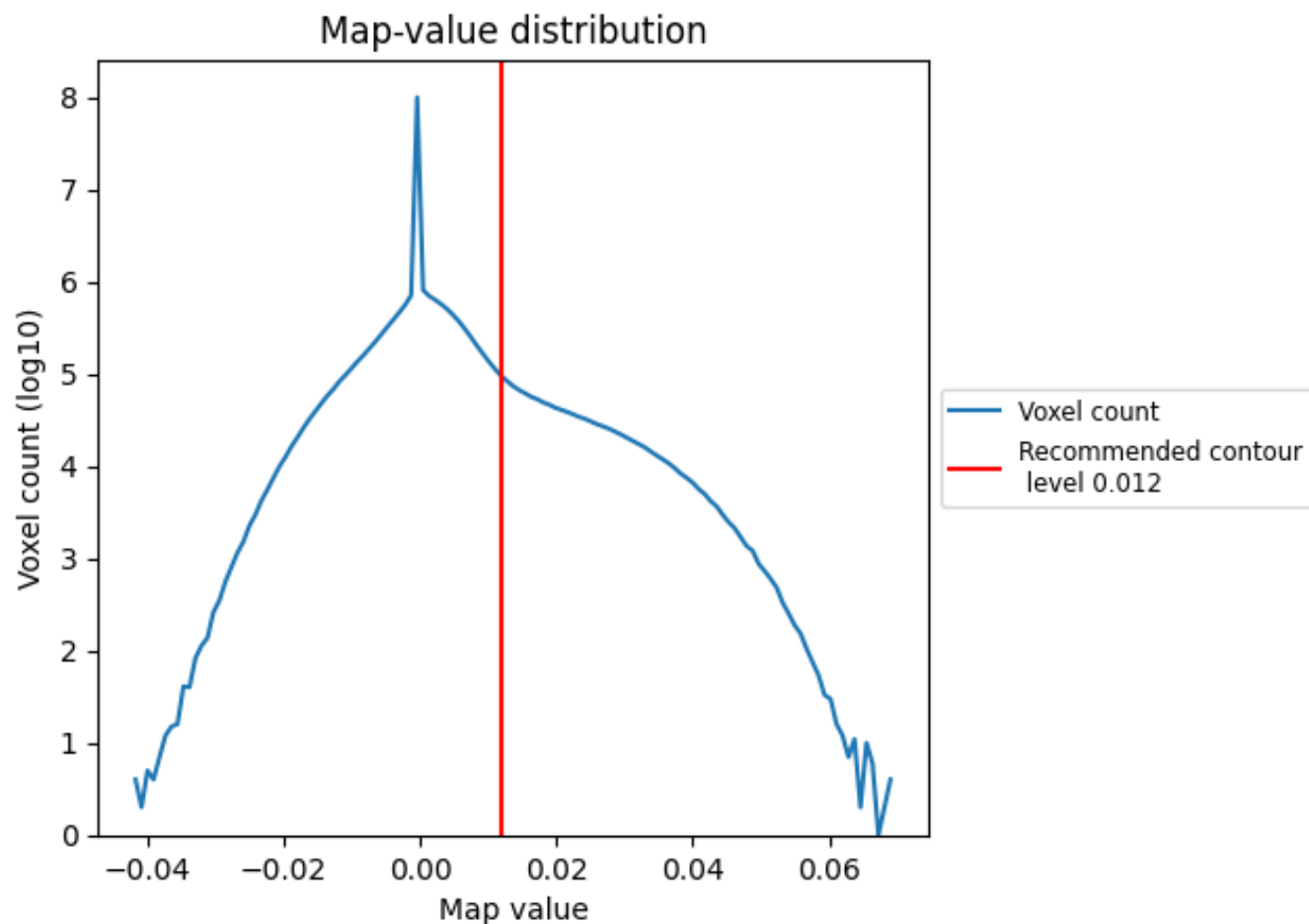
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

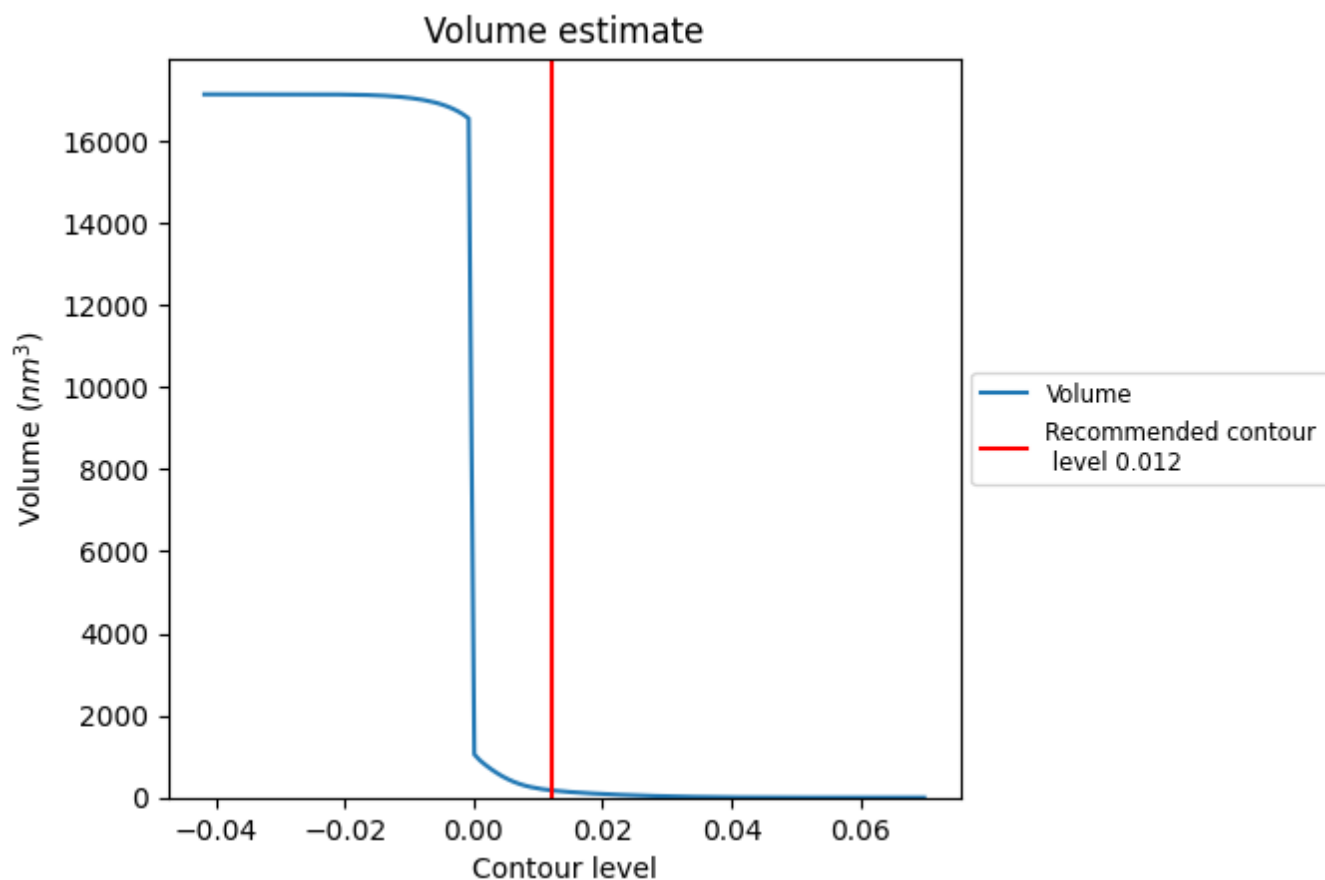
This section contains the results of statistical analysis of the map.

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.

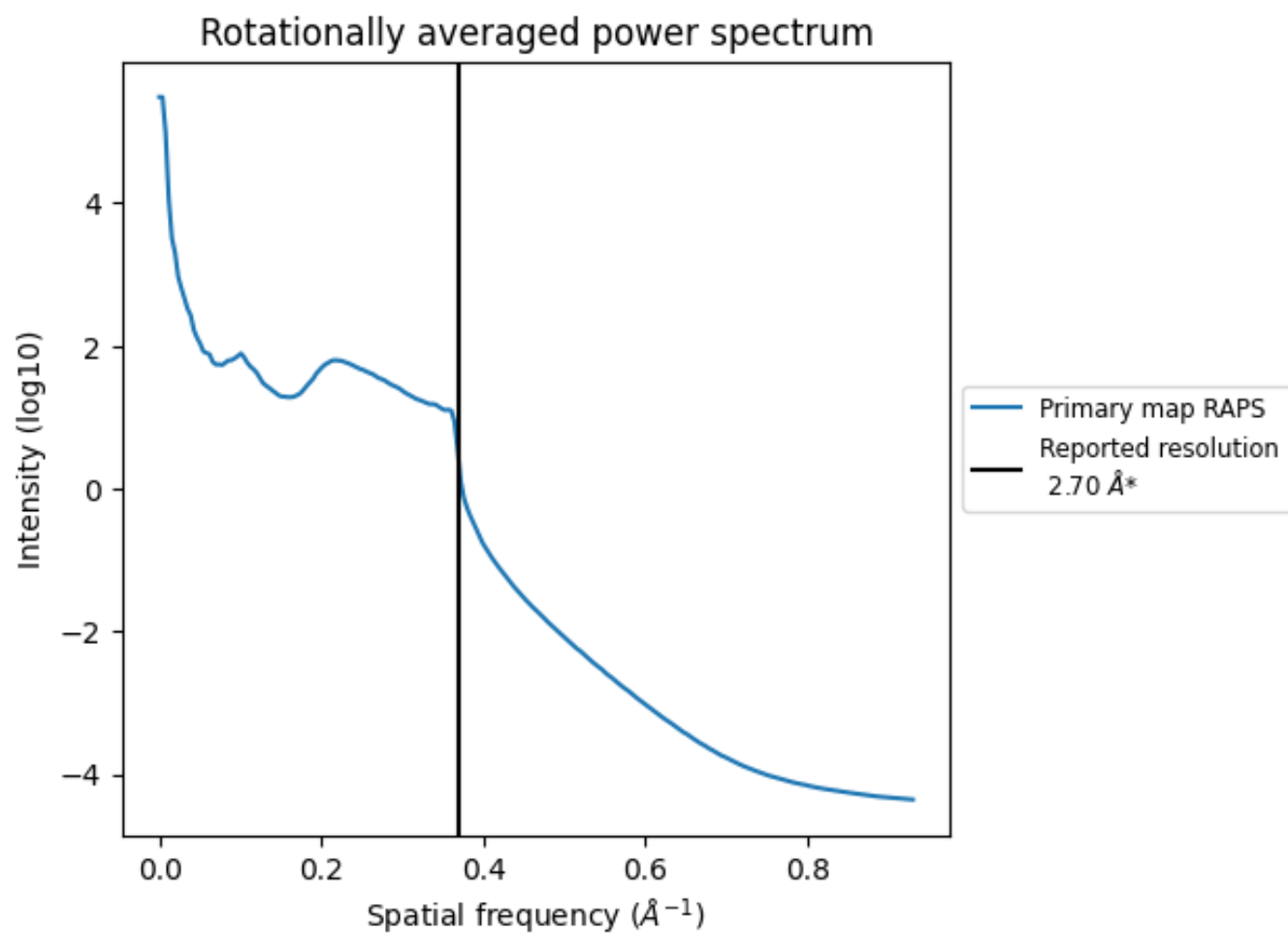
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178 nm³; this corresponds to an approximate mass of 161 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 0.370 Å⁻¹

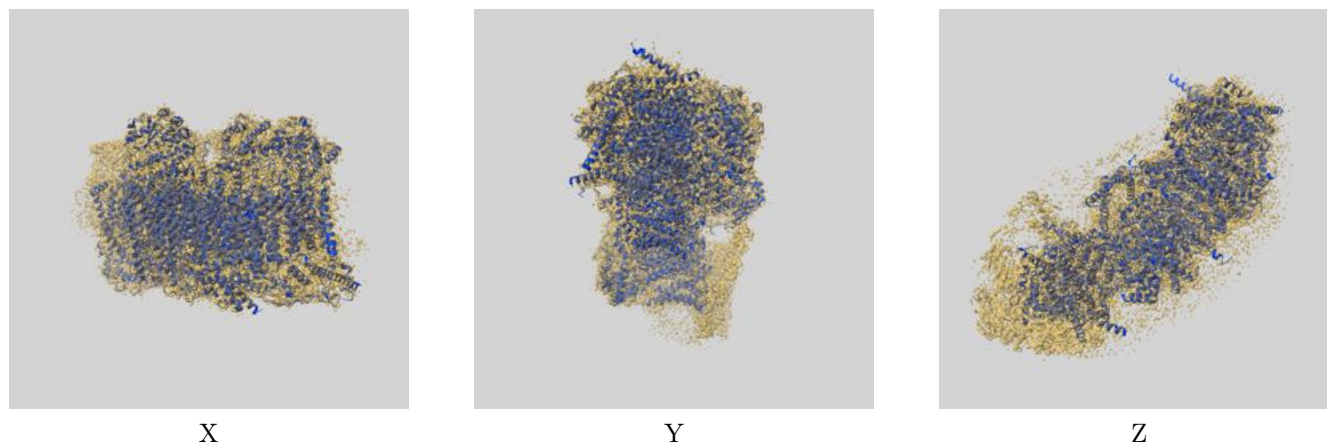
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

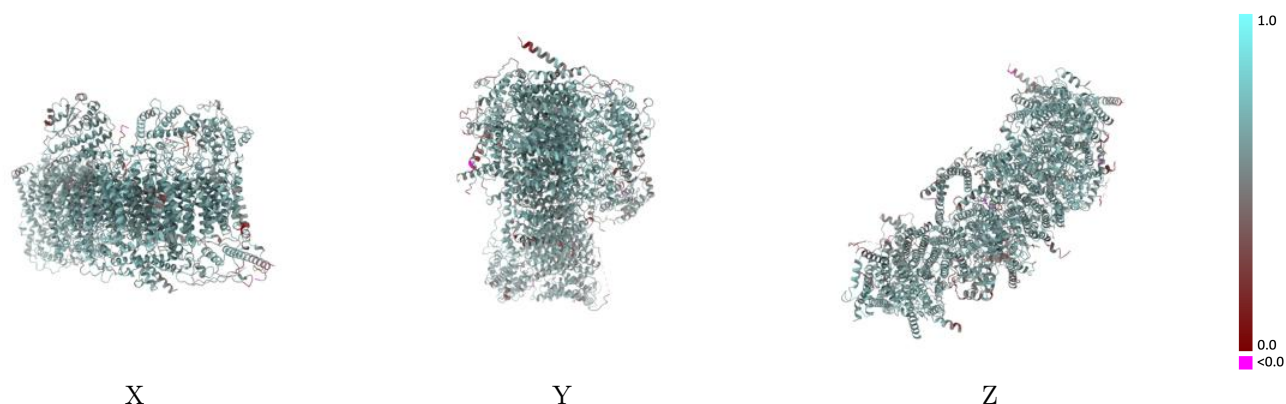
This section contains information regarding the fit between EMDB map EMD-32155 and PDB model 7VWL. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



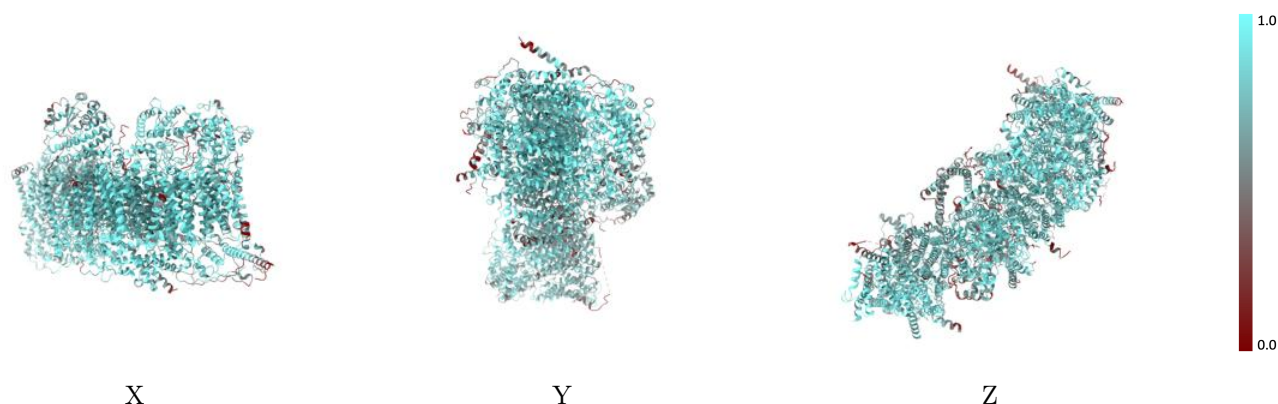
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



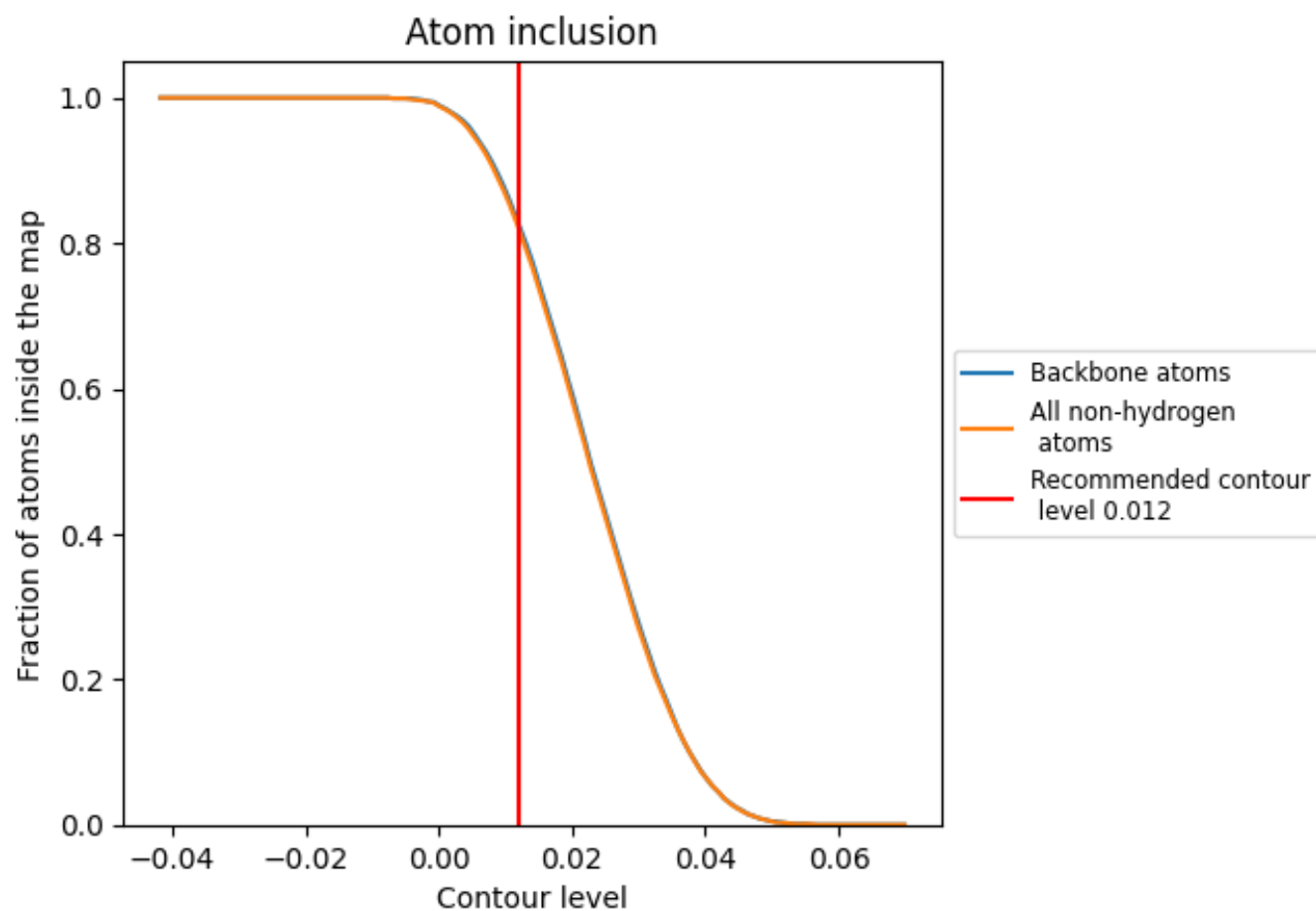
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8200	 0.5990
Q	 0.6410	 0.5390
S	 0.8610	 0.6060
U	 0.8080	 0.5850
V	 0.5990	 0.5300
W	 0.8580	 0.6160
X	 0.7800	 0.5690
Y	 0.6870	 0.5400
Z	 0.6460	 0.5100
a	 0.8690	 0.6300
b	 0.7160	 0.5440
c	 0.8410	 0.6040
d	 0.8320	 0.6060
e	 0.7610	 0.5650
f	 0.7340	 0.5530
g	 0.9030	 0.6290
h	 0.8610	 0.6100
i	 0.9080	 0.6370
j	 0.6850	 0.5540
k	 0.8140	 0.5920
l	 0.8830	 0.6320
m	 0.7560	 0.5640
n	 0.7470	 0.5730
o	 0.8310	 0.5990
p	 0.8440	 0.6100
r	 0.9080	 0.6360
s	 0.8560	 0.6100
u	 0.8150	 0.5960
v	 0.7150	 0.5410
w	 0.7400	 0.5620

