



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:32 AM UTC

PDB ID : 7VBP / pdb_00007vbp
EMDB ID : EMD-31884
Title : Membrane arm of deactive state CI from DQ-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-09-01
Resolution : 2.80 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:

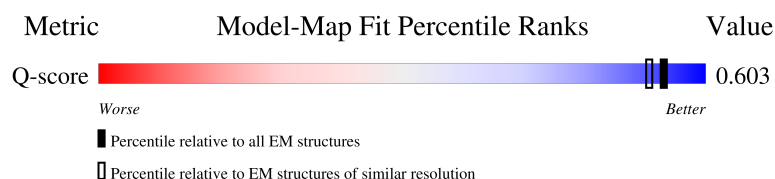
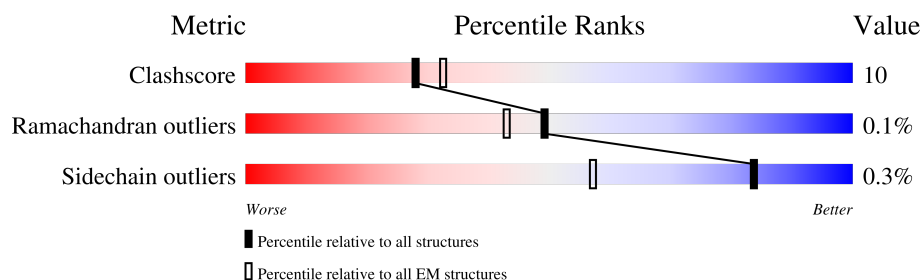
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11806 (2.30 - 3.30)

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

Mol	Chain	Length	Quality of chain
1	Q	40	48% 72% 25% .
2	S	70	6% 87% 13%
3	U	83	11% 89% 11%
4	V	140	73% 84% 14% .

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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
31	CDL	a	201	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 39022 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
			707	455	104	143	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
			342	225	58	59		

- 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
			4761	3155	740	817	49		

- 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
			939	628	137	166	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
			479	311	88	79	1		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	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
			1022	639	192	182	9		

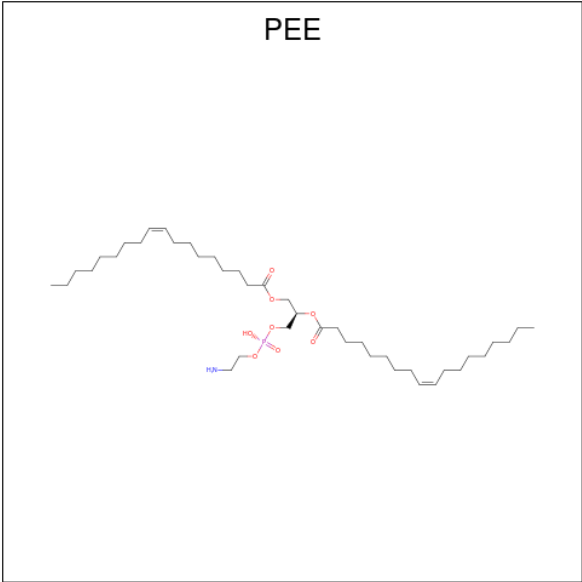
There is a discrepancy between the modelled and reference sequences:

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

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

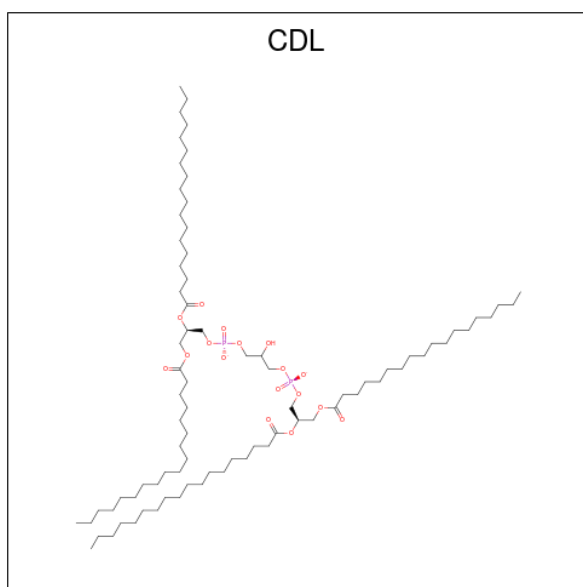
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2586	1646	439	491	10		

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



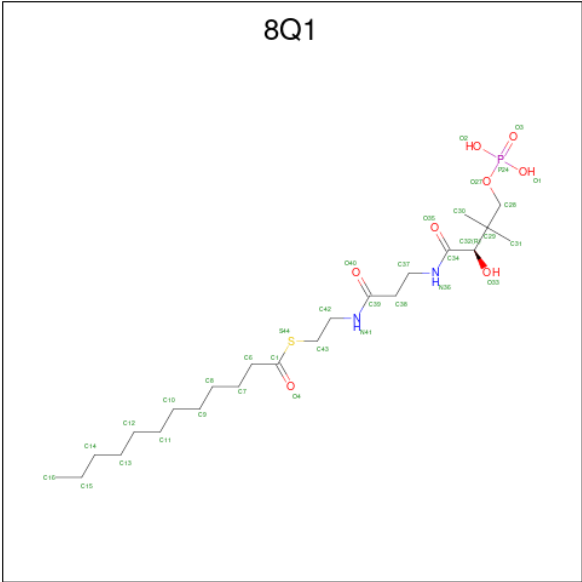
Mol	Chain	Residues	Atoms					AltConf
30	Q	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	r	1	Total	C	N	O	P	0
			41	31	1	8	1	
30	s	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 31 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



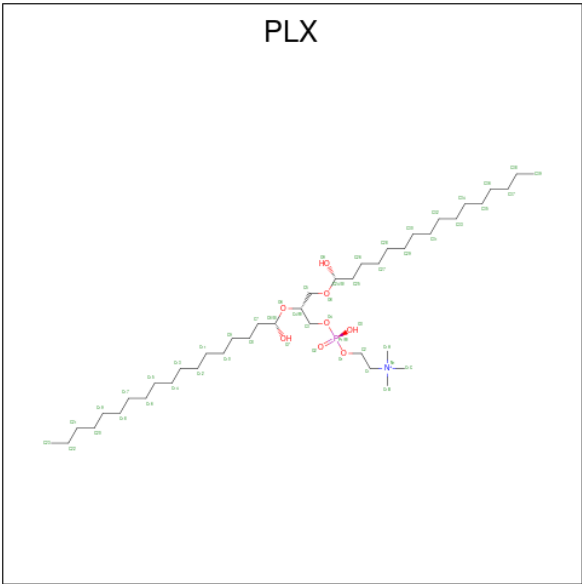
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			71	52	17	2	
31	a	1	Total	C	O	P	0
			91	72	17	2	
31	g	1	Total	C	O	P	0
			62	43	17	2	
31	l	1	Total	C	O	P	0
			99	80	17	2	
31	l	1	Total	C	O	P	0
			100	81	17	2	
31	r	1	Total	C	O	P	0
			100	81	17	2	

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



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

- Molecule 33 is (9R,11S)-9-([[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOX (CCD ID: PLX) (formula: C₄₂H₈₉NO₈P) (labeled as "Ligand of Interest" by depositor).



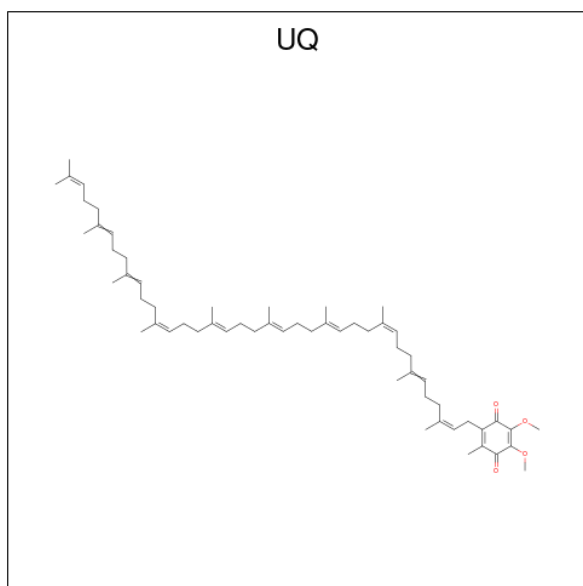
Mol	Chain	Residues	Atoms					AltConf
33	a	1	Total	C	N	O	P	0
			52	42	1	8	1	

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

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



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

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

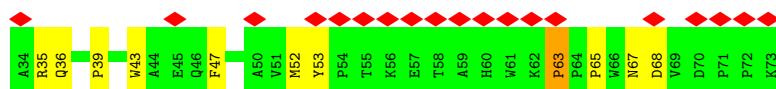
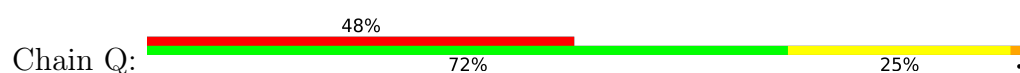
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Mol	Chain	Residues	Atoms		AltConf
36	j	14	Total 14	O 14	0
36	k	16	Total 16	O 16	0
36	l	55	Total 55	O 55	0
36	m	10	Total 10	O 10	0
36	n	1	Total 1	O 1	0
36	p	2	Total 2	O 2	0
36	r	86	Total 86	O 86	0
36	s	68	Total 68	O 68	0
36	w	3	Total 3	O 3	0

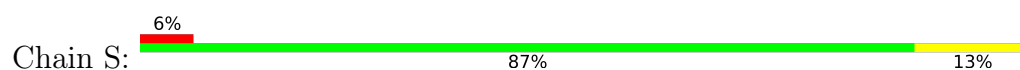
3 Residue-property plots

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

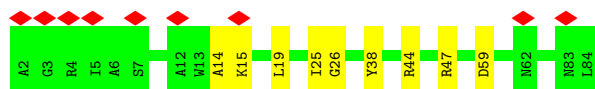
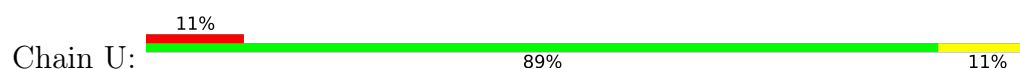
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



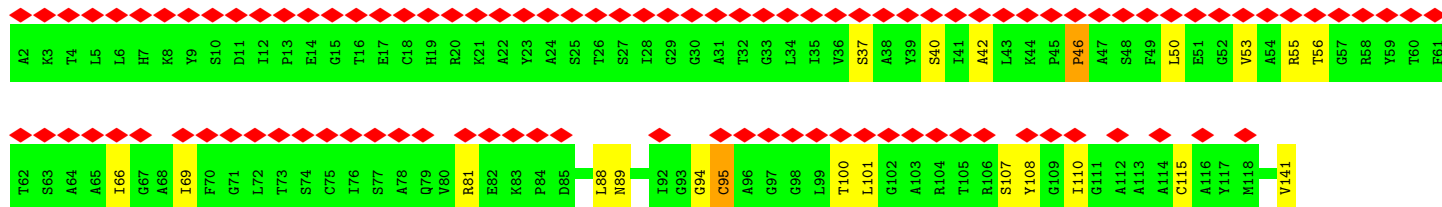
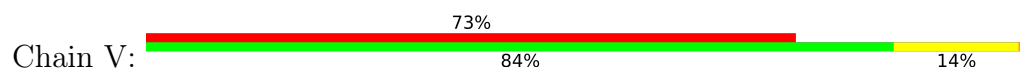
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



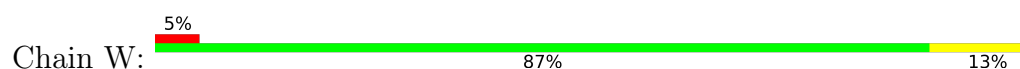
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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

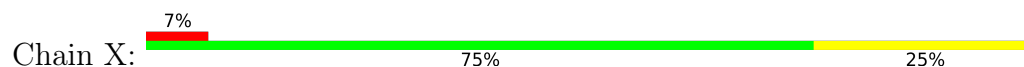


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

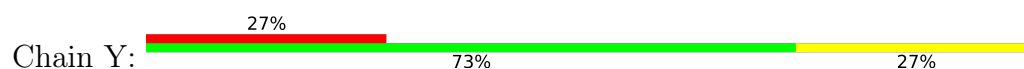




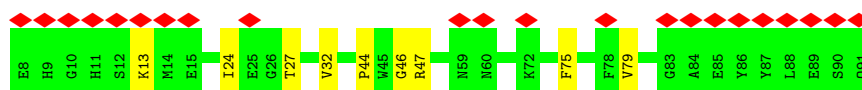
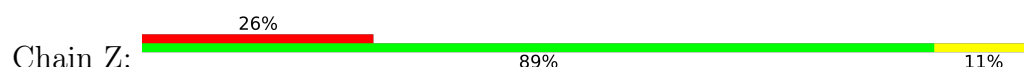
- Molecule 6: Acyl carrier protein, mitochondrial



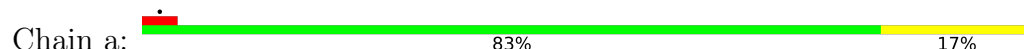
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



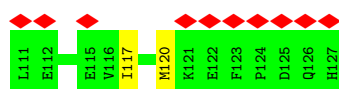
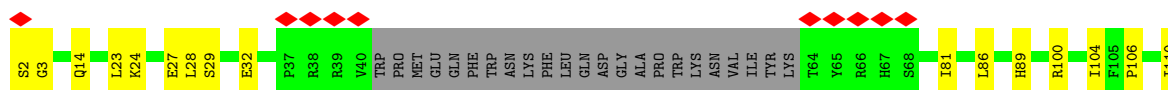
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



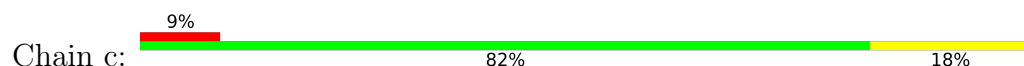
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

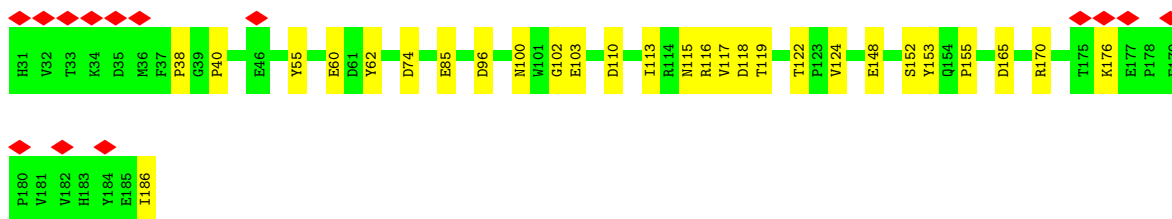


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

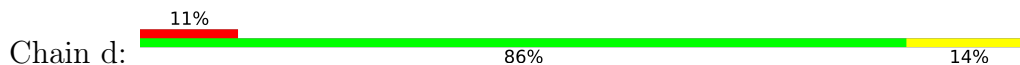


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

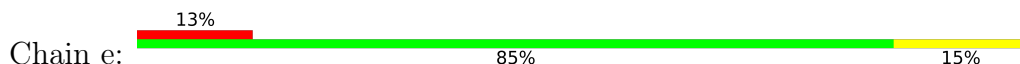




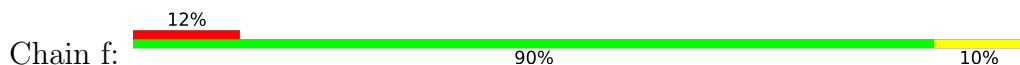
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



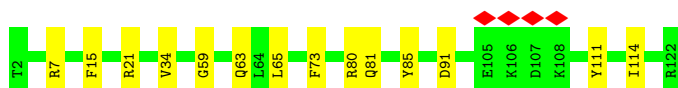
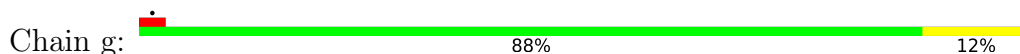
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



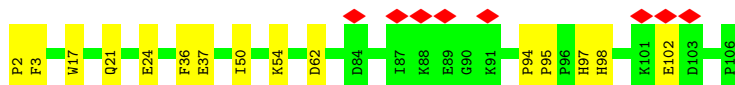
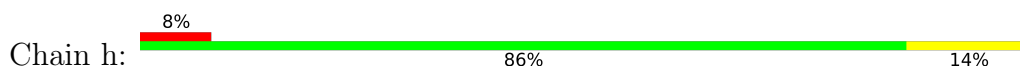
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



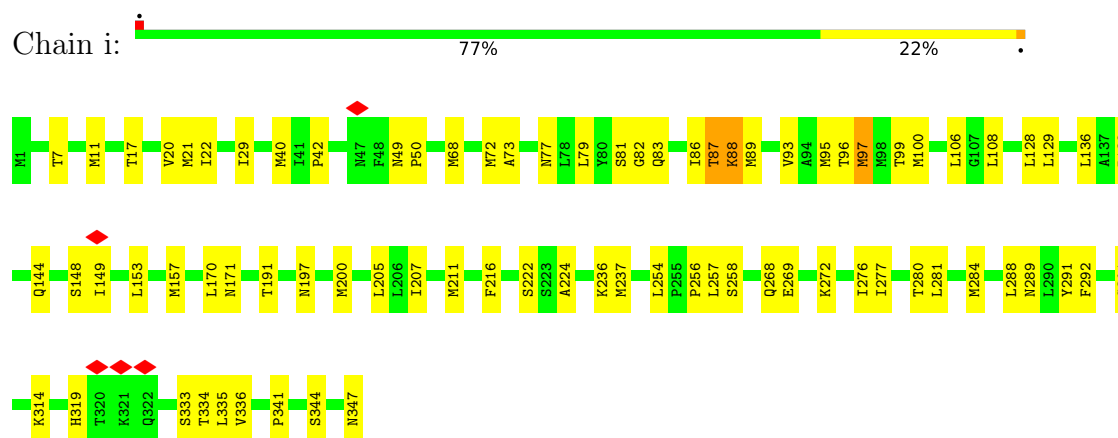
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2



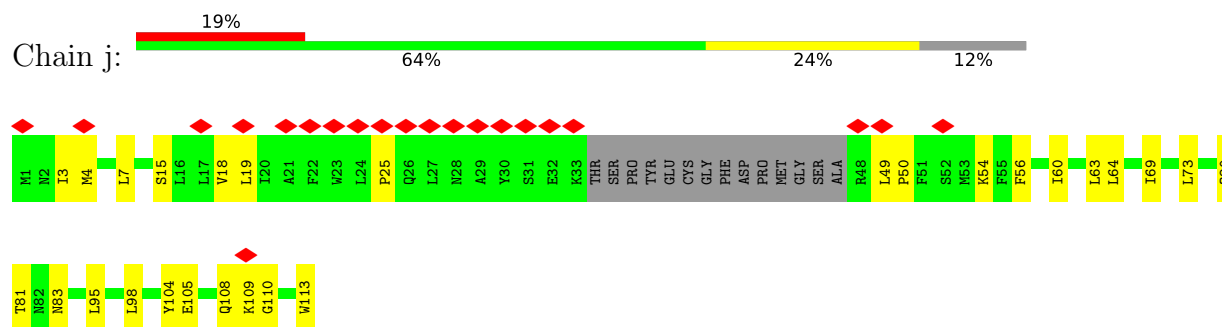
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



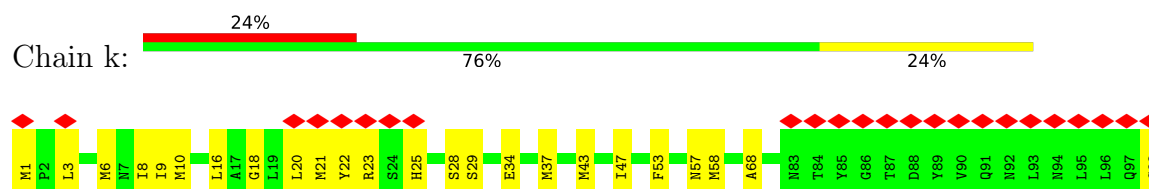
- Molecule 17: NADH-ubiquinone oxidoreductase chain 2



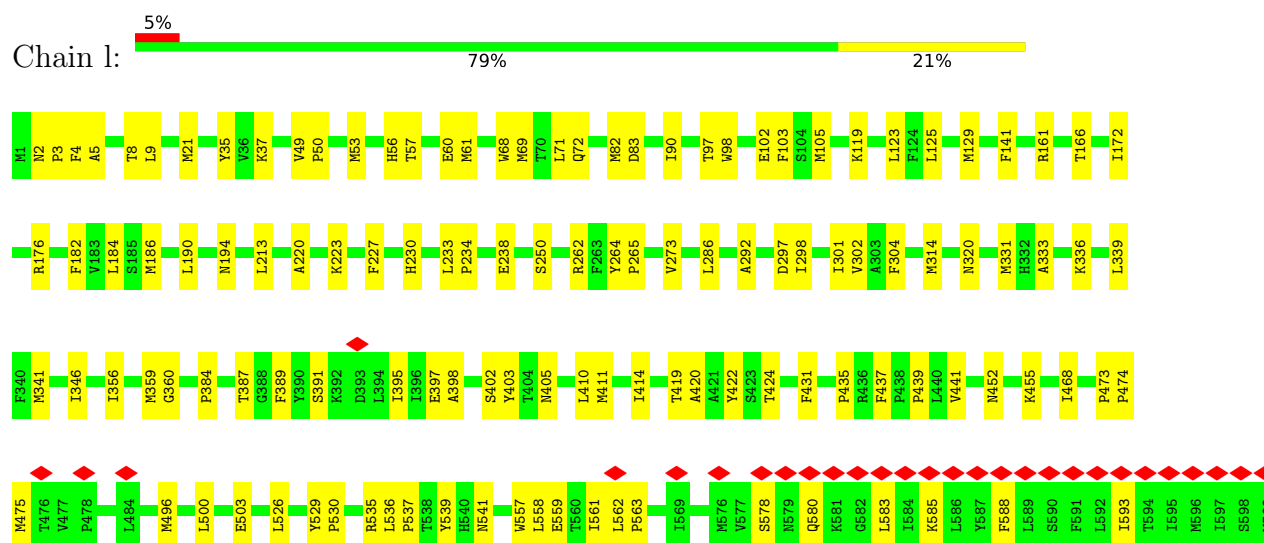
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3



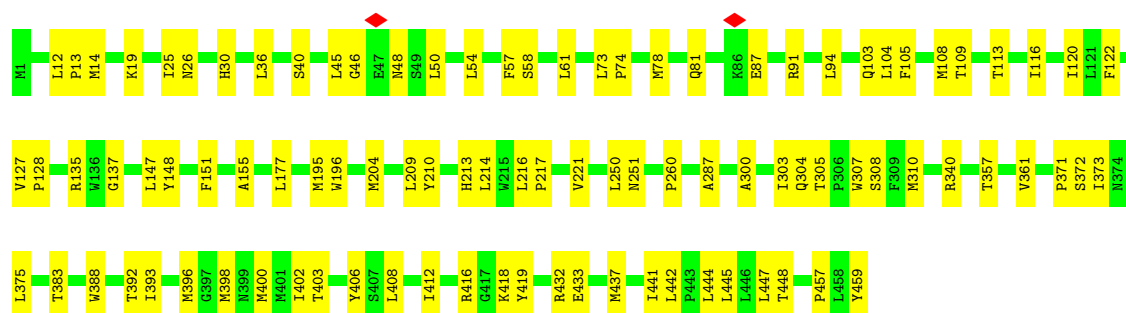
- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L



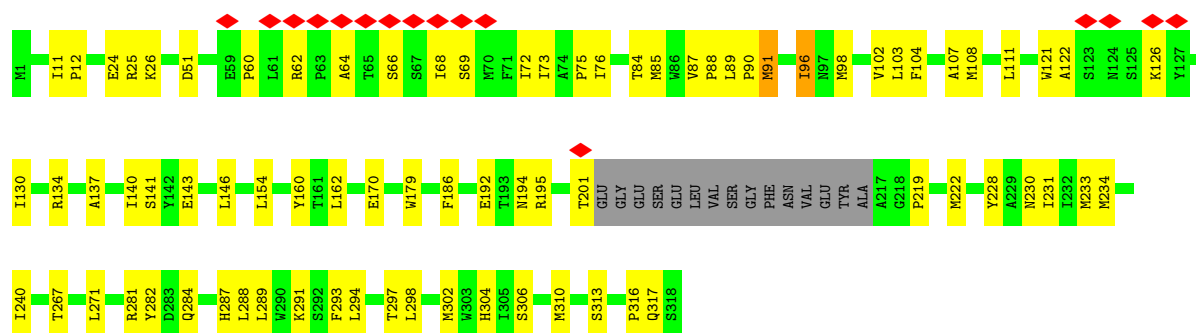
- Molecule 20: NADH-ubiquinone oxidoreductase chain 5



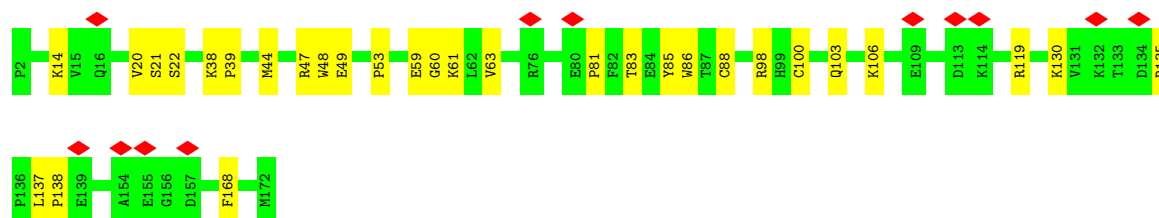
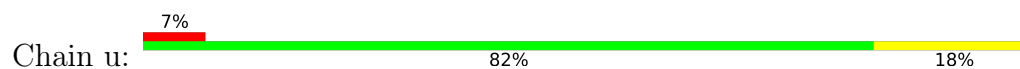




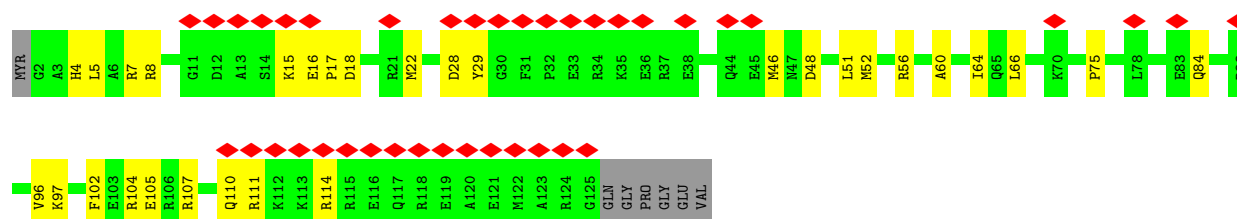
- Molecule 26: NADH-ubiquinone oxidoreductase chain 1



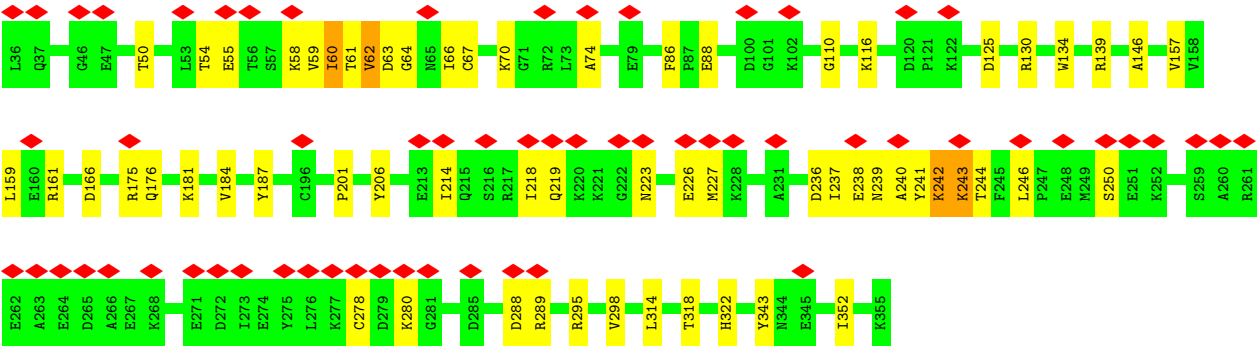
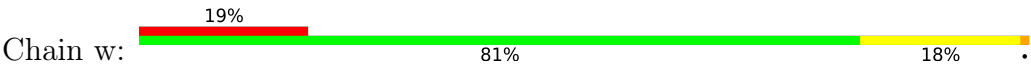
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



- 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	387112	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	0.067	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0123	Depositor
Map size (Å)	274.9952, 274.9952, 274.9952	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.5371, 0.5371, 0.5371	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	Q	0.50	1/350 (0.3%)	0.95	4/483 (0.8%)
2	S	0.18	0/582	0.39	0/783
3	U	0.14	0/664	0.35	0/912
4	V	0.20	0/1042	0.44	3/1411 (0.2%)
5	W	0.17	0/973	0.33	0/1312
6	X	0.19	0/719	0.40	0/972
7	Y	0.18	0/626	0.35	0/857
8	Z	0.14	0/695	0.30	0/939
9	a	0.20	0/1199	0.37	0/1623
10	b	0.17	0/906	0.40	0/1232
11	c	0.18	0/1371	0.33	0/1875
12	d	0.18	0/1494	0.35	0/2015
13	e	0.18	0/916	0.37	0/1246
14	f	0.14	0/350	0.28	0/473
15	g	0.18	0/1031	0.33	0/1394
16	h	0.17	0/889	0.31	0/1190
17	i	0.20	0/2773	0.39	0/3768
18	j	0.22	0/819	0.43	0/1117
19	k	0.22	0/759	0.46	0/1029
20	l	0.21	0/4889	0.43	0/6652
21	m	0.23	0/959	0.44	0/1300
22	n	0.23	0/491	0.56	1/663 (0.2%)
23	o	0.17	0/1092	0.36	0/1481
24	p	0.21	0/1590	0.40	0/2155
25	r	0.21	0/3723	0.39	0/5078
26	s	0.21	0/2464	0.43	0/3369
27	u	0.18	0/1436	0.38	0/1938
28	v	0.16	0/1046	0.42	0/1404
29	w	0.16	0/2646	0.38	0/3584
All	All	0.20	1/38494 (0.0%)	0.40	8/52255 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	63	PRO	CG-CD	-7.77	1.24	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	63	PRO	N-CD-CG	-13.21	83.39	103.20
1	Q	63	PRO	CA-CB-CG	-12.65	80.46	104.50
4	V	95	CYS	CA-CB-SG	6.91	130.28	114.40
4	V	94	GLY	CA-C-N	-6.50	111.81	122.54
4	V	94	GLY	C-N-CA	-6.50	111.81	122.54
22	n	16	LEU	N-CA-C	5.59	117.37	111.28
1	Q	63	PRO	CA-N-CD	-5.11	104.85	112.00
1	Q	63	PRO	N-CA-CB	-5.02	100.38	103.19

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	11	0
2	S	567	0	565	8	0
3	U	643	0	642	8	0
4	V	1021	0	1027	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	W	949	0	935	13	0
6	X	707	0	697	15	0
7	Y	600	0	539	14	0
8	Z	674	0	643	7	0
9	a	1165	0	1174	21	0
10	b	879	0	899	17	0
11	c	1315	0	1208	24	0
12	d	1461	0	1429	23	0
13	e	890	0	837	14	0
14	f	342	0	341	3	0
15	g	1000	0	994	11	0
16	h	867	0	871	13	0
17	i	2710	0	2874	75	0
18	j	800	0	855	25	0
19	k	748	0	799	22	0
20	l	4761	0	4882	110	0
21	m	939	0	952	45	0
22	n	479	0	486	25	0
23	o	1062	0	1072	10	0
24	p	1534	0	1470	22	0
25	r	3631	0	3839	85	0
26	s	2394	0	2508	69	0
27	u	1398	0	1378	22	0
28	v	1022	0	969	25	0
29	w	2586	0	2542	45	0
30	Q	47	0	71	17	0
30	U	51	0	82	8	0
30	b	46	0	69	15	0
30	l	46	0	69	6	0
30	m	41	0	59	14	0
30	r	41	0	59	14	0
30	s	51	0	82	5	0
31	V	71	0	92	5	0
31	a	91	0	132	25	0
31	g	62	0	68	20	0
31	l	199	0	307	21	0
31	r	100	0	156	6	0
32	X	35	0	0	1	0
33	a	52	0	88	13	0
33	g	52	0	88	9	0
33	m	52	0	88	2	0
33	r	104	0	176	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	s	28	0	31	4	0
35	w	27	0	11	4	0
36	Q	6	0	0	3	0
36	S	3	0	0	0	0
36	U	3	0	0	2	0
36	V	2	0	0	0	0
36	W	1	0	0	0	0
36	a	2	0	0	0	0
36	c	2	0	0	0	0
36	d	3	0	0	1	0
36	e	2	0	0	1	0
36	h	4	0	0	5	0
36	i	66	0	0	4	0
36	j	14	0	0	1	0
36	k	16	0	0	1	0
36	l	55	0	0	7	0
36	m	10	0	0	3	0
36	n	1	0	0	1	0
36	p	2	0	0	0	0
36	r	86	0	0	5	0
36	s	68	0	0	5	0
36	w	3	0	0	0	0
All	All	39022	0	39456	746	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 10.

All (746) 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)
22:n:13:VAL:CG1	25:r:14:MET:HG2	1.59	1.30
26:s:84:THR:O	26:s:87:VAL:HG22	1.36	1.21
36:h:204:HOH:O	17:i:88:LYS:CG	1.95	1.14
30:Q:101:PEE:H28	30:Q:101:PEE:H36	1.25	1.14
31:a:201:CDL:H521	30:b:201:PEE:H13	1.29	1.10
26:s:87:VAL:HG23	26:s:88:PRO:CD	1.85	1.06
20:l:397:GLU:OE2	36:l:801:HOH:O	1.74	1.05
26:s:87:VAL:CG2	26:s:88:PRO:HD3	1.87	1.04
31:a:201:CDL:H251	31:a:201:CDL:H211	1.35	1.03
30:m:202:PEE:H25	30:m:202:PEE:H56	1.41	1.01
22:n:13:VAL:HG13	25:r:14:MET:HG2	1.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:119:LYS:NZ	31:l:701:CDL:H512	1.78	0.99
20:l:2:ASN:OD1	20:l:3:PRO:HD2	1.62	0.98
29:w:66:ILE:O	35:w:401:ADP:O2A	1.81	0.97
22:n:13:VAL:HG12	25:r:14:MET:HG2	1.47	0.96
1:Q:53:TYR:OH	30:Q:101:PEE:O3	1.84	0.95
10:b:100:ARG:HB2	20:l:60:GLU:HB2	1.47	0.94
26:s:87:VAL:HG23	26:s:88:PRO:HD3	0.95	0.93
29:w:175:ARG:HH12	29:w:240:ALA:HB2	1.35	0.92
31:a:201:CDL:H521	30:b:201:PEE:C11	2.00	0.92
4:V:95:CYS:HB2	4:V:115:CYS:HA	1.49	0.91
31:a:201:CDL:H322	30:b:201:PEE:C38	2.01	0.91
31:g:202:CDL:H601	17:i:256:PRO:CB	2.02	0.89
30:Q:101:PEE:H28	30:Q:101:PEE:C22	2.03	0.89
9:a:95:GLU:OE2	31:a:201:CDL:O1	1.90	0.89
33:a:202:PLX:H282	33:a:202:PLX:H322	1.54	0.89
1:Q:53:TYR:OH	30:Q:101:PEE:C3	2.22	0.88
31:g:202:CDL:HB21	22:n:34:LYS:NZ	1.90	0.87
31:a:201:CDL:H322	30:b:201:PEE:H62	1.55	0.86
29:w:239:ASN:OD1	29:w:243:LYS:HD3	1.77	0.84
36:h:204:HOH:O	17:i:88:LYS:CD	2.20	0.84
30:m:202:PEE:H10	30:m:202:PEE:H2	1.60	0.84
36:h:204:HOH:O	17:i:88:LYS:CB	2.18	0.83
20:l:119:LYS:HZ2	31:l:701:CDL:H512	1.43	0.83
31:a:201:CDL:H211	31:a:201:CDL:C25	2.09	0.82
36:h:204:HOH:O	17:i:88:LYS:HG3	1.68	0.82
18:j:4:MET:SD	30:m:202:PEE:H21	2.21	0.81
30:m:202:PEE:H10	30:m:202:PEE:C1	2.11	0.81
30:r:501:PEE:C15	30:r:501:PEE:H30	2.12	0.80
31:g:202:CDL:H601	17:i:256:PRO:HB2	1.65	0.78
26:s:146:LEU:HD11	26:s:192:GLU:HG3	1.65	0.78
30:b:201:PEE:O1P	30:b:201:PEE:H8	1.83	0.78
31:g:202:CDL:HB21	22:n:34:LYS:HZ3	1.47	0.77
17:i:281:LEU:CD2	30:r:501:PEE:C37	2.63	0.77
19:k:34:GLU:OE1	36:k:101:HOH:O	2.02	0.77
9:a:97:GLU:OE1	12:d:60:ARG:NH2	2.18	0.76
9:a:127:ASP:OD1	33:a:202:PLX:H12	1.86	0.76
17:i:281:LEU:HD23	30:r:501:PEE:C37	2.16	0.76
17:i:277:ILE:HG23	30:r:501:PEE:H58	1.67	0.75
31:g:202:CDL:H542	31:g:202:CDL:C58	2.16	0.75
23:o:23:TYR:OH	24:p:68:GLU:OE1	2.03	0.75
26:s:84:THR:O	26:s:87:VAL:CG2	2.29	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:g:202:CDL:H601	17:i:256:PRO:HB3	1.68	0.75
29:w:242:LYS:HA	29:w:246:LEU:HD23	1.69	0.75
4:V:95:CYS:HB2	4:V:115:CYS:CA	2.15	0.74
9:a:131:LYS:NZ	22:n:32:ASP:OD2	2.20	0.74
31:g:202:CDL:C12	31:g:202:CDL:H762	2.18	0.73
30:m:202:PEE:H56	30:m:202:PEE:C17	2.17	0.73
20:l:397:GLU:CG	36:l:801:HOH:O	2.35	0.73
24:p:139:GLN:NE2	24:p:143:GLU:OE1	2.22	0.72
30:Q:101:PEE:H32	20:l:562:LEU:HG	1.70	0.72
3:U:25:ILE:HG12	30:s:401:PEE:H38	1.70	0.72
26:s:288:LEU:CD1	30:s:401:PEE:H7	2.20	0.72
31:a:201:CDL:H191	31:a:201:CDL:H732	1.70	0.71
31:l:701:CDL:H382	25:r:372:SER:HB3	1.73	0.71
21:m:31:LEU:HA	21:m:34:ILE:HD12	1.72	0.71
25:r:81:GLN:NE2	36:r:604:HOH:O	2.24	0.71
17:i:82:GLY:O	36:i:401:HOH:O	2.07	0.71
30:m:202:PEE:H7	30:m:202:PEE:O4	1.91	0.70
25:r:210:TYR:O	25:r:213:HIS:ND1	2.25	0.70
20:l:227:PHE:O	20:l:230:HIS:ND1	2.23	0.70
21:m:57:PHE:HZ	26:s:111:LEU:HD11	1.56	0.70
36:Q:203:HOH:O	17:i:49:ASN:HB2	1.92	0.69
31:a:201:CDL:H322	30:b:201:PEE:C37	2.22	0.69
16:h:37:GLU:OE2	36:i:401:HOH:O	2.10	0.69
20:l:223:LYS:HG3	36:l:832:HOH:O	1.89	0.69
10:b:89:HIS:CE1	30:b:201:PEE:H50	2.28	0.69
20:l:119:LYS:NZ	31:l:701:CDL:C51	2.54	0.69
12:d:57:ALA:HA	12:d:60:ARG:HD3	1.75	0.69
1:Q:53:TYR:OH	30:Q:101:PEE:H8	1.91	0.69
17:i:88:LYS:HE3	17:i:148:SER:OG	1.92	0.68
30:m:202:PEE:H53	30:m:202:PEE:H24	1.75	0.68
17:i:77:ASN:OD1	17:i:89:MET:O	2.11	0.68
25:r:418:LYS:O	36:r:601:HOH:O	2.12	0.68
17:i:108:LEU:HD11	17:i:191:THR:HG21	1.75	0.68
30:b:201:PEE:O5	30:b:201:PEE:H1	1.93	0.67
25:r:74:PRO:O	25:r:78:MET:HG3	1.94	0.67
30:r:501:PEE:H30	30:r:501:PEE:H22	1.76	0.67
28:v:15:LYS:HE3	28:v:110:GLN:HE22	1.58	0.67
7:Y:43:ARG:HG3	7:Y:46:GLN:HB2	1.75	0.67
17:i:207:ILE:HG22	17:i:211:MET:HE2	1.75	0.67
25:r:403:THR:HA	25:r:406:TYR:CE2	2.30	0.67
20:l:8:THR:HB	20:l:82:MET:HE3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:161:ARG:NH1	20:l:238:GLU:OE2	2.26	0.67
19:k:10:MET:HE3	21:m:14:VAL:HG11	1.75	0.67
29:w:125:ASP:O	29:w:130:ARG:NH2	2.28	0.66
10:b:100:ARG:HH11	20:l:60:GLU:HG3	1.61	0.66
1:Q:47:PHE:HD1	1:Q:52:MET:HE1	1.60	0.66
20:l:190:LEU:HD23	25:r:383:THR:HG21	1.78	0.66
10:b:29:SER:OG	10:b:32:GLU:OE1	2.13	0.65
17:i:281:LEU:HD21	30:r:501:PEE:C37	2.26	0.65
21:m:23:LYS:O	36:m:301:HOH:O	2.13	0.65
28:v:22:MET:HE1	28:v:102:PHE:HA	1.79	0.65
22:n:15:ILE:C	22:n:15:ILE:HD12	2.20	0.65
18:j:63:LEU:HD12	36:j:209:HOH:O	1.97	0.65
17:i:72:MET:HE1	19:k:9:ILE:HG12	1.79	0.65
31:a:201:CDL:H382	12:d:48:ALA:HB2	1.78	0.65
23:o:31:LYS:O	23:o:35:GLU:HG3	1.97	0.65
12:d:97:LYS:NZ	25:r:46:GLY:HA3	2.12	0.65
26:s:24:GLU:HG3	26:s:271:LEU:HD22	1.79	0.64
29:w:237:ILE:O	29:w:241:TYR:HB2	1.96	0.64
10:b:106:PRO:HG2	10:b:120:MET:HE2	1.79	0.64
17:i:95:MET:HE2	17:i:149:ILE:HG22	1.79	0.64
20:l:250:SER:HB2	20:l:333:ALA:HA	1.78	0.64
36:Q:203:HOH:O	17:i:50:PRO:HD2	1.97	0.64
9:a:141:GLN:O	9:a:145:GLU:HG3	1.97	0.64
11:c:117:VAL:HG21	20:l:539:TYR:HB2	1.80	0.64
30:r:501:PEE:H30	30:r:501:PEE:H21	1.80	0.63
33:a:202:PLX:H282	33:a:202:PLX:C32	2.26	0.63
26:s:25:ARG:NH2	34:s:402:UQ:O2	2.32	0.63
26:s:62:ARG:HH21	26:s:68:ILE:HB	1.64	0.63
20:l:119:LYS:HZ1	31:l:701:CDL:H512	1.60	0.63
21:m:57:PHE:CZ	26:s:111:LEU:HD11	2.32	0.63
29:w:250:SER:O	29:w:280:LYS:NZ	2.31	0.63
4:V:107:SER:HB3	4:V:110:ILE:HG22	1.81	0.62
11:c:62:TYR:OH	11:c:74:ASP:OD1	2.16	0.62
4:V:37:SER:HB3	4:V:56:THR:HG22	1.81	0.62
4:V:81:ARG:NH1	4:V:89:ASN:OD1	2.32	0.62
33:g:201:PLX:H1B3	16:h:2:PRO:HD2	1.81	0.61
26:s:304:HIS:O	36:s:501:HOH:O	2.16	0.61
17:i:335:LEU:HD21	31:r:504:CDL:H402	1.82	0.61
19:k:8:ILE:HG21	19:k:43:MET:HB2	1.83	0.61
18:j:18:VAL:HG22	26:s:222:MET:HE3	1.82	0.61
26:s:281:ARG:HB2	26:s:284:GLN:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:60:GLU:OE1	20:l:83:ASP:HA	2.00	0.61
17:i:276:ILE:HG21	30:r:501:PEE:H14	1.83	0.61
20:l:123:LEU:HD13	31:l:701:CDL:H121	1.83	0.61
31:r:504:CDL:H331	31:r:504:CDL:H202	1.81	0.61
30:Q:101:PEE:C20	20:l:562:LEU:HG	2.30	0.61
30:U:101:PEE:C10	30:U:101:PEE:H49	2.31	0.61
33:g:201:PLX:H393	33:g:201:PLX:H211	1.82	0.61
30:U:101:PEE:H49	30:U:101:PEE:C11	2.31	0.60
10:b:81:ILE:HG23	30:b:201:PEE:H58	1.82	0.60
20:l:56:HIS:CD2	20:l:57:THR:HG23	2.36	0.60
25:r:260:PRO:HG3	33:r:502:PLX:H132	1.83	0.60
12:d:33:LEU:HD12	12:d:36:ILE:HD11	1.82	0.60
20:l:119:LYS:HZ1	31:l:701:CDL:C51	2.14	0.60
4:V:88:LEU:HD12	33:r:502:PLX:H24	1.82	0.60
12:d:71:VAL:HG11	12:d:87:GLU:HB3	1.82	0.60
18:j:64:LEU:HD13	21:m:165:VAL:HG22	1.82	0.60
30:Q:101:PEE:H31	20:l:562:LEU:HD21	1.82	0.60
11:c:116:ARG:HG2	30:l:703:PEE:H49	1.82	0.60
29:w:66:ILE:O	35:w:401:ADP:PA	2.59	0.60
30:b:201:PEE:H8	30:b:201:PEE:P	2.42	0.59
20:l:496:MET:HE1	31:l:702:CDL:H591	1.84	0.59
31:g:202:CDL:H542	31:g:202:CDL:H582	1.82	0.59
28:v:17:PRO:HB3	28:v:105:GLU:OE1	2.02	0.59
7:Y:51:THR:HG22	7:Y:53:SER:H	1.67	0.59
29:w:88:GLU:OE2	29:w:161:ARG:NH1	2.35	0.59
8:Z:24:ILE:O	8:Z:27:THR:OG1	2.21	0.59
31:a:201:CDL:H761	31:a:201:CDL:H201	1.84	0.59
6:X:69:SER:OG	6:X:70:ASP:N	2.36	0.59
5:W:85:GLN:NE2	5:W:89:GLU:OE2	2.34	0.59
28:v:29:TYR:OH	28:v:111:ARG:NH2	2.35	0.59
31:l:701:CDL:H311	31:l:701:CDL:H552	1.83	0.59
25:r:251:ASN:HD21	25:r:304:GLN:HE22	1.50	0.59
15:g:59:GLY:O	15:g:63:GLN:HG3	2.03	0.58
18:j:18:VAL:HA	26:s:222:MET:HE3	1.85	0.58
20:l:4:PHE:HB2	20:l:53:MET:CE	2.32	0.58
26:s:24:GLU:HA	26:s:271:LEU:HD13	1.85	0.58
29:w:50:THR:OG1	29:w:288:ASP:OD1	2.21	0.58
31:g:202:CDL:H622	31:g:202:CDL:H581	1.84	0.58
18:j:7:LEU:HD21	30:m:202:PEE:H59	1.85	0.58
22:n:17:VAL:HG21	25:r:30:HIS:HB3	1.84	0.58
4:V:69:ILE:HG13	4:V:100:THR:HG21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:69:SER:O	26:s:73:ILE:HG12	2.03	0.58
17:i:334:THR:HG21	31:r:504:CDL:H391	1.86	0.58
33:a:202:PLX:H102	25:r:40:SER:HB3	1.86	0.57
20:l:103:PHE:HB2	20:l:341:MET:HE3	1.87	0.57
13:e:89:VAL:HG21	25:r:25:ILE:HG23	1.85	0.57
31:g:202:CDL:H542	31:g:202:CDL:H581	1.84	0.57
2:S:5:ILE:HG12	26:s:26:LYS:HG2	1.85	0.57
17:i:268:GLN:HE22	17:i:272:LYS:HE3	1.69	0.57
31:V:201:CDL:H831	23:o:94:GLY:HA3	1.86	0.57
36:U:202:HOH:O	18:j:80:GLN:HB3	2.03	0.57
3:U:59:ASP:HB2	27:u:130:LYS:HB2	1.86	0.57
18:j:95:LEU:HD23	18:j:98:LEU:HD23	1.86	0.57
20:l:161:ARG:NH2	24:p:88:GLY:O	2.37	0.57
29:w:146:ALA:HB1	29:w:157:VAL:HG21	1.87	0.57
29:w:239:ASN:O	29:w:243:LYS:HG3	2.05	0.57
20:l:473:PRO:HG2	20:l:475:MET:HE3	1.86	0.57
29:w:139:ARG:NH1	29:w:166:ASP:OD2	2.37	0.57
30:Q:101:PEE:C25	30:Q:101:PEE:H34	2.35	0.56
12:d:33:LEU:HD21	20:l:49:VAL:HG22	1.87	0.56
20:l:166:THR:CG2	30:l:703:PEE:H2	2.36	0.56
20:l:562:LEU:HB3	20:l:563:PRO:HD3	1.87	0.56
5:W:86:MET:HE2	5:W:124:LEU:HB3	1.88	0.56
26:s:24:GLU:OE1	26:s:228:TYR:OH	2.16	0.56
3:U:26:GLY:HA3	30:U:101:PEE:H37	1.87	0.56
19:k:98:CYS:HB2	20:l:580:GLN:HB2	1.88	0.56
27:u:137:LEU:HD12	27:u:138:PRO:HD2	1.88	0.56
11:c:55:TYR:OH	11:c:74:ASP:O	2.19	0.56
17:i:268:GLN:NE2	17:i:272:LYS:HE3	2.21	0.56
22:n:13:VAL:HG13	25:r:14:MET:CG	2.25	0.56
31:g:202:CDL:H581	31:g:202:CDL:C62	2.36	0.56
31:a:201:CDL:H322	30:b:201:PEE:H60	1.86	0.56
20:l:391:SER:O	20:l:395:ILE:HG12	2.06	0.56
24:p:29:SER:HB3	24:p:76:HIS:CD2	2.40	0.55
10:b:86:LEU:HD11	20:l:9:LEU:HD12	1.88	0.55
11:c:113:ILE:HD11	11:c:116:ARG:HD2	1.88	0.55
25:r:412:ILE:HA	25:r:416:ARG:HG3	1.87	0.55
26:s:316:PRO:O	36:s:503:HOH:O	2.18	0.55
33:a:202:PLX:H212	13:e:104:THR:CG2	2.35	0.55
13:e:112:TYR:HB3	25:r:45:LEU:HD23	1.89	0.55
19:k:25:HIS:O	19:k:28:SER:N	2.39	0.55
9:a:139:ILE:HG23	25:r:54:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:27:ILE:HD13	26:s:121:TRP:CZ3	2.42	0.55
25:r:204:MET:HG3	25:r:209:LEU:HB2	1.89	0.55
5:W:130:ASN:HB3	21:m:1:MET:H1	1.72	0.55
26:s:62:ARG:HD3	26:s:64:ALA:H	1.71	0.55
6:X:125:GLU:HG2	20:l:439:PRO:HG2	1.89	0.55
17:i:211:MET:HG2	17:i:333:SER:HB2	1.89	0.55
17:i:301:SER:O	25:r:135:ARG:NH1	2.40	0.55
25:r:50:LEU:HB2	25:r:58:SER:HB3	1.87	0.55
20:l:176:ARG:NH2	36:l:809:HOH:O	2.40	0.54
12:d:97:LYS:HZ1	25:r:46:GLY:HA3	1.73	0.54
10:b:104:ILE:HB	28:v:48:ASP:HB3	1.89	0.54
12:d:46:THR:O	12:d:50:GLU:HG3	2.08	0.54
17:i:22:ILE:O	36:i:403:HOH:O	2.18	0.54
19:k:18:GLY:HA2	19:k:21:MET:HE2	1.87	0.54
20:l:397:GLU:CD	36:l:801:HOH:O	2.33	0.54
22:n:17:VAL:HB	22:n:18:PRO:HD3	1.89	0.54
26:s:287:HIS:CD2	26:s:291:LYS:HD2	2.42	0.54
22:n:13:VAL:CG1	25:r:14:MET:CG	2.56	0.54
20:l:286:LEU:HD22	20:l:411:MET:SD	2.48	0.54
30:m:202:PEE:C1	30:m:202:PEE:C4	2.86	0.54
7:Y:45:ARG:HG2	20:l:439:PRO:HB3	1.90	0.54
17:i:68:MET:HE1	19:k:37:MET:HB3	1.90	0.54
27:u:49:GLU:OE1	27:u:135:ARG:NH2	2.40	0.54
33:a:202:PLX:C32	33:a:202:PLX:C28	2.86	0.54
17:i:170:LEU:HD11	17:i:288:LEU:HD22	1.88	0.54
20:l:559:GLU:O	20:l:563:PRO:HD2	2.08	0.54
28:v:51:LEU:O	28:v:52:MET:HG3	2.08	0.54
6:X:116:VAL:HG12	6:X:120:MET:HE2	1.90	0.54
2:S:43:TYR:CZ	5:W:68:ARG:HG3	2.43	0.54
11:c:155:PRO:HG3	28:v:4:HIS:CD2	2.42	0.54
20:l:331:MET:SD	20:l:387:THR:OG1	2.62	0.53
22:n:14:HIS:CE1	25:r:26:ASN:ND2	2.76	0.53
26:s:186:PHE:HB2	30:s:401:PEE:H76	1.90	0.53
18:j:73:LEU:HD13	21:m:55:MET:HE1	1.91	0.53
22:n:8:VAL:O	22:n:12:TRP:HB3	2.08	0.53
1:Q:68:ASP:O	17:i:49:ASN:ND2	2.42	0.53
31:a:201:CDL:OA7	31:a:201:CDL:HA61	2.06	0.53
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.43	0.53
27:u:100:CYS:HB2	27:u:103:GLN:OE1	2.07	0.53
28:v:111:ARG:HA	28:v:114:ARG:HE	1.74	0.53
31:a:201:CDL:H541	30:b:201:PEE:H15	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:122:THR:OG1	11:c:124:VAL:O	2.26	0.53
25:r:340:ARG:NH1	36:r:610:HOH:O	2.41	0.53
9:a:96:ALA:HB2	12:d:61:TYR:CE2	2.43	0.53
31:a:201:CDL:H541	30:b:201:PEE:C12	2.38	0.53
21:m:57:PHE:HD2	26:s:107:ALA:HB1	1.73	0.53
12:d:101:GLU:OE2	36:d:201:HOH:O	2.19	0.53
30:Q:101:PEE:H34	30:Q:101:PEE:H41	1.91	0.53
20:l:141:PHE:HE2	25:r:375:LEU:HD11	1.73	0.53
17:i:171:ASN:ND2	20:l:578:SER:OG	2.26	0.53
21:m:23:LYS:HB3	36:m:301:HOH:O	2.09	0.53
25:r:445:LEU:O	25:r:448:THR:HG22	2.09	0.53
12:d:26:LEU:HD22	28:v:75:PRO:HB2	1.91	0.52
18:j:3:ILE:HG21	30:m:202:PEE:H13	1.89	0.52
5:W:128:ARG:NH1	16:h:102:GLU:OE2	2.37	0.52
6:X:90:TYR:HE1	8:Z:44:PRO:HB2	1.74	0.52
19:k:22:TYR:HB2	20:l:585:LYS:HA	1.90	0.52
26:s:317:GLN:HB2	36:s:551:HOH:O	2.08	0.52
19:k:58:MET:HE2	21:m:146:LEU:HA	1.91	0.52
10:b:28:LEU:HD22	10:b:32:GLU:HG2	1.90	0.52
24:p:26:HIS:CD2	24:p:79:PRO:HB3	2.44	0.52
29:w:176:GLN:NE2	29:w:236:ASP:OD2	2.41	0.52
7:Y:97:LEU:HD23	28:v:107:ARG:HD2	1.92	0.52
21:m:17:PHE:HA	21:m:20:PHE:CE2	2.44	0.52
24:p:47:ARG:NH2	24:p:70:GLU:OE1	2.43	0.52
28:v:15:LYS:HG3	28:v:110:GLN:OE1	2.09	0.52
4:V:95:CYS:CB	4:V:115:CYS:HA	2.30	0.52
12:d:43:ARG:HB3	12:d:44:PRO:HD3	1.91	0.52
33:a:202:PLX:O1	33:a:202:PLX:H1A2	2.09	0.52
26:s:288:LEU:HD13	30:s:401:PEE:H7	1.92	0.52
4:V:66:ILE:HD11	4:V:101:LEU:HD13	1.93	0.51
26:s:170:GLU:OE1	27:u:98:ARG:NH1	2.41	0.51
1:Q:35:ARG:HD3	29:w:322:HIS:CE1	2.45	0.51
12:d:160:LYS:NZ	15:g:114:ILE:O	2.42	0.51
20:l:5:ALA:HB2	20:l:61:MET:SD	2.49	0.51
20:l:346:ILE:HD11	20:l:431:PHE:CZ	2.45	0.51
28:v:60:ALA:O	28:v:64:ILE:HG12	2.11	0.51
5:W:63:GLU:OE2	27:u:119:ARG:NH2	2.42	0.51
20:l:419:THR:HA	20:l:422:TYR:CE2	2.45	0.51
27:u:83:THR:HA	27:u:86:TRP:CD1	2.45	0.51
29:w:59:VAL:HG13	29:w:201:PRO:HA	1.91	0.51
29:w:86:PHE:HB2	29:w:159:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:136:THR:HG21	25:r:48:ASN:HD22	1.76	0.51
9:a:187:PRO:HA	27:u:48:TRP:CD1	2.44	0.51
20:l:220:ALA:HB1	20:l:314:MET:HE1	1.92	0.51
26:s:219:PRO:HA	26:s:222:MET:HE2	1.93	0.51
17:i:100:MET:HE3	17:i:153:LEU:HD21	1.92	0.51
20:l:500:LEU:HD22	31:l:702:CDL:H551	1.93	0.51
30:Q:101:PEE:C22	30:Q:101:PEE:C18	2.85	0.51
27:u:14:LYS:O	27:u:61:LYS:NZ	2.43	0.51
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.93	0.51
12:d:102:ILE:HD11	13:e:125:LEU:HD23	1.92	0.51
13:e:152:ASP:OD1	13:e:153:GLU:N	2.43	0.51
33:g:201:PLX:H301	17:i:347:ASN:HB3	1.93	0.51
20:l:526:LEU:HD12	20:l:530:PRO:HG2	1.92	0.51
30:Q:101:PEE:H31	20:l:562:LEU:CD2	2.41	0.50
5:W:80:ASP:HB3	27:u:53:PRO:HB3	1.93	0.50
16:h:21:GLN:HA	19:k:53:PHE:CE1	2.46	0.50
21:m:45:LEU:HD23	21:m:50:SER:HA	1.93	0.50
5:W:62:ILE:O	5:W:66:GLU:HG2	2.11	0.50
29:w:54:THR:O	29:w:55:GLU:HG3	2.11	0.50
20:l:97:THR:HG21	20:l:125:LEU:HD22	1.92	0.50
29:w:64:GLY:HA2	29:w:206:TYR:CE1	2.45	0.50
7:Y:97:LEU:HG	28:v:104:ARG:HB2	1.93	0.50
33:a:202:PLX:H212	13:e:104:THR:HG22	1.93	0.50
26:s:87:VAL:CG2	26:s:88:PRO:CD	2.66	0.50
29:w:67:CYS:HB3	29:w:214:ILE:HG23	1.94	0.50
30:Q:101:PEE:H2	30:Q:101:PEE:H10	1.93	0.50
10:b:32:GLU:HG3	24:p:115:TYR:HD1	1.77	0.50
21:m:133:SER:OG	21:m:138:GLU:OE2	2.23	0.50
29:w:223:ASN:HB3	29:w:226:GLU:HB3	1.94	0.50
11:c:96:ASP:OD2	36:r:601:HOH:O	2.18	0.50
12:d:107:GLN:OE1	20:l:194:ASN:ND2	2.39	0.50
18:j:15:SER:HA	26:s:76:ILE:HD12	1.93	0.50
20:l:119:LYS:HZ2	31:l:701:CDL:C51	2.19	0.50
30:Q:101:PEE:H10	30:Q:101:PEE:C1	2.42	0.50
7:Y:87:PRO:HG3	28:v:96:VAL:HG22	1.94	0.50
21:m:175:ASN:OD1	29:w:289:ARG:NH2	2.44	0.50
17:i:269:GLU:OE2	36:i:404:HOH:O	2.19	0.50
26:s:89:LEU:O	36:s:502:HOH:O	2.18	0.50
16:h:50:ILE:HG22	16:h:54:LYS:HE2	1.94	0.49
17:i:197:ASN:HD22	17:i:200:MET:HG2	1.77	0.49
21:m:175:ASN:CG	29:w:289:ARG:HH22	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:81:PRO:HG3	27:u:106:LYS:HE2	1.94	0.49
29:w:59:VAL:HG23	29:w:157:VAL:HG23	1.94	0.49
8:Z:24:ILE:HD11	8:Z:46:GLY:C	2.37	0.49
20:l:557:TRP:O	20:l:561:ILE:HG12	2.11	0.49
17:i:68:MET:CE	19:k:37:MET:HB3	2.42	0.49
20:l:233:LEU:HB3	20:l:234:PRO:HD3	1.93	0.49
21:m:10:SER:O	21:m:14:VAL:HG23	2.12	0.49
7:Y:50:LEU:HD22	7:Y:54:GLN:NE2	2.28	0.49
17:i:42:PRO:HG2	21:m:167:VAL:HG22	1.94	0.49
20:l:500:LEU:HD22	31:l:702:CDL:H542	1.95	0.49
33:g:201:PLX:H231	17:i:207:ILE:HD13	1.94	0.49
30:l:703:PEE:H7	30:l:703:PEE:C11	2.43	0.49
29:w:239:ASN:O	29:w:243:LYS:HB2	2.13	0.49
2:S:1:MET:HB2	2:S:3:PHE:CE1	2.47	0.49
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.95	0.49
13:e:143:ASP:HB3	13:e:146:LYS:HE3	1.93	0.49
24:p:100:PRO:HG3	25:r:419:TYR:CE1	2.48	0.49
30:U:101:PEE:C31	30:U:101:PEE:H1	2.40	0.49
18:j:73:LEU:O	26:s:160:TYR:OH	2.28	0.49
23:o:65:LEU:O	23:o:69:THR:HG23	2.12	0.49
25:r:122:PHE:O	36:r:602:HOH:O	2.20	0.49
26:s:51:ASP:HB3	34:s:402:UQ:H8	1.93	0.49
31:a:201:CDL:OB7	31:a:201:CDL:HB61	2.13	0.49
18:j:54:LYS:HD3	18:j:113:TRP:HA	1.94	0.49
31:l:701:CDL:H581	31:l:701:CDL:H811	1.95	0.49
31:l:701:CDL:H601	31:l:701:CDL:H772	1.94	0.49
30:l:703:PEE:H7	30:l:703:PEE:H14	1.94	0.49
25:r:13:PRO:HB3	31:r:504:CDL:H581	1.95	0.49
29:w:58:LYS:NZ	29:w:278:CYS:HB2	2.28	0.49
19:k:68:ALA:HB2	21:m:64:MET:HE2	1.95	0.48
25:r:251:ASN:HD21	25:r:304:GLN:NE2	2.11	0.48
20:l:536:LEU:HB3	20:l:537:PRO:HD3	1.94	0.48
17:i:95:MET:CE	17:i:149:ILE:HG22	2.42	0.48
7:Y:105:ASP:N	7:Y:105:ASP:OD1	2.45	0.48
20:l:72:GLN:NE2	25:r:459:TYR:O	2.46	0.48
25:r:12:LEU:HB2	25:r:13:PRO:HD3	1.96	0.48
29:w:110:GLY:HA2	29:w:134:TRP:CD2	2.48	0.48
32:X:201:8Q1:N36	32:X:201:8Q1:O40	2.45	0.48
7:Y:100:LEU:O	7:Y:102:ASP:N	2.41	0.48
15:g:7:ARG:NH1	15:g:91:ASP:OD1	2.47	0.48
20:l:172:ILE:HG21	25:r:408:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:o:57:LEU:HD23	23:o:57:LEU:O	2.14	0.48
1:Q:47:PHE:CD1	1:Q:52:MET:HE1	2.46	0.48
4:V:108:TYR:HB2	31:V:201:CDL:HB32	1.96	0.48
20:l:37:LYS:HE2	20:l:105:MET:HE1	1.94	0.48
20:l:68:TRP:CH2	20:l:69:MET:HE2	2.49	0.48
20:l:292:ALA:HB2	20:l:304:PHE:HB3	1.95	0.48
9:a:120:TRP:O	9:a:124:THR:HG22	2.13	0.48
16:h:97:HIS:HA	16:h:102:GLU:HB3	1.96	0.48
25:r:216:LEU:HD23	25:r:287:ALA:HB1	1.96	0.48
25:r:373:ILE:HD11	25:r:444:LEU:HD23	1.95	0.48
26:s:293:PHE:O	26:s:297:THR:OG1	2.23	0.48
26:s:126:LYS:O	26:s:130:ILE:HG12	2.14	0.48
28:v:18:ASP:O	28:v:22:MET:HG3	2.14	0.48
29:w:62:VAL:HG21	29:w:74:ALA:HB2	1.95	0.48
33:a:202:PLX:H142	25:r:36:LEU:HD11	1.95	0.48
15:g:15:PHE:O	15:g:80:ARG:NH1	2.46	0.48
20:l:541:ASN:HD22	30:l:703:PEE:H57	1.78	0.48
21:m:25:SER:O	21:m:27:ILE:N	2.46	0.48
34:s:402:UQ:H72	34:s:402:UQ:H111	1.70	0.48
2:S:47:LEU:HD22	27:u:22:SER:HB2	1.94	0.48
7:Y:94:ASP:HB3	7:Y:99:ILE:HB	1.95	0.48
9:a:87:THR:HG23	31:a:201:CDL:OA7	2.13	0.48
9:a:94:GLY:HA2	9:a:116:PRO:HG3	1.96	0.48
10:b:24:LYS:NZ	10:b:27:GLU:OE1	2.35	0.48
18:j:110:GLY:HA3	21:m:169:MET:HE1	1.96	0.48
20:l:298:ILE:O	20:l:302:VAL:HG23	2.14	0.48
25:r:105:PHE:O	25:r:109:THR:OG1	2.22	0.48
26:s:134:ARG:O	26:s:282:TYR:OH	2.30	0.48
19:k:3:LEU:HD13	19:k:6:MET:HE3	1.95	0.47
20:l:398:ALA:O	20:l:402:SER:OG	2.25	0.47
26:s:288:LEU:HD11	30:s:401:PEE:H7	1.93	0.47
15:g:34:VAL:HG12	31:g:202:CDL:H771	1.96	0.47
17:i:236:LYS:NZ	17:i:314:LYS:O	2.43	0.47
26:s:317:GLN:CB	36:s:551:HOH:O	2.62	0.47
29:w:66:ILE:C	35:w:401:ADP:O2A	2.55	0.47
13:e:70:ASN:O	13:e:73:SER:HB2	2.14	0.47
29:w:314:LEU:O	29:w:318:THR:HG22	2.14	0.47
30:Q:101:PEE:H37	30:Q:101:PEE:H60	1.95	0.47
3:U:14:ALA:O	3:U:15:LYS:HG2	2.15	0.47
25:r:196:TRP:CD1	25:r:250:LEU:HB3	2.49	0.47
31:a:201:CDL:H791	31:a:201:CDL:H221	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:85:GLU:OE2	11:c:119:THR:OG1	2.33	0.47
31:g:202:CDL:H592	25:r:120:ILE:HG21	1.96	0.47
25:r:116:ILE:HG13	27:u:168:PHE:CD1	2.49	0.47
2:S:69:ILE:HD13	27:u:20:VAL:HG13	1.97	0.47
3:U:19:LEU:HG	36:U:201:HOH:O	2.13	0.47
15:g:73:PHE:HE2	33:g:201:PLX:H392	1.79	0.47
17:i:222:SER:O	17:i:224:ALA:N	2.47	0.47
26:s:195:ARG:HD3	26:s:231:ILE:HD11	1.97	0.47
29:w:58:LYS:HZ3	29:w:278:CYS:HB2	1.79	0.47
29:w:116:LYS:NZ	29:w:125:ASP:OD2	2.47	0.47
5:W:130:ASN:HB3	21:m:1:MET:N	2.29	0.47
9:a:136:THR:HG21	25:r:48:ASN:ND2	2.28	0.47
33:a:202:PLX:H81	25:r:40:SER:OG	2.15	0.47
15:g:85:TYR:CZ	17:i:344:SER:HB3	2.50	0.47
17:i:81:SER:O	17:i:83:GLN:N	2.43	0.47
18:j:105:GLU:HA	21:m:169:MET:HE2	1.97	0.47
20:l:49:VAL:HB	20:l:50:PRO:HD3	1.95	0.47
20:l:384:PRO:HA	20:l:389:PHE:CD1	2.50	0.47
20:l:583:LEU:HD12	36:l:850:HOH:O	2.14	0.47
21:m:8:ILE:O	21:m:12:ILE:HG12	2.15	0.47
26:s:66:SER:HB2	26:s:122:ALA:O	2.14	0.47
34:s:402:UQ:H72	34:s:402:UQ:HM53	1.68	0.47
16:h:3:PHE:HB2	17:i:144:GLN:CD	2.40	0.47
18:j:49:LEU:N	18:j:50:PRO:HD2	2.29	0.47
19:k:16:LEU:O	19:k:20:LEU:HG	2.14	0.47
21:m:25:SER:O	21:m:28:TYR:N	2.41	0.47
8:Z:75:PHE:O	8:Z:79:VAL:HG23	2.14	0.47
25:r:104:LEU:HG	25:r:108:MET:HE2	1.98	0.47
18:j:25:PRO:HB2	26:s:60:PRO:HD3	1.96	0.46
1:Q:65:PRO:HB2	1:Q:67:ASN:O	2.15	0.46
11:c:148:GLU:OE1	20:l:405:ASN:ND2	2.37	0.46
13:e:71:PRO:O	13:e:72:ASP:HB2	2.15	0.46
18:j:56:PHE:N	21:m:74:MET:HE1	2.30	0.46
31:l:702:CDL:H232	31:l:702:CDL:H873	1.96	0.46
25:r:433:GLU:O	25:r:437:MET:HG2	2.15	0.46
1:Q:47:PHE:O	36:Q:201:HOH:O	2.20	0.46
17:i:89:MET:HG2	17:i:95:MET:HA	1.97	0.46
21:m:35:VAL:HA	30:m:202:PEE:H40	1.97	0.46
25:r:398:MET:O	25:r:402:ILE:HG13	2.14	0.46
29:w:58:LYS:O	29:w:60:ILE:HG13	2.15	0.46
21:m:23:LYS:CB	36:m:301:HOH:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:U:101:PEE:H49	30:U:101:PEE:H13	1.98	0.46
7:Y:43:ARG:CG	7:Y:46:GLN:HB2	2.44	0.46
36:h:204:HOH:O	17:i:88:LYS:HB3	2.01	0.46
20:l:474:PRO:O	20:l:475:MET:HE2	2.15	0.46
25:r:57:PHE:CD1	25:r:113:THR:HG22	2.51	0.46
25:r:300:ALA:O	25:r:308:SER:HB3	2.16	0.46
26:s:102:VAL:HG11	26:s:154:LEU:HD11	1.98	0.46
6:X:91:ASP:HB3	8:Z:47:ARG:NH1	2.31	0.46
11:c:165:ASP:OD2	11:c:170:ARG:NH2	2.49	0.46
20:l:69:MET:HG3	20:l:71:LEU:CD2	2.45	0.46
25:r:303:ILE:HD12	25:r:388:TRP:CD1	2.50	0.46
9:a:133:TYR:OH	12:d:87:GLU:OE1	2.19	0.46
18:j:15:SER:O	18:j:19:LEU:HG	2.14	0.46
19:k:23:ARG:NH1	21:m:23:LYS:O	2.49	0.46
20:l:182:PHE:HD1	20:l:186:MET:HE2	1.80	0.46
27:u:85:TYR:O	27:u:88:CYS:HB2	2.15	0.46
28:v:46:MET:HE2	28:v:56:ARG:CB	2.46	0.46
29:w:223:ASN:O	29:w:227:MET:HG2	2.15	0.46
11:c:118:ASP:O	20:l:535:ARG:HD3	2.16	0.46
20:l:264:TYR:CD2	20:l:265:PRO:HD3	2.51	0.46
20:l:420:ALA:O	20:l:424:THR:HG22	2.16	0.46
25:r:127:VAL:HB	25:r:128:PRO:HD3	1.97	0.46
26:s:96:ILE:HG21	26:s:98:MET:HE3	1.97	0.46
1:Q:39:PRO:HB3	1:Q:43:TRP:CD1	2.50	0.46
5:W:51:MET:HA	26:s:313:SER:HB2	1.98	0.46
21:m:70:TYR:CE1	21:m:74:MET:HE3	2.50	0.46
4:V:141:VAL:O	9:a:169:TYR:OH	2.20	0.45
7:Y:43:ARG:NH2	7:Y:49:GLN:HB2	2.31	0.45
9:a:140:LEU:HD21	25:r:177:LEU:HB3	1.98	0.45
20:l:558:LEU:HB3	25:r:214:LEU:HD11	1.98	0.45
18:j:104:TYR:O	18:j:108:GLN:HG2	2.15	0.45
20:l:182:PHE:CD1	20:l:186:MET:HE2	2.51	0.45
20:l:541:ASN:ND2	30:l:703:PEE:H57	2.30	0.45
25:r:195:MET:HG3	30:r:501:PEE:O4	2.16	0.45
26:s:233:MET:HE3	26:s:233:MET:HB3	1.86	0.45
27:u:60:GLY:O	27:u:63:VAL:HG22	2.16	0.45
1:Q:36:GLN:NE2	25:r:137:GLY:O	2.49	0.45
31:a:201:CDL:H432	12:d:44:PRO:HB3	1.97	0.45
21:m:3:MET:HG2	21:m:8:ILE:HD11	1.97	0.45
22:n:10:ASP:OD1	25:r:19:LYS:HD2	2.16	0.45
26:s:104:PHE:CE1	26:s:108:MET:HE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:92:PHE:O	13:e:96:SER:HB2	2.15	0.45
18:j:69:ILE:O	18:j:73:LEU:HG	2.16	0.45
24:p:19:LEU:HD22	24:p:64:LEU:HD12	1.97	0.45
24:p:119:PHE:O	24:p:123:GLU:OE1	2.33	0.45
31:a:201:CDL:C32	30:b:201:PEE:H62	2.36	0.45
21:m:51:PHE:O	21:m:55:MET:HG2	2.16	0.45
21:m:57:PHE:CD1	21:m:61:LEU:HD12	2.52	0.45
16:h:24:GLU:O	16:h:24:GLU:HG3	2.16	0.45
8:Z:13:LYS:HA	8:Z:13:LYS:HD2	1.77	0.45
12:d:140:GLN:HG3	12:d:144:SER:HB3	1.99	0.45
36:e:201:HOH:O	25:r:432:ARG:HA	2.17	0.45
17:i:17:THR:O	17:i:21:MET:HG3	2.17	0.45
17:i:280:THR:O	17:i:284:MET:HG2	2.16	0.45
30:r:501:PEE:C15	30:r:501:PEE:C19	2.86	0.45
29:w:66:ILE:HG23	35:w:401:ADP:O2A	2.17	0.45
29:w:343:TYR:HA	29:w:352:ILE:HD12	1.97	0.45
30:b:201:PEE:H10	33:r:503:PLX:O2	2.17	0.45
11:c:113:ILE:C	11:c:115:ASN:H	2.25	0.45
19:k:22:TYR:HE1	19:k:29:SER:HG	1.64	0.45
20:l:102:GLU:HA	20:l:105:MET:HE2	1.99	0.45
33:r:502:PLX:H1C3	33:r:502:PLX:H22	1.75	0.45
29:w:295:ARG:HA	29:w:298:VAL:HG22	1.99	0.45
31:V:201:CDL:H562	31:V:201:CDL:H721	1.98	0.45
17:i:40:MET:HE1	17:i:129:LEU:HD23	1.98	0.45
11:c:186:ILE:O	28:v:97:LYS:NZ	2.49	0.45
33:m:201:PLX:H341	33:m:201:PLX:H151	1.98	0.45
31:r:504:CDL:H161	31:r:504:CDL:H132	1.69	0.45
26:s:137:ALA:HB3	26:s:282:TYR:OH	2.16	0.45
3:U:44:ARG:HG2	3:U:47:ARG:NH2	2.31	0.44
17:i:128:LEU:HD12	17:i:216:PHE:HB3	2.00	0.44
23:o:114:LYS:NZ	23:o:118:GLU:OE2	2.42	0.44
28:v:66:LEU:HD12	28:v:84:GLN:HA	1.97	0.44
6:X:155:TYR:CE1	10:b:23:LEU:HB3	2.52	0.44
17:i:254:LEU:O	17:i:257:LEU:HB2	2.18	0.44
9:a:114:LYS:HG3	12:d:63:TYR:CE1	2.53	0.44
33:a:202:PLX:H212	13:e:104:THR:HG21	1.99	0.44
20:l:360:GLY:HA3	20:l:435:PRO:HA	2.00	0.44
20:l:2:ASN:HD22	20:l:61:MET:CE	2.31	0.44
26:s:141:SER:HB3	26:s:289:LEU:HD22	1.99	0.44
28:v:51:LEU:HD21	28:v:64:ILE:HD13	1.98	0.44
31:a:201:CDL:H761	31:a:201:CDL:C20	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:110:ILE:HD11	10:b:117:ILE:HD11	1.98	0.44
21:m:55:MET:HE1	26:s:103:LEU:HD11	1.99	0.44
31:r:504:CDL:H362	31:r:504:CDL:H392	1.74	0.44
29:w:166:ASP:OD1	29:w:187:TYR:OH	2.27	0.44
29:w:242:LYS:HE2	29:w:242:LYS:HB3	1.60	0.44
13:e:73:SER:O	13:e:75:GLY:N	2.51	0.44
14:f:72:ARG:NH1	15:g:21:ARG:HB2	2.33	0.44
20:l:452:ASN:HA	20:l:455:LYS:HG2	1.99	0.44
24:p:71:PHE:O	24:p:75:GLN:HB3	2.18	0.44
26:s:267:THR:O	26:s:271:LEU:HG	2.17	0.44
30:U:101:PEE:H35	30:U:101:PEE:H30	1.68	0.44
9:a:108:GLU:HB2	9:a:111:GLU:HG3	1.99	0.44
31:g:202:CDL:HB21	22:n:34:LYS:HZ1	1.76	0.44
24:p:29:SER:HB3	24:p:76:HIS:HD2	1.81	0.44
24:p:63:LEU:O	24:p:64:LEU:HB3	2.17	0.44
22:n:17:VAL:HG23	36:n:101:HOH:O	2.18	0.44
26:s:294:LEU:O	26:s:298:LEU:HG	2.18	0.44
9:a:184:LYS:C	9:a:186:THR:H	2.26	0.43
10:b:100:ARG:HD3	20:l:60:GLU:HG3	2.00	0.43
17:i:79:LEU:HB2	19:k:47:ILE:HD13	2.00	0.43
19:k:57:ASN:HB3	21:m:143:ILE:HG13	1.99	0.43
4:V:141:VAL:HG11	17:i:272:LYS:HB3	1.99	0.43
6:X:87:LEU:HD23	6:X:87:LEU:HA	1.84	0.43
17:i:86:ILE:O	17:i:87:THR:HG23	2.19	0.43
17:i:276:ILE:CG2	30:r:501:PEE:H14	2.48	0.43
20:l:356:ILE:HA	20:l:359:MET:HG2	1.99	0.43
20:l:529:TYR:HB3	20:l:530:PRO:HD3	2.00	0.43
21:m:38:GLY:HA3	30:m:202:PEE:H35	2.00	0.43
31:a:201:CDL:C25	31:a:201:CDL:C21	2.86	0.43
31:a:201:CDL:H372	31:a:201:CDL:H341	1.86	0.43
31:g:202:CDL:H741	31:g:202:CDL:H712	1.85	0.43
17:i:96:THR:O	17:i:100:MET:HG2	2.19	0.43
33:m:201:PLX:H342	33:m:201:PLX:H372	1.77	0.43
5:W:68:ARG:NH2	21:m:134:GLY:HA2	2.34	0.43
6:X:129:GLU:HB3	24:p:82:PHE:CD2	2.54	0.43
17:i:277:ILE:O	17:i:281:LEU:HG	2.19	0.43
18:j:3:ILE:CG2	30:m:202:PEE:H13	2.48	0.43
26:s:194:ASN:ND2	26:s:201:THR:OG1	2.49	0.43
20:l:69:MET:HG3	20:l:71:LEU:HD21	1.99	0.43
20:l:437:PHE:HE2	20:l:441:VAL:HG22	1.84	0.43
26:s:72:ILE:O	26:s:76:ILE:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:40:PRO:O	11:c:74:ASP:HB2	2.19	0.43
25:r:19:LYS:HB3	25:r:19:LYS:HE3	1.77	0.43
26:s:90:PRO:HD2	26:s:240:ILE:HD13	2.00	0.43
27:u:47:ARG:NH2	27:u:53:PRO:HG3	2.34	0.43
2:S:54:ILE:HD11	27:u:21:SER:HA	2.00	0.43
30:U:101:PEE:H39	26:s:302:MET:HE1	2.01	0.43
17:i:277:ILE:HG23	30:r:501:PEE:C36	2.42	0.43
18:j:109:LYS:N	18:j:109:LYS:HD2	2.34	0.43
27:u:38:LYS:HB3	27:u:39:PRO:HD3	2.00	0.43
28:v:46:MET:HE2	28:v:56:ARG:HB3	2.00	0.43
31:V:201:CDL:H792	20:l:561:ILE:HD11	2.01	0.43
22:n:14:HIS:HE1	25:r:26:ASN:ND2	2.16	0.43
31:g:202:CDL:C63	25:r:108:MET:HE1	2.48	0.43
17:i:7:THR:HG22	17:i:11:MET:HE2	2.00	0.43
24:p:63:LEU:C	24:p:65:ARG:H	2.26	0.43
33:r:502:PLX:H331	33:r:502:PLX:H301	1.52	0.43
3:U:26:GLY:HA3	30:U:101:PEE:C23	2.49	0.42
7:Y:68:TRP:CZ2	7:Y:72:ARG:HD2	2.54	0.42
31:a:201:CDL:H201	31:a:201:CDL:C76	2.49	0.42
21:m:57:PHE:CD2	26:s:107:ALA:HB1	2.52	0.42
23:o:84:PRO:O	23:o:88:LEU:HD23	2.19	0.42
4:V:42:ALA:HB2	20:l:593:ILE:HD12	2.01	0.42
6:X:105:MET:HE1	6:X:112:SER:HA	2.01	0.42
17:i:99:THR:HG22	17:i:157:MET:HE1	2.00	0.42
22:n:39:ARG:HG3	22:n:57:TRP:CE2	2.54	0.42
24:p:28:GLU:HB3	24:p:37:TYR:CE1	2.54	0.42
17:i:136:LEU:HD23	17:i:205:LEU:HD21	2.00	0.42
20:l:83:ASP:CG	20:l:262:ARG:HH12	2.27	0.42
22:n:17:VAL:HG21	25:r:30:HIS:CB	2.49	0.42
24:p:170:ILE:O	24:p:173:ARG:HD3	2.19	0.42
25:r:87:GLU:OE2	25:r:91:ARG:HD2	2.19	0.42
25:r:357:THR:O	25:r:361:VAL:HG23	2.19	0.42
26:s:72:ILE:O	26:s:75:PRO:HD2	2.20	0.42
4:V:46:PRO:HB3	4:V:55:ARG:NH2	2.34	0.42
6:X:104:PHE:HD1	6:X:108:LEU:HD12	1.85	0.42
13:e:73:SER:C	13:e:75:GLY:H	2.27	0.42
31:g:202:CDL:H752	31:g:202:CDL:H781	1.61	0.42
17:i:276:ILE:HG21	30:r:501:PEE:H7	2.02	0.42
5:W:43:LEU:HG	26:s:179:TRP:HE1	1.84	0.42
31:a:201:CDL:H412	31:a:201:CDL:H381	1.91	0.42
11:c:152:SER:O	20:l:403:TYR:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:g:202:CDL:CB2	22:n:34:LYS:NZ	2.73	0.42
16:h:17:TRP:CD1	16:h:17:TRP:H	2.38	0.42
17:i:20:VAL:HG13	17:i:29:ILE:HG23	2.02	0.42
10:b:32:GLU:HG3	24:p:115:TYR:HA	2.02	0.42
14:f:55:TRP:O	14:f:59:ILE:HG12	2.19	0.42
17:i:291:TYR:HA	25:r:151:PHE:HZ	1.84	0.42
19:k:1:MET:HE2	19:k:6:MET:HG3	2.02	0.42
19:k:20:LEU:HA	20:l:588:PHE:HB3	2.01	0.42
19:k:57:ASN:ND2	21:m:139:GLU:HA	2.35	0.42
20:l:320:ASN:OD1	36:l:802:HOH:O	2.22	0.42
30:Q:101:PEE:H33	25:r:155:ALA:HB2	2.02	0.42
14:f:47:THR:HG23	15:g:65:LEU:HD22	2.01	0.42
33:g:201:PLX:H351	17:i:336:VAL:HB	2.01	0.42
30:r:501:PEE:H21	30:r:501:PEE:C19	2.44	0.42
25:r:221:VAL:O	25:r:340:ARG:NH1	2.53	0.42
12:d:79:GLU:O	15:g:111:TYR:OH	2.30	0.42
17:i:86:ILE:C	17:i:87:THR:HG23	2.45	0.42
31:l:701:CDL:H582	31:l:701:CDL:H551	1.72	0.42
27:u:59:GLU:O	27:u:63:VAL:HG13	2.20	0.42
29:w:243:LYS:HB3	29:w:243:LYS:HE2	1.64	0.42
6:X:94:ASP:HA	6:X:95:PRO:HD3	1.96	0.42
11:c:102:GLY:HA3	23:o:43:LEU:HD22	2.00	0.42
18:j:60:ILE:HG21	21:m:168:ILE:HG21	2.02	0.42
28:v:28:ASP:OD1	28:v:28:ASP:N	2.50	0.42
17:i:106:LEU:HG	17:i:138:PRO:HB2	2.01	0.41
17:i:268:GLN:HG3	27:u:168:PHE:CZ	2.55	0.41
20:l:90:ILE:HG12	20:l:129:MET:SD	2.60	0.41
25:r:94:LEU:HD23	25:r:94:LEU:HA	1.94	0.41
25:r:441:ILE:HG23	25:r:442:LEU:HD12	2.01	0.41
5:W:129:THR:HG22	5:W:132:GLU:OE2	2.20	0.41
10:b:2:SER:OG	10:b:3:GLY:N	2.53	0.41
13:e:108:TYR:CE1	33:r:503:PLX:H1B2	2.55	0.41
31:g:202:CDL:H781	31:g:202:CDL:H812	1.79	0.41
31:g:202:CDL:CB2	22:n:34:LYS:HZ3	2.26	0.41
20:l:286:LEU:HD21	31:l:702:CDL:H812	2.02	0.41
25:r:73:LEU:HD22	25:r:103:GLN:OE1	2.19	0.41
26:s:140:ILE:O	26:s:143:GLU:HG2	2.20	0.41
26:s:306:SER:O	26:s:310:MET:HG3	2.21	0.41
2:S:34:LYS:HE3	2:S:34:LYS:HB2	1.87	0.41
6:X:84:LEU:O	6:X:88:LYS:HG3	2.21	0.41
33:a:202:PLX:H22	33:a:202:PLX:H1C3	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:n:17:VAL:HG21	25:r:30:HIS:CG	2.54	0.41
25:r:303:ILE:HG22	25:r:305:THR:HG23	2.01	0.41
33:g:201:PLX:H1C2	16:h:2:PRO:HD2	2.02	0.41
20:l:213:LEU:HB3	20:l:273:VAL:HG11	2.01	0.41
31:l:701:CDL:H391	25:r:371:PRO:HD2	2.03	0.41
26:s:85:MET:SD	26:s:108:MET:HB2	2.61	0.41
26:s:141:SER:HB3	26:s:289:LEU:CD2	2.50	0.41
28:v:7:ARG:NE	28:v:16:GLU:OE2	2.33	0.41
29:w:219:GLN:HA	29:w:227:MET:SD	2.61	0.41
10:b:14:GLN:NE2	24:p:157:ALA:HB3	2.36	0.41
12:d:69:ARG:HD2	22:n:43:LEU:O	2.21	0.41
16:h:95:PRO:HD2	16:h:98:HIS:HD2	1.86	0.41
31:l:701:CDL:H452	25:r:445:LEU:HB3	2.01	0.41
33:r:503:PLX:H121	33:r:503:PLX:H152	1.84	0.41
28:v:4:HIS:CE1	28:v:5:LEU:HG	2.56	0.41
3:U:38:TYR:HB2	26:s:310:MET:O	2.21	0.41
9:a:106:VAL:CG2	22:n:50:ARG:HE	2.34	0.41
11:c:186:ILE:H	28:v:97:LYS:NZ	2.18	0.41
15:g:81:GLN:HE21	17:i:341:PRO:HB2	1.85	0.41
16:h:36:PHE:CD1	16:h:62:ASP:HB3	2.56	0.41
20:l:184:LEU:HB2	25:r:393:ILE:HG12	2.03	0.41
20:l:190:LEU:HD21	25:r:307:TRP:CH2	2.56	0.41
20:l:331:MET:HE1	20:l:468:ILE:HD12	2.03	0.41
22:n:29:ARG:O	22:n:33:GLU:HG3	2.20	0.41
26:s:230:ASN:O	26:s:234:MET:HG2	2.20	0.41
11:c:38:PRO:HD2	23:o:70:TYR:CD2	2.55	0.41
20:l:71:LEU:HD12	25:r:310:MET:HE1	2.02	0.41
21:m:17:PHE:CD1	21:m:20:PHE:HE2	2.39	0.41
25:r:216:LEU:HB3	25:r:217:PRO:HD3	2.02	0.41
29:w:218:ILE:HG23	29:w:226:GLU:HG3	2.02	0.41
2:S:41:PHE:HB3	21:m:135:PHE:C	2.46	0.41
31:V:201:CDL:H671	31:V:201:CDL:H642	1.88	0.41
6:X:133:ILE:HG12	24:p:4:SER:OG	2.20	0.41
11:c:60:GLU:OE1	11:c:60:GLU:N	2.47	0.41
33:g:201:PLX:H22	33:g:201:PLX:H1C3	1.80	0.41
20:l:4:PHE:CD1	20:l:4:PHE:C	2.98	0.41
20:l:37:LYS:HD3	20:l:98:TRP:HE1	1.86	0.41
21:m:55:MET:HE3	26:s:103:LEU:HD21	2.03	0.41
30:m:202:PEE:H27	30:m:202:PEE:H22	1.75	0.41
26:s:90:PRO:HG3	26:s:162:LEU:HB3	2.03	0.41
29:w:238:GLU:O	29:w:242:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Q:101:PEE:C20	20:l:562:LEU:CG	2.98	0.41
11:c:176:LYS:HA	11:c:176:LYS:HD2	1.79	0.41
18:j:81:THR:C	18:j:83:ASN:H	2.29	0.41
20:l:503:GLU:OE1	20:l:503:GLU:HA	2.21	0.41
7:Y:89:PRO:HA	7:Y:92:TRP:CE3	2.57	0.40
11:c:100:ASN:HB2	11:c:103:GLU:CD	2.46	0.40
11:c:153:TYR:OH	28:v:8:ARG:NH1	2.37	0.40
12:d:51:PHE:O	12:d:55:GLN:HG2	2.21	0.40
16:h:94:PRO:HA	16:h:95:PRO:HD3	1.93	0.40
20:l:559:GLU:OE2	25:r:148:TYR:OH	2.29	0.40
31:l:702:CDL:H541	31:l:702:CDL:H572	1.41	0.40
25:r:447:LEU:HD11	33:r:503:PLX:H393	2.02	0.40
26:s:11:ILE:HB	26:s:12:PRO:HD3	2.02	0.40
29:w:181:LYS:O	29:w:184:VAL:HG22	2.21	0.40
9:a:124:THR:O	33:a:202:PLX:H1A3	2.21	0.40
17:i:347:ASN:OD1	17:i:347:ASN:N	2.54	0.40
20:l:410:LEU:O	20:l:414:ILE:HG13	2.22	0.40
31:l:701:CDL:H582	31:l:701:CDL:H791	2.02	0.40
23:o:50:GLN:O	23:o:56:ARG:HD3	2.21	0.40
27:u:44:MET:O	27:u:48:TRP:HE3	2.04	0.40
29:w:63:ASP:O	29:w:70:LYS:HD3	2.22	0.40
4:V:40:SER:OG	4:V:55:ARG:NH1	2.55	0.40
8:Z:32:VAL:HG21	24:p:35:ASP:HB2	2.03	0.40
11:c:110:ASP:OD1	11:c:110:ASP:N	2.54	0.40
17:i:73:ALA:HB2	17:i:97:MET:HB3	2.04	0.40
17:i:237:MET:HE1	17:i:319:HIS:NE2	2.36	0.40
17:i:258:SER:OG	17:i:336:VAL:HG22	2.21	0.40
20:l:21:MET:SD	20:l:35:TYR:OH	2.72	0.40
20:l:336:LYS:HD3	20:l:339:LEU:HD12	2.04	0.40
25:r:396:MET:O	25:r:400:MET:HG3	2.21	0.40
4:V:50:LEU:HA	4:V:53:VAL:HG12	2.03	0.40
25:r:61:LEU:HB2	25:r:457:PRO:HD3	2.02	0.40
25:r:392:THR:O	25:r:396:MET:HG2	2.20	0.40
33:g:201:PLX:H72	33:g:201:PLX:H101	1.82	0.40
20:l:297:ASP:O	20:l:301:ILE:HG13	2.22	0.40
21:m:23:LYS:N	21:m:24:PRO:HD3	2.36	0.40
24:p:157:ALA:HB1	24:p:162:ASP:HB3	2.03	0.40
25:r:147:LEU:HD22	25:r:151:PHE:HE2	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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	47
5	W	111/113 (98%)	109 (98%)	2 (2%)	0	100	100
6	X	86/88 (98%)	84 (98%)	2 (2%)	0	100	100
7	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
8	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
9	a	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
10	b	99/126 (79%)	93 (94%)	6 (6%)	0	100	100
11	c	154/156 (99%)	146 (95%)	8 (5%)	0	100	100
12	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
13	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
14	f	40/42 (95%)	38 (95%)	2 (5%)	0	100	100
15	g	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
16	h	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
17	i	345/347 (99%)	334 (97%)	10 (3%)	1 (0%)	36	66
18	j	95/113 (84%)	90 (95%)	5 (5%)	0	100	100
19	k	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
20	l	601/603 (100%)	574 (96%)	27 (4%)	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%)	119 (94%)	7 (6%)	0	100	100
24	p	176/178 (99%)	167 (95%)	8 (4%)	1 (1%)	21	51
25	r	457/459 (100%)	444 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	s	299/318 (94%)	285 (95%)	14 (5%)	0	100	100
27	u	169/171 (99%)	162 (96%)	7 (4%)	0	100	100
28	v	122/131 (93%)	113 (93%)	9 (7%)	0	100	100
29	w	318/320 (99%)	301 (95%)	17 (5%)	0	100	100
All	All	4586/4757 (96%)	4388 (96%)	195 (4%)	3 (0%)	49	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	i	87	THR
4	V	46	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%)	33 (97%)	1 (3%)	37	73
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%)	101 (100%)	0	100	100
5	W	99/99 (100%)	99 (100%)	0	100	100
6	X	80/81 (99%)	80 (100%)	0	100	100
7	Y	63/63 (100%)	63 (100%)	0	100	100
8	Z	65/65 (100%)	65 (100%)	0	100	100
9	a	122/122 (100%)	122 (100%)	0	100	100
10	b	98/119 (82%)	98 (100%)	0	100	100
11	c	141/141 (100%)	141 (100%)	0	100	100
12	d	155/155 (100%)	155 (100%)	0	100	100
13	e	99/99 (100%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	f	35/38 (92%)	35 (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%)	308 (99%)	3 (1%)	68	88
18	j	88/99 (89%)	88 (100%)	0	100	100
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	529/537 (98%)	529 (100%)	0	100	100
21	m	97/141 (69%)	97 (100%)	0	100	100
22	n	53/53 (100%)	52 (98%)	1 (2%)	50	81
23	o	113/113 (100%)	113 (100%)	0	100	100
24	p	159/159 (100%)	159 (100%)	0	100	100
25	r	410/410 (100%)	410 (100%)	0	100	100
26	s	263/275 (96%)	261 (99%)	2 (1%)	73	90
27	u	153/153 (100%)	153 (100%)	0	100	100
28	v	103/115 (90%)	103 (100%)	0	100	100
29	w	282/283 (100%)	276 (98%)	6 (2%)	47	79
All	All	4066/4179 (97%)	4053 (100%)	13 (0%)	84	95

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	63	PRO
17	i	88	LYS
17	i	93	VAL
17	i	97	MET
22	n	15	ILE
26	s	91	MET
26	s	96	ILE
29	w	60	ILE
29	w	61	THR
29	w	62	VAL
29	w	242	LYS
29	w	243	LYS
29	w	244	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
4	V	129	GLN
9	a	170	GLN
9	a	189	ASN
10	b	83	HIS
11	c	84	GLN
11	c	100	ASN
13	e	56	GLN
14	f	61	GLN
14	f	62	HIS
15	g	18	ASN
15	g	81	GLN
16	h	34	HIS
16	h	82	GLN
17	i	120	GLN
17	i	144	GLN
17	i	186	HIS
17	i	268	GLN
19	k	50	ASN
20	l	165	ASN
20	l	192	HIS
20	l	210	ASN
20	l	270	ASN
20	l	274	GLN
20	l	296	ASN
20	l	446	ASN
20	l	541	ASN
20	l	580	GLN
22	n	3	ASN
22	n	11	HIS
22	n	14	HIS
23	o	52	ASN
23	o	75	ASN
24	p	26	HIS
24	p	51	HIS
24	p	62	GLN
24	p	75	GLN
24	p	78	GLN
25	r	26	ASN
25	r	251	ASN
26	s	124	ASN
27	u	30	HIS
27	u	35	GLN
27	u	64	ASN

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Mol	Chain	Res	Type
27	u	65	GLN
27	u	143	HIS
28	v	4	HIS
28	v	82	HIS
29	w	322	HIS

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](#)

21 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	PEE	s	401	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
31	CDL	l	702	-	99,99,99	1.11	9 (9%)	105,111,111	0.87	4 (3%)
31	CDL	l	701	-	98,98,99	1.11	8 (8%)	104,110,111	0.90	4 (3%)
30	PEE	U	101	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
30	PEE	l	703	-	45,45,50	1.24	6 (13%)	48,50,55	1.01	2 (4%)
30	PEE	b	201	-	45,45,50	1.24	6 (13%)	48,50,55	0.99	2 (4%)
30	PEE	r	501	-	40,40,50	1.17	5 (12%)	43,45,55	0.99	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PLX	a	202	-	51,51,51	0.60	0	53,59,59	0.70	0
30	PEE	Q	101	-	46,46,50	1.22	6 (13%)	49,51,55	1.02	3 (6%)
31	CDL	V	201	-	70,70,99	1.23	8 (11%)	76,82,111	0.94	4 (5%)
33	PLX	g	201	-	51,51,51	1.18	3 (5%)	53,59,59	0.70	1 (1%)
34	UQ	s	402	-	28,28,63	3.31	7 (25%)	36,37,79	2.84	12 (33%)
33	PLX	r	502	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
31	CDL	r	504	-	99,99,99	1.11	8 (8%)	105,111,111	0.85	4 (3%)
32	8Q1	X	201	-	32,34,34	2.20	7 (21%)	39,43,43	1.73	9 (23%)
30	PEE	m	202	-	40,40,50	1.17	5 (12%)	43,45,55	0.99	2 (4%)
31	CDL	a	201	-	90,90,99	0.97	4 (4%)	96,102,111	1.07	5 (5%)
33	PLX	r	503	-	51,51,51	1.19	4 (7%)	53,59,59	0.61	1 (1%)
33	PLX	m	201	-	51,51,51	1.20	4 (7%)	53,59,59	0.61	1 (1%)
35	ADP	w	401	-	28,29,29	3.18	9 (32%)	43,45,45	1.88	8 (18%)
31	CDL	g	202	-	61,61,99	1.17	4 (6%)	67,73,111	1.10	4 (5%)

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	PEE	s	401	-	-	27/54/54/54	-
31	CDL	l	702	-	-	58/110/110/110	-
31	CDL	l	701	-	-	56/109/109/110	-
30	PEE	U	101	-	-	24/54/54/54	-
30	PEE	l	703	-	-	26/49/49/54	-
30	PEE	b	201	-	-	33/49/49/54	-
30	PEE	r	501	-	-	27/44/44/54	-
33	PLX	a	202	-	-	9/55/55/55	-
30	PEE	Q	101	-	-	22/50/50/54	-
31	CDL	V	201	-	-	39/81/81/110	-
33	PLX	g	201	-	-	27/55/55/55	-
34	UQ	s	402	-	-	10/21/45/87	0/1/1/1
33	PLX	r	502	-	-	31/55/55/55	-
31	CDL	r	504	-	-	59/110/110/110	-
32	8Q1	X	201	-	-	20/41/41/41	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PEE	m	202	-	-	20/44/44/54	-
31	CDL	a	201	-	-	27/101/101/110	-
33	PLX	r	503	-	-	34/55/55/55	-
33	PLX	m	201	-	-	29/55/55/55	-
35	ADP	w	401	-	-	4/16/32/32	0/3/3/3
31	CDL	g	202	-	-	17/72/72/110	-

All (119) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	402	UQ	C13-C14	9.60	1.55	1.33
34	s	402	UQ	C8-C9	9.22	1.54	1.33
35	w	401	ADP	C3'-C4'	-8.98	1.30	1.53
34	s	402	UQ	C18-C19	7.89	1.56	1.32
35	w	401	ADP	O4'-C4'	7.82	1.62	1.45
32	X	201	8Q1	P24-O27	7.28	1.83	1.60
35	w	401	ADP	PA-O3A	6.55	1.66	1.59
35	w	401	ADP	C6-N6	5.45	1.48	1.34
32	X	201	8Q1	C28-C29	4.91	1.60	1.52
35	w	401	ADP	O4'-C1'	-4.47	1.31	1.42
31	a	201	CDL	OA8-CA7	4.28	1.45	1.33
31	a	201	CDL	OB8-CB7	4.26	1.45	1.33
31	g	202	CDL	OA8-CA7	4.25	1.45	1.33
31	g	202	CDL	OB8-CB7	4.23	1.45	1.33
31	g	202	CDL	OB6-CB5	4.15	1.46	1.34
31	g	202	CDL	OA6-CA5	4.14	1.46	1.34
31	a	201	CDL	OB6-CB5	4.09	1.45	1.34
31	a	201	CDL	OA6-CA5	4.06	1.45	1.34
32	X	201	8Q1	C1-S44	3.92	1.85	1.76
30	s	401	PEE	C18-C19	3.85	1.53	1.31
30	l	703	PEE	C18-C19	3.84	1.53	1.31
30	b	201	PEE	C18-C19	3.83	1.53	1.31
30	m	202	PEE	C18-C19	3.83	1.53	1.31
30	r	501	PEE	C18-C19	3.82	1.53	1.31
30	U	101	PEE	C18-C19	3.81	1.53	1.31
30	Q	101	PEE	C18-C19	3.78	1.53	1.31
30	l	703	PEE	C39-C38	3.74	1.53	1.31
30	b	201	PEE	C39-C38	3.74	1.52	1.31
30	U	101	PEE	C39-C38	3.73	1.52	1.31
30	Q	101	PEE	C39-C38	3.71	1.52	1.31
30	s	401	PEE	C39-C38	3.71	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	201	8Q1	O27-C28	-3.52	1.32	1.43
31	V	201	CDL	OA8-CA7	3.42	1.43	1.33
31	r	504	CDL	OA8-CA7	3.41	1.43	1.33
32	X	201	8Q1	C34-N36	3.38	1.41	1.33
31	l	701	CDL	OA8-CA7	3.37	1.43	1.33
31	l	702	CDL	OA8-CA7	3.36	1.43	1.33
35	w	401	ADP	C8-N9	-3.33	1.31	1.37
35	w	401	ADP	O2'-C2'	-3.13	1.35	1.43
32	X	201	8Q1	C6-C1	3.03	1.53	1.50
31	l	701	CDL	OB6-CB5	3.02	1.42	1.34
31	l	702	CDL	OA6-CA5	3.02	1.42	1.34
31	l	701	CDL	OB8-CB7	3.00	1.42	1.33
35	w	401	ADP	O3'-C3'	3.00	1.50	1.43
31	r	504	CDL	OB6-CB5	2.98	1.42	1.34
31	V	201	CDL	OA6-CA5	2.98	1.42	1.34
31	r	504	CDL	OA6-CA5	2.98	1.42	1.34
33	r	503	PLX	O6-C4	-2.98	1.40	1.44
31	l	702	CDL	OB6-CB5	2.96	1.42	1.34
31	l	702	CDL	OB8-CB7	2.96	1.42	1.33
31	V	201	CDL	OB6-CB5	2.93	1.42	1.34
33	g	201	PLX	O6-C4	-2.91	1.40	1.44
31	r	504	CDL	OB8-CB7	2.91	1.41	1.33
31	V	201	CDL	OB8-CB7	2.88	1.41	1.33
31	l	701	CDL	OA6-CA5	2.87	1.42	1.34
33	m	201	PLX	O6-C4	-2.85	1.41	1.44
32	X	201	8Q1	C39-N41	2.81	1.40	1.33
30	Q	101	PEE	O2-C2	-2.66	1.40	1.46
34	s	402	UQ	C6-C1	2.63	1.53	1.46
30	s	401	PEE	O2-C2	-2.62	1.40	1.46
31	l	701	CDL	OA6-CA4	-2.62	1.40	1.46
33	r	502	PLX	C7-C6	2.60	1.56	1.50
31	r	504	CDL	OA6-CA4	-2.57	1.40	1.46
30	U	101	PEE	O2-C2	-2.56	1.40	1.46
30	l	703	PEE	O2-C2	-2.55	1.40	1.46
30	r	501	PEE	O2-C2	-2.55	1.40	1.46
33	r	502	PLX	O6-C4	-2.51	1.41	1.44
31	V	201	CDL	OA6-CA4	-2.50	1.40	1.46
30	b	201	PEE	O2-C2	-2.49	1.40	1.46
30	m	202	PEE	O2-C2	-2.49	1.40	1.46
30	Q	101	PEE	O3-C30	2.49	1.40	1.33
30	b	201	PEE	O3-C30	2.48	1.40	1.33
30	U	101	PEE	O3-C30	2.47	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	l	702	CDL	OA6-CA4	-2.47	1.40	1.46
31	V	201	CDL	OB6-CB4	-2.44	1.40	1.46
30	l	703	PEE	O3-C30	2.42	1.40	1.33
31	l	702	CDL	OB6-CB4	-2.40	1.41	1.46
31	l	701	CDL	OB6-CB4	-2.40	1.41	1.46
30	s	401	PEE	O3-C30	2.39	1.40	1.33
35	w	401	ADP	C5-N7	-2.39	1.34	1.39
33	r	503	PLX	C7-C6	2.38	1.55	1.50
30	r	501	PEE	O3-C30	2.38	1.40	1.33
33	m	201	PLX	C7-C6	2.34	1.55	1.50
30	b	201	PEE	O2-C10	2.33	1.40	1.34
30	m	202	PEE	O3-C30	2.31	1.40	1.33
31	r	504	CDL	OB6-CB4	-2.31	1.41	1.46
34	s	402	UQ	O4-C4	-2.31	1.18	1.23
30	U	101	PEE	O2-C10	2.30	1.40	1.34
31	r	504	CDL	PB2-OB5	2.29	1.68	1.59
30	m	202	PEE	O2-C10	2.28	1.40	1.34
33	g	201	PLX	C7-C6	2.26	1.55	1.50
31	V	201	CDL	PB2-OB2	2.26	1.68	1.59
31	r	504	CDL	PB2-OB2	2.25	1.68	1.59
30	r	501	PEE	O2-C10	2.25	1.40	1.34
30	m	202	PEE	O3-C3	-2.22	1.40	1.45
31	l	701	CDL	PB2-OB5	2.21	1.68	1.59
30	l	703	PEE	O2-C10	2.21	1.40	1.34
30	l	703	PEE	O3-C3	-2.21	1.40	1.45
31	l	702	CDL	PB2-OB5	2.19	1.68	1.59
31	V	201	CDL	PB2-OB5	2.18	1.67	1.59
33	r	502	PLX	P1-O4	2.18	1.67	1.59
31	l	701	CDL	PB2-OB2	2.18	1.67	1.59
30	r	501	PEE	O3-C3	-2.18	1.40	1.45
31	l	702	CDL	PB2-OB2	2.17	1.67	1.59
33	m	201	PLX	P1-O4	2.16	1.67	1.59
30	s	401	PEE	O2-C10	2.15	1.40	1.34
30	Q	101	PEE	O2-C10	2.13	1.40	1.34
30	U	101	PEE	O3-C3	-2.13	1.40	1.45
30	b	201	PEE	O3-C3	-2.11	1.40	1.45
30	s	401	PEE	O3-C3	-2.09	1.40	1.45
33	m	201	PLX	P1-O1	2.09	1.67	1.59
34	s	402	UQ	O3-CM3	-2.06	1.40	1.45
33	g	201	PLX	P1-O4	2.05	1.67	1.59
33	r	502	PLX	P1-O1	2.05	1.67	1.59
33	r	503	PLX	P1-O4	2.05	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Q	101	PEE	O3-C3	-2.04	1.40	1.45
33	r	503	PLX	P1-O1	2.02	1.67	1.59
31	l	702	CDL	C11-CA5	2.02	1.56	1.50
34	s	402	UQ	O1-C1	-2.02	1.18	1.23

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	402	UQ	C7-C8-C9	-9.90	109.78	126.83
34	s	402	UQ	C12-C13-C14	-6.36	113.07	127.62
35	w	401	ADP	C5-C4-N3	-5.45	119.22	126.72
32	X	201	8Q1	C6-C1-S44	4.86	119.20	113.40
35	w	401	ADP	N3-C2-N1	-4.58	121.64	128.58
34	s	402	UQ	C10-C9-C8	-4.58	111.88	123.63
34	s	402	UQ	C11-C9-C8	-4.52	111.03	121.17
34	s	402	UQ	C17-C18-C19	-4.31	113.27	127.64
35	w	401	ADP	N3-C4-N9	4.29	134.46	127.17
34	s	402	UQ	C15-C14-C13	-4.08	113.15	123.63
31	r	504	CDL	OB6-CB5-C51	4.05	120.24	111.48
31	l	701	CDL	OA6-CA5-C11	4.04	120.21	111.48
30	Q	101	PEE	O2-C10-C11	4.04	120.21	111.48
30	s	401	PEE	O2-C10-C11	4.03	120.20	111.48
30	l	703	PEE	O2-C10-C11	4.03	120.20	111.48
30	m	202	PEE	O2-C10-C11	4.02	120.17	111.48
31	l	702	CDL	OB6-CB5-C51	4.00	120.13	111.48
31	a	201	CDL	OB6-CB5-C51	4.00	120.12	111.48
31	V	201	CDL	OB6-CB5-C51	3.98	120.09	111.48
30	r	501	PEE	O2-C10-C11	3.97	120.06	111.48
31	g	202	CDL	OB6-CB5-C51	3.96	120.04	111.48
31	l	702	CDL	OA6-CA5-C11	3.94	119.99	111.48
30	b	201	PEE	O2-C10-C11	3.88	119.87	111.48
31	l	701	CDL	OB6-CB5-C51	3.87	119.86	111.48
30	U	101	PEE	O2-C10-C11	3.87	119.84	111.48
31	a	201	CDL	OA6-CA5-C11	3.74	119.58	111.48
31	r	504	CDL	OA6-CA5-C11	3.69	119.46	111.48
34	s	402	UQ	C7-C6-C5	-3.59	118.74	124.89
35	w	401	ADP	C2-N3-C4	3.58	120.57	111.83
34	s	402	UQ	C16-C14-C13	-3.55	113.20	121.17
35	w	401	ADP	N9-C8-N7	-3.49	108.98	113.94
32	X	201	8Q1	C43-S44-C1	3.32	111.67	101.84
34	s	402	UQ	C21-C19-C18	-3.21	113.01	122.66
35	w	401	ADP	C5-N7-C8	3.18	108.45	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	w	401	ADP	C4-N9-C8	3.16	109.06	105.74
32	X	201	8Q1	O35-C34-N36	-3.13	116.36	122.98
34	s	402	UQ	CM5-C5-C6	-3.07	119.41	124.45
34	s	402	UQ	C20-C19-C18	-3.04	113.52	122.66
31	a	201	CDL	OB8-CB7-C71	3.02	121.06	111.83
32	X	201	8Q1	O2-P24-O27	-2.98	98.89	106.67
35	w	401	ADP	C4-C5-N7	-2.97	107.19	110.58
30	s	401	PEE	O3-C30-C31	2.96	120.85	111.83
31	a	201	CDL	OA8-CA7-C31	2.89	120.63	111.83
30	l	703	PEE	O3-C30-C31	2.86	120.55	111.83
33	g	201	PLX	C1A-N1-C1	2.82	121.13	109.91
31	V	201	CDL	OB8-CB7-C71	2.81	120.42	111.83
31	r	504	CDL	OA8-CA7-C31	2.79	120.35	111.83
31	l	701	CDL	OB8-CB7-C71	2.76	120.26	111.83
31	g	202	CDL	OA8-CA7-C31	2.75	120.22	111.83
30	r	501	PEE	O3-C30-C31	2.73	120.16	111.83
31	l	702	CDL	OB8-CB7-C71	2.71	120.09	111.83
30	b	201	PEE	O3-C30-C31	2.68	120.00	111.83
30	Q	101	PEE	O3-C30-C31	2.66	119.95	111.83
30	U	101	PEE	O3-C30-C31	2.65	119.93	111.83
31	g	202	CDL	OB8-CB7-C71	2.64	119.88	111.83
31	l	701	CDL	OA8-CA7-C31	2.63	119.84	111.83
31	r	504	CDL	OB8-CB7-C71	2.63	119.84	111.83
31	l	702	CDL	OA8-CA7-C31	2.60	119.75	111.83
32	X	201	8Q1	O4-C1-S44	-2.59	119.39	122.68
30	m	202	PEE	O3-C30-C31	2.55	119.62	111.83
31	g	202	CDL	OA6-CA5-C11	2.52	120.17	110.93
31	V	201	CDL	OA8-CA7-C31	2.51	119.49	111.83
33	r	503	PLX	C1A-N1-C1	2.50	119.83	109.91
32	X	201	8Q1	O40-C39-N41	-2.49	118.15	123.03
31	a	201	CDL	CB4-OB6-CB5	-2.48	111.86	117.80
33	r	502	PLX	C1A-N1-C1	2.47	119.72	109.91
31	V	201	CDL	OA6-CA5-C11	2.43	119.86	110.93
34	s	402	UQ	C7-C6-C1	2.42	121.33	118.52
32	X	201	8Q1	O1-P24-O2	2.38	116.73	107.80
33	m	201	PLX	C1A-N1-C1	2.34	119.22	109.91
32	X	201	8Q1	C32-C34-N36	2.29	120.83	116.48
32	X	201	8Q1	O4-C1-C6	-2.22	121.42	123.98
30	Q	101	PEE	C2-O2-C10	-2.02	112.96	117.80

There are no chirality outliers.

All (599) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	Q	101	PEE	C4-O4P-P-O3P
30	Q	101	PEE	C4-O4P-P-O2P
30	Q	101	PEE	C4-O4P-P-O1P
30	U	101	PEE	C19-C20-C21-C22
30	U	101	PEE	C11-C10-O2-C2
30	U	101	PEE	O4-C10-O2-C2
30	U	101	PEE	C1-O3P-P-O1P
30	U	101	PEE	C1-O3P-P-O4P
30	b	201	PEE	C4-O4P-P-O3P
30	b	201	PEE	C4-O4P-P-O2P
30	b	201	PEE	C4-O4P-P-O1P
30	l	703	PEE	C11-C10-O2-C2
30	l	703	PEE	C4-O4P-P-O3P
30	l	703	PEE	C4-O4P-P-O2P
30	l	703	PEE	C4-O4P-P-O1P
30	m	202	PEE	C11-C10-O2-C2
30	m	202	PEE	C4-O4P-P-O3P
30	m	202	PEE	C4-O4P-P-O2P
30	m	202	PEE	C4-O4P-P-O1P
30	m	202	PEE	O4P-C4-C5-N
30	r	501	PEE	C1-O3P-P-O2P
30	r	501	PEE	C1-O3P-P-O1P
30	r	501	PEE	C1-O3P-P-O4P
30	r	501	PEE	C4-O4P-P-O3P
30	r	501	PEE	C4-O4P-P-O2P
30	s	401	PEE	O4P-C4-C5-N
31	V	201	CDL	CA2-OA2-PA1-OA4
31	V	201	CDL	CA2-OA2-PA1-OA5
31	V	201	CDL	CB3-OB5-PB2-OB2
31	V	201	CDL	CB3-OB5-PB2-OB3
31	V	201	CDL	CB3-OB5-PB2-OB4
31	a	201	CDL	CA2-OA2-PA1-OA3
31	a	201	CDL	CA2-OA2-PA1-OA4
31	a	201	CDL	CA2-OA2-PA1-OA5
31	a	201	CDL	CA3-OA5-PA1-OA2
31	a	201	CDL	CA3-OA5-PA1-OA4
31	a	201	CDL	CB2-OB2-PB2-OB3
31	a	201	CDL	CB2-OB2-PB2-OB5
31	g	202	CDL	CA2-OA2-PA1-OA4
31	g	202	CDL	CA2-OA2-PA1-OA5
31	g	202	CDL	CB2-OB2-PB2-OB5
31	l	701	CDL	CA2-OA2-PA1-OA3
31	l	701	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
31	l	701	CDL	CA2-OA2-PA1-OA5
31	l	701	CDL	CA3-OA5-PA1-OA3
31	l	701	CDL	CB2-OB2-PB2-OB3
31	l	701	CDL	CB2-OB2-PB2-OB4
31	l	701	CDL	CB2-OB2-PB2-OB5
31	l	702	CDL	O1-C1-CB2-OB2
31	l	702	CDL	CA2-C1-CB2-OB2
31	l	702	CDL	CA2-OA2-PA1-OA3
31	l	702	CDL	CA2-OA2-PA1-OA5
31	l	702	CDL	CB2-OB2-PB2-OB4
31	l	702	CDL	CB2-OB2-PB2-OB5
31	l	702	CDL	OB6-CB4-CB6-OB8
31	r	504	CDL	CB2-C1-CA2-OA2
31	r	504	CDL	CA2-OA2-PA1-OA3
31	r	504	CDL	CA2-OA2-PA1-OA4
31	r	504	CDL	CA2-OA2-PA1-OA5
31	r	504	CDL	CB2-OB2-PB2-OB3
31	r	504	CDL	CB2-OB2-PB2-OB5
31	r	504	CDL	CB3-OB5-PB2-OB2
31	r	504	CDL	CB3-OB5-PB2-OB4
31	r	504	CDL	C51-CB5-OB6-CB4
32	X	201	8Q1	C1-C6-C7-C8
32	X	201	8Q1	O4-C1-S44-C43
32	X	201	8Q1	C6-C1-S44-C43
32	X	201	8Q1	C28-C29-C32-C34
32	X	201	8Q1	C28-C29-C32-O33
32	X	201	8Q1	C30-C29-C32-C34
32	X	201	8Q1	C30-C29-C32-O33
32	X	201	8Q1	C31-C29-C32-C34
32	X	201	8Q1	C31-C29-C32-O33
32	X	201	8Q1	N36-C37-C38-C39
32	X	201	8Q1	C28-O27-P24-O3
32	X	201	8Q1	C28-O27-P24-O2
32	X	201	8Q1	C28-O27-P24-O1
33	a	202	PLX	O7-C6-O6-C4
33	a	202	PLX	C3-O4-P1-O1
33	a	202	PLX	C2-O1-P1-O2
33	g	201	PLX	O7-C6-O6-C4
33	g	201	PLX	C3-O4-P1-O1
33	m	201	PLX	O7-C6-C7-C8
33	m	201	PLX	O7-C6-O6-C4
33	m	201	PLX	C25-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
33	m	201	PLX	O9-C24-C25-C26
33	r	502	PLX	O7-C6-O6-C4
33	r	502	PLX	C5-C4-O6-C6
33	r	502	PLX	C2-O1-P1-O2
33	r	502	PLX	O9-C24-C25-C26
33	r	503	PLX	O7-C6-O6-C4
33	r	503	PLX	C2-O1-P1-O4
33	r	503	PLX	C2-O1-P1-O2
33	r	503	PLX	C2-O1-P1-O3
33	r	503	PLX	O9-C24-O8-C5
33	r	503	PLX	O9-C24-C25-C26
34	s	402	UQ	C7-C8-C9-C10
34	s	402	UQ	C7-C8-C9-C11
34	s	402	UQ	C12-C13-C14-C16
35	w	401	ADP	C5'-O5'-PA-O2A
31	l	701	CDL	OA9-CA7-OA8-CA6
30	U	101	PEE	C2-C3-O3-C30
31	l	701	CDL	C31-CA7-OA8-CA6
30	b	201	PEE	O4-C10-O2-C2
30	m	202	PEE	O4-C10-O2-C2
30	r	501	PEE	O4-C10-O2-C2
31	r	504	CDL	OB7-CB5-OB6-CB4
30	U	101	PEE	C31-C30-O3-C3
30	m	202	PEE	C31-C30-O3-C3
31	l	702	CDL	C71-CB7-OB8-CB6
30	b	201	PEE	C11-C10-O2-C2
34	s	402	UQ	C12-C11-C9-C10
30	b	201	PEE	C31-C30-O3-C3
31	r	504	CDL	C71-CB7-OB8-CB6
30	U	101	PEE	O5-C30-O3-C3
31	l	702	CDL	OB9-CB7-OB8-CB6
30	l	703	PEE	O4-C10-O2-C2
30	b	201	PEE	C2-C3-O3-C30
31	g	202	CDL	O1-C1-CB2-OB2
31	l	701	CDL	O1-C1-CB2-OB2
30	b	201	PEE	O5-C30-O3-C3
30	m	202	PEE	O5-C30-O3-C3
30	Q	101	PEE	C11-C10-O2-C2
30	r	501	PEE	C11-C10-O2-C2
31	r	504	CDL	OB9-CB7-OB8-CB6
30	Q	101	PEE	O4-C10-O2-C2
34	s	402	UQ	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	r	502	PLX	C9-C10-C11-C12
34	s	402	UQ	C17-C18-C19-C21
33	g	201	PLX	C7-C8-C9-C10
30	U	101	PEE	C17-C18-C19-C20
30	r	501	PEE	C17-C18-C19-C20
31	V	201	CDL	CA2-C1-CB2-OB2
31	g	202	CDL	CA2-C1-CB2-OB2
30	l	703	PEE	C31-C30-O3-C3
33	m	201	PLX	C15-C16-C17-C18
31	l	702	CDL	C11-C12-C13-C14
31	l	702	CDL	C35-C36-C37-C38
31	l	702	CDL	C54-C55-C56-C57
33	r	502	PLX	C30-C31-C32-C33
30	l	703	PEE	O5-C30-O3-C3
31	V	201	CDL	OB6-CB4-CB6-OB8
31	l	702	CDL	OA6-CA4-CA6-OA8
30	b	201	PEE	C10-C11-C12-C13
31	l	702	CDL	CB5-C51-C52-C53
30	b	201	PEE	C37-C38-C39-C40
33	m	201	PLX	C28-C29-C30-C31
31	r	504	CDL	CB5-C51-C52-C53
31	l	701	CDL	CB5-C51-C52-C53
31	l	701	CDL	CB7-C71-C72-C73
31	l	701	CDL	C20-C21-C22-C23
31	V	201	CDL	O1-C1-CB2-OB2
31	r	504	CDL	O1-C1-CA2-OA2
30	l	703	PEE	C37-C38-C39-C40
30	s	401	PEE	C37-C38-C39-C40
31	l	701	CDL	C71-CB7-OB8-CB6
31	l	701	CDL	CA2-C1-CB2-OB2
31	l	702	CDL	C39-C40-C41-C42
30	U	101	PEE	C40-C41-C42-C43
33	r	503	PLX	O8-C24-C25-C26
31	g	202	CDL	C11-CA5-OA6-CA4
31	g	202	CDL	OA7-CA5-OA6-CA4
31	a	201	CDL	O1-C1-CA2-OA2
31	l	701	CDL	C55-C56-C57-C58
31	g	202	CDL	CA6-CA4-OA6-CA5
30	m	202	PEE	C13-C14-C15-C16
31	r	504	CDL	C20-C21-C22-C23
31	r	504	CDL	C74-C75-C76-C77
31	l	701	CDL	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
30	m	202	PEE	C31-C32-C33-C34
30	s	401	PEE	C31-C30-O3-C3
30	m	202	PEE	C22-C23-C24-C25
31	l	701	CDL	OB9-CB7-OB8-CB6
31	l	701	CDL	C71-C72-C73-C74
31	l	702	CDL	C37-C38-C39-C40
31	l	702	CDL	C60-C61-C62-C63
33	r	503	PLX	C10-C11-C12-C13
31	r	504	CDL	C32-C33-C34-C35
33	r	503	PLX	C25-C26-C27-C28
31	l	702	CDL	C53-C54-C55-C56
31	r	504	CDL	C12-C13-C14-C15
33	g	201	PLX	C11-C10-C9-C8
33	r	503	PLX	C11-C12-C13-C14
31	l	701	CDL	C82-C83-C84-C85
31	r	504	CDL	C43-C44-C45-C46
33	r	502	PLX	C27-C28-C29-C30
31	V	201	CDL	C74-C75-C76-C77
31	l	701	CDL	O1-C1-CA2-OA2
31	l	701	CDL	C62-C63-C64-C65
31	l	702	CDL	C33-C34-C35-C36
33	r	502	PLX	C15-C16-C17-C18
30	r	501	PEE	C10-C11-C12-C13
31	l	701	CDL	C36-C37-C38-C39
31	r	504	CDL	C55-C56-C57-C58
33	m	201	PLX	C26-C27-C28-C29
33	m	201	PLX	C10-C11-C12-C13
33	r	502	PLX	C7-C8-C9-C10
30	l	703	PEE	C21-C22-C23-C24
30	l	703	PEE	C31-C32-C33-C34
31	l	701	CDL	C73-C74-C75-C76
33	g	201	PLX	C10-C11-C12-C13
33	g	201	PLX	C27-C28-C29-C30
33	m	201	PLX	C12-C13-C14-C15
33	r	502	PLX	C12-C13-C14-C15
31	l	701	CDL	C56-C57-C58-C59
31	l	701	CDL	C75-C76-C77-C78
33	g	201	PLX	C28-C29-C30-C31
33	m	201	PLX	C7-C8-C9-C10
33	m	201	PLX	C25-C26-C27-C28
33	r	502	PLX	C28-C29-C30-C31
31	l	702	CDL	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
31	r	504	CDL	C76-C77-C78-C79
33	r	502	PLX	C16-C17-C18-C19
31	l	701	CDL	C14-C15-C16-C17
31	l	702	CDL	C56-C57-C58-C59
33	r	503	PLX	C30-C31-C32-C33
30	b	201	PEE	C31-C32-C33-C34
31	l	702	CDL	C62-C63-C64-C65
31	V	201	CDL	C55-C56-C57-C58
33	m	201	PLX	C27-C28-C29-C30
30	s	401	PEE	C30-C31-C32-C33
33	m	201	PLX	C9-C10-C11-C12
30	s	401	PEE	O5-C30-O3-C3
30	b	201	PEE	C13-C14-C15-C16
34	s	402	UQ	C12-C11-C9-C8
34	s	402	UQ	C13-C14-C16-C17
30	s	401	PEE	C34-C35-C36-C37
31	V	201	CDL	C77-C78-C79-C80
31	l	702	CDL	C22-C23-C24-C25
31	V	201	CDL	C84-C85-C86-C87
31	r	504	CDL	C71-C72-C73-C74
33	g	201	PLX	C25-C26-C27-C28
31	l	701	CDL	C35-C36-C37-C38
31	l	701	CDL	C54-C55-C56-C57
31	r	504	CDL	C73-C74-C75-C76
31	V	201	CDL	C59-C60-C61-C62
31	l	701	CDL	C74-C75-C76-C77
31	l	702	CDL	C52-C53-C54-C55
33	m	201	PLX	C14-C15-C16-C17
30	b	201	PEE	C33-C34-C35-C36
31	a	201	CDL	C51-CB5-OB6-CB4
31	l	701	CDL	C51-CB5-OB6-CB4
31	l	701	CDL	C40-C41-C42-C43
31	r	504	CDL	C41-C42-C43-C44
31	r	504	CDL	C75-C76-C77-C78
33	r	502	PLX	C13-C14-C15-C16
31	r	504	CDL	C14-C15-C16-C17
33	r	503	PLX	C31-C32-C33-C34
33	r	503	PLX	C2-C1-N1-C1C
30	r	501	PEE	C12-C13-C14-C15
33	g	201	PLX	C30-C31-C32-C33
33	r	503	PLX	C28-C29-C30-C31
33	r	503	PLX	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
30	Q	101	PEE	C34-C35-C36-C37
31	r	504	CDL	C60-C61-C62-C63
31	l	702	CDL	C14-C15-C16-C17
31	V	201	CDL	C51-CB5-OB6-CB4
32	X	201	8Q1	C9-C10-C11-C12
30	U	101	PEE	C34-C35-C36-C37
31	l	702	CDL	C55-C56-C57-C58
30	r	501	PEE	C19-C20-C21-C22
31	V	201	CDL	C56-C57-C58-C59
33	g	201	PLX	C35-C36-C37-C38
31	r	504	CDL	C72-C73-C74-C75
33	r	502	PLX	C31-C32-C33-C34
33	r	503	PLX	C14-C15-C16-C17
31	V	201	CDL	C71-C72-C73-C74
30	r	501	PEE	C13-C14-C15-C16
31	l	702	CDL	C73-C74-C75-C76
30	r	501	PEE	C31-C30-O3-C3
31	V	201	CDL	C64-C65-C66-C67
31	l	701	CDL	C52-C53-C54-C55
33	g	201	PLX	C9-C10-C11-C12
33	r	503	PLX	C2-C1-N1-C1A
30	r	501	PEE	C32-C33-C34-C35
30	s	401	PEE	C33-C34-C35-C36
30	s	401	PEE	C35-C36-C37-C38
30	Q	101	PEE	C31-C32-C33-C34
30	b	201	PEE	C11-C12-C13-C14
33	g	201	PLX	C14-C15-C16-C17
31	a	201	CDL	OB7-CB5-OB6-CB4
33	m	201	PLX	O8-C24-C25-C26
31	V	201	CDL	CA7-C31-C32-C33
31	l	701	CDL	C32-C33-C34-C35
33	g	201	PLX	C32-C33-C34-C35
30	b	201	PEE	C1-C2-C3-O3
30	r	501	PEE	C1-C2-C3-O3
31	V	201	CDL	CB3-CB4-CB6-OB8
31	g	202	CDL	CA3-CA4-CA6-OA8
31	l	702	CDL	CA3-CA4-CA6-OA8
31	r	504	CDL	CA3-CA4-CA6-OA8
33	r	502	PLX	C3-C4-C5-O8
31	a	201	CDL	C31-C32-C33-C34
30	s	401	PEE	C15-C16-C17-C18
31	l	701	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
30	Q	101	PEE	C22-C23-C24-C25
30	s	401	PEE	C13-C14-C15-C16
31	g	202	CDL	C75-C76-C77-C78
31	r	504	CDL	C56-C57-C58-C59
31	V	201	CDL	OB7-CB5-OB6-CB4
33	r	502	PLX	C33-C34-C35-C36
30	s	401	PEE	C23-C24-C25-C26
33	m	201	PLX	C34-C35-C36-C37
30	b	201	PEE	C32-C33-C34-C35
31	r	504	CDL	C52-C53-C54-C55
30	r	501	PEE	O5-C30-O3-C3
30	s	401	PEE	C17-C18-C19-C20
31	r	504	CDL	C13-C14-C15-C16
30	U	101	PEE	C36-C37-C38-C39
30	s	401	PEE	C32-C33-C34-C35
31	a	201	CDL	CB2-C1-CA2-OA2
31	V	201	CDL	C52-C53-C54-C55
33	r	503	PLX	C27-C28-C29-C30
30	m	202	PEE	O2-C2-C3-O3
31	r	504	CDL	OA6-CA4-CA6-OA8
33	m	201	PLX	O6-C4-C5-O8
33	r	503	PLX	C36-C37-C38-C39
30	r	501	PEE	C22-C23-C24-C25
32	X	201	8Q1	C13-C14-C15-C16
30	Q	101	PEE	C24-C25-C26-C27
30	s	401	PEE	C14-C15-C16-C17
33	r	503	PLX	C16-C17-C18-C19
33	r	503	PLX	C13-C14-C15-C16
31	l	702	CDL	C12-C13-C14-C15
33	r	503	PLX	C9-C10-C11-C12
33	r	503	PLX	C32-C33-C34-C35
31	r	504	CDL	C31-C32-C33-C34
30	U	101	PEE	C42-C43-C44-C45
31	a	201	CDL	C37-C38-C39-C40
31	a	201	CDL	C71-C72-C73-C74
31	l	702	CDL	C40-C41-C42-C43
31	l	701	CDL	OB7-CB5-OB6-CB4
31	r	504	CDL	C62-C63-C64-C65
33	r	502	PLX	C10-C11-C12-C13
30	Q	101	PEE	O3P-C1-C2-C3
30	s	401	PEE	C11-C10-O2-C2
33	r	503	PLX	C2-C1-N1-C1B

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Mol	Chain	Res	Type	Atoms
31	l	701	CDL	C59-C60-C61-C62
31	r	504	CDL	C59-C60-C61-C62
31	l	701	CDL	C81-C82-C83-C84
30	s	401	PEE	C21-C22-C23-C24
30	s	401	PEE	C10-C11-C12-C13
30	Q	101	PEE	C1-C2-C3-O3
30	U	101	PEE	C1-C2-C3-O3
32	X	201	8Q1	O33-C32-C34-N36
33	g	201	PLX	C3-C4-C5-O8
31	r	504	CDL	C17-C18-C19-C20
31	V	201	CDL	C82-C83-C84-C85
31	r	504	CDL	C79-C80-C81-C82
30	m	202	PEE	C11-C12-C13-C14
30	r	501	PEE	O3P-C1-C2-O2
31	l	701	CDL	OB5-CB3-CB4-OB6
31	l	702	CDL	OA5-CA3-CA4-OA6
34	s	402	UQ	C17-C18-C19-C20
30	l	703	PEE	C13-C14-C15-C16
33	r	502	PLX	C29-C30-C31-C32
31	g	202	CDL	C58-C59-C60-C61
31	l	702	CDL	C64-C65-C66-C67
30	b	201	PEE	C30-C31-C32-C33
33	m	201	PLX	C33-C34-C35-C36
30	U	101	PEE	C38-C39-C40-C41
30	b	201	PEE	C18-C19-C20-C21
33	a	202	PLX	C11-C12-C13-C14
31	V	201	CDL	C75-C76-C77-C78
30	U	101	PEE	C21-C22-C23-C24
34	s	402	UQ	C9-C11-C12-C13
31	l	702	CDL	C84-C85-C86-C87
31	l	702	CDL	C57-C58-C59-C60
30	b	201	PEE	C14-C15-C16-C17
31	l	701	CDL	C51-C52-C53-C54
31	l	702	CDL	C59-C60-C61-C62
31	V	201	CDL	CB2-C1-CA2-OA2
30	Q	101	PEE	C11-C12-C13-C14
30	b	201	PEE	O3P-C1-C2-C3
30	r	501	PEE	O3P-C1-C2-C3
31	V	201	CDL	OB5-CB3-CB4-CB6
30	Q	101	PEE	C18-C19-C20-C21
33	m	201	PLX	C31-C32-C33-C34
33	m	201	PLX	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	l	701	CDL	C37-C38-C39-C40
33	g	201	PLX	C12-C13-C14-C15
30	m	202	PEE	C3-C2-O2-C10
30	l	703	PEE	C32-C33-C34-C35
31	V	201	CDL	C62-C63-C64-C65
30	s	401	PEE	O4-C10-O2-C2
30	Q	101	PEE	O3P-C1-C2-O2
30	b	201	PEE	O3P-C1-C2-O2
30	l	703	PEE	O3P-C1-C2-O2
30	m	202	PEE	O3P-C1-C2-O2
31	a	201	CDL	OA5-CA3-CA4-OA6
31	r	504	CDL	OB5-CB3-CB4-OB6
30	s	401	PEE	C1-C2-C3-O3
31	l	702	CDL	CB3-CB4-CB6-OB8
33	r	503	PLX	C3-C4-C5-O8
33	r	502	PLX	C14-C15-C16-C17
30	U	101	PEE	O2-C2-C3-O3
33	g	201	PLX	O6-C4-C5-O8
33	r	502	PLX	O6-C4-C5-O8
30	s	401	PEE	C24-C25-C26-C27
30	Q	101	PEE	C32-C33-C34-C35
33	r	503	PLX	C34-C35-C36-C37
33	m	201	PLX	C7-C6-O6-C4
30	s	401	PEE	C20-C21-C22-C23
33	g	201	PLX	C33-C34-C35-C36
33	a	202	PLX	C13-C14-C15-C16
33	r	503	PLX	C17-C18-C19-C20
30	Q	101	PEE	C21-C22-C23-C24
33	g	201	PLX	O9-C24-C25-C26
31	r	504	CDL	C78-C79-C80-C81
31	l	702	CDL	C20-C21-C22-C23
30	b	201	PEE	C34-C35-C36-C37
31	a	201	CDL	C71-CB7-OB8-CB6
30	s	401	PEE	C39-C40-C41-C42
31	r	504	CDL	C36-C37-C38-C39
30	m	202	PEE	O3P-C1-C2-C3
31	r	504	CDL	OB5-CB3-CB4-CB6
33	m	201	PLX	O4-C3-C4-C5
31	l	702	CDL	C82-C83-C84-C85
33	r	503	PLX	C11-C10-C9-C8
31	V	201	CDL	O1-C1-CA2-OA2
31	V	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
31	r	504	CDL	C40-C41-C42-C43
31	r	504	CDL	C84-C85-C86-C87
32	X	201	8Q1	C42-C43-S44-C1
30	U	101	PEE	C12-C13-C14-C15
33	g	201	PLX	O8-C24-C25-C26
33	m	201	PLX	O6-C6-C7-C8
30	s	401	PEE	O3P-C1-C2-O2
31	V	201	CDL	OB5-CB3-CB4-OB6
31	V	201	CDL	OB9-CB7-OB8-CB6
31	g	202	CDL	C78-C79-C80-C81
31	V	201	CDL	C12-C11-CA5-OA7
30	U	101	PEE	C22-C23-C24-C25
30	Q	101	PEE	O2-C2-C3-O3
30	r	501	PEE	O2-C2-C3-O3
31	g	202	CDL	OA6-CA4-CA6-OA8
33	r	503	PLX	O6-C4-C5-O8
33	g	201	PLX	C17-C18-C19-C20
30	m	202	PEE	C1-C2-C3-O3
33	m	201	PLX	C3-C4-C5-O8
33	g	201	PLX	C13-C14-C15-C16
33	m	201	PLX	C13-C14-C15-C16
30	U	101	PEE	C1-O3P-P-O2P
30	b	201	PEE	C1-O3P-P-O1P
30	l	703	PEE	C1-O3P-P-O2P
30	l	703	PEE	O4P-C4-C5-N
31	V	201	CDL	CA3-OA5-PA1-OA2
31	V	201	CDL	CA3-OA5-PA1-OA3
31	V	201	CDL	CA3-OA5-PA1-OA4
31	V	201	CDL	CB2-OB2-PB2-OB3
31	a	201	CDL	CB2-OB2-PB2-OB4
31	a	201	CDL	CB3-OB5-PB2-OB3
31	g	202	CDL	CB2-OB2-PB2-OB3
31	l	701	CDL	CB3-OB5-PB2-OB4
31	l	702	CDL	CB2-OB2-PB2-OB3
31	l	702	CDL	CB3-OB5-PB2-OB2
31	l	702	CDL	CB3-OB5-PB2-OB3
31	l	702	CDL	CB3-OB5-PB2-OB4
31	r	504	CDL	CB3-OB5-PB2-OB3
33	a	202	PLX	C3-O4-P1-O2
33	g	201	PLX	C3-O4-P1-O2
33	r	502	PLX	C3-O4-P1-O1
33	r	502	PLX	C3-O4-P1-O2

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Mol	Chain	Res	Type	Atoms
33	r	502	PLX	C3-O4-P1-O3
33	r	502	PLX	C2-O1-P1-O4
33	r	502	PLX	C2-O1-P1-O3
33	r	503	PLX	C3-O4-P1-O2
35	w	401	ADP	C5'-O5'-PA-O1A
35	w	401	ADP	C5'-O5'-PA-O3A
31	l	702	CDL	CB7-C71-C72-C73
31	V	201	CDL	C12-C11-CA5-OA6
31	r	504	CDL	C82-C83-C84-C85
30	b	201	PEE	C2-C1-O3P-P
30	Q	101	PEE	C38-C39-C40-C41
30	l	703	PEE	C30-C31-C32-C33
33	r	503	PLX	C12-C13-C14-C15
30	l	703	PEE	C1-C2-O2-C10
30	l	703	PEE	C3-C2-O2-C10
31	a	201	CDL	CA6-CA4-OA6-CA5
33	g	201	PLX	C18-C19-C20-C21
30	s	401	PEE	O3P-C1-C2-C3
31	l	702	CDL	OA5-CA3-CA4-CA6
33	m	201	PLX	C30-C31-C32-C33
33	m	201	PLX	O4-C3-C4-O6
31	a	201	CDL	OB9-CB7-OB8-CB6
31	l	702	CDL	C34-C35-C36-C37
31	r	504	CDL	C64-C65-C66-C67
31	l	702	CDL	C75-C76-C77-C78
31	r	504	CDL	CB4-CB3-OB5-PB2
30	b	201	PEE	O2-C2-C3-O3
30	s	401	PEE	O2-C2-C3-O3
31	V	201	CDL	C72-C73-C74-C75
30	b	201	PEE	C22-C23-C24-C25
31	l	702	CDL	C44-C45-C46-C47
30	Q	101	PEE	C10-C11-C12-C13
30	m	202	PEE	C18-C19-C20-C21
30	r	501	PEE	C20-C21-C22-C23
31	g	202	CDL	C53-C54-C55-C56
33	r	503	PLX	C26-C27-C28-C29
31	V	201	CDL	C32-C31-CA7-OA8
31	l	701	CDL	OA6-CA4-CA6-OA8
31	l	702	CDL	C72-C73-C74-C75
31	l	701	CDL	C38-C39-C40-C41
30	b	201	PEE	C36-C37-C38-C39
33	g	201	PLX	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
31	l	702	CDL	C31-C32-C33-C34
30	b	201	PEE	C38-C39-C40-C41
31	r	504	CDL	OB6-CB4-CB6-OB8
31	l	702	CDL	C83-C84-C85-C86
31	r	504	CDL	C58-C59-C60-C61
30	Q	101	PEE	C35-C36-C37-C38
31	a	201	CDL	CA2-C1-CB2-OB2
33	r	502	PLX	O8-C24-C25-C26
30	m	202	PEE	O3-C30-C31-C32
31	r	504	CDL	C44-C45-C46-C47
31	l	702	CDL	C15-C16-C17-C18
30	Q	101	PEE	C2-C1-O3P-P
31	a	201	CDL	CA4-CA3-OA5-PA1
33	a	202	PLX	C14-C15-C16-C17
33	r	502	PLX	C26-C27-C28-C29
31	l	701	CDL	C60-C61-C62-C63
31	r	504	CDL	C35-C36-C37-C38
30	r	501	PEE	C30-C31-C32-C33
30	l	703	PEE	O3P-C1-C2-C3
31	a	201	CDL	OA5-CA3-CA4-CA6
30	l	703	PEE	O2-C2-C3-O3
31	l	701	CDL	OB6-CB4-CB6-OB8
30	s	401	PEE	C36-C37-C38-C39
30	l	703	PEE	C14-C15-C16-C17
30	b	201	PEE	C17-C18-C19-C20
33	r	502	PLX	C25-C26-C27-C28
30	U	101	PEE	C30-C31-C32-C33
30	l	703	PEE	C36-C37-C38-C39
31	l	701	CDL	C44-C45-C46-C47
31	r	504	CDL	C57-C58-C59-C60
31	V	201	CDL	C80-C81-C82-C83
30	l	703	PEE	C16-C17-C18-C19
30	s	401	PEE	C31-C32-C33-C34
30	r	501	PEE	C2-C1-O3P-P
30	U	101	PEE	C44-C45-C46-C47
33	a	202	PLX	O4-C3-C4-O6
31	l	702	CDL	C13-C14-C15-C16
30	Q	101	PEE	C36-C37-C38-C39
30	r	501	PEE	C16-C17-C18-C19
33	g	201	PLX	C16-C17-C18-C19
30	r	501	PEE	C11-C12-C13-C14
30	b	201	PEE	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
30	l	703	PEE	C18-C19-C20-C21
30	r	501	PEE	C18-C19-C20-C21
31	l	702	CDL	C32-C31-CA7-OA8
31	l	701	CDL	OB5-CB3-CB4-CB6
31	r	504	CDL	OA5-CA3-CA4-CA6
31	a	201	CDL	C72-C73-C74-C75
31	l	701	CDL	C76-C77-C78-C79
31	g	202	CDL	C12-C11-CA5-OA6
33	r	502	PLX	C11-C12-C13-C14
31	a	201	CDL	O1-C1-CB2-OB2
31	l	701	CDL	C72-C71-CB7-OB8
32	X	201	8Q1	C29-C32-C34-O35
30	r	501	PEE	C15-C16-C17-C18
31	a	201	CDL	C58-C59-C60-C61
31	r	504	CDL	C42-C43-C44-C45
30	l	703	PEE	C1-C2-C3-O3
33	g	201	PLX	C25-C24-O8-C5
33	r	503	PLX	C25-C24-O8-C5
31	r	504	CDL	C52-C51-CB5-OB6
31	l	702	CDL	C41-C42-C43-C44
30	b	201	PEE	C16-C17-C18-C19
33	a	202	PLX	C6-C7-C8-C9
33	r	503	PLX	C24-C25-C26-C27
31	l	702	CDL	C12-C11-CA5-OA6
30	U	101	PEE	O2-C10-C11-C12
31	r	504	CDL	C11-C12-C13-C14
30	b	201	PEE	C1-C2-O2-C10
31	l	702	CDL	C32-C31-CA7-OA9
32	X	201	8Q1	C29-C32-C34-N36
31	l	701	CDL	C16-C17-C18-C19
33	r	502	PLX	C4-C3-O4-P1
31	l	701	CDL	C72-C71-CB7-OB9
31	a	201	CDL	CA5-C11-C12-C13
31	r	504	CDL	C33-C34-C35-C36
31	l	701	CDL	C11-CA5-OA6-CA4
31	g	202	CDL	C71-C72-C73-C74
32	X	201	8Q1	C7-C8-C9-C10
30	l	703	PEE	C34-C35-C36-C37
30	U	101	PEE	C23-C24-C25-C26
33	g	201	PLX	O9-C24-O8-C5
33	m	201	PLX	O9-C24-O8-C5
33	r	502	PLX	O9-C24-O8-C5

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Mol	Chain	Res	Type	Atoms
33	m	201	PLX	C19-C20-C21-C22
31	l	701	CDL	OA7-CA5-OA6-CA4
31	l	702	CDL	C80-C81-C82-C83
31	l	702	CDL	C12-C11-CA5-OA7
31	r	504	CDL	C52-C51-CB5-OB7
30	m	202	PEE	C23-C24-C25-C26
31	l	701	CDL	C12-C11-CA5-OA6
31	l	701	CDL	CA7-C31-C32-C33
30	b	201	PEE	O2-C10-C11-C12
35	w	401	ADP	PB-O3A-PA-O2A

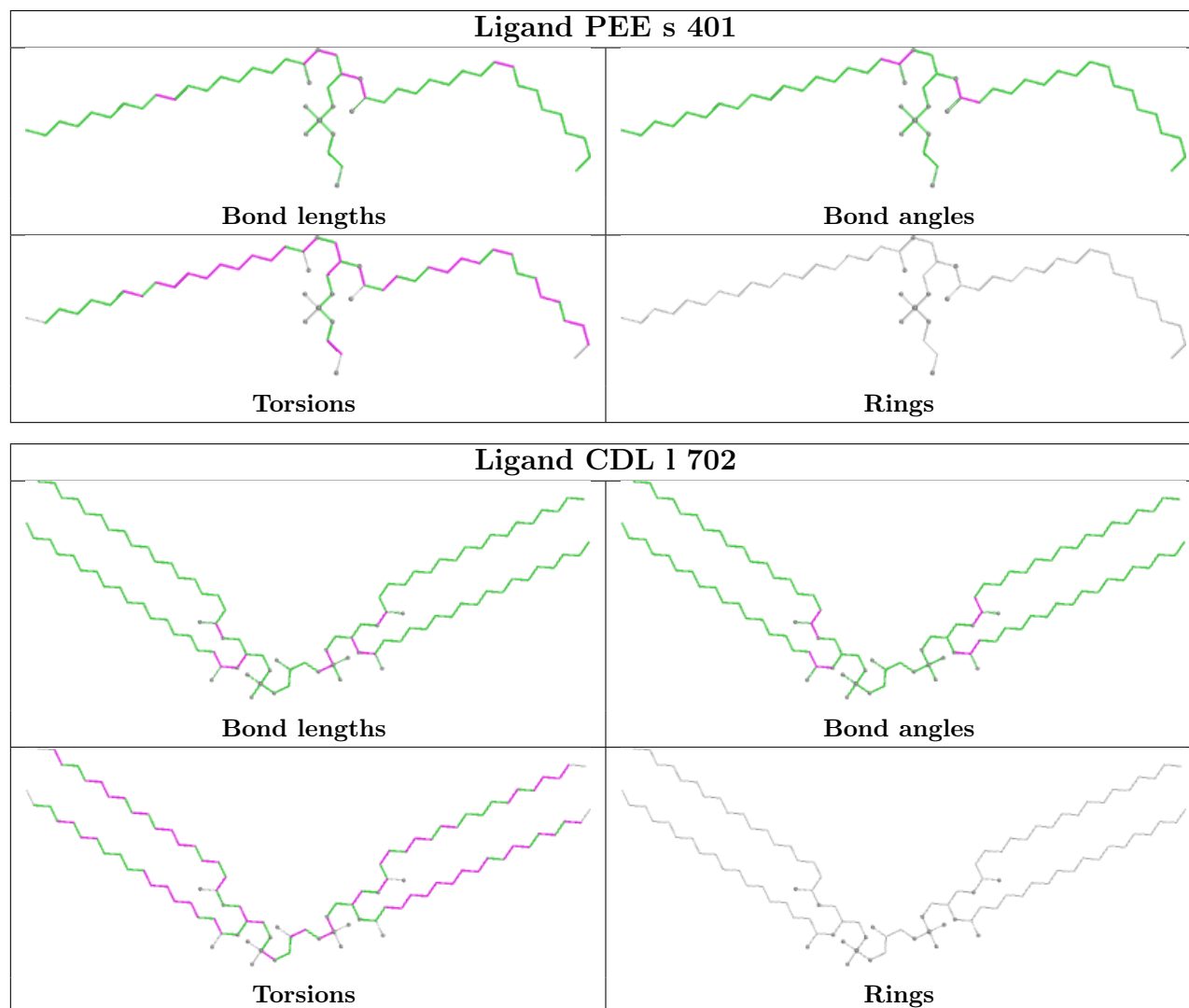
There are no ring outliers.

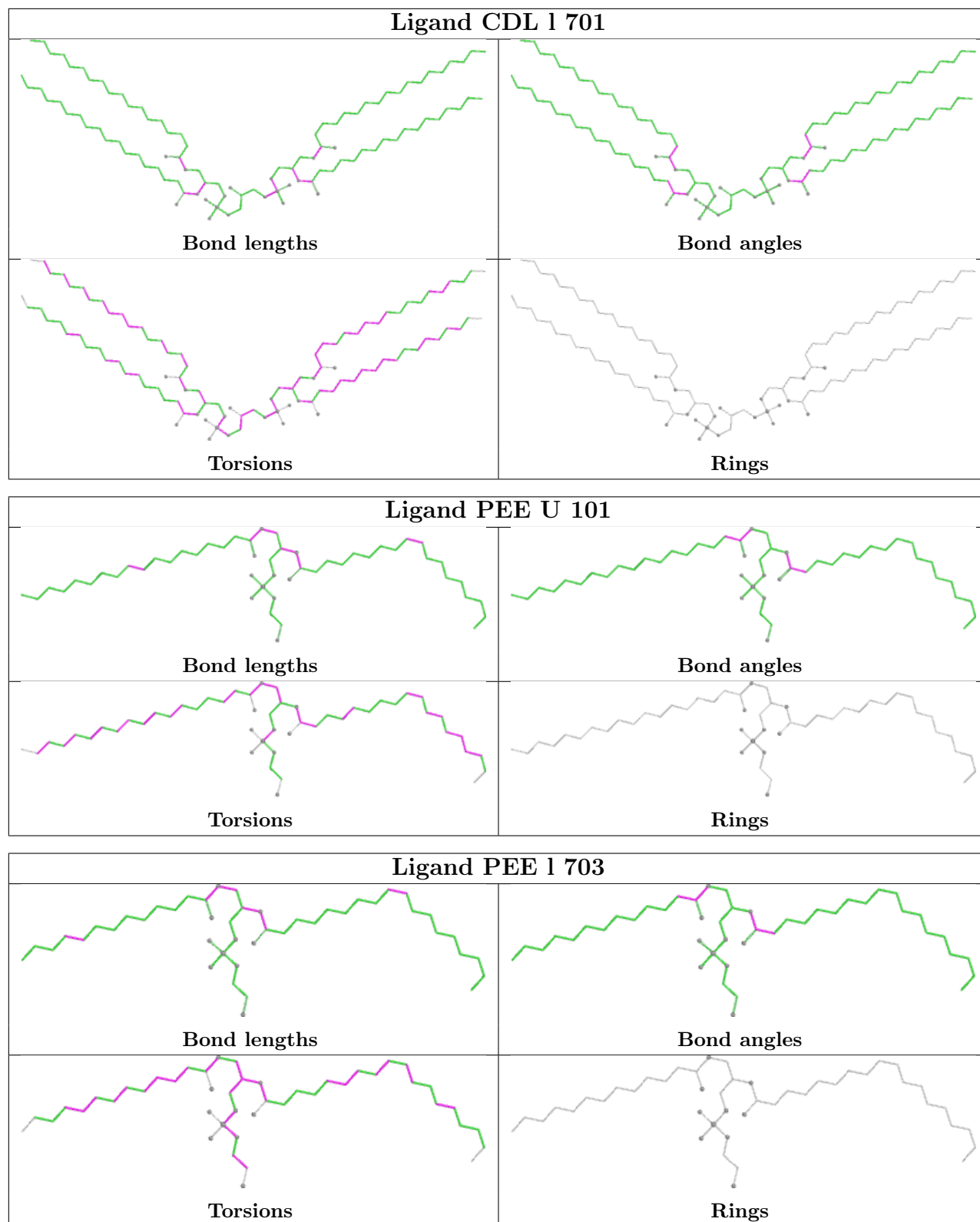
21 monomers are involved in 187 short contacts:

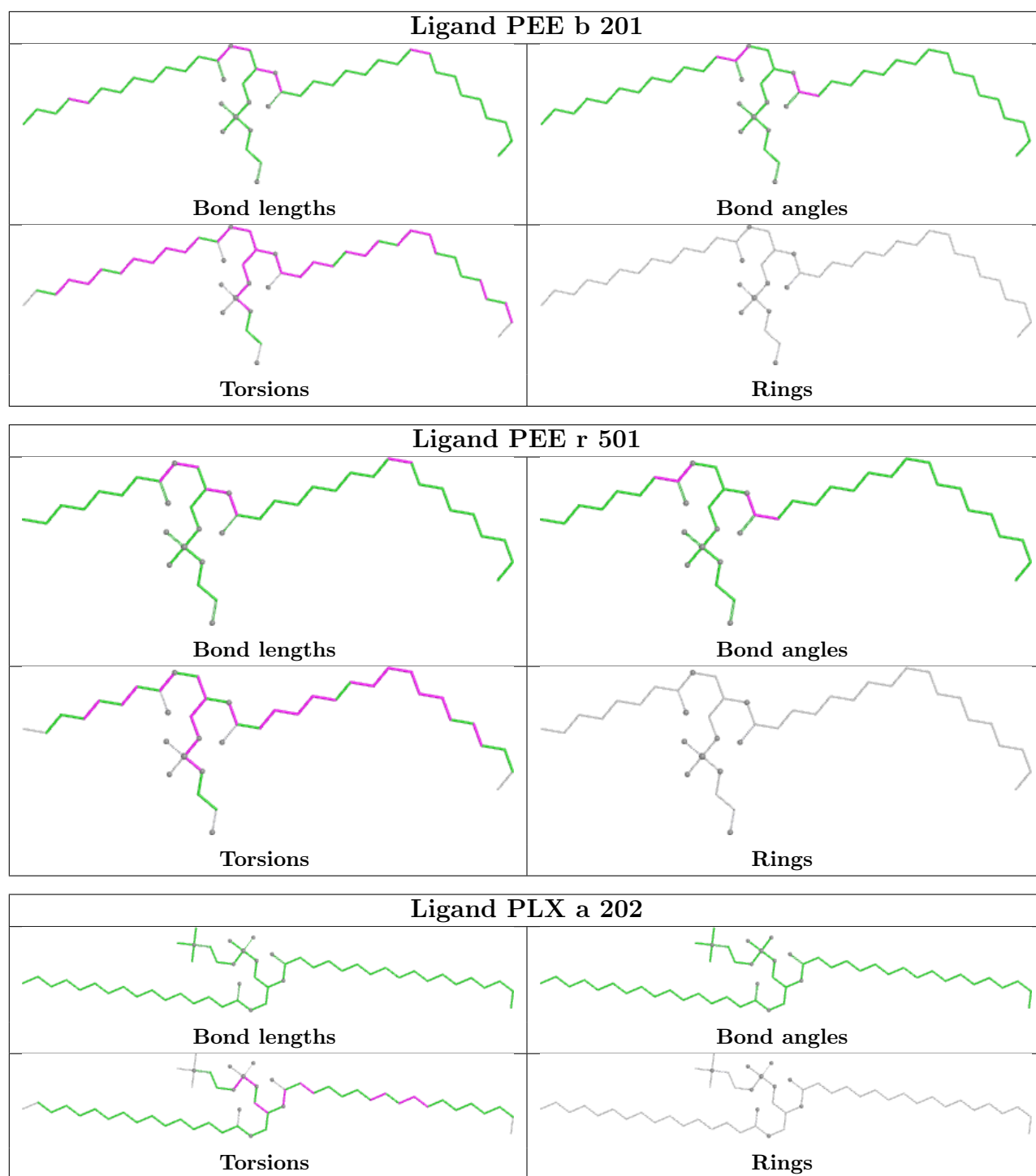
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	s	401	PEE	5	0
31	l	702	CDL	6	0
31	l	701	CDL	15	0
30	U	101	PEE	8	0
30	l	703	PEE	6	0
30	b	201	PEE	15	0
30	r	501	PEE	14	0
33	a	202	PLX	13	0
30	Q	101	PEE	17	0
31	V	201	CDL	5	0
33	g	201	PLX	9	0
34	s	402	UQ	4	0
33	r	502	PLX	4	0
31	r	504	CDL	6	0
32	X	201	8Q1	1	0
30	m	202	PEE	14	0
31	a	201	CDL	25	0
33	r	503	PLX	4	0
33	m	201	PLX	2	0
35	w	401	ADP	4	0
31	g	202	CDL	20	0

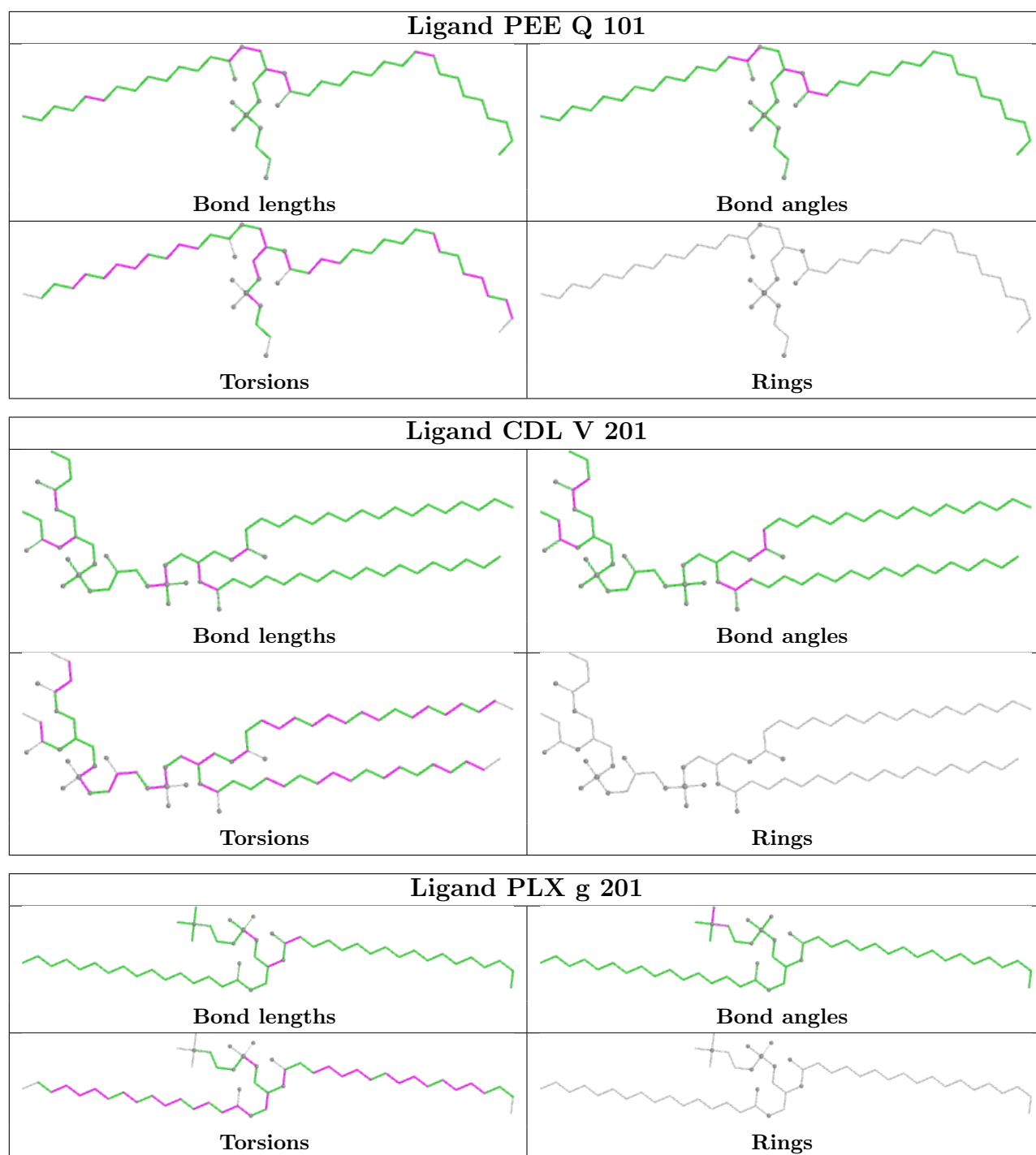
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

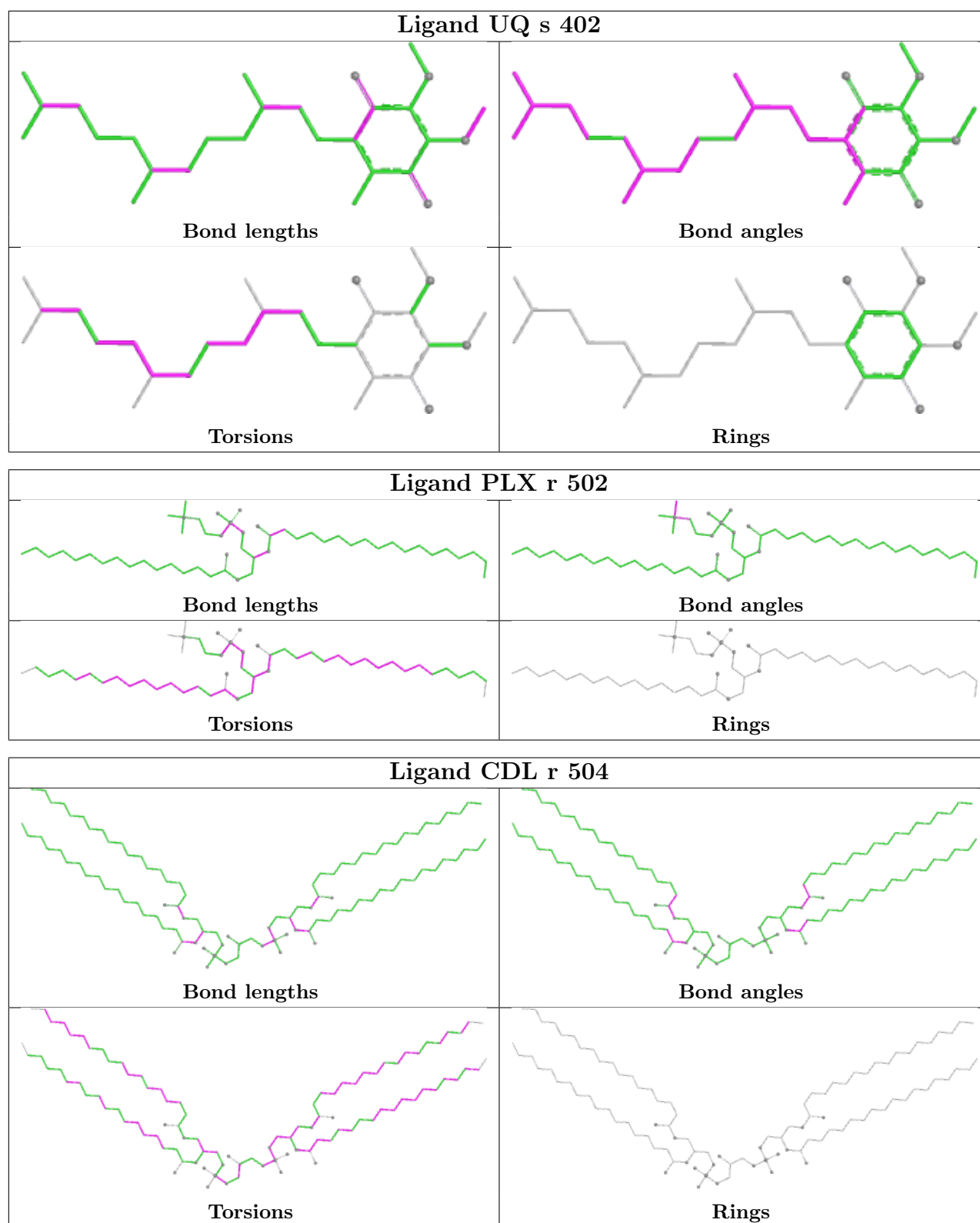
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

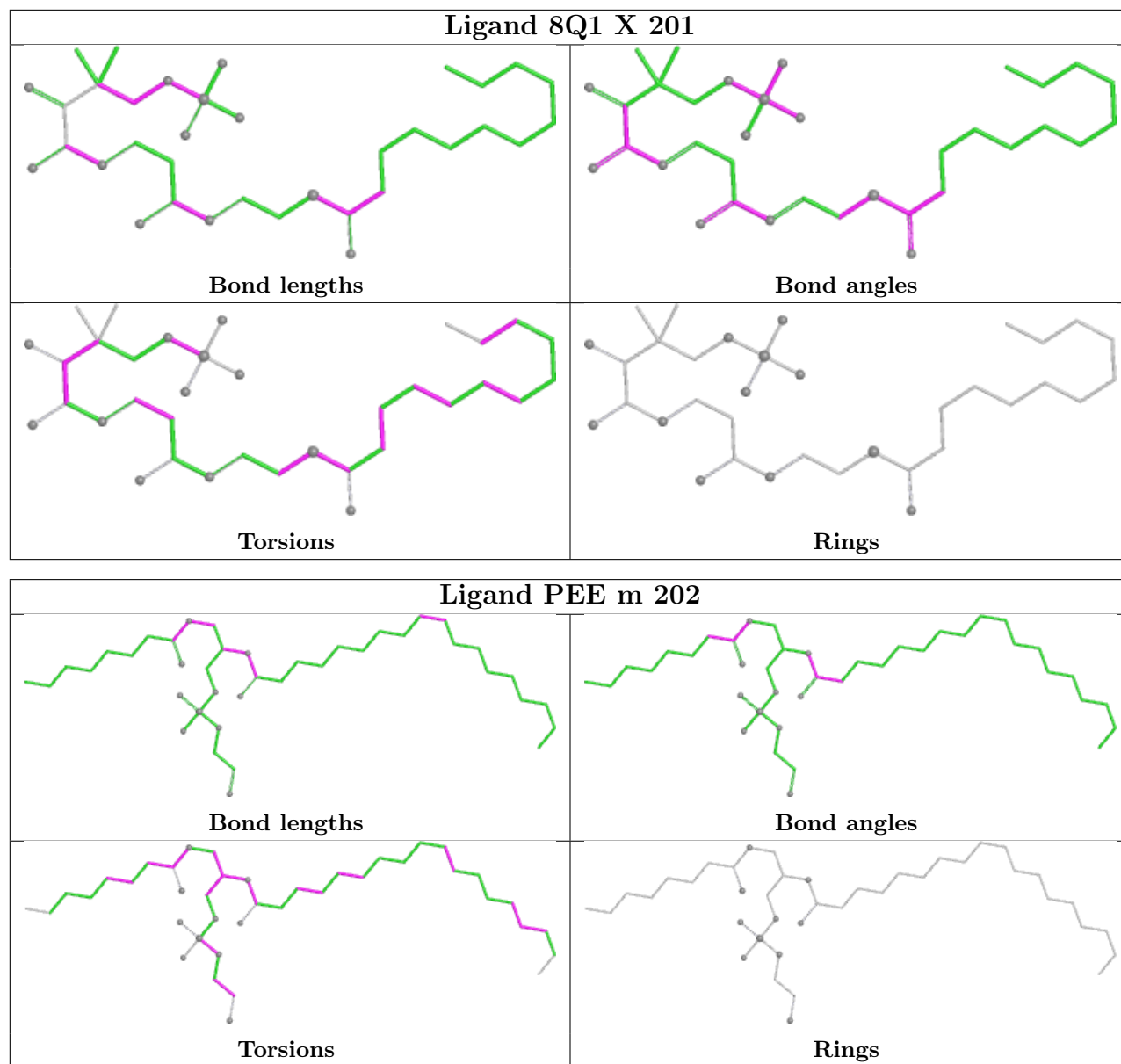


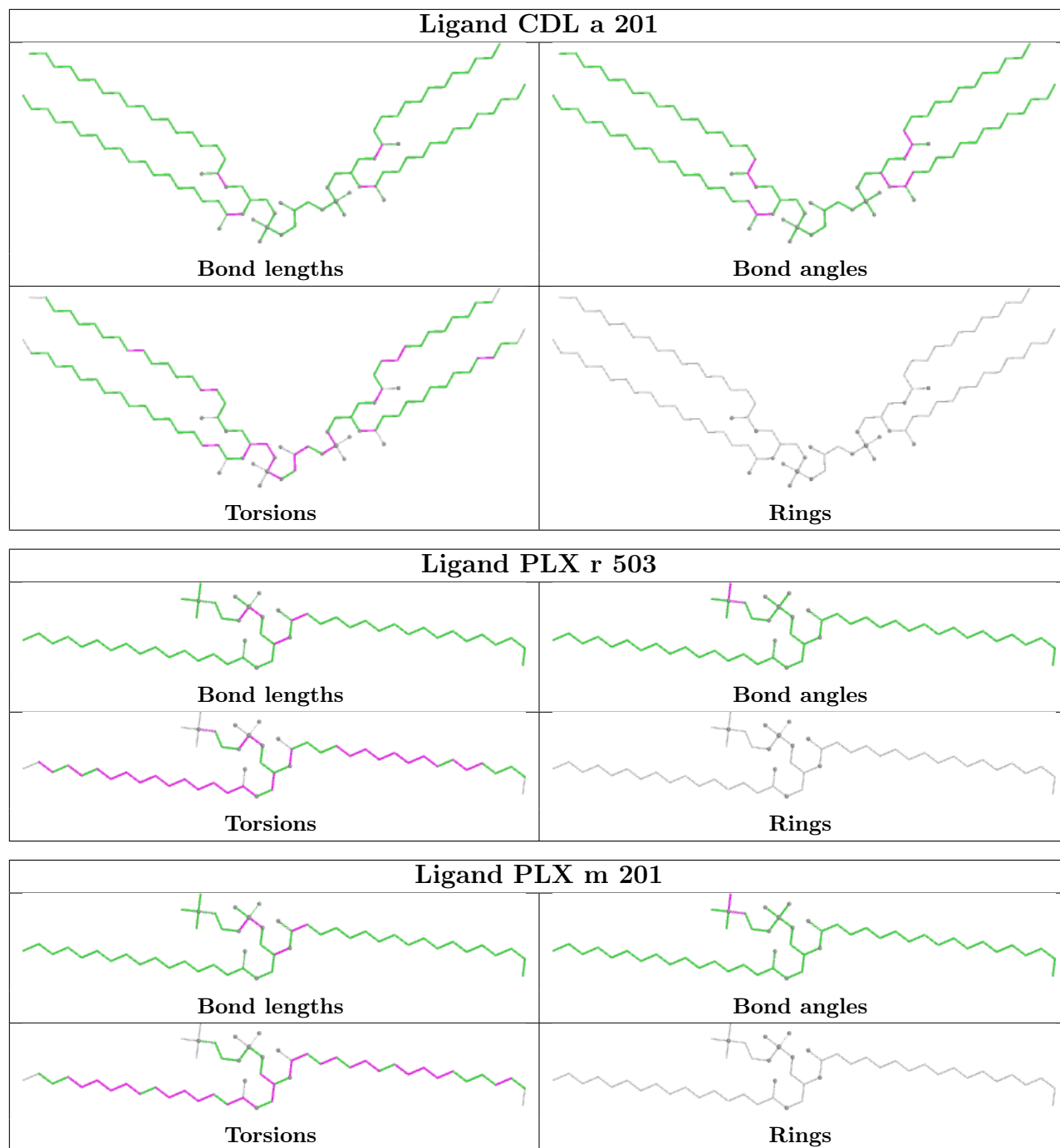


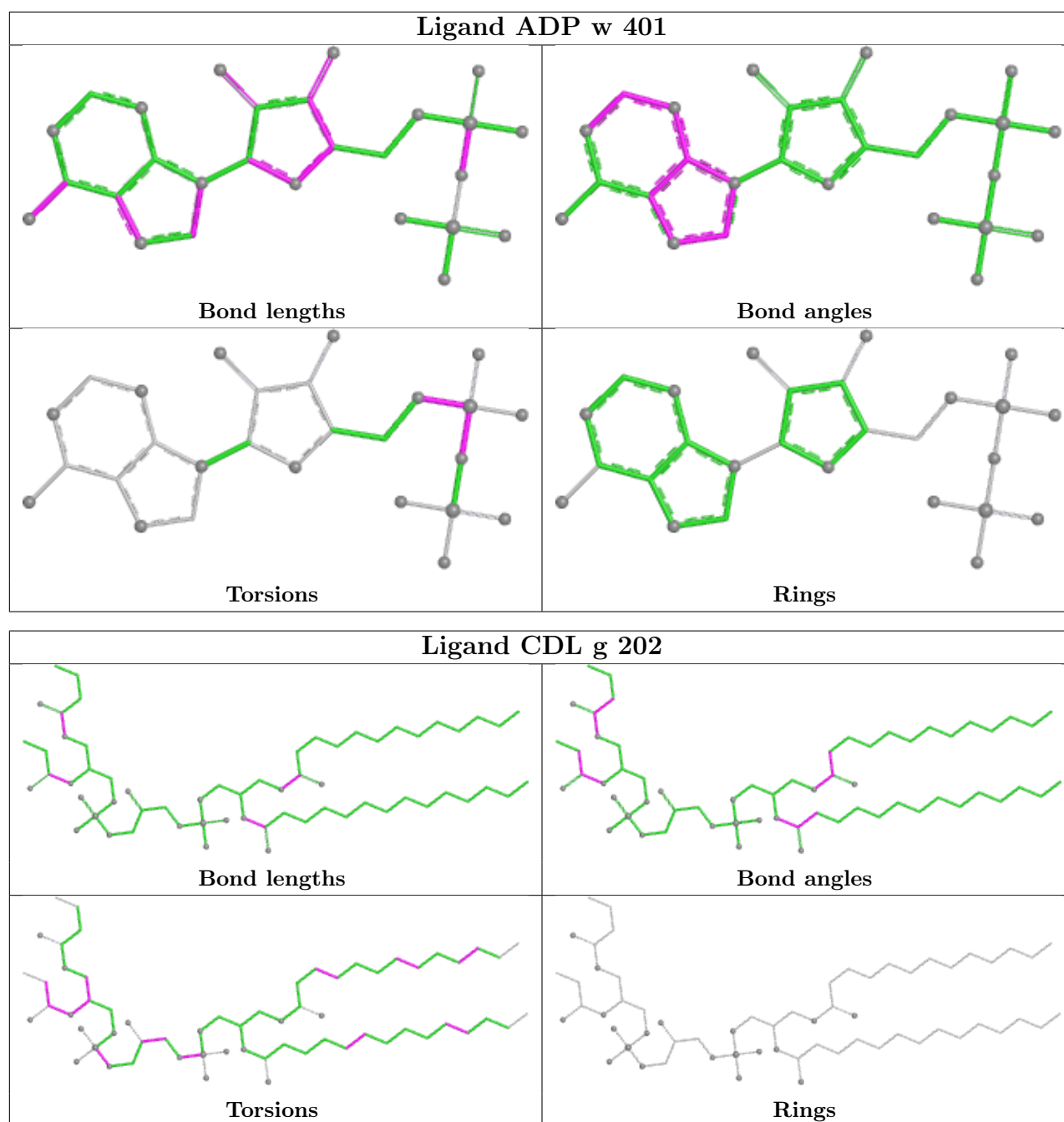












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

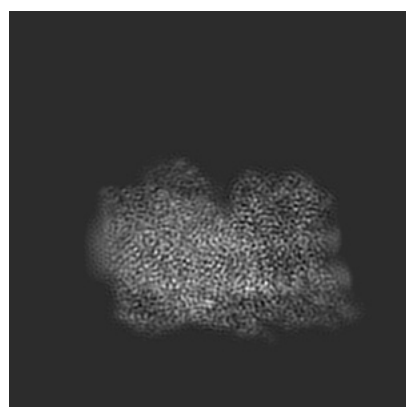
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31884. These allow visual inspection of the internal detail of the map and identification of artifacts.

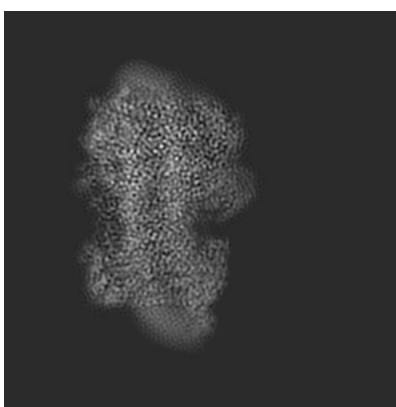
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

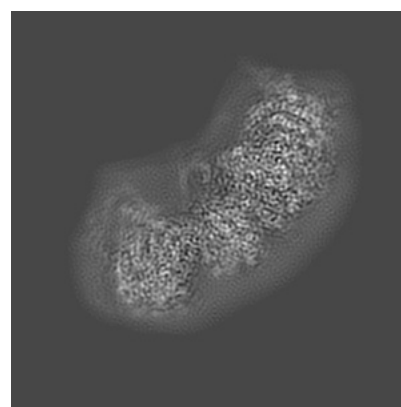
6.1.1 Primary map



X



Y

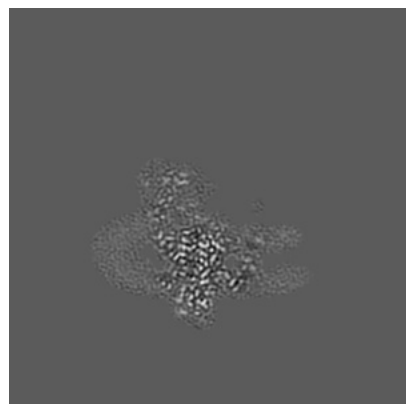


Z

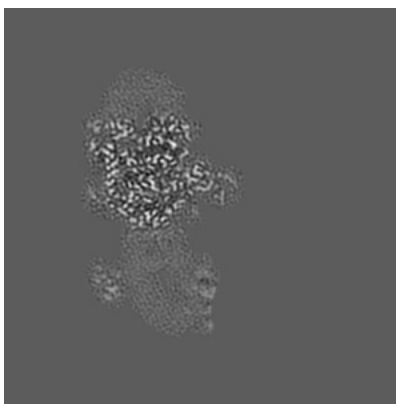
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

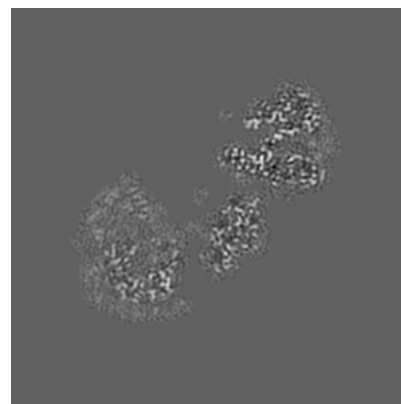
6.2.1 Primary map



X Index: 256



Y Index: 256

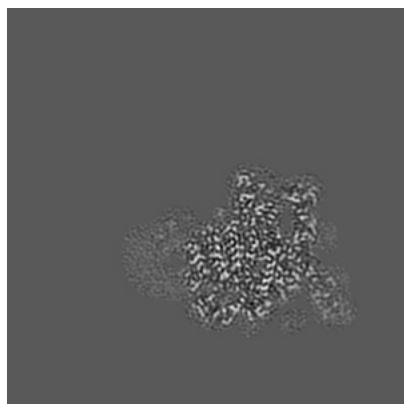


Z Index: 256

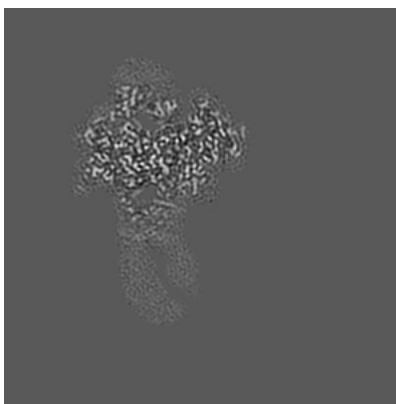
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

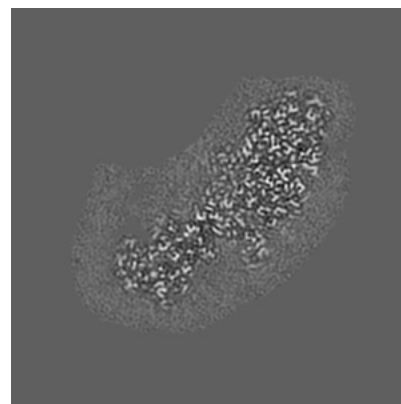
6.3.1 Primary map



X Index: 331



Y Index: 306

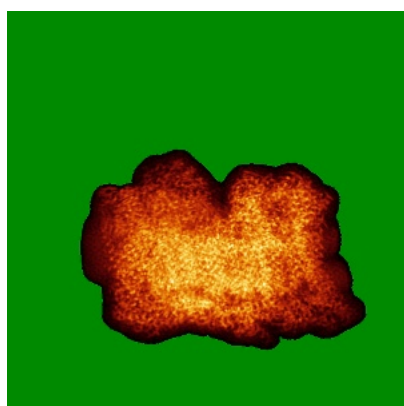


Z Index: 210

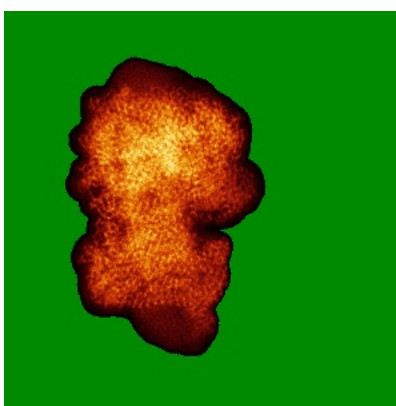
The images above show the largest variance slices of the map in three orthogonal directions.

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

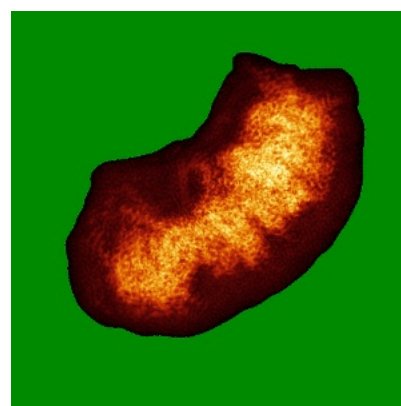
6.4.1 Primary map



X



Y

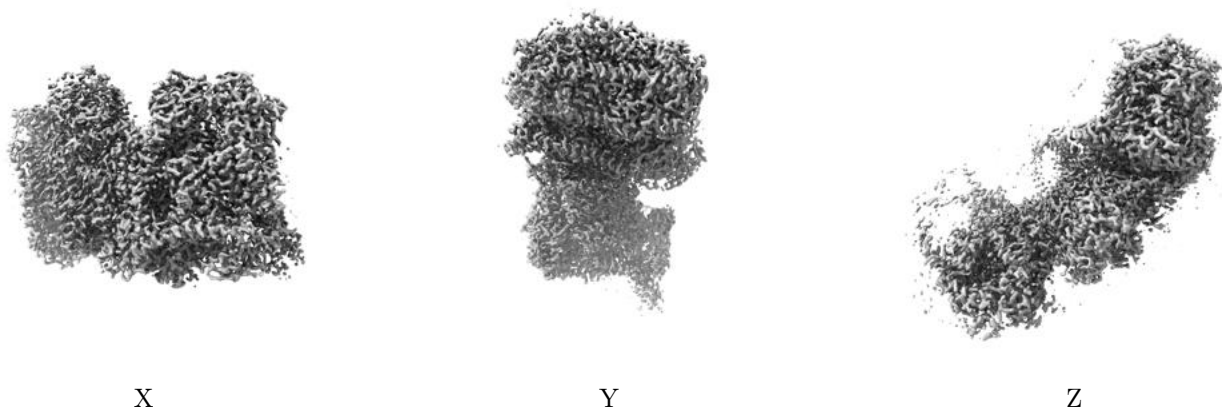


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0123. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

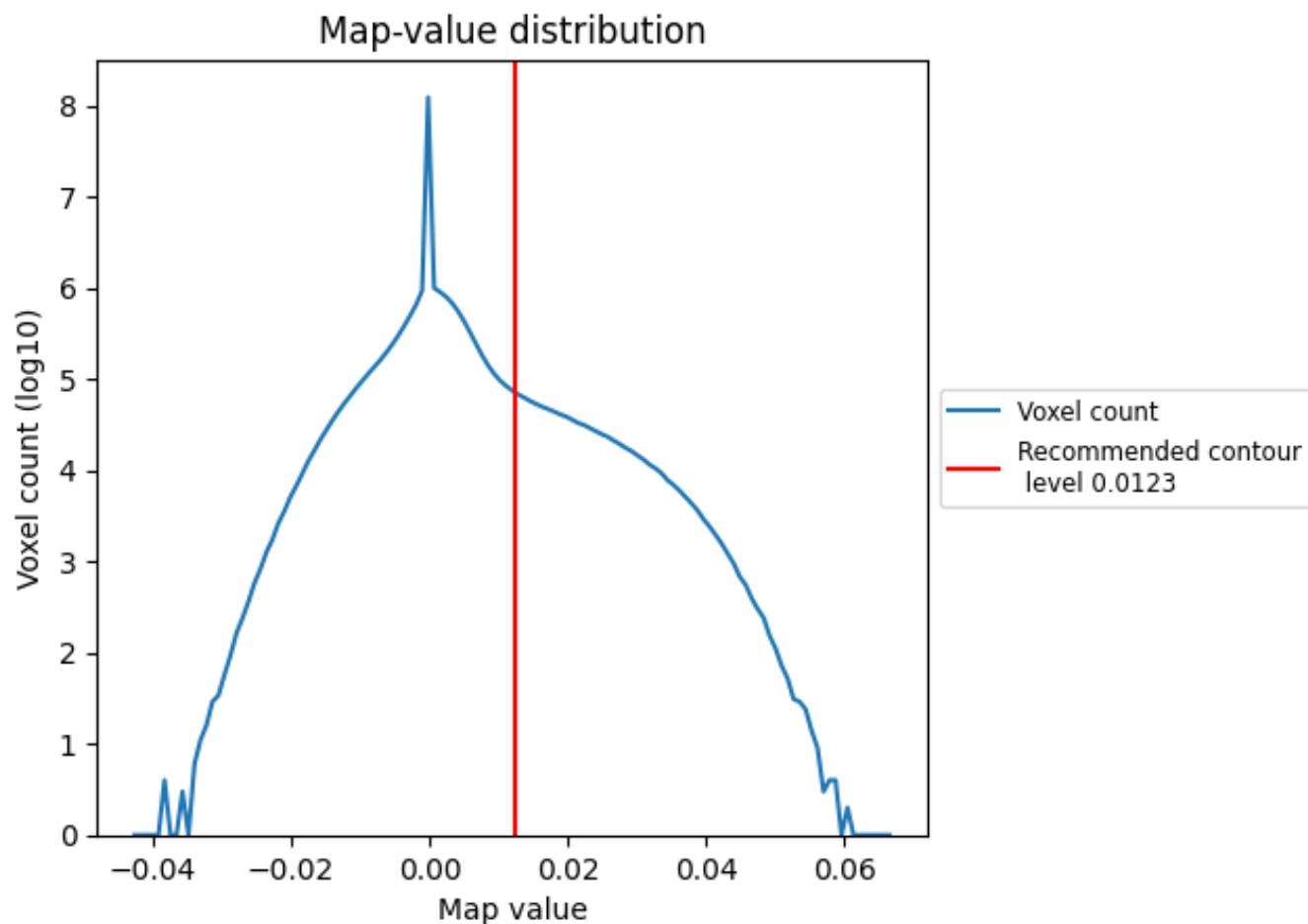
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

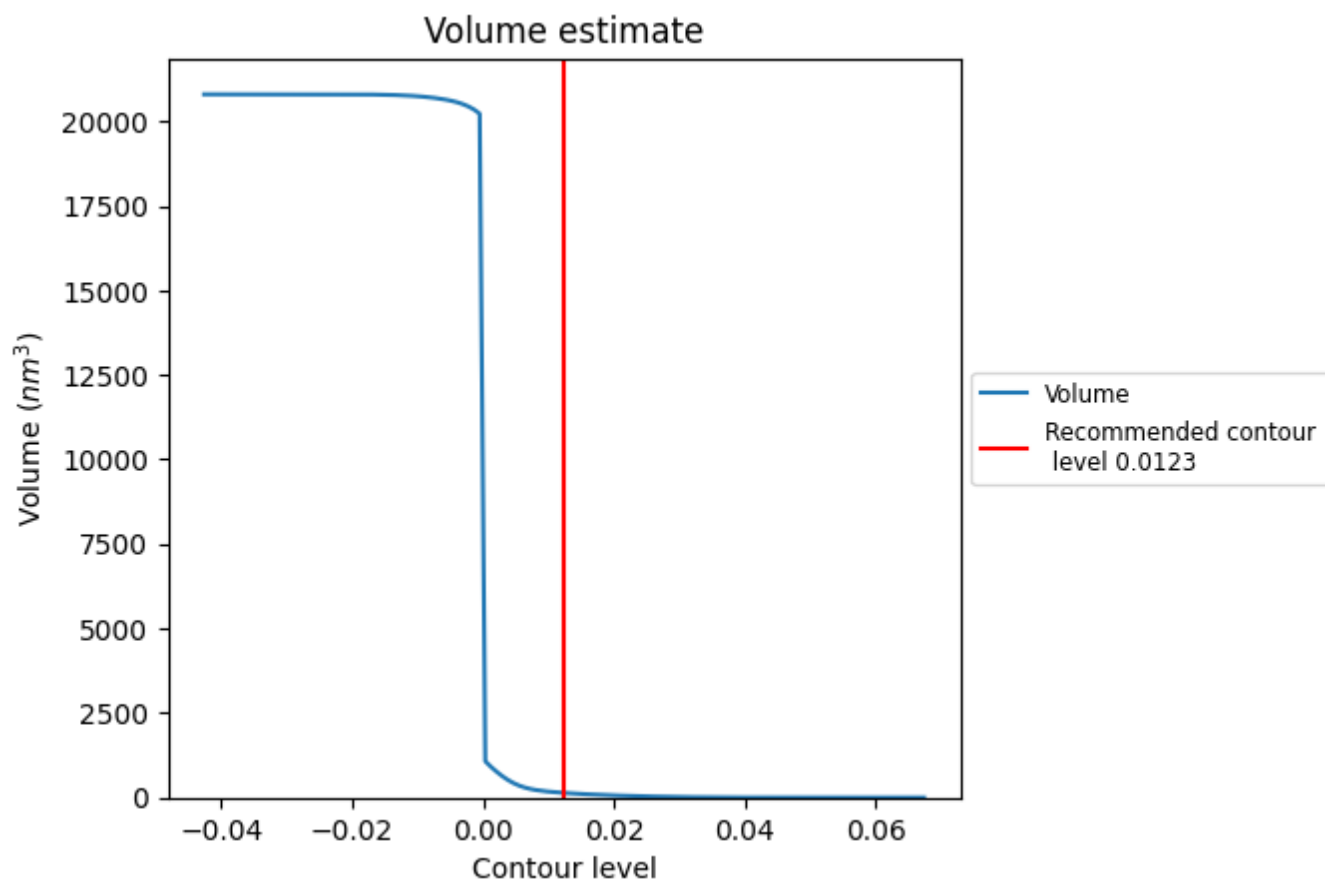
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

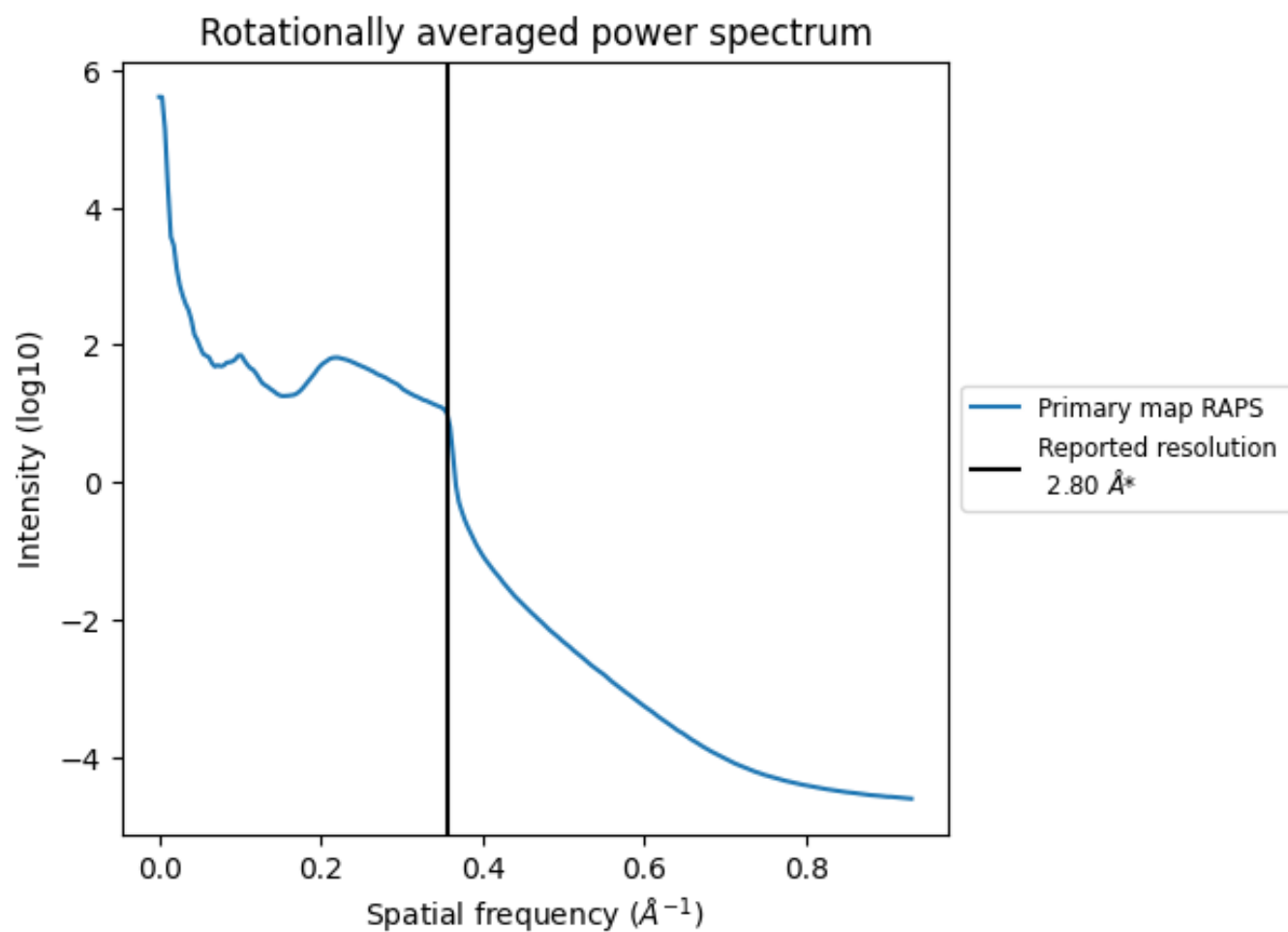
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 138 nm³; this corresponds to an approximate mass of 125 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 0.357 Å⁻¹

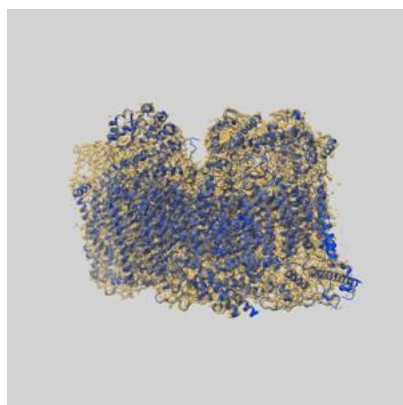
8 Fourier-Shell correlation ⓘ

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

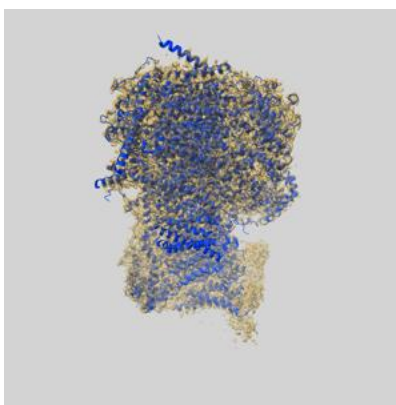
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31884 and PDB model 7VBP. Per-residue inclusion information can be found in section 3 on page 16.

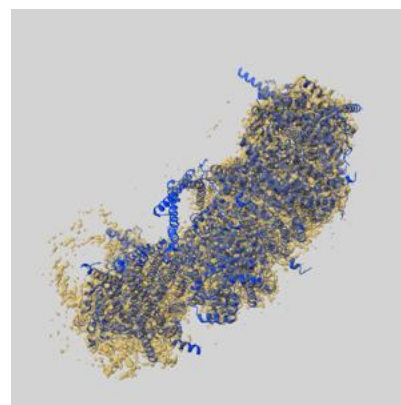
9.1 Map-model overlay [i](#)



X



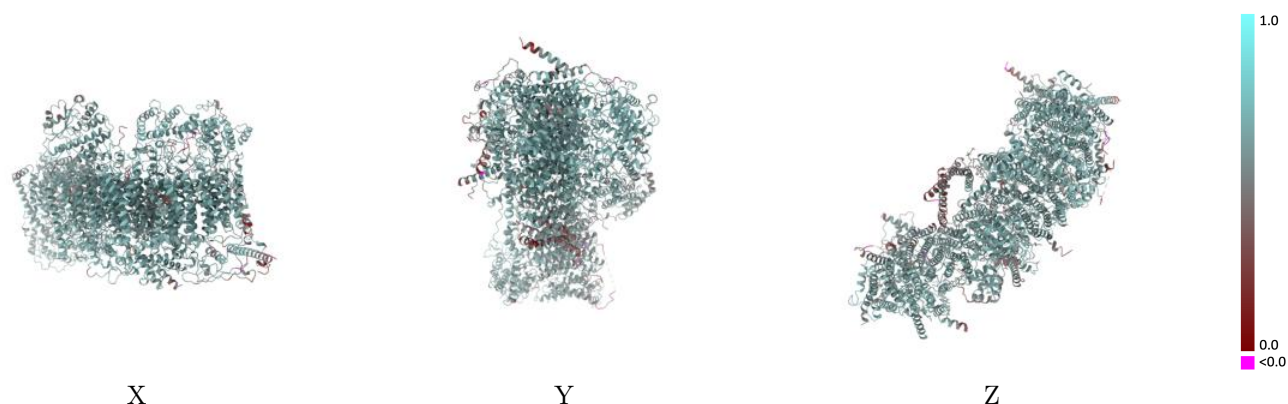
Y



Z

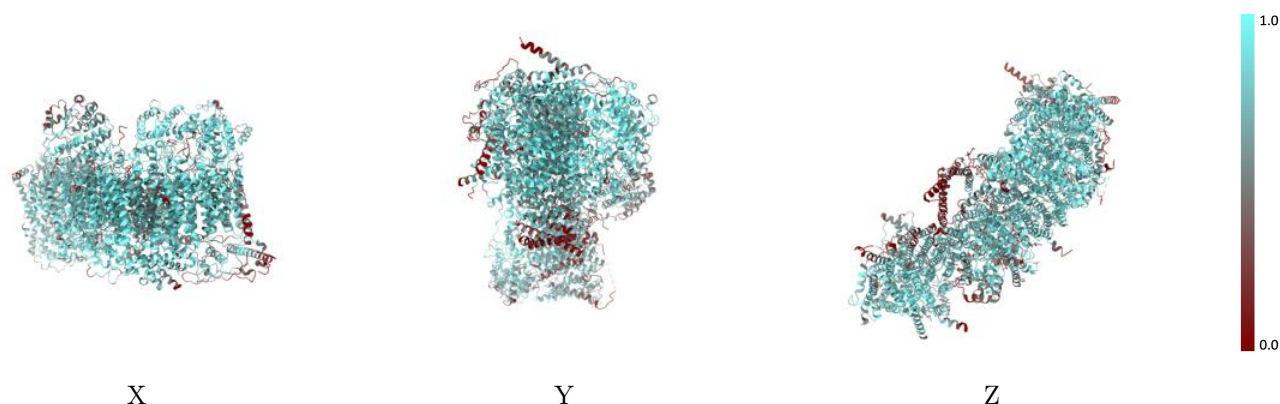
The images above show the 3D surface view of the map at the recommended contour level 0.0123 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



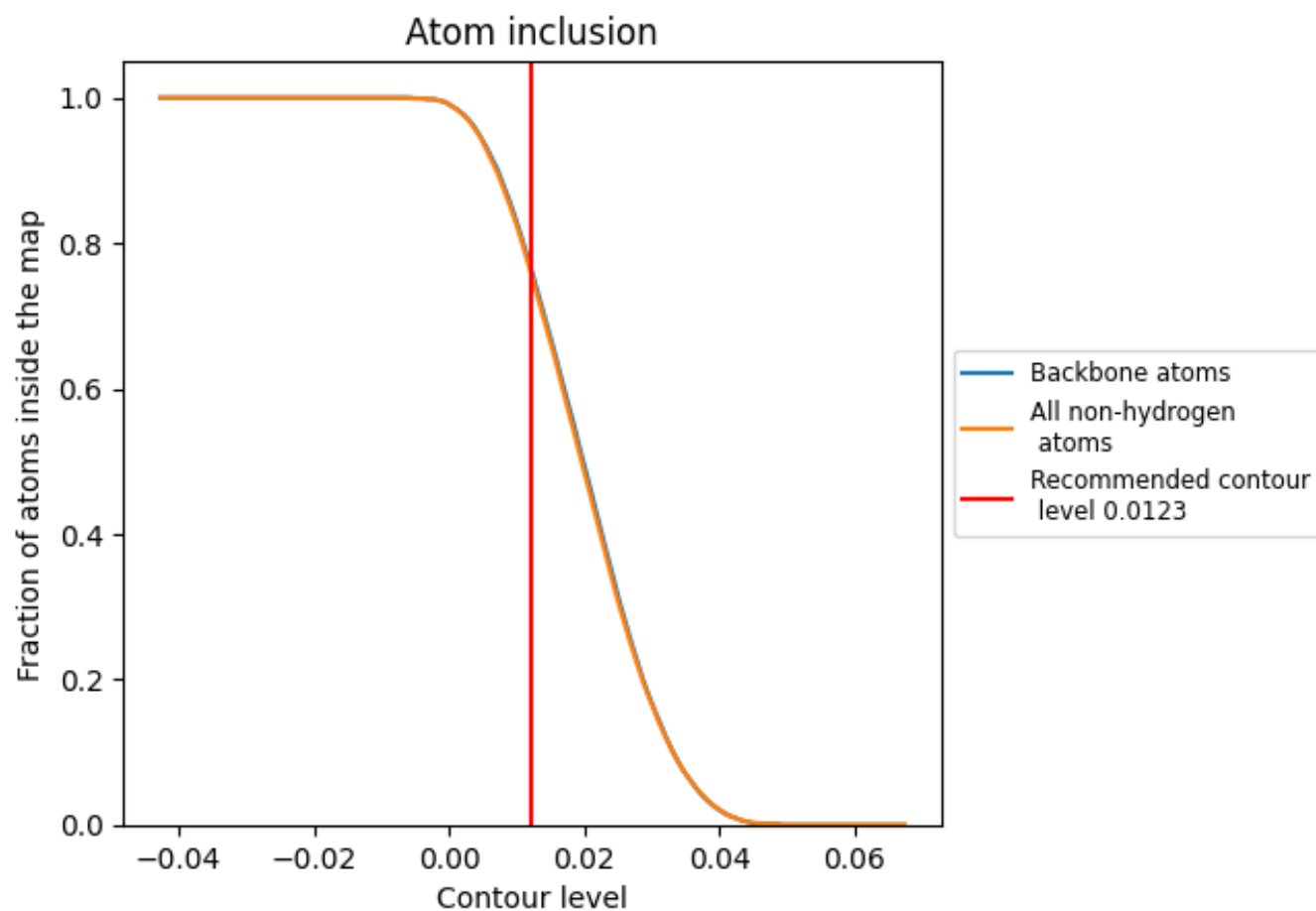
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0123).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 75% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7540	 0.6030
Q	 0.4180	 0.5380
S	 0.7740	 0.6110
U	 0.6990	 0.5860
V	 0.2780	 0.4410
W	 0.7980	 0.6210
X	 0.7660	 0.6000
Y	 0.6100	 0.5510
Z	 0.5750	 0.5190
a	 0.8120	 0.6210
b	 0.6470	 0.5550
c	 0.7910	 0.6140
d	 0.7600	 0.6060
e	 0.7420	 0.5990
f	 0.6710	 0.5760
g	 0.8210	 0.6260
h	 0.7980	 0.6170
i	 0.9050	 0.6480
j	 0.6620	 0.5670
k	 0.6480	 0.5720
l	 0.8200	 0.6270
m	 0.6270	 0.5550
n	 0.6880	 0.5750
o	 0.8040	 0.6130
p	 0.8410	 0.6240
r	 0.8950	 0.6450
s	 0.7980	 0.6130
u	 0.7470	 0.6030
v	 0.5820	 0.5380
w	 0.6660	 0.5910

