



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 08:03 AM UTC

PDB ID : 7VYE / pdb_00007vye
EMDB ID : EMD-32202
Title : Membrane arm of deactive state CI from Q10-NADH dataset
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-14
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

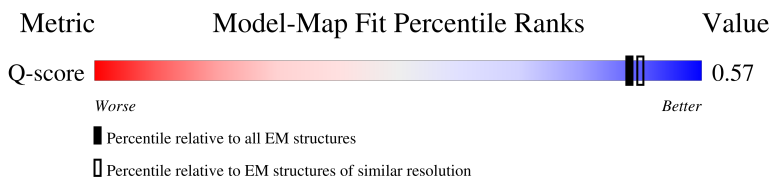
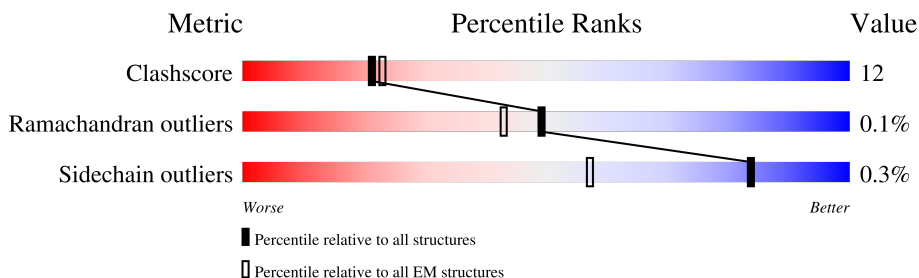
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 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.



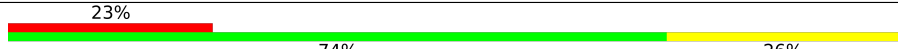
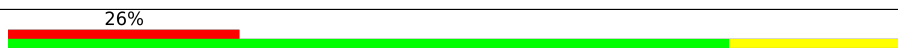
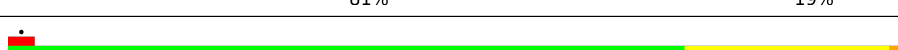
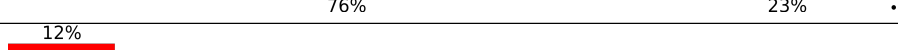
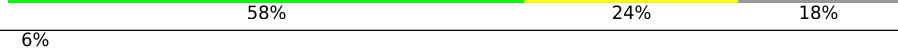
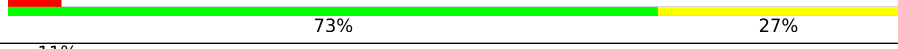
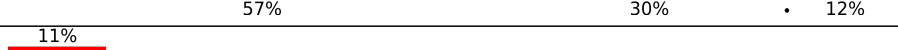
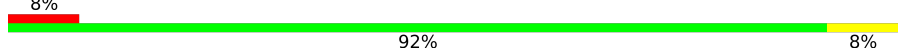
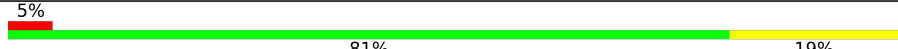
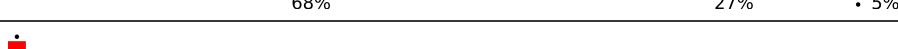
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	Q	40	
2	S	70	
3	U	83	
4	V	140	

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Mol	Chain	Length	Quality of chain
5	W	113	
6	X	88	
7	Y	70	
8	Z	84	
9	a	140	
10	b	126	
11	c	156	
12	d	175	
13	e	107	
14	f	42	
15	g	121	
16	h	105	
17	i	347	
18	j	113	
19	k	98	
20	l	603	
21	m	175	
22	n	56	
23	o	128	
24	p	178	
25	r	459	
26	s	318	
27	u	171	
28	v	126	
29	w	320	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	PEE	r	501	-	-	X	-
31	CDL	l	701	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 38846 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.

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
			1015	648	171	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
			945	612	160	165	8		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	88	Total	C	N	O	S	0	0
			699	449	103	142	5		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase AGGG subunit.

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-ubiquinone oxidoreductase B12 subunit.

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-ubiquinone oxidoreductase SGDHD subunit.

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-ubiquinone oxidoreductase KFYI subunit.

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
			4785	3173	741	820	51		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	n	56	Total	C	N	O	S	0	0
			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 sub-

unit 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-ubiquinone oxidoreductase B18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	124	Total	C	N	O	S	0	0
			1012	633	188	182	9		

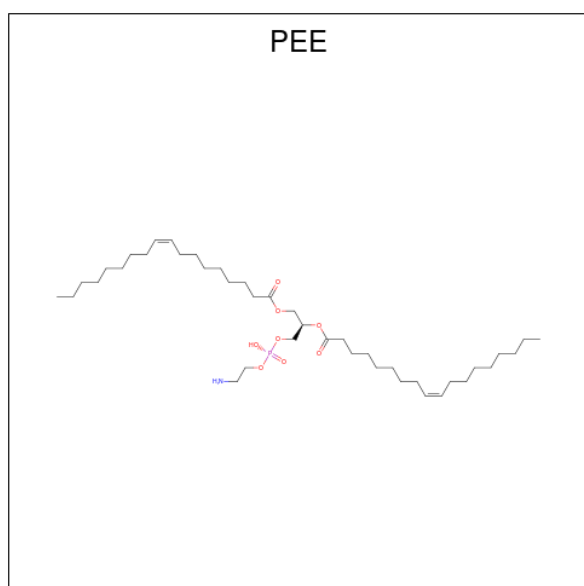
There is a discrepancy between the modelled and reference sequences:

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.

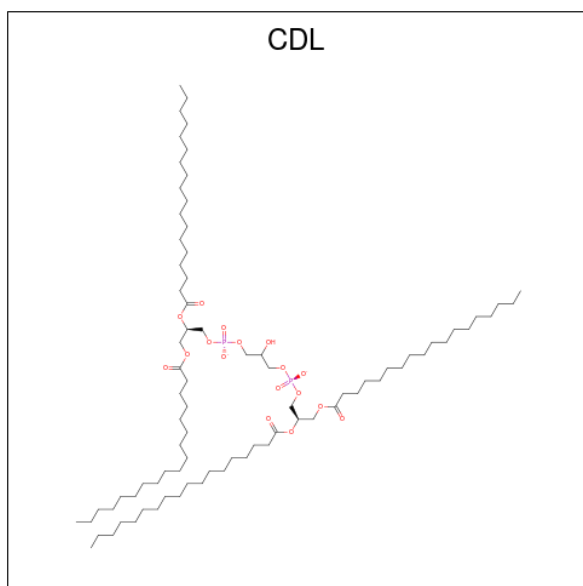
Mol	Chain	Residues	Atoms					AltConf	Trace
29	w	320	Total	C	N	O	S	0	0
			2583	1646	437	491	9		

- Molecule 30 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
30	U	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	V	1	Total	C	N	O	P	0
			40	30	1	8	1	
30	b	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
30	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
30	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
30	s	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: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



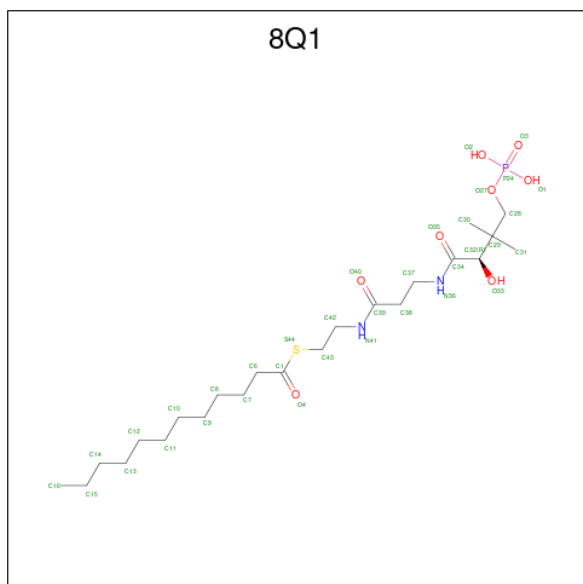
Mol	Chain	Residues	Atoms				AltConf
31	V	1	Total	C	O	P	0
			94	75	17	2	
31	a	1	Total	C	O	P	0
			91	72	17	2	
31	g	1	Total	C	O	P	0
			97	78	17	2	

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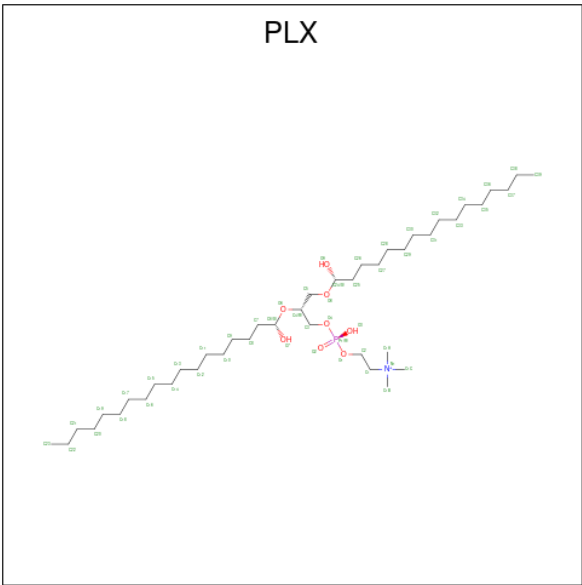
Mol	Chain	Residues	Atoms				AltConf
31	i	1	Total	C	O	P	0
			66	47	17	2	
31	l	1	Total	C	O	P	0
			99	80	17	2	
31	l	1	Total	C	O	P	0
			100	81	17	2	
31	o	1	Total	C	O	P	0
			68	49	17	2	
31	u	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 32 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS) (labeled as "Ligand of Interest" by depositor).



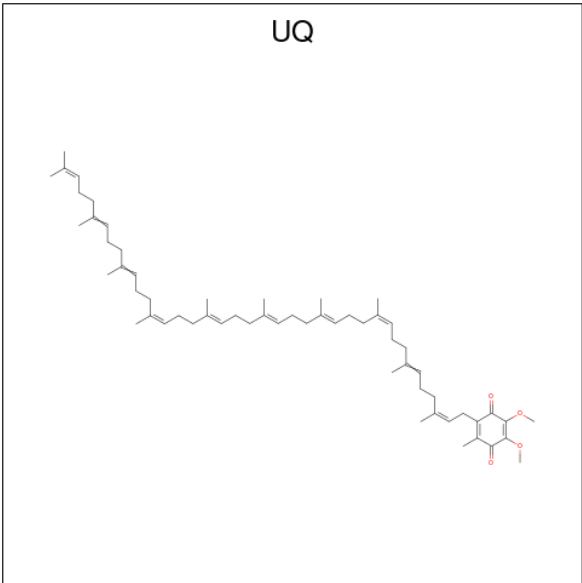
Mol	Chain	Residues	Atoms						AltConf
32	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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



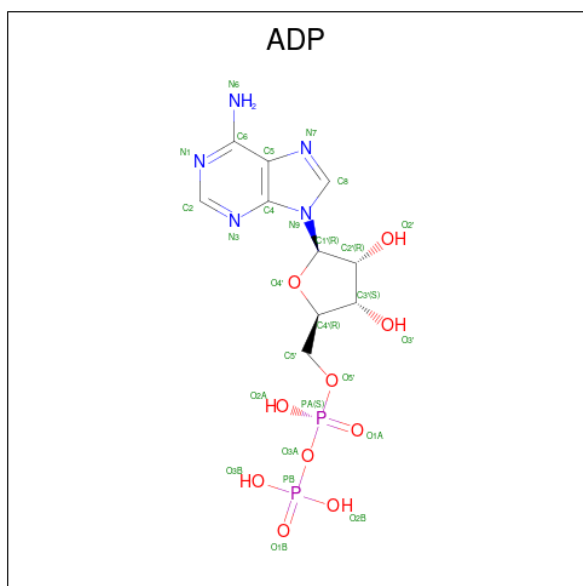
Mol	Chain	Residues	Atoms					AltConf
33	a	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	j	1	Total	C	N	O	P	0
			52	42	1	8	1	
33	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- 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: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

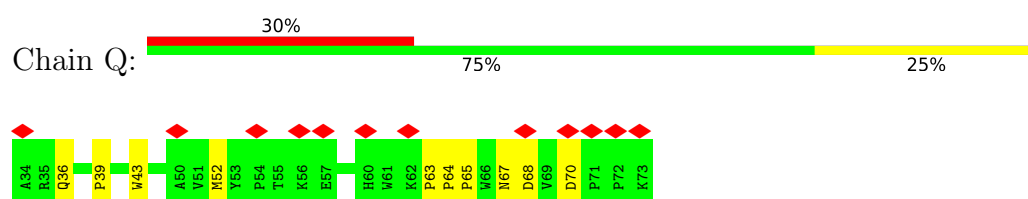


Mol	Chain	Residues	Atoms					AltConf
35	w	1	Total	C	N	O	P	0
			27	10	5	10	2	

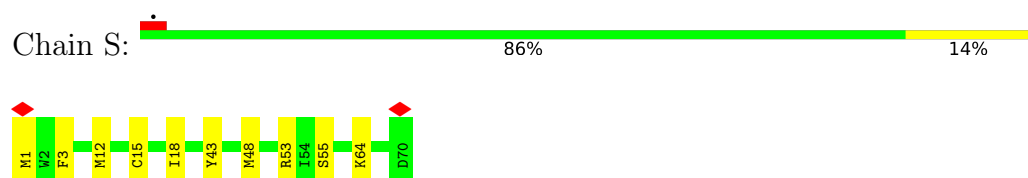
3 Residue-property plots [i](#)

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

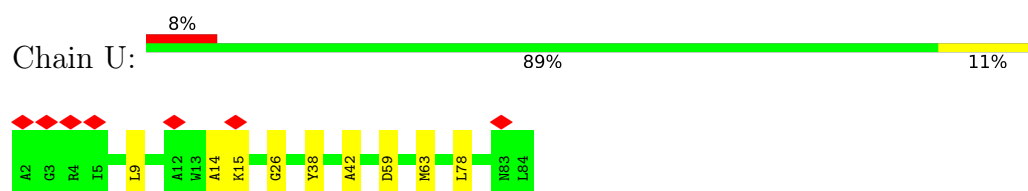
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2



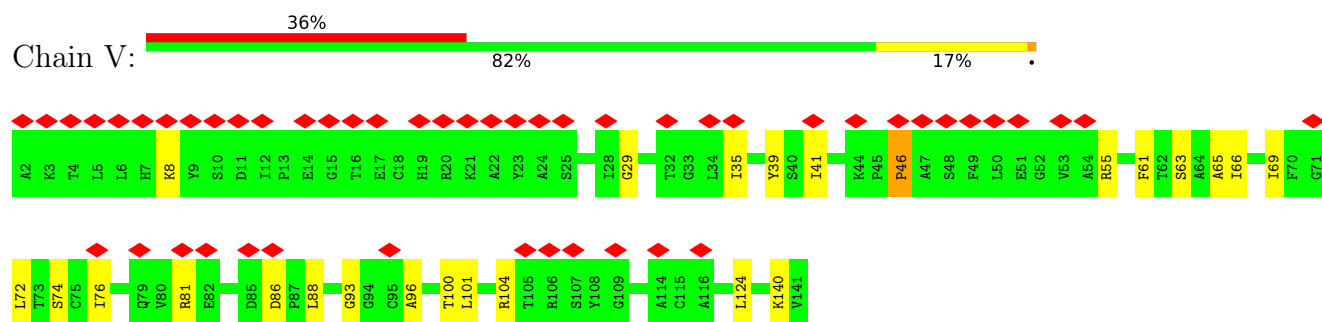
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



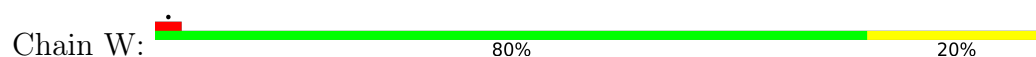
- Molecule 3: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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

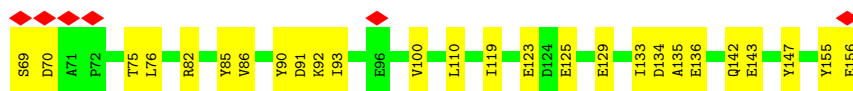


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

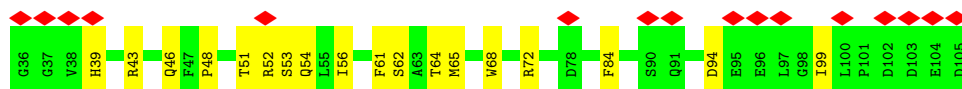




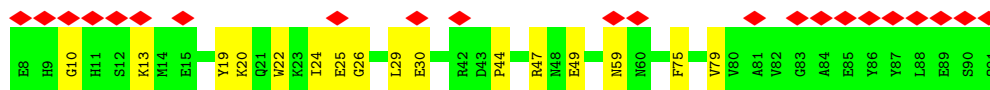
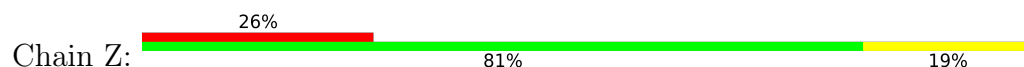
- Molecule 6: Acyl carrier protein



- Molecule 7: NADH-ubiquinone oxidoreductase AGGG subunit



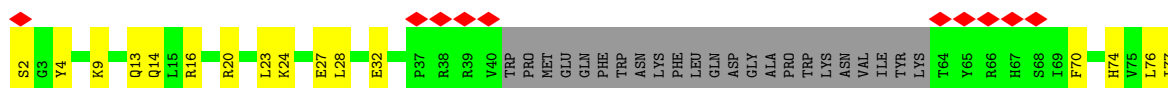
- Molecule 8: NADH-ubiquinone oxidoreductase B12 subunit



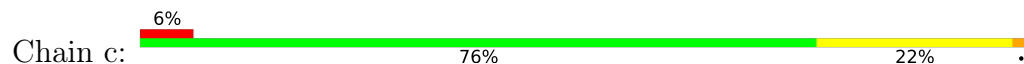
- Molecule 9: NADH-ubiquinone oxidoreductase SGD subunit

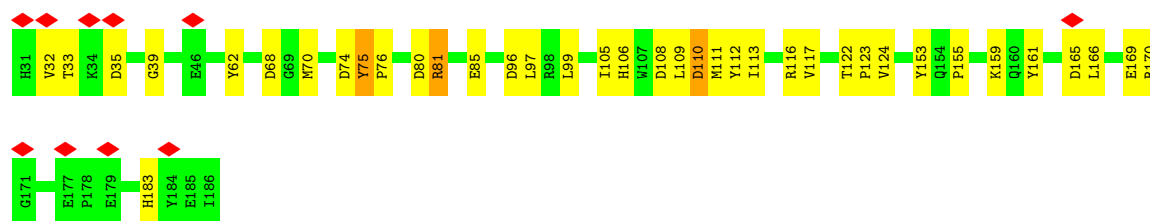


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

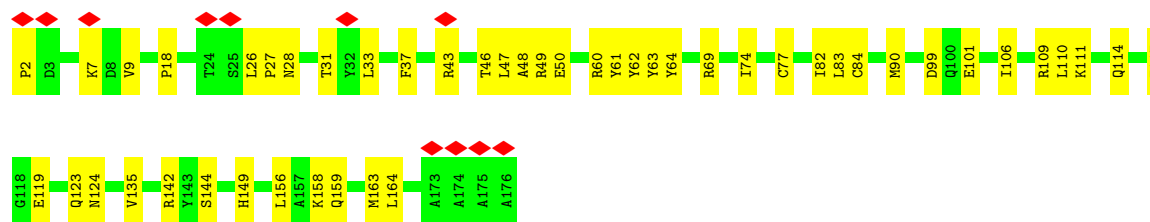
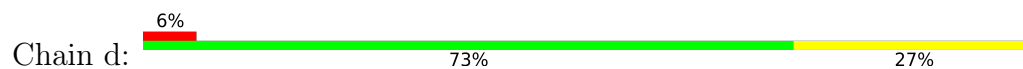


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

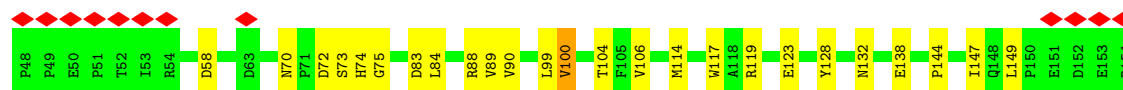
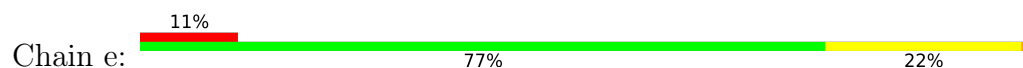




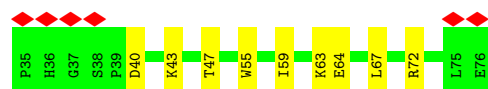
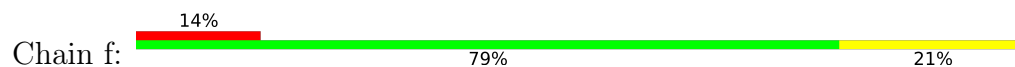
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



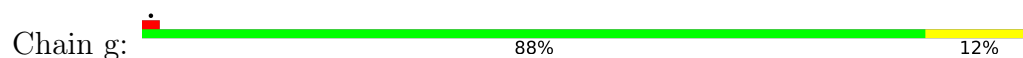
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



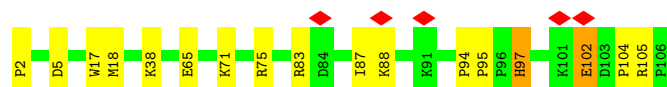
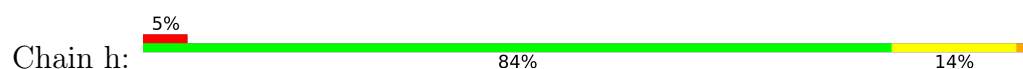
- Molecule 14: NADH-ubiquinone oxidoreductase KFYI subunit



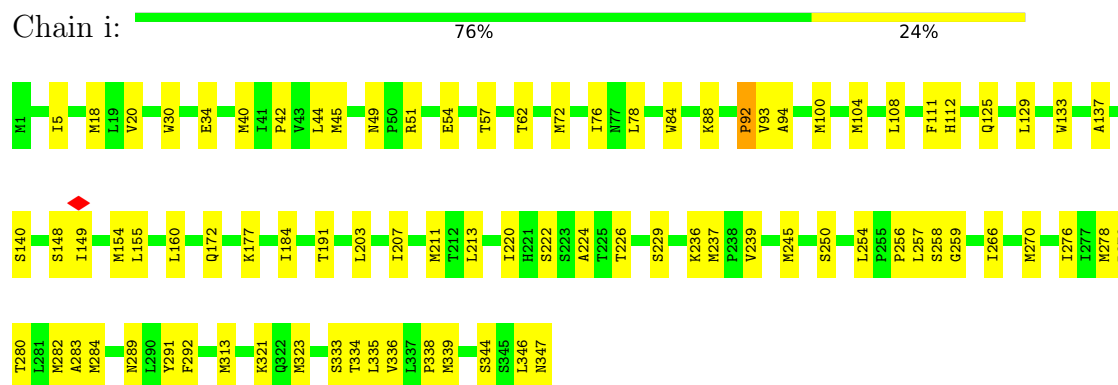
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2



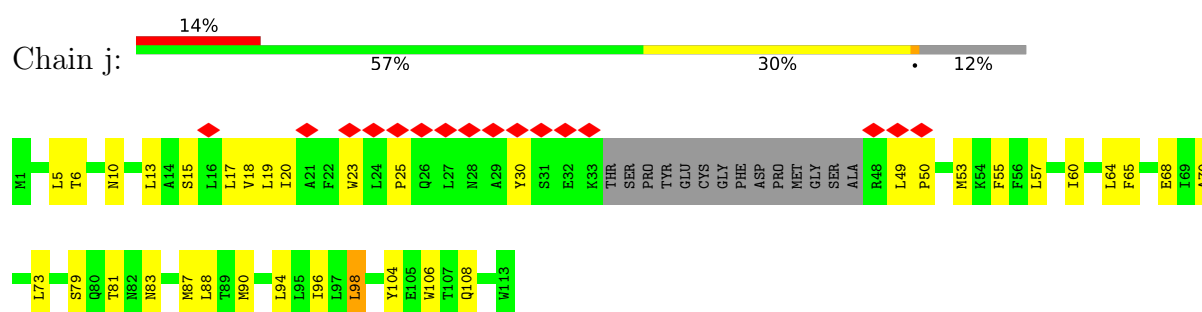
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



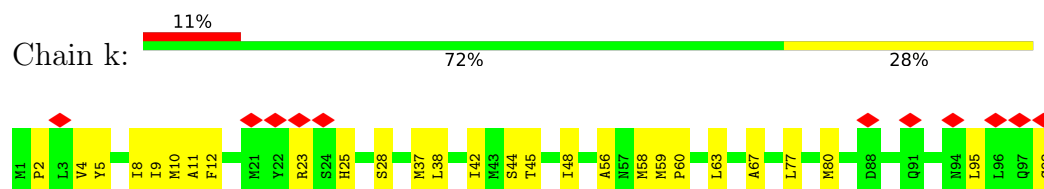
- Molecule 17: NADH-ubiquinone oxidoreductase chain 2



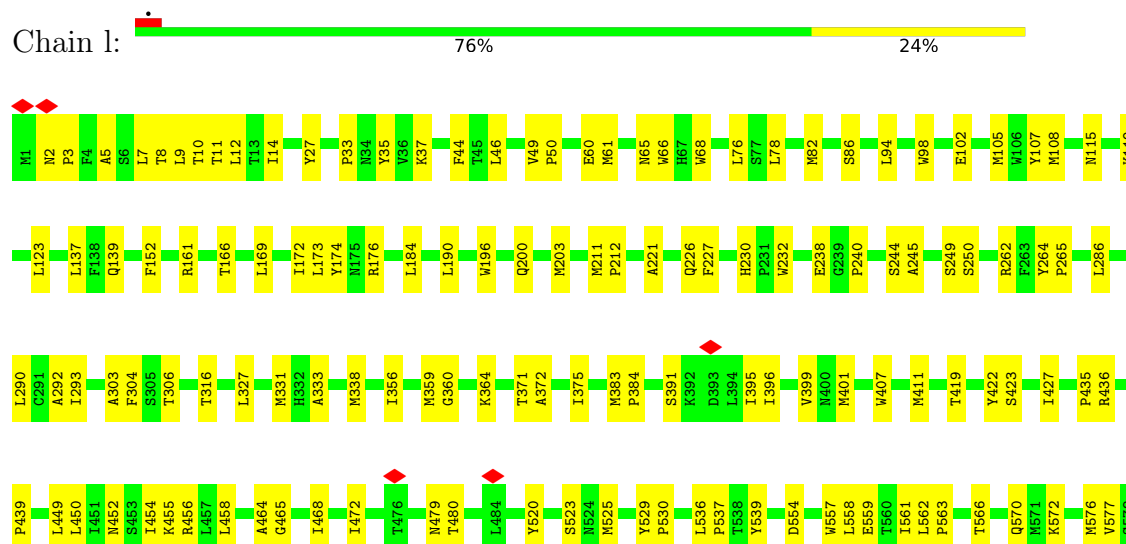
- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

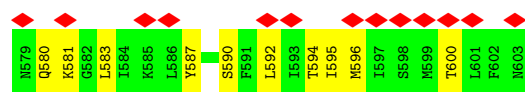


- Molecule 19: NADH-ubiquinone oxidoreductase chain 4L

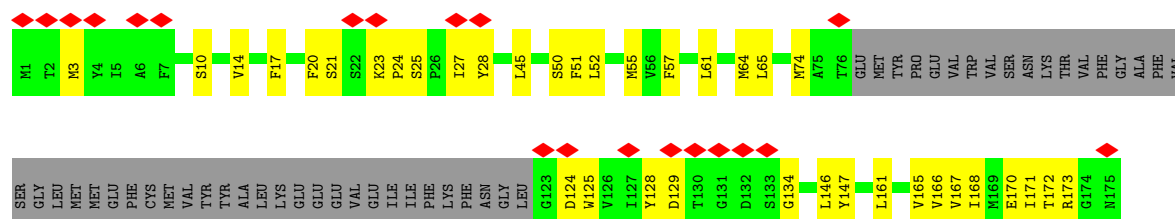


- Molecule 20: NADH-ubiquinone oxidoreductase chain 5

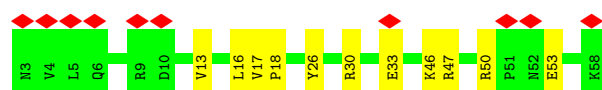
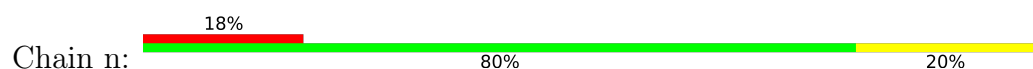




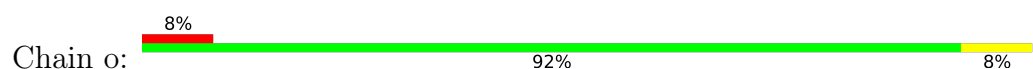
- Molecule 21: NADH-ubiquinone oxidoreductase chain 6



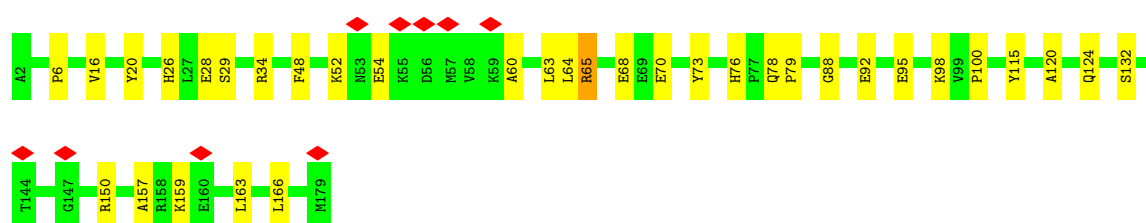
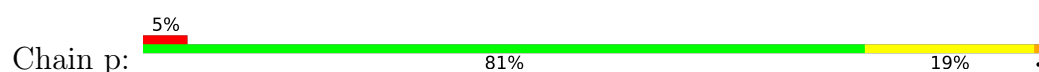
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



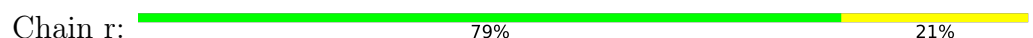
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

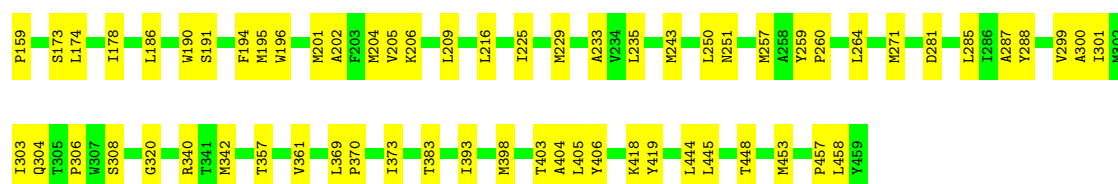


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

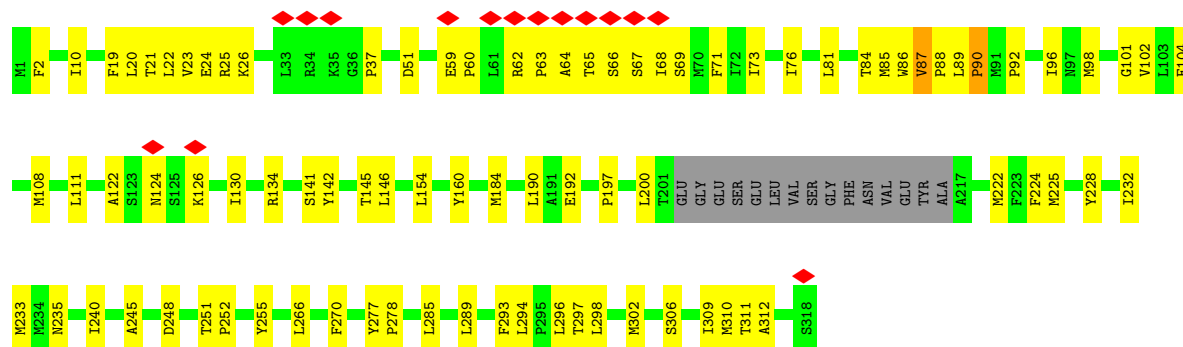


- Molecule 25: NADH-ubiquinone oxidoreductase chain 4

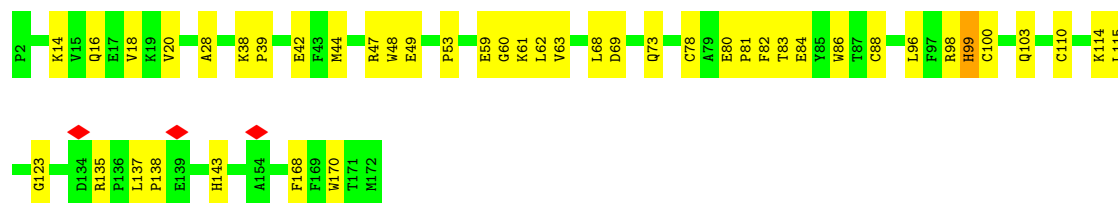




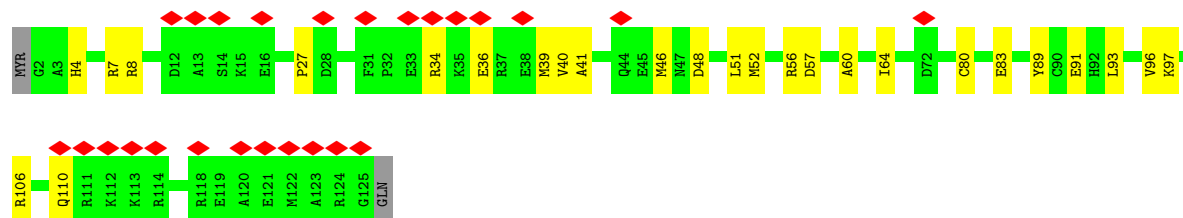
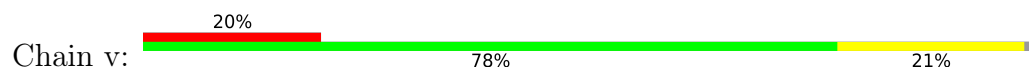
• Molecule 26: NADH-ubiquinone oxidoreductase chain 1



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

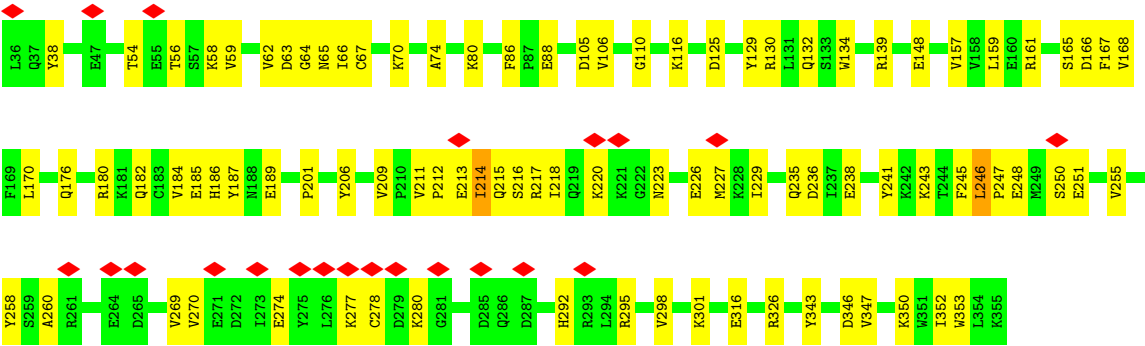


• Molecule 28: NADH-ubiquinone oxidoreductase B18 subunit



• 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	104881	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	0.157	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0306	Depositor
Map size ($\text{\AA}$)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.15	0/350	0.33	0/483
2	S	0.21	0/582	0.42	0/783
3	U	0.16	0/664	0.31	0/912
4	V	0.22	0/1036	0.53	2/1404 (0.1%)
5	W	0.23	0/969	0.41	0/1307
6	X	0.17	0/711	0.37	0/963
7	Y	0.15	0/626	0.34	0/857
8	Z	0.16	0/695	0.35	0/939
9	a	0.23	0/1199	0.62	2/1623 (0.1%)
10	b	0.21	0/906	0.54	1/1232 (0.1%)
11	c	0.23	0/1371	0.52	2/1875 (0.1%)
12	d	0.16	0/1494	0.29	0/2015
13	e	0.21	0/916	0.54	2/1246 (0.2%)
14	f	0.15	0/350	0.30	0/473
15	g	0.18	0/1031	0.32	0/1394
16	h	0.22	0/889	0.51	0/1190
17	i	0.21	0/2773	0.39	0/3768
18	j	0.28	0/819	0.48	0/1117
19	k	0.22	0/759	0.39	0/1029
20	l	0.20	0/4914	0.39	0/6683
21	m	0.21	0/973	0.41	0/1320
22	n	0.22	0/491	0.59	1/663 (0.2%)
23	o	0.17	0/1092	0.33	0/1481
24	p	0.18	0/1590	0.38	1/2155 (0.0%)
25	r	0.23	0/3723	0.42	0/5078
26	s	0.25	0/2464	0.53	2/3369 (0.1%)
27	u	0.23	0/1436	0.52	1/1938 (0.1%)
28	v	0.17	0/1036	0.48	0/1393
29	w	0.20	0/2643	0.45	1/3580 (0.0%)
All	All	0.21	0/38502	0.44	15/52270 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	a	94	GLY	N-CA-C	10.19	123.28	111.36
9	a	92	PHE	N-CA-C	8.66	120.80	111.36
11	c	75	TYR	CA-C-N	8.26	128.19	119.85
11	c	75	TYR	C-N-CA	8.26	128.19	119.85
26	s	87	VAL	CA-C-N	8.07	127.65	118.85
26	s	87	VAL	C-N-CA	8.07	127.65	118.85
13	e	100	VAL	N-CA-C	6.75	116.88	110.53
4	V	86	ASP	CA-C-N	6.50	126.26	119.05
4	V	86	ASP	C-N-CA	6.50	126.26	119.05
10	b	76	LEU	N-CA-C	6.12	118.03	111.36
29	w	243	LYS	N-CA-C	6.03	117.93	111.36
22	n	16	LEU	N-CA-C	5.85	117.66	111.28
27	u	99	HIS	N-CA-C	5.33	117.09	111.28
13	e	99	LEU	N-CA-C	5.32	116.88	111.14
24	p	65	ARG	N-CA-C	-5.20	105.23	112.45

There are no chirality outliers.

There are no planarity outliers.

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	7	0
2	S	567	0	565	7	0
3	U	643	0	642	9	0
4	V	1015	0	1016	25	0
5	W	945	0	931	27	0
6	X	699	0	674	19	0
7	Y	600	0	539	12	0
8	Z	674	0	643	12	0
9	a	1165	0	1174	38	0
10	b	879	0	899	34	0
11	c	1315	0	1208	35	0
12	d	1461	0	1429	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	e	890	0	837	19	0
14	f	342	0	341	6	0
15	g	1000	0	994	14	0
16	h	867	0	871	16	0
17	i	2710	0	2874	78	0
18	j	800	0	855	38	0
19	k	748	0	799	23	0
20	l	4785	0	4933	117	0
21	m	951	0	962	38	0
22	n	479	0	486	14	0
23	o	1062	0	1072	9	0
24	p	1534	0	1470	30	0
25	r	3631	0	3839	93	0
26	s	2394	0	2508	76	0
27	u	1398	0	1378	35	0
28	v	1012	0	947	21	0
29	w	2583	0	2539	63	0
30	U	51	0	82	6	0
30	V	40	0	54	6	0
30	b	46	0	69	18	0
30	i	47	0	71	10	0
30	l	46	0	69	8	0
30	r	51	0	82	21	0
30	s	92	0	141	10	0
31	V	94	0	138	19	0
31	a	91	0	132	16	0
31	g	97	0	147	8	0
31	i	66	0	76	16	0
31	l	199	0	307	46	0
31	o	68	0	83	14	0
31	u	78	0	103	13	0
32	X	35	0	0	2	0
33	a	52	0	88	9	0
33	g	52	0	88	1	0
33	j	52	0	88	2	0
33	r	52	0	88	7	0
34	s	28	0	31	5	0
35	w	27	0	11	4	0
All	All	38846	0	39674	928	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (928) 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)
9:a:96:ALA:HB2	12:d:61:TYR:CE2	1.52	1.41
31:V:202:CDL:H601	31:V:202:CDL:H732	1.24	1.18
30:i:402:PEE:H36	30:i:402:PEE:H28	1.25	1.17
25:r:201:MET:CE	30:r:501:PEE:H78	1.75	1.15
31:o:201:CDL:H112	31:o:201:CDL:H342	1.26	1.13
31:l:701:CDL:H842	31:l:701:CDL:H631	1.14	1.13
25:r:201:MET:HE2	30:r:501:PEE:H77	1.14	1.12
31:l:701:CDL:H791	31:l:701:CDL:H611	1.33	1.11
31:l:701:CDL:H601	31:l:701:CDL:H772	1.26	1.09
25:r:201:MET:HE2	30:r:501:PEE:C45	1.82	1.09
22:n:13:VAL:CG1	25:r:14:MET:HG2	1.82	1.09
26:s:87:VAL:HG23	26:s:88:PRO:HD3	1.21	1.09
30:V:201:PEE:H2	30:V:201:PEE:H9	1.25	1.07
25:r:251:ASN:HD21	25:r:304:GLN:NE2	1.52	1.07
31:l:701:CDL:H541	31:l:701:CDL:HA62	1.35	1.06
24:p:64:LEU:O	24:p:68:GLU:HG2	1.55	1.06
31:l:701:CDL:H422	25:r:448:THR:HG21	1.36	1.06
29:w:67:CYS:CB	29:w:218:ILE:HD11	1.85	1.06
22:n:13:VAL:HG12	25:r:14:MET:HG2	1.08	1.03
18:j:68:GLU:OE2	18:j:98:LEU:HD22	1.60	1.01
25:r:201:MET:CE	30:r:501:PEE:H77	1.91	0.99
9:a:96:ALA:CB	12:d:61:TYR:CE2	2.45	0.99
31:l:701:CDL:H312	31:l:701:CDL:H742	1.01	0.98
31:o:201:CDL:H791	31:o:201:CDL:H832	1.42	0.98
31:l:701:CDL:H742	31:l:701:CDL:C31	1.93	0.97
31:a:201:CDL:H521	30:b:201:PEE:H13	1.47	0.96
31:l:701:CDL:H842	31:l:701:CDL:C63	1.96	0.96
17:i:133:TRP:HE3	31:i:401:CDL:H392	1.31	0.96
4:V:61:PHE:HD2	4:V:104:ARG:HH12	0.98	0.95
25:r:201:MET:CE	30:r:501:PEE:C46	2.45	0.95
4:V:66:ILE:HD11	4:V:101:LEU:HD13	1.48	0.94
26:s:87:VAL:CG2	26:s:88:PRO:HD3	1.97	0.94
5:W:98:MET:HE2	5:W:104:TRP:CE2	2.04	0.93
26:s:84:THR:O	26:s:87:VAL:HG22	1.69	0.92
31:a:201:CDL:H521	30:b:201:PEE:C11	1.99	0.91
25:r:251:ASN:HD21	25:r:304:GLN:HE22	0.94	0.91
17:i:133:TRP:CE3	31:i:401:CDL:H392	2.06	0.90
30:V:201:PEE:H2	30:V:201:PEE:C4	2.00	0.90
9:a:96:ALA:HB2	12:d:61:TYR:HE2	1.31	0.89
31:l:701:CDL:H791	31:l:701:CDL:C61	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:i:402:PEE:H28	30:i:402:PEE:C22	2.03	0.89
26:s:87:VAL:HG23	26:s:88:PRO:CD	2.04	0.88
25:r:201:MET:HE3	30:r:501:PEE:H78	1.55	0.88
4:V:69:ILE:HG13	4:V:100:THR:HG21	1.55	0.87
31:l:701:CDL:H312	31:l:701:CDL:C74	1.97	0.87
30:l:703:PEE:H7	30:l:703:PEE:C11	2.04	0.87
25:r:201:MET:CE	30:r:501:PEE:C45	2.52	0.87
31:a:201:CDL:H251	31:a:201:CDL:H211	1.57	0.87
31:a:201:CDL:H532	30:b:201:PEE:H56	1.55	0.86
19:k:37:MET:HE1	21:m:64:MET:HE1	1.56	0.86
31:o:201:CDL:H112	31:o:201:CDL:C34	2.05	0.86
5:W:85:GLN:O	5:W:89:GLU:HG2	1.76	0.86
17:i:321:LYS:HE3	31:i:401:CDL:OA4	1.77	0.85
31:l:701:CDL:HA62	31:l:701:CDL:C54	2.07	0.84
27:u:96:LEU:HD12	27:u:99:HIS:CD2	2.12	0.84
29:w:67:CYS:CB	29:w:218:ILE:CD1	2.56	0.83
4:V:61:PHE:HD2	4:V:104:ARG:NH1	1.77	0.83
31:o:201:CDL:H342	31:o:201:CDL:C11	2.07	0.83
30:s:401:PEE:H54	30:s:401:PEE:H25	1.58	0.82
5:W:98:MET:HE2	5:W:104:TRP:CD2	2.14	0.82
22:n:13:VAL:HG12	25:r:14:MET:CG	2.02	0.82
31:V:202:CDL:H211	31:V:202:CDL:H452	1.61	0.81
25:r:251:ASN:ND2	25:r:304:GLN:HE22	1.77	0.81
31:u:201:CDL:H581	31:u:201:CDL:H542	1.61	0.81
25:r:201:MET:HE2	30:r:501:PEE:C46	2.09	0.81
9:a:127:ASP:OD1	33:a:202:PLX:H1C2	1.81	0.80
6:X:91:ASP:HB3	8:Z:47:ARG:HH12	1.46	0.79
18:j:68:GLU:HG2	21:m:161:LEU:HD13	1.64	0.79
17:i:133:TRP:HE3	31:i:401:CDL:C39	1.96	0.78
31:V:202:CDL:H611	31:V:202:CDL:C74	2.13	0.78
18:j:18:VAL:HG22	26:s:222:MET:HG3	1.66	0.77
24:p:64:LEU:O	24:p:68:GLU:CG	2.31	0.77
31:l:701:CDL:H541	31:l:701:CDL:CA6	2.13	0.77
31:u:201:CDL:H542	31:u:201:CDL:C58	2.15	0.77
20:l:286:LEU:HD22	20:l:411:MET:HE3	1.68	0.76
5:W:98:MET:CE	5:W:104:TRP:CD2	2.69	0.76
9:a:126:TYR:O	33:a:202:PLX:H1B3	1.85	0.76
31:l:701:CDL:H772	31:l:701:CDL:C60	2.12	0.76
9:a:96:ALA:HB2	12:d:61:TYR:CD2	2.20	0.75
26:s:87:VAL:N	26:s:88:PRO:HD2	2.02	0.75
20:l:356:ILE:HA	20:l:359:MET:HE3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:l:701:CDL:H871	31:l:701:CDL:H642	1.70	0.73
11:c:116:ARG:HG2	30:l:703:PEE:H49	1.68	0.73
9:a:179:ILE:HG21	16:h:38:LYS:HG3	1.70	0.73
11:c:75:TYR:OH	11:c:105:ILE:O	2.05	0.73
11:c:108:ASP:HB3	11:c:111:MET:HE2	1.71	0.73
25:r:195:MET:HB2	30:r:501:PEE:O4	1.90	0.72
25:r:191:SER:HB3	30:r:501:PEE:H3	1.73	0.71
32:X:201:8Q1:O27	32:X:201:8Q1:O33	2.05	0.71
18:j:96:ILE:HD13	26:s:302:MET:HE1	1.72	0.71
31:V:202:CDL:H601	31:V:202:CDL:C73	2.14	0.71
29:w:211:VAL:HG21	29:w:235:GLN:NE2	2.05	0.71
17:i:129:LEU:CD1	31:i:401:CDL:H341	2.21	0.70
5:W:100:ASP:OD1	5:W:101:VAL:N	2.25	0.70
20:l:359:MET:O	20:l:436:ARG:NH2	2.25	0.70
29:w:165:SER:HB3	29:w:245:PHE:CE1	2.26	0.70
17:i:125:GLN:HG2	31:i:401:CDL:OA3	1.90	0.70
10:b:16:ARG:HD3	10:b:20:ARG:NH1	2.07	0.70
18:j:96:ILE:CD1	26:s:302:MET:HE1	2.21	0.70
29:w:250:SER:O	29:w:280:LYS:NZ	2.22	0.70
10:b:16:ARG:HD3	10:b:20:ARG:HH12	1.57	0.70
29:w:88:GLU:OE2	29:w:161:ARG:NH1	2.25	0.70
17:i:129:LEU:HD12	31:i:401:CDL:H341	1.74	0.70
30:l:703:PEE:H7	30:l:703:PEE:H14	1.74	0.70
20:l:227:PHE:O	20:l:230:HIS:ND1	2.24	0.69
29:w:246:LEU:HD12	29:w:255:VAL:HG11	1.73	0.69
31:u:201:CDL:H581	31:u:201:CDL:C54	2.20	0.69
20:l:596:MET:O	20:l:600:THR:HG23	1.92	0.69
17:i:92:PRO:O	17:i:94:ALA:N	2.26	0.69
31:l:701:CDL:H581	31:l:701:CDL:H622	1.73	0.69
20:l:558:LEU:HD21	31:o:201:CDL:H852	1.74	0.69
11:c:161:TYR:HB3	11:c:166:LEU:HG	1.74	0.68
31:l:701:CDL:H631	31:l:701:CDL:C84	2.08	0.68
17:i:125:GLN:CG	31:i:401:CDL:OA3	2.42	0.68
20:l:250:SER:HB2	20:l:333:ALA:HA	1.75	0.68
31:l:701:CDL:H792	31:l:701:CDL:H552	1.75	0.68
26:s:87:VAL:CG2	26:s:88:PRO:CD	2.68	0.68
10:b:14:GLN:HE22	24:p:157:ALA:HB3	1.56	0.67
29:w:139:ARG:NH1	29:w:166:ASP:OD1	2.27	0.67
6:X:155:TYR:CE1	10:b:23:LEU:HB3	2.29	0.67
31:V:202:CDL:H611	31:V:202:CDL:H741	1.75	0.67
31:V:202:CDL:OA7	31:V:202:CDL:HA62	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:184:MET:HE1	26:s:296:LEU:HB2	1.75	0.67
11:c:165:ASP:OD2	11:c:170:ARG:NH2	2.27	0.67
28:v:39:MET:HE3	28:v:41:ALA:H	1.58	0.67
14:f:40:ASP:OD2	14:f:43:LYS:NZ	2.27	0.67
7:Y:43:ARG:HB3	7:Y:46:GLN:HG2	1.77	0.67
17:i:321:LYS:CE	31:i:401:CDL:OA4	2.43	0.67
25:r:251:ASN:ND2	25:r:304:GLN:NE2	2.36	0.67
4:V:72:LEU:O	4:V:76:ILE:HG12	1.95	0.66
6:X:76:LEU:HD21	10:b:20:ARG:HH21	1.60	0.66
12:d:69:ARG:HH22	22:n:46:LYS:HB3	1.59	0.66
10:b:104:ILE:HB	28:v:48:ASP:HB3	1.76	0.66
18:j:25:PRO:HB2	26:s:60:PRO:HD3	1.76	0.66
20:l:401:MET:SD	20:l:479:ASN:ND2	2.66	0.66
10:b:28:LEU:HG	10:b:32:GLU:HG2	1.78	0.66
18:j:60:ILE:HG21	21:m:168:ILE:HG21	1.78	0.66
26:s:51:ASP:HB3	34:s:403:UQ:H8	1.77	0.66
27:u:103:GLN:N	27:u:103:GLN:OE1	2.28	0.66
29:w:125:ASP:O	29:w:130:ARG:NH2	2.29	0.66
29:w:63:ASP:OD2	29:w:245:PHE:CZ	2.49	0.65
25:r:191:SER:CB	30:r:501:PEE:H3	2.26	0.65
27:u:44:MET:HB3	27:u:48:TRP:HZ3	1.62	0.65
30:l:703:PEE:H64	30:l:703:PEE:H22	1.79	0.65
10:b:109:THR:HG22	10:b:116:VAL:HG22	1.78	0.65
30:b:201:PEE:O2P	30:b:201:PEE:N	2.21	0.65
17:i:100:MET:HE1	20:l:595:ILE:HG23	1.78	0.65
17:i:108:LEU:HD11	17:i:191:THR:HG21	1.79	0.65
31:l:701:CDL:C84	31:l:701:CDL:H651	2.27	0.64
6:X:92:LYS:HG2	6:X:110:LEU:HD21	1.79	0.64
26:s:235:ASN:HD21	26:s:270:PHE:HE2	1.45	0.64
7:Y:62:SER:HG	20:l:371:THR:HG1	1.45	0.64
4:V:81:ARG:NH2	4:V:88:LEU:HD22	2.12	0.64
11:c:109:LEU:O	11:c:113:ILE:HG23	1.96	0.64
31:l:701:CDL:H601	31:l:701:CDL:C77	2.16	0.64
12:d:119:GLU:HG2	28:v:52:MET:HA	1.81	0.63
13:e:89:VAL:HG21	25:r:25:ILE:HG23	1.79	0.63
27:u:96:LEU:HD12	27:u:99:HIS:NE2	2.13	0.63
26:s:235:ASN:ND2	26:s:270:PHE:HE2	1.96	0.63
12:d:111:LYS:NZ	20:l:200:GLN:OE1	2.32	0.63
18:j:94:LEU:HD12	21:m:147:TYR:HE1	1.62	0.63
29:w:246:LEU:N	29:w:247:PRO:HD2	2.13	0.63
31:V:202:CDL:H732	31:V:202:CDL:C60	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:201:PEE:H3	33:r:502:PLX:O2	1.98	0.63
11:c:80:ASP:O	11:c:81:ARG:C	2.40	0.62
4:V:69:ILE:CG1	4:V:100:THR:HG21	2.29	0.62
16:h:97:HIS:HA	16:h:102:GLU:HB3	1.81	0.62
20:l:391:SER:O	20:l:395:ILE:HG12	1.99	0.62
20:l:407:TRP:O	20:l:411:MET:HG2	1.99	0.62
25:r:48:ASN:OD1	25:r:49:SER:N	2.30	0.62
29:w:38:TYR:HH	29:w:292:HIS:HD1	1.48	0.62
26:s:62:ARG:HD3	26:s:64:ALA:H	1.63	0.62
9:a:96:ALA:CB	12:d:61:TYR:CD2	2.81	0.62
9:a:95:GLU:HG3	9:a:114:LYS:HE3	1.82	0.61
31:l:701:CDL:H652	33:r:502:PLX:H122	1.81	0.61
26:s:184:MET:HE2	26:s:293:PHE:HA	1.83	0.61
30:b:201:PEE:H23	33:r:502:PLX:H102	1.83	0.61
18:j:79:SER:HA	18:j:87:MET:HE2	1.81	0.61
15:g:34:VAL:HG21	31:u:201:CDL:OA7	1.99	0.61
33:a:202:PLX:H212	13:e:104:THR:HG21	1.81	0.61
12:d:2:PRO:O	12:d:7:LYS:NZ	2.33	0.61
27:u:80:GLU:O	27:u:84:GLU:HG3	2.01	0.61
20:l:119:LYS:NZ	31:l:701:CDL:H512	2.16	0.61
20:l:590:SER:O	20:l:594:THR:HG23	2.01	0.61
26:s:235:ASN:HD22	26:s:266:LEU:HB3	1.66	0.61
30:s:401:PEE:H25	30:s:401:PEE:C34	2.27	0.61
31:l:701:CDL:H651	31:l:701:CDL:H841	1.83	0.61
24:p:29:SER:HB3	24:p:76:HIS:HD2	1.66	0.61
26:s:69:SER:O	26:s:73:ILE:HG12	2.00	0.61
26:s:146:LEU:HD11	26:s:192:GLU:HG3	1.83	0.60
6:X:85:TYR:OH	8:Z:22:TRP:NE1	2.28	0.60
30:r:501:PEE:H7	30:r:501:PEE:H14	1.82	0.60
16:h:18:MET:HE3	19:k:56:ALA:HA	1.83	0.60
17:i:276:ILE:HG21	30:r:501:PEE:H14	1.84	0.60
17:i:149:ILE:HD13	17:i:154:MET:HE3	1.84	0.60
21:m:21:SER:O	21:m:23:LYS:NZ	2.34	0.60
21:m:25:SER:O	21:m:28:TYR:N	2.34	0.60
31:g:202:CDL:H311	17:i:239:VAL:HG23	1.83	0.60
25:r:191:SER:HB3	30:r:501:PEE:C1	2.32	0.60
19:k:10:MET:HE3	21:m:14:VAL:HG11	1.82	0.60
26:s:102:VAL:HG11	26:s:154:LEU:HD11	1.83	0.60
30:b:201:PEE:H47	20:l:68:TRP:CE3	2.37	0.59
18:j:6:THR:HG21	26:s:87:VAL:HG11	1.84	0.59
30:b:201:PEE:H9	33:r:502:PLX:O2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:g:202:CDL:H742	31:g:202:CDL:H271	1.83	0.59
17:i:213:LEU:HD13	31:i:401:CDL:H141	1.84	0.59
6:X:100:VAL:HG22	6:X:142:GLN:HB2	1.84	0.59
31:l:701:CDL:H422	25:r:448:THR:CG2	2.22	0.59
13:e:106:VAL:HG13	25:r:453:MET:HE2	1.84	0.59
31:l:701:CDL:H581	31:l:701:CDL:H872	1.85	0.59
24:p:95:GLU:OE1	24:p:98:LYS:NZ	2.29	0.59
26:s:62:ARG:HH21	26:s:68:ILE:HB	1.67	0.59
31:V:202:CDL:H611	31:V:202:CDL:H742	1.85	0.59
9:a:93:ILE:HG22	9:a:93:ILE:O	2.00	0.59
31:V:202:CDL:H741	31:V:202:CDL:C61	2.33	0.59
19:k:98:CYS:HB2	20:l:580:GLN:HB2	1.85	0.58
11:c:153:TYR:OH	28:v:8:ARG:NH1	2.32	0.58
28:v:93:LEU:O	28:v:97:LYS:HG3	2.02	0.58
2:S:15:CYS:HA	2:S:18:ILE:HD12	1.85	0.58
29:w:59:VAL:HG13	29:w:201:PRO:HA	1.86	0.58
17:i:278:MET:O	17:i:282:MET:HG3	2.04	0.58
30:U:101:PEE:H20	18:j:106:TRP:CE3	2.39	0.58
6:X:69:SER:OG	6:X:70:ASP:N	2.36	0.58
18:j:90:MET:HE2	18:j:90:MET:HA	1.85	0.58
31:a:201:CDL:H521	30:b:201:PEE:H14	1.83	0.58
30:b:201:PEE:H38	20:l:66:TRP:HZ3	1.69	0.58
18:j:70:ALA:HA	18:j:73:LEU:HD12	1.85	0.58
10:b:74:HIS:NE2	20:l:35:TYR:CE1	2.71	0.58
8:Z:26:GLY:N	8:Z:30:GLU:OE2	2.34	0.58
6:X:125:GLU:HG2	20:l:439:PRO:HG2	1.84	0.57
25:r:201:MET:HE1	30:r:501:PEE:H78	1.77	0.57
25:r:373:ILE:HD11	25:r:444:LEU:HD23	1.86	0.57
3:U:9:LEU:HD11	30:U:101:PEE:H68	1.85	0.57
15:g:12:PRO:HB3	16:h:5:ASP:HB3	1.86	0.57
20:l:360:GLY:HA3	20:l:435:PRO:HA	1.86	0.57
26:s:104:PHE:HE1	30:s:401:PEE:H52	1.70	0.57
29:w:132:GLN:OE1	35:w:401:ADP:N6	2.37	0.57
20:l:559:GLU:O	20:l:563:PRO:HD2	2.04	0.57
24:p:63:LEU:C	24:p:65:ARG:H	2.12	0.57
4:V:69:ILE:HG21	4:V:100:THR:HG21	1.86	0.57
19:k:5:TYR:O	19:k:9:ILE:HG12	2.04	0.57
28:v:4:HIS:HA	28:v:7:ARG:HE	1.69	0.57
31:l:701:CDL:H351	25:r:361:VAL:HG13	1.85	0.57
21:m:45:LEU:HD23	21:m:50:SER:HA	1.86	0.57
6:X:155:TYR:HE1	10:b:23:LEU:HB3	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:196:TRP:CD1	25:r:250:LEU:HB3	2.40	0.57
17:i:133:TRP:CE3	31:i:401:CDL:C39	2.79	0.57
26:s:25:ARG:HD2	34:s:403:UQ:HM21	1.87	0.57
26:s:66:SER:HA	26:s:124:ASN:OD1	2.05	0.57
27:u:80:GLU:HB2	27:u:81:PRO:HD3	1.87	0.57
20:l:290:LEU:O	20:l:523:SER:OG	2.22	0.57
18:j:88:LEU:HD13	26:s:309:ILE:HD12	1.86	0.56
5:W:74:LEU:O	5:W:78:GLU:HG3	2.05	0.56
10:b:74:HIS:NE2	20:l:35:TYR:OH	2.24	0.56
17:i:42:PRO:HG2	21:m:167:VAL:HG22	1.87	0.56
31:u:201:CDL:H762	31:u:201:CDL:H121	1.87	0.56
9:a:115:HIS:NE2	31:a:201:CDL:OB4	2.38	0.56
11:c:110:ASP:OD1	11:c:110:ASP:N	2.37	0.56
18:j:68:GLU:OE2	18:j:98:LEU:CD2	2.46	0.56
20:l:119:LYS:NZ	31:l:701:CDL:OA3	2.37	0.56
25:r:14:MET:SD	25:r:26:ASN:HB3	2.46	0.56
25:r:225:ILE:HG13	25:r:229:MET:HE2	1.88	0.56
25:r:19:LYS:HD2	25:r:22:MET:HG3	1.86	0.56
26:s:277:TYR:HE2	30:s:402:PEE:H58	1.70	0.56
4:V:69:ILE:HG21	4:V:100:THR:CG2	2.36	0.56
10:b:104:ILE:HD13	12:d:18:PRO:HG3	1.88	0.56
19:k:2:PRO:HD2	19:k:5:TYR:CD2	2.40	0.56
31:o:201:CDL:H801	31:o:201:CDL:H842	1.88	0.56
28:v:51:LEU:O	28:v:52:MET:HG3	2.05	0.56
17:i:62:THR:HG23	17:i:104:MET:HE2	1.88	0.56
7:Y:94:ASP:HB3	7:Y:99:ILE:HB	1.88	0.56
29:w:80:LYS:HE3	29:w:270:VAL:HG21	1.87	0.56
30:i:402:PEE:H47	30:r:501:PEE:H40	1.88	0.55
20:l:566:THR:O	20:l:570:GLN:HG2	2.05	0.55
31:l:701:CDL:H851	31:l:701:CDL:H811	1.87	0.55
23:o:3:PHE:CZ	24:p:70:GLU:HG3	2.40	0.55
29:w:274:GLU:O	29:w:277:LYS:NZ	2.39	0.55
18:j:64:LEU:HD13	21:m:165:VAL:HG22	1.88	0.55
19:k:23:ARG:HD3	21:m:23:LYS:HB2	1.87	0.55
11:c:80:ASP:HA	11:c:106:HIS:HE2	1.71	0.55
30:i:402:PEE:C25	30:i:402:PEE:H34	2.35	0.55
18:j:73:LEU:HD13	21:m:55:MET:HE1	1.86	0.55
20:l:464:ALA:O	20:l:468:ILE:HG12	2.07	0.55
30:s:401:PEE:O4	30:s:401:PEE:H7	2.05	0.55
31:a:201:CDL:OA7	31:a:201:CDL:HA61	2.06	0.55
20:l:562:LEU:HB3	20:l:563:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:110:CYS:O	27:u:114:LYS:HG2	2.06	0.55
20:l:11:THR:HG23	20:l:12:LEU:HD12	1.89	0.55
31:o:201:CDL:C36	31:o:201:CDL:H322	2.36	0.55
29:w:185:GLU:O	29:w:189:GLU:HG3	2.06	0.55
25:r:14:MET:O	25:r:18:SER:OG	2.22	0.55
25:r:186:LEU:HD11	25:r:195:MET:HE1	1.88	0.55
28:v:46:MET:HE2	28:v:56:ARG:HG2	1.89	0.55
7:Y:51:THR:HG22	7:Y:53:SER:H	1.72	0.54
22:n:50:ARG:HB2	22:n:53:GLU:HB2	1.88	0.54
25:r:398:MET:HA	25:r:398:MET:HE2	1.89	0.54
10:b:99:GLU:OE2	20:l:2:ASN:ND2	2.39	0.54
11:c:75:TYR:CG	11:c:76:PRO:HD2	2.42	0.54
29:w:116:LYS:NZ	29:w:125:ASP:OD2	2.39	0.54
29:w:105:ASP:OD1	29:w:106:VAL:N	2.40	0.54
4:V:46:PRO:HB3	4:V:55:ARG:NH2	2.23	0.54
31:a:201:CDL:H211	31:a:201:CDL:C25	2.34	0.54
11:c:161:TYR:O	11:c:183:HIS:NE2	2.38	0.54
20:l:419:THR:HA	20:l:422:TYR:CE2	2.43	0.54
26:s:225:MET:HE2	34:s:403:UQ:H153	1.90	0.54
30:b:201:PEE:H5	30:b:201:PEE:P	2.30	0.54
11:c:80:ASP:HA	11:c:106:HIS:NE2	2.22	0.54
20:l:7:LEU:HD22	20:l:46:LEU:HD11	1.89	0.54
11:c:96:ASP:OD1	11:c:97:LEU:N	2.40	0.54
29:w:132:GLN:CD	35:w:401:ADP:HN62	2.16	0.54
20:l:172:ILE:O	20:l:176:ARG:HG2	2.08	0.54
10:b:4:TYR:HB2	10:b:9:LYS:HE3	1.88	0.54
30:s:401:PEE:H25	30:s:401:PEE:C35	2.37	0.54
27:u:49:GLU:OE1	27:u:135:ARG:NH2	2.40	0.54
12:d:28:ASN:HD21	12:d:31:THR:HG23	1.73	0.53
18:j:30:TYR:CE2	26:s:59:GLU:HB2	2.43	0.53
26:s:90:PRO:HD2	26:s:240:ILE:HD13	1.90	0.53
11:c:159:LYS:NZ	28:v:57:ASP:OD2	2.40	0.53
4:V:96:ALA:O	4:V:100:THR:HG23	2.08	0.53
33:a:202:PLX:O7	33:a:202:PLX:H92	2.07	0.53
12:d:114:GLN:HG3	20:l:203:MET:HG2	1.91	0.53
12:d:144:SER:O	12:d:158:LYS:NZ	2.40	0.53
16:h:102:GLU:O	16:h:102:GLU:HG3	2.09	0.53
18:j:73:LEU:O	26:s:160:TYR:OH	2.26	0.53
10:b:74:HIS:NE2	20:l:35:TYR:HE1	2.07	0.53
15:g:36:MET:HE2	17:i:339:MET:HE2	1.90	0.53
1:Q:39:PRO:HB3	1:Q:43:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:68:ASP:O	17:i:49:ASN:ND2	2.42	0.53
7:Y:43:ARG:HG3	7:Y:48:PRO:HA	1.91	0.53
31:i:401:CDL:H331	31:i:401:CDL:OA9	2.09	0.53
29:w:216:SER:O	29:w:220:LYS:HG2	2.08	0.53
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.91	0.53
29:w:226:GLU:O	29:w:229:ILE:HG13	2.08	0.53
31:g:202:CDL:H391	17:i:334:THR:HG21	1.89	0.53
20:l:86:SER:OG	20:l:262:ARG:NH2	2.42	0.53
20:l:102:GLU:OE2	20:l:456:ARG:NH2	2.32	0.53
11:c:80:ASP:O	11:c:81:ARG:O	2.27	0.52
12:d:26:LEU:HD12	12:d:27:PRO:HD2	1.90	0.52
15:g:36:MET:HE3	15:g:74:GLY:HA2	1.90	0.52
17:i:270:MET:HE1	17:i:282:MET:SD	2.49	0.52
20:l:8:THR:HG23	20:l:82:MET:HE3	1.91	0.52
19:k:11:ALA:HB1	21:m:17:PHE:CD2	2.44	0.52
26:s:20:LEU:HD22	26:s:232:ILE:HD11	1.92	0.52
17:i:289:ASN:HA	17:i:292:PHE:CE2	2.45	0.52
20:l:5:ALA:HB2	20:l:61:MET:SD	2.49	0.52
20:l:66:TRP:O	20:l:78:LEU:N	2.37	0.52
22:n:30:ARG:O	22:n:33:GLU:HG2	2.10	0.52
9:a:152:LYS:HD3	15:g:96:VAL:HG21	1.91	0.52
18:j:87:MET:HE1	26:s:309:ILE:HD11	1.91	0.52
26:s:130:ILE:O	26:s:134:ARG:HG3	2.09	0.52
6:X:93:ILE:HD11	6:X:110:LEU:HD11	1.92	0.52
29:w:176:GLN:NE2	29:w:236:ASP:OD2	2.43	0.52
20:l:27:TYR:O	20:l:115:ASN:ND2	2.36	0.52
8:Z:25:GLU:HA	8:Z:30:GLU:OE2	2.10	0.52
19:k:23:ARG:HG2	21:m:23:LYS:HE2	1.91	0.52
21:m:17:PHE:CD1	21:m:20:PHE:HE1	2.27	0.52
31:o:201:CDL:H781	31:o:201:CDL:H822	1.91	0.52
26:s:200:LEU:HD11	26:s:285:LEU:HD21	1.90	0.52
2:S:55:SER:O	2:S:64:LYS:NZ	2.43	0.52
4:V:81:ARG:HH22	4:V:88:LEU:HD22	1.75	0.52
33:g:201:PLX:H301	17:i:347:ASN:HB3	1.91	0.52
17:i:40:MET:HE3	17:i:44:LEU:HD21	1.92	0.52
17:i:220:ILE:HB	17:i:323:MET:HE1	1.92	0.52
19:k:37:MET:SD	19:k:67:ALA:HB3	2.50	0.52
27:u:137:LEU:HD12	27:u:138:PRO:HD2	1.92	0.52
25:r:403:THR:HA	25:r:406:TYR:CE2	2.45	0.51
20:l:161:ARG:NH2	24:p:88:GLY:O	2.43	0.51
21:m:125:TRP:HA	21:m:128:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:28:ALA:HB2	27:u:82:PHE:HE1	1.76	0.51
20:l:161:ARG:NH1	20:l:238:GLU:OE2	2.40	0.51
17:i:236:LYS:HD3	17:i:237:MET:HE2	1.92	0.51
31:l:701:CDL:H611	31:l:701:CDL:H811	1.92	0.51
9:a:78:THR:HG22	13:e:100:VAL:HG11	1.92	0.51
30:i:402:PEE:H34	30:i:402:PEE:H41	1.91	0.51
29:w:129:TYR:OH	29:w:186:HIS:ND1	2.27	0.51
12:d:60:ARG:NH2	12:d:62:TYR:OH	2.43	0.51
12:d:106:ILE:HG13	12:d:135:VAL:HG21	1.93	0.51
29:w:295:ARG:HA	29:w:298:VAL:HG22	1.92	0.51
29:w:343:TYR:HA	29:w:352:ILE:HD12	1.93	0.51
5:W:85:GLN:OE1	16:h:105:ARG:NH1	2.44	0.51
31:l:701:CDL:H632	33:r:502:PLX:H131	1.93	0.51
9:a:127:ASP:CG	33:a:202:PLX:H1C2	2.35	0.51
28:v:27:PRO:HB2	28:v:34:ARG:HE	1.76	0.51
31:a:201:CDL:H382	12:d:48:ALA:HB2	1.93	0.50
10:b:85:TYR:CE1	30:b:201:PEE:H48	2.45	0.50
18:j:68:GLU:HB2	18:j:98:LEU:CD2	2.41	0.50
20:l:264:TYR:CD2	20:l:265:PRO:HD3	2.46	0.50
24:p:92:GLU:HB3	24:p:95:GLU:HG3	1.92	0.50
30:s:401:PEE:O4	30:s:401:PEE:H18	2.11	0.50
6:X:90:TYR:HE1	8:Z:44:PRO:HB2	1.76	0.50
25:r:299:VAL:O	25:r:303:ILE:HG12	2.10	0.50
20:l:76:LEU:HD21	20:l:196:TRP:HE3	1.76	0.50
31:l:701:CDL:H842	31:l:701:CDL:C64	2.40	0.50
30:l:703:PEE:H7	30:l:703:PEE:H13	1.90	0.50
21:m:61:LEU:HD23	21:m:65:LEU:HD12	1.93	0.50
28:v:39:MET:HE3	28:v:41:ALA:N	2.26	0.50
17:i:88:LYS:HD2	17:i:148:SER:OG	2.12	0.50
30:i:402:PEE:C1	30:i:402:PEE:H10	2.42	0.50
21:m:125:TRP:HA	21:m:128:TYR:HD2	1.76	0.50
25:r:103:GLN:HE21	25:r:107:ILE:HD11	1.76	0.50
1:Q:36:GLN:NE2	25:r:135:ARG:O	2.43	0.50
3:U:14:ALA:O	3:U:15:LYS:HG2	2.12	0.50
5:W:53:TRP:HH2	27:u:98:ARG:HH11	1.59	0.50
9:a:66:ARG:NH1	13:e:72:ASP:OD1	2.44	0.50
31:a:201:CDL:HB21	30:b:201:PEE:H51	1.94	0.50
3:U:59:ASP:HA	3:U:63:MET:HE2	1.93	0.50
20:l:290:LEU:O	20:l:293:ILE:HG22	2.12	0.50
4:V:61:PHE:CD2	4:V:104:ARG:NH1	2.64	0.50
11:c:123:PRO:HD2	20:l:525:MET:HE1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:110:LEU:HD11	20:l:203:MET:HE2	1.93	0.50
18:j:104:TYR:O	18:j:108:GLN:HG2	2.11	0.50
31:l:701:CDL:H331	31:l:701:CDL:OA9	2.10	0.50
25:r:300:ALA:O	25:r:308:SER:HB3	2.12	0.50
4:V:65:ALA:O	4:V:69:ILE:HG12	2.12	0.50
27:u:44:MET:HE3	27:u:48:TRP:CH2	2.47	0.50
5:W:88:ARG:HH11	5:W:91:LEU:HD23	1.77	0.50
16:h:97:HIS:HA	16:h:102:GLU:HG2	1.94	0.50
19:k:4:VAL:O	19:k:8:ILE:HG12	2.11	0.50
20:l:557:TRP:O	20:l:561:ILE:HG12	2.12	0.50
9:a:61:GLY:O	9:a:65:ARG:HG3	2.11	0.49
9:a:168:TRP:CD2	15:g:2:THR:HG23	2.47	0.49
11:c:81:ARG:NE	11:c:85:GLU:OE1	2.42	0.49
11:c:166:LEU:HD22	11:c:169:GLU:OE2	2.12	0.49
29:w:211:VAL:HG21	29:w:235:GLN:HE21	1.74	0.49
24:p:16:VAL:HG22	24:p:64:LEU:HD13	1.93	0.49
31:o:201:CDL:H832	31:o:201:CDL:C79	2.18	0.49
26:s:96:ILE:HG22	26:s:98:MET:HG3	1.94	0.49
9:a:71:MET:O	9:a:75:ILE:HG13	2.13	0.49
31:o:201:CDL:C79	31:o:201:CDL:C83	2.86	0.49
28:v:60:ALA:O	28:v:64:ILE:HG12	2.12	0.49
25:r:204:MET:HG3	25:r:209:LEU:HB2	1.94	0.49
11:c:33:THR:OG1	11:c:35:ASP:OD1	2.26	0.49
19:k:45:THR:HG23	21:m:52:LEU:HD13	1.95	0.49
20:l:536:LEU:HB3	20:l:537:PRO:HD3	1.93	0.49
17:i:84:TRP:HH2	19:k:59:MET:HE2	1.77	0.49
20:l:173:LEU:HD13	25:r:405:LEU:HD21	1.94	0.49
29:w:63:ASP:HB3	29:w:241:TYR:CE1	2.47	0.49
29:w:63:ASP:O	29:w:206:TYR:HD1	1.96	0.49
26:s:235:ASN:ND2	26:s:266:LEU:HB3	2.28	0.49
29:w:62:VAL:HG21	29:w:74:ALA:HB2	1.95	0.49
20:l:49:VAL:HB	20:l:50:PRO:HD3	1.94	0.49
23:o:48:LEU:HB3	24:p:166:LEU:HD13	1.95	0.49
25:r:271:MET:HE2	25:r:271:MET:HA	1.94	0.49
26:s:86:TRP:NE1	26:s:233:MET:HB2	2.26	0.49
27:u:83:THR:HA	27:u:86:TRP:CD1	2.47	0.49
30:i:402:PEE:H10	30:i:402:PEE:H2	1.94	0.49
22:n:13:VAL:HG13	25:r:14:MET:HA	1.95	0.49
29:w:213:GLU:HG2	29:w:217:ARG:HD2	1.93	0.49
24:p:100:PRO:HG3	25:r:419:TYR:CE1	2.47	0.48
27:u:78:CYS:CB	27:u:110:CYS:SG	3.00	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:V:201:PEE:O4	30:V:201:PEE:H10	2.13	0.48
30:i:402:PEE:H37	30:i:402:PEE:H60	1.95	0.48
25:r:159:PRO:HG2	30:r:501:PEE:H35	1.94	0.48
29:w:170:LEU:HD21	29:w:184:VAL:HG23	1.94	0.48
18:j:49:LEU:N	18:j:50:PRO:HD2	2.28	0.48
20:l:105:MET:HB2	20:l:449:LEU:HD13	1.95	0.48
21:m:25:SER:O	21:m:27:ILE:N	2.46	0.48
23:o:113:GLU:O	23:o:117:GLN:HG2	2.13	0.48
26:s:66:SER:HB3	26:s:122:ALA:O	2.12	0.48
29:w:110:GLY:HA2	29:w:134:TRP:CD2	2.47	0.48
20:l:221:ALA:HA	20:l:226:GLN:HG2	1.95	0.48
16:h:88:LYS:HB3	16:h:88:LYS:HE2	1.63	0.48
12:d:159:GLN:O	12:d:163:MET:HG3	2.12	0.48
13:e:70:ASN:O	13:e:73:SER:HB2	2.14	0.48
18:j:13:LEU:HD13	26:s:10:ILE:HG21	1.96	0.48
19:k:25:HIS:O	19:k:28:SER:N	2.40	0.48
1:Q:65:PRO:HB2	1:Q:67:ASN:O	2.13	0.48
5:W:66:GLU:OE1	27:u:123:GLY:N	2.43	0.48
9:a:80:ILE:HB	9:a:81:PRO:HD3	1.95	0.48
9:a:83:ALA:HA	31:a:201:CDL:H161	1.96	0.48
31:a:201:CDL:H772	31:a:201:CDL:H201	1.94	0.48
30:l:703:PEE:C11	30:l:703:PEE:C3	2.85	0.48
28:v:106:ARG:O	28:v:110:GLN:HG2	2.14	0.48
10:b:106:PRO:HA	10:b:117:ILE:HG22	1.96	0.48
18:j:15:SER:HA	26:s:76:ILE:HD12	1.95	0.48
25:r:14:MET:HE3	25:r:14:MET:HB3	1.83	0.48
29:w:148:GLU:OE1	29:w:301:LYS:NZ	2.40	0.48
5:W:114:THR:OG1	27:u:143:HIS:ND1	2.35	0.48
31:a:201:CDL:H191	31:a:201:CDL:H732	1.95	0.48
17:i:222:SER:O	17:i:224:ALA:N	2.47	0.48
26:s:21:THR:CG2	26:s:224:PHE:HE1	2.27	0.48
26:s:277:TYR:HE2	30:s:402:PEE:C36	2.27	0.48
27:u:18:VAL:HG12	27:u:20:VAL:HG22	1.96	0.48
21:m:17:PHE:O	21:m:21:SER:HB2	2.14	0.48
29:w:58:LYS:HZ3	29:w:278:CYS:HB2	1.79	0.48
17:i:321:LYS:NZ	31:i:401:CDL:OA4	2.46	0.47
27:u:114:LYS:HB2	27:u:115:LEU:HD12	1.95	0.47
13:e:144:PRO:HA	13:e:147:ILE:HD12	1.96	0.47
31:g:202:CDL:H402	17:i:335:LEU:HD21	1.96	0.47
20:l:78:LEU:HD11	31:l:701:CDL:H251	1.95	0.47
20:l:152:PHE:HB2	20:l:172:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:70:ASP:OD2	17:i:51:ARG:NH1	2.48	0.47
26:s:22:LEU:HD12	26:s:22:LEU:O	2.13	0.47
29:w:64:GLY:N	29:w:70:LYS:HD3	2.29	0.47
29:w:132:GLN:HE22	35:w:401:ADP:N6	2.12	0.47
10:b:85:TYR:CD1	30:b:201:PEE:H48	2.49	0.47
17:i:20:VAL:HG11	17:i:137:ALA:HB1	1.97	0.47
20:l:166:THR:CG2	30:l:703:PEE:H2	2.44	0.47
2:S:53:ARG:HB3	16:h:104:PRO:HB2	1.96	0.47
9:a:187:PRO:HA	27:u:48:TRP:CD1	2.49	0.47
12:d:164:LEU:HD12	13:e:149:LEU:HD22	1.97	0.47
18:j:17:LEU:HA	18:j:20:ILE:HG12	1.96	0.47
18:j:53:MET:HG3	18:j:57:LEU:HD23	1.95	0.47
20:l:372:ALA:HA	20:l:458:LEU:HD21	1.97	0.47
29:w:161:ARG:HD3	29:w:241:TYR:OH	2.14	0.47
11:c:39:GLY:O	11:c:74:ASP:HB2	2.15	0.47
14:f:47:THR:HG23	15:g:65:LEU:HD22	1.96	0.47
17:i:40:MET:HE1	17:i:129:LEU:HD23	1.97	0.47
24:p:120:ALA:O	24:p:124:GLN:HG2	2.13	0.47
26:s:20:LEU:HD23	26:s:228:TYR:CD2	2.49	0.47
26:s:85:MET:SD	26:s:108:MET:HB2	2.55	0.47
29:w:65:ASN:ND2	29:w:238:GLU:HB2	2.30	0.47
31:V:202:CDL:C74	31:V:202:CDL:C61	2.88	0.47
10:b:14:GLN:NE2	24:p:157:ALA:HB3	2.26	0.47
14:f:63:LYS:O	14:f:67:LEU:HD13	2.15	0.47
19:k:58:MET:SD	21:m:146:LEU:HA	2.55	0.47
26:s:62:ARG:HH11	26:s:64:ALA:HA	1.79	0.47
10:b:70:PHE:O	10:b:74:HIS:HB2	2.15	0.47
17:i:203:LEU:HB2	17:i:347:ASN:HD21	1.78	0.47
20:l:292:ALA:HB2	20:l:304:PHE:HB3	1.97	0.47
6:X:75:THR:OG1	6:X:156:GLU:O	2.25	0.47
25:r:122:PHE:CZ	25:r:206:LYS:HD3	2.49	0.47
31:u:201:CDL:H781	31:u:201:CDL:H752	1.62	0.47
28:v:93:LEU:HA	28:v:96:VAL:HG22	1.97	0.47
10:b:13:GLN:HA	10:b:16:ARG:HH11	1.80	0.47
12:d:82:ILE:HG23	12:d:83:LEU:HD22	1.96	0.47
20:l:450:LEU:O	20:l:454:ILE:HG12	2.14	0.47
29:w:86:PHE:HB2	29:w:159:LEU:HD23	1.96	0.47
2:S:1:MET:HB2	2:S:3:PHE:CE2	2.50	0.46
7:Y:52:ARG:O	7:Y:56:ILE:HG23	2.15	0.46
24:p:132:SER:HB2	24:p:163:LEU:HD13	1.97	0.46
25:r:281:ASP:OD1	25:r:340:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:143:GLU:OE1	10:b:9:LYS:HE2	2.14	0.46
10:b:24:LYS:O	10:b:27:GLU:HG3	2.15	0.46
20:l:245:ALA:O	20:l:249:SER:OG	2.24	0.46
26:s:233:MET:HE3	26:s:233:MET:HB3	1.78	0.46
3:U:9:LEU:CD1	30:U:101:PEE:H68	2.45	0.46
15:g:7:ARG:NH1	15:g:91:ASP:OD1	2.48	0.46
19:k:80:MET:HE3	21:m:172:THR:HA	1.98	0.46
31:u:201:CDL:C58	31:u:201:CDL:C54	2.86	0.46
28:v:80:CYS:HB3	28:v:83:GLU:OE1	2.16	0.46
3:U:38:TYR:HB2	26:s:310:MET:O	2.16	0.46
4:V:29:GLY:O	4:V:63:SER:OG	2.33	0.46
7:Y:39:HIS:NE2	8:Z:10:GLY:HA2	2.31	0.46
26:s:87:VAL:N	26:s:88:PRO:CD	2.74	0.46
31:V:202:CDL:H532	20:l:577:VAL:HA	1.96	0.46
20:l:331:MET:CE	20:l:465:GLY:HA2	2.46	0.46
20:l:529:TYR:HB3	20:l:530:PRO:HD3	1.98	0.46
20:l:581:LYS:HB3	20:l:583:LEU:HD23	1.98	0.46
33:a:202:PLX:H212	13:e:104:THR:CG2	2.45	0.46
10:b:86:LEU:HD11	20:l:9:LEU:HD12	1.97	0.46
10:b:93:LYS:HE2	10:b:93:LYS:HB2	1.73	0.46
20:l:33:PRO:HB2	20:l:105:MET:HE3	1.98	0.46
20:l:592:LEU:O	20:l:596:MET:HG3	2.15	0.46
27:u:69:ASP:O	27:u:73:GLN:HG3	2.16	0.46
29:w:248:GLU:O	29:w:251:GLU:HG2	2.16	0.46
7:Y:65:MET:SD	20:l:375:ILE:HG12	2.55	0.46
9:a:168:TRP:HB3	15:g:2:THR:O	2.16	0.46
11:c:62:TYR:OH	11:c:74:ASP:O	2.30	0.46
25:r:41:LEU:O	25:r:44:GLN:NE2	2.49	0.46
3:U:9:LEU:HD11	30:U:101:PEE:C41	2.46	0.46
17:i:72:MET:HE3	17:i:76:ILE:HG13	1.98	0.46
31:l:702:CDL:H421	31:l:702:CDL:H391	1.64	0.46
21:m:170:GLU:HG3	21:m:173:ARG:HH21	1.81	0.46
26:s:92:PRO:HG3	26:s:252:PRO:CB	2.46	0.46
29:w:214:ILE:CG2	29:w:215:GLN:N	2.79	0.46
29:w:258:TYR:CE2	29:w:269:VAL:HG22	2.51	0.46
4:V:8:LYS:N	4:V:8:LYS:HD2	2.31	0.45
6:X:119:ILE:HG21	6:X:135:ALA:HB1	1.98	0.45
26:s:19:PHE:O	26:s:23:VAL:HG23	2.15	0.45
11:c:165:ASP:O	11:c:170:ARG:NH2	2.48	0.45
12:d:142:ARG:NH1	13:e:138:GLU:O	2.42	0.45
13:e:119:ARG:O	13:e:123:GLU:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:96:ILE:HD11	26:s:302:MET:HE1	1.97	0.45
20:l:480:THR:HG21	28:v:91:GLU:HB2	1.97	0.45
25:r:74:PRO:O	25:r:78:MET:HG3	2.16	0.45
2:S:43:TYR:CZ	5:W:68:ARG:HG3	2.52	0.45
9:a:101:ILE:HG12	12:d:64:TYR:HB3	1.98	0.45
21:m:166:VAL:O	21:m:170:GLU:OE1	2.33	0.45
24:p:76:HIS:O	24:p:78:GLN:N	2.49	0.45
11:c:68:ASP:CG	11:c:70:MET:HG2	2.41	0.45
17:i:313:MET:HE2	17:i:313:MET:HB3	1.79	0.45
19:k:44:SER:O	19:k:48:ILE:HG12	2.17	0.45
26:s:306:SER:O	26:s:310:MET:HG3	2.17	0.45
12:d:99:ASP:OD2	12:d:142:ARG:NH2	2.49	0.45
13:e:128:TYR:O	13:e:132:ASN:ND2	2.41	0.45
25:r:12:LEU:HB2	25:r:13:PRO:HD3	1.97	0.45
25:r:206:LYS:HB3	25:r:206:LYS:HE2	1.70	0.45
10:b:123:PHE:HD2	28:v:40:VAL:HG11	1.82	0.45
19:k:38:LEU:O	19:k:42:ILE:HG12	2.17	0.45
7:Y:68:TRP:CZ2	7:Y:72:ARG:HD2	2.52	0.45
17:i:222:SER:O	17:i:222:SER:OG	2.32	0.45
31:l:701:CDL:H762	31:l:701:CDL:H311	1.98	0.45
25:r:457:PRO:HG2	25:r:458:LEU:HD12	1.99	0.45
31:u:201:CDL:H741	31:u:201:CDL:H712	1.76	0.45
29:w:180:ARG:NH2	29:w:182:GLN:OE1	2.50	0.45
4:V:124:LEU:HD11	30:r:501:PEE:H58	1.98	0.45
31:V:202:CDL:H512	20:l:580:GLN:HE22	1.82	0.45
5:W:68:ARG:CZ	5:W:72:MET:HE2	2.46	0.45
8:Z:13:LYS:HD2	8:Z:13:LYS:HA	1.75	0.45
25:r:112:ALA:HB1	25:r:118:PHE:HB2	1.98	0.45
2:S:48:MET:HE1	5:W:143:TYR:CZ	2.51	0.45
8:Z:19:TYR:CZ	8:Z:20:LYS:HE2	2.51	0.45
10:b:32:GLU:HG3	24:p:115:TYR:HA	1.99	0.45
10:b:87:LYS:NZ	10:b:88:TYR:OH	2.45	0.45
17:i:250:SER:O	17:i:259:GLY:HA3	2.17	0.45
31:l:702:CDL:H591	31:l:702:CDL:H622	1.50	0.45
10:b:77:ILE:HB	10:b:78:PRO:HD3	1.99	0.45
25:r:116:ILE:HG13	27:u:168:PHE:CD1	2.52	0.45
25:r:357:THR:O	25:r:361:VAL:HG23	2.16	0.45
26:s:248:ASP:OD2	26:s:251:THR:HG22	2.17	0.45
29:w:246:LEU:N	29:w:247:PRO:CD	2.79	0.45
6:X:134:ASP:HB3	6:X:147:TYR:CE2	2.52	0.44
13:e:58:ASP:OD2	29:w:326:ARG:NE	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:h:2:PRO:HA	17:i:140:SER:HB2	1.99	0.44
20:l:174:TYR:CD2	20:l:232:TRP:HB3	2.52	0.44
24:p:26:HIS:CD2	24:p:79:PRO:HB3	2.52	0.44
29:w:180:ARG:NH1	29:w:316:GLU:OE2	2.47	0.44
7:Y:61:PHE:HA	7:Y:64:THR:HG22	1.99	0.44
15:g:85:TYR:CZ	17:i:344:SER:HB3	2.52	0.44
31:g:202:CDL:H392	31:g:202:CDL:H362	1.49	0.44
20:l:37:LYS:HD3	20:l:98:TRP:HE1	1.81	0.44
20:l:190:LEU:HD22	25:r:383:THR:HG21	1.99	0.44
25:r:418:LYS:HE2	25:r:419:TYR:CE2	2.52	0.44
13:e:84:LEU:HG	13:e:88:ARG:NH1	2.33	0.44
17:i:254:LEU:O	17:i:257:LEU:HB2	2.17	0.44
20:l:338:MET:HE2	20:l:338:MET:HB3	1.91	0.44
8:Z:49:GLU:OE2	24:p:34:ARG:HB3	2.16	0.44
13:e:114:MET:HB3	13:e:117:TRP:HB3	1.98	0.44
17:i:338:PRO:HG3	31:u:201:CDL:H601	1.99	0.44
25:r:196:TRP:CE3	25:r:257:MET:HE2	2.53	0.44
11:c:117:VAL:HG21	20:l:539:TYR:HB2	1.99	0.44
22:n:26:TYR:CZ	22:n:30:ARG:HD3	2.53	0.44
26:s:81:LEU:O	26:s:85:MET:HG2	2.17	0.44
4:V:35:ILE:HG22	31:V:202:CDL:H761	1.98	0.44
9:a:80:ILE:N	9:a:81:PRO:CD	2.80	0.44
11:c:32:VAL:HG13	23:o:61:GLU:OE1	2.17	0.44
11:c:122:THR:OG1	11:c:124:VAL:O	2.29	0.44
17:i:256:PRO:HB2	31:u:201:CDL:H612	2.00	0.44
20:l:65:ASN:OD1	20:l:66:TRP:N	2.48	0.44
23:o:4:PRO:HD2	24:p:73:TYR:CE2	2.53	0.44
28:v:34:ARG:NH1	28:v:36:GLU:OE1	2.51	0.44
3:U:26:GLY:HA3	30:U:101:PEE:H37	1.99	0.44
17:i:18:MET:HE2	17:i:18:MET:HA	1.99	0.44
17:i:42:PRO:HG3	21:m:167:VAL:HG13	1.99	0.44
18:j:94:LEU:HD12	21:m:147:TYR:CE1	2.48	0.44
22:n:17:VAL:HB	22:n:18:PRO:HD3	2.00	0.44
23:o:82:PRO:O	31:o:201:CDL:OB7	2.35	0.44
24:p:150:ARG:HD2	24:p:150:ARG:HA	1.85	0.44
26:s:141:SER:HB3	26:s:289:LEU:HD22	1.98	0.44
30:s:401:PEE:H18	30:s:401:PEE:H24	1.87	0.44
27:u:38:LYS:HB3	27:u:39:PRO:HD3	1.99	0.44
29:w:209:VAL:HG22	29:w:260:ALA:HB2	2.00	0.44
30:V:201:PEE:C4	30:V:201:PEE:C1	2.85	0.44
32:X:201:8Q1:C30	24:p:52:LYS:HG3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:72:MET:HE3	17:i:76:ILE:CG1	2.47	0.44
17:i:270:MET:HE3	17:i:279:PRO:HG3	2.00	0.44
20:l:316:THR:OG1	20:l:395:ILE:HD12	2.17	0.44
31:o:201:CDL:H873	25:r:264:LEU:HD21	2.00	0.44
25:r:201:MET:HE1	30:r:501:PEE:C46	2.42	0.44
26:s:293:PHE:O	26:s:297:THR:OG1	2.23	0.44
28:v:83:GLU:OE1	28:v:83:GLU:N	2.39	0.44
11:c:105:ILE:CG2	11:c:109:LEU:HD22	2.48	0.43
12:d:37:PHE:CE2	20:l:3:PRO:HB3	2.53	0.43
20:l:554:ASP:OD2	25:r:288:TYR:OH	2.32	0.43
22:n:17:VAL:HG21	25:r:30:HIS:CG	2.53	0.43
26:s:26:LYS:HE2	26:s:37:PRO:O	2.18	0.43
27:u:16:GLN:O	27:u:68:LEU:HD11	2.18	0.43
27:u:44:MET:HB3	27:u:48:TRP:CZ3	2.48	0.43
31:u:201:CDL:H601	31:u:201:CDL:H572	1.75	0.43
4:V:39:TYR:OH	20:l:594:THR:HG22	2.18	0.43
31:V:202:CDL:H322	20:l:576:MET:HE1	1.99	0.43
9:a:96:ALA:O	12:d:63:TYR:HD1	2.01	0.43
9:a:126:TYR:C	9:a:127:ASP:OD1	2.61	0.43
17:i:30:TRP:O	17:i:34:GLU:HG2	2.17	0.43
19:k:98:CYS:SG	20:l:587:TYR:OH	2.75	0.43
20:l:383:MET:SD	20:l:384:PRO:HD2	2.58	0.43
23:o:3:PHE:CE2	24:p:70:GLU:HG3	2.52	0.43
26:s:63:PRO:C	26:s:65:THR:H	2.26	0.43
27:u:14:LYS:O	27:u:61:LYS:NZ	2.51	0.43
9:a:126:TYR:O	33:a:202:PLX:C1B	2.63	0.43
17:i:280:THR:O	17:i:284:MET:HG2	2.19	0.43
1:Q:63:PRO:HA	1:Q:64:PRO:HD3	1.93	0.43
17:i:226:THR:HG23	17:i:229:SER:H	1.84	0.43
20:l:78:LEU:HA	20:l:139:GLN:HE21	1.82	0.43
21:m:129:ASP:OD1	21:m:129:ASP:N	2.47	0.43
31:u:201:CDL:H171	31:u:201:CDL:H201	1.84	0.43
10:b:88:TYR:CZ	12:d:49:ARG:HG2	2.54	0.43
20:l:244:SER:O	20:l:249:SER:HB3	2.18	0.43
31:l:702:CDL:H181	31:l:702:CDL:H212	1.76	0.43
27:u:28:ALA:HB2	27:u:82:PHE:CE1	2.54	0.43
9:a:184:LYS:O	9:a:185:THR:OG1	2.29	0.43
31:i:401:CDL:OA7	31:i:401:CDL:HA62	2.16	0.43
20:l:102:GLU:HA	20:l:105:MET:HG3	2.00	0.43
20:l:108:MET:HE1	20:l:240:PRO:HB3	1.99	0.43
21:m:3:MET:N	21:m:3:MET:SD	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:m:10:SER:O	21:m:14:VAL:HG23	2.18	0.43
30:r:501:PEE:H32	30:r:501:PEE:H25	1.70	0.43
26:s:294:LEU:O	26:s:298:LEU:HG	2.18	0.43
27:u:38:LYS:NZ	27:u:42:GLU:OE2	2.51	0.43
5:W:104:TRP:CH2	16:h:75:ARG:HG3	2.54	0.43
13:e:74:HIS:HB2	13:e:83:ASP:OD2	2.19	0.43
17:i:57:THR:HA	19:k:77:LEU:HD13	2.01	0.43
29:w:258:TYR:HE2	29:w:269:VAL:HG13	1.83	0.43
5:W:128:ARG:HB3	5:W:132:GLU:OE2	2.18	0.43
31:a:201:CDL:OB7	30:b:201:PEE:H14	2.19	0.43
13:e:73:SER:C	13:e:75:GLY:H	2.26	0.43
13:e:90:VAL:HG22	25:r:28:THR:HG21	1.99	0.43
17:i:172:GLN:OE1	17:i:177:LYS:HD3	2.19	0.43
18:j:81:THR:C	18:j:83:ASN:H	2.26	0.43
5:W:98:MET:HE2	5:W:104:TRP:CZ2	2.49	0.43
11:c:62:TYR:HE1	11:c:76:PRO:HB3	1.83	0.43
12:d:37:PHE:CD2	20:l:3:PRO:HB3	2.54	0.43
20:l:452:ASN:HA	20:l:455:LYS:HG2	2.00	0.43
31:l:701:CDL:C85	31:l:701:CDL:C81	2.97	0.43
24:p:20:TYR:HB2	24:p:48:PHE:CZ	2.54	0.43
31:V:202:CDL:C51	20:l:580:GLN:HE22	2.31	0.43
18:j:90:MET:HE2	18:j:90:MET:CA	2.47	0.43
27:u:59:GLU:HA	27:u:62:LEU:HD12	2.00	0.43
9:a:96:ALA:O	12:d:63:TYR:CD1	2.72	0.42
31:g:202:CDL:H542	31:g:202:CDL:H511	1.79	0.42
21:m:57:PHE:CE1	26:s:111:LEU:HD11	2.54	0.42
22:n:47:ARG:HG2	22:n:47:ARG:HH11	1.84	0.42
25:r:71:TRP:O	25:r:74:PRO:HD2	2.19	0.42
27:u:44:MET:HE3	27:u:48:TRP:CZ3	2.54	0.42
5:W:86:MET:HE2	5:W:124:LEU:HB3	2.01	0.42
9:a:139:ILE:HG23	25:r:54:LEU:HD23	2.01	0.42
12:d:46:THR:O	12:d:50:GLU:HG3	2.20	0.42
26:s:190:LEU:HD23	26:s:270:PHE:CD1	2.53	0.42
34:s:403:UQ:H152	34:s:403:UQ:H101	2.01	0.42
33:a:202:PLX:H102	25:r:40:SER:HB3	2.01	0.42
12:d:61:TYR:C	12:d:62:TYR:HD1	2.27	0.42
12:d:117:GLU:HG3	12:d:124:ASN:HB2	2.02	0.42
31:g:202:CDL:H772	31:g:202:CDL:H741	1.81	0.42
17:i:104:MET:HG3	17:i:111:PHE:HB3	2.01	0.42
20:l:119:LYS:HZ1	31:l:701:CDL:H512	1.81	0.42
25:r:306:PRO:HA	25:r:458:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:88:LEU:O	4:V:88:LEU:HD23	2.19	0.42
9:a:78:THR:C	9:a:81:PRO:HD2	2.44	0.42
31:l:702:CDL:H382	31:l:702:CDL:H351	1.74	0.42
25:r:178:ILE:HD12	25:r:178:ILE:H	1.84	0.42
25:r:190:TRP:O	25:r:194:PHE:HD2	2.02	0.42
29:w:59:VAL:HG23	29:w:157:VAL:HG23	2.01	0.42
29:w:66:ILE:O	29:w:214:ILE:CD1	2.67	0.42
5:W:53:TRP:HH2	27:u:98:ARG:NH1	2.17	0.42
31:a:201:CDL:H211	31:a:201:CDL:H182	1.71	0.42
14:f:64:GLU:OE1	14:f:64:GLU:HA	2.20	0.42
17:i:154:MET:HE2	17:i:154:MET:HB2	1.96	0.42
17:i:211:MET:HG2	17:i:333:SER:HB2	2.01	0.42
18:j:5:LEU:HD23	26:s:2:PHE:HD2	1.85	0.42
18:j:65:PHE:CD2	18:j:98:LEU:HD11	2.55	0.42
20:l:173:LEU:HD23	30:l:703:PEE:H15	2.01	0.42
23:o:94:GLY:HA3	31:o:201:CDL:H811	2.00	0.42
24:p:28:GLU:OE2	24:p:34:ARG:NH1	2.46	0.42
29:w:211:VAL:N	29:w:212:PRO:CD	2.83	0.42
5:W:68:ARG:NH2	21:m:134:GLY:HA2	2.34	0.42
8:Z:75:PHE:O	8:Z:79:VAL:HG13	2.20	0.42
11:c:62:TYR:CE1	11:c:76:PRO:HB3	2.54	0.42
11:c:97:LEU:HB3	11:c:99:LEU:HD12	2.00	0.42
20:l:107:TYR:HD1	20:l:108:MET:HE2	1.85	0.42
25:r:115:LEU:HD12	25:r:174:LEU:HD22	2.01	0.42
26:s:126:LYS:O	26:s:130:ILE:HG12	2.18	0.42
5:W:91:LEU:HD11	5:W:106:VAL:HG12	2.00	0.42
5:W:98:MET:HE3	5:W:104:TRP:CD2	2.53	0.42
8:Z:59:ASN:HB3	20:l:364:LYS:NZ	2.34	0.42
11:c:155:PRO:HG3	28:v:4:HIS:CE1	2.54	0.42
16:h:83:ARG:O	16:h:87:ILE:HG12	2.20	0.42
22:n:47:ARG:HH22	22:n:53:GLU:CD	2.25	0.42
25:r:445:LEU:O	25:r:448:THR:HG22	2.19	0.42
31:V:202:CDL:H621	17:i:160:LEU:HD11	2.01	0.42
17:i:266:ILE:HG22	17:i:270:MET:HE2	2.01	0.42
20:l:520:TYR:CE1	31:l:702:CDL:HB22	2.54	0.42
21:m:23:LYS:N	21:m:24:PRO:HD3	2.35	0.42
24:p:54:GLU:OE1	24:p:60:ALA:HB2	2.20	0.42
29:w:214:ILE:HG22	29:w:215:GLN:N	2.34	0.42
7:Y:84:PHE:CE2	28:v:89:TYR:HA	2.55	0.42
31:a:201:CDL:OB7	30:b:201:PEE:C11	2.68	0.42
17:i:278:MET:HE3	17:i:278:MET:HB3	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:l:701:CDL:H842	31:l:701:CDL:H651	2.00	0.42
25:r:285:LEU:HD13	25:r:342:MET:HE1	2.02	0.42
26:s:63:PRO:HG2	26:s:66:SER:HB2	2.01	0.42
27:u:170:TRP:HA	31:u:201:CDL:OB7	2.20	0.42
5:W:51:MET:HE2	26:s:311:THR:HB	2.02	0.42
9:a:147:ALA:HB2	25:r:173:SER:HB2	2.01	0.42
33:j:201:PLX:H372	33:j:201:PLX:H342	1.61	0.42
31:l:702:CDL:H112	31:l:702:CDL:H142	1.72	0.42
34:s:403:UQ:H72	34:s:403:UQ:H111	1.88	0.42
1:Q:52:MET:HE3	1:Q:52:MET:HB3	1.84	0.41
31:V:202:CDL:H512	20:l:580:GLN:NE2	2.34	0.41
9:a:50:HIS:HB3	9:a:52:LYS:HE2	2.02	0.41
9:a:136:THR:HG21	25:r:48:ASN:ND2	2.35	0.41
11:c:111:MET:HE3	11:c:112:TYR:CZ	2.54	0.41
11:c:169:GLU:HA	12:d:123:GLN:HB2	2.02	0.41
12:d:149:HIS:HD2	25:r:304:GLN:NE2	2.17	0.41
15:g:48:ASN:HB3	15:g:55:VAL:HA	2.02	0.41
19:k:60:PRO:O	19:k:63:LEU:HB3	2.19	0.41
26:s:89:LEU:HA	26:s:90:PRO:HD3	1.90	0.41
26:s:197:PRO:HB3	26:s:278:PRO:O	2.20	0.41
30:U:101:PEE:H35	30:U:101:PEE:H30	1.50	0.41
5:W:105:LYS:HE2	5:W:105:LYS:HB2	1.90	0.41
9:a:106:VAL:HG13	22:n:50:ARG:NH2	2.35	0.41
30:b:201:PEE:H33	31:l:701:CDL:H241	2.02	0.41
12:d:9:VAL:O	12:d:109:ARG:NH2	2.45	0.41
16:h:94:PRO:HA	16:h:95:PRO:HD3	1.79	0.41
17:i:207:ILE:O	17:i:211:MET:HG3	2.20	0.41
17:i:283:ALA:HB1	25:r:158:LEU:HD13	2.00	0.41
18:j:55:PHE:HB2	21:m:74:MET:HE1	2.01	0.41
20:l:303:ALA:O	20:l:306:THR:HG22	2.20	0.41
20:l:468:ILE:O	20:l:472:ILE:HG12	2.21	0.41
25:r:121:LEU:O	25:r:125:THR:HG23	2.20	0.41
25:r:257:MET:HE3	25:r:257:MET:HB3	1.94	0.41
33:r:502:PLX:H301	33:r:502:PLX:H331	1.60	0.41
29:w:170:LEU:HD22	29:w:187:TYR:CD1	2.54	0.41
29:w:223:ASN:O	29:w:227:MET:HG3	2.20	0.41
31:V:202:CDL:H342	31:V:202:CDL:H371	1.92	0.41
17:i:5:ILE:HG21	21:m:170:GLU:OE2	2.20	0.41
31:l:701:CDL:H851	31:l:701:CDL:C81	2.50	0.41
26:s:98:MET:HE1	26:s:104:PHE:CG	2.56	0.41
29:w:167:PHE:O	29:w:170:LEU:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:76:LEU:HD23	9:a:76:LEU:HA	1.93	0.41
11:c:81:ARG:HB3	11:c:85:GLU:OE1	2.20	0.41
12:d:33:LEU:HD23	12:d:33:LEU:HA	1.85	0.41
14:f:72:ARG:HE	15:g:22:SER:HB3	1.85	0.41
16:h:17:TRP:CD1	16:h:17:TRP:H	2.39	0.41
17:i:245:MET:HE3	17:i:245:MET:HB3	1.92	0.41
3:U:78:LEU:HD23	3:U:78:LEU:HA	1.94	0.41
4:V:124:LEU:CD1	30:r:501:PEE:H58	2.51	0.41
5:W:98:MET:CE	5:W:104:TRP:CE3	3.03	0.41
5:W:98:MET:HE3	5:W:104:TRP:CG	2.56	0.41
9:a:98:LEU:HA	12:d:63:TYR:O	2.21	0.41
9:a:101:ILE:HA	9:a:102:PRO:HD3	1.92	0.41
30:b:201:PEE:H3	30:b:201:PEE:O4	2.20	0.41
17:i:112:HIS:HB2	17:i:184:ILE:HD13	2.01	0.41
33:j:201:PLX:H312	33:j:201:PLX:H282	1.83	0.41
29:w:54:THR:C	29:w:56:THR:H	2.27	0.41
29:w:346:ASP:OD1	29:w:347:VAL:N	2.53	0.41
7:Y:51:THR:O	7:Y:54:GLN:HG2	2.20	0.41
17:i:129:LEU:HD13	31:i:401:CDL:H341	2.01	0.41
30:i:402:PEE:H32	20:l:562:LEU:HG	2.02	0.41
20:l:44:PHE:HB2	20:l:94:LEU:HB3	2.02	0.41
20:l:107:TYR:CD1	20:l:108:MET:HE2	2.55	0.41
22:n:47:ARG:NH2	22:n:53:GLU:OE2	2.46	0.41
25:r:233:ALA:HA	25:r:320:GLY:HA2	2.03	0.41
26:s:142:TYR:O	26:s:145:THR:HG22	2.21	0.41
27:u:60:GLY:O	27:u:63:VAL:HG22	2.21	0.41
29:w:63:ASP:OD2	29:w:245:PHE:CE2	2.74	0.41
12:d:77:CYS:SG	12:d:84:CYS:HB3	2.60	0.41
17:i:291:TYR:HA	25:r:151:PHE:HZ	1.85	0.41
20:l:105:MET:HE2	20:l:105:MET:HB3	1.93	0.41
20:l:211:MET:N	20:l:212:PRO:HD2	2.36	0.41
20:l:423:SER:O	20:l:427:ILE:HG12	2.20	0.41
21:m:51:PHE:CZ	21:m:55:MET:HE3	2.56	0.41
21:m:124:ASP:N	21:m:124:ASP:OD1	2.48	0.41
25:r:216:LEU:HD23	25:r:287:ALA:HB1	2.01	0.41
25:r:243:MET:HB3	25:r:301:ILE:HG21	2.03	0.41
6:X:136:GLU:O	10:b:2:SER:OG	2.38	0.41
17:i:45:MET:HE1	21:m:171:ILE:HG23	2.02	0.41
17:i:344:SER:C	17:i:346:LEU:H	2.29	0.41
20:l:123:LEU:CD1	31:l:701:CDL:OA7	2.68	0.41
25:r:369:LEU:HD12	25:r:370:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:245:ALA:HB3	26:s:255:TYR:CE2	2.56	0.41
4:V:74:SER:OG	4:V:93:GLY:HA3	2.20	0.41
8:Z:24:ILE:HG23	8:Z:29:LEU:HB2	2.02	0.41
33:a:202:PLX:H111	33:a:202:PLX:H81	1.60	0.41
14:f:55:TRP:O	14:f:59:ILE:HG12	2.20	0.41
15:g:2:THR:HG22	15:g:4:MET:HG3	2.03	0.41
15:g:60:LEU:HD13	29:w:353:TRP:HB2	2.03	0.41
31:g:202:CDL:H812	31:g:202:CDL:H241	2.03	0.41
20:l:10:THR:O	20:l:14:ILE:HG12	2.21	0.41
20:l:94:LEU:HD23	20:l:94:LEU:HA	1.92	0.41
20:l:169:LEU:HD12	20:l:169:LEU:HA	1.88	0.41
20:l:559:GLU:OE2	25:r:148:TYR:OH	2.26	0.41
23:o:84:PRO:O	23:o:88:LEU:HG	2.21	0.41
24:p:29:SER:HB3	24:p:76:HIS:CD2	2.52	0.41
25:r:67:VAL:HG12	33:r:502:PLX:H382	2.02	0.41
25:r:235:LEU:HD23	25:r:235:LEU:HA	1.92	0.41
27:u:96:LEU:HB2	27:u:99:HIS:HD2	1.86	0.41
6:X:82:ARG:O	6:X:86:VAL:HG23	2.21	0.41
12:d:74:ILE:HG23	12:d:156:LEU:HD22	2.02	0.41
12:d:90:MET:SD	25:r:47:GLU:HB3	2.61	0.41
16:h:65:GLU:OE2	16:h:71:LYS:HB2	2.21	0.41
17:i:72:MET:HG2	19:k:12:PHE:CE2	2.56	0.41
18:j:65:PHE:CE2	18:j:98:LEU:CD1	3.03	0.41
31:o:201:CDL:C36	31:o:201:CDL:C32	2.98	0.41
30:s:401:PEE:H25	30:s:401:PEE:H56	2.03	0.41
27:u:47:ARG:NH2	27:u:53:PRO:HG3	2.36	0.41
10:b:32:GLU:HG3	24:p:115:TYR:CD1	2.56	0.40
16:h:97:HIS:HA	16:h:102:GLU:CB	2.51	0.40
20:l:137:LEU:HD23	20:l:137:LEU:HA	1.96	0.40
29:w:350:LYS:HA	29:w:350:LYS:HD3	1.86	0.40
3:U:42:ALA:HB2	26:s:312:ALA:HA	2.03	0.40
4:V:41:ILE:HD13	4:V:55:ARG:HH11	1.86	0.40
4:V:88:LEU:HD23	4:V:88:LEU:C	2.45	0.40
5:W:86:MET:HE2	5:W:86:MET:HB3	1.91	0.40
10:b:100:ARG:HB3	20:l:60:GLU:HB2	2.03	0.40
17:i:125:GLN:HG3	31:i:401:CDL:OA3	2.20	0.40
17:i:155:LEU:HD22	17:i:278:MET:HE2	2.03	0.40
18:j:68:GLU:HB2	18:j:98:LEU:HD23	2.03	0.40
20:l:572:LYS:HA	20:l:572:LYS:HD2	1.91	0.40
24:p:159:LYS:HE3	24:p:159:LYS:HB2	1.84	0.40
17:i:78:LEU:HD22	17:i:84:TRP:CZ2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:6:THR:O	18:j:10:ASN:ND2	2.54	0.40
20:l:327:LEU:O	20:l:331:MET:HG2	2.21	0.40
25:r:22:MET:HE3	25:r:22:MET:HB3	1.85	0.40
25:r:259:TYR:HB2	25:r:260:PRO:HD3	2.03	0.40
29:w:132:GLN:NE2	35:w:401:ADP:HN62	2.20	0.40
2:s:12:MET:SD	26:s:20:LEU:HA	2.61	0.40
30:V:201:PEE:H12	31:V:202:CDL:OA5	2.21	0.40
10:b:77:ILE:N	10:b:78:PRO:CD	2.84	0.40
12:d:101:GLU:OE1	13:e:119:ARG:NH1	2.52	0.40
17:i:49:ASN:ND2	17:i:51:ARG:HB2	2.37	0.40
17:i:258:SER:OG	17:i:336:VAL:HG22	2.22	0.40
30:i:402:PEE:C20	20:l:562:LEU:HG	2.52	0.40
18:j:19:LEU:O	18:j:23:TRP:HD1	2.04	0.40
20:l:396:ILE:HA	20:l:399:VAL:HG12	2.04	0.40
25:r:202:ALA:O	25:r:205:VAL:HG12	2.22	0.40
25:r:403:THR:O	25:r:404:ALA:C	2.65	0.40
26:s:67:SER:O	26:s:71:PHE:HB2	2.22	0.40
26:s:98:MET:HE2	26:s:101:GLY:HA2	2.02	0.40
4:V:140:LYS:H	4:V:140:LYS:HG2	1.75	0.40
30:V:201:PEE:H20	30:V:201:PEE:H14	1.56	0.40
6:X:133:ILE:HD11	24:p:6:PRO:HA	2.03	0.40
12:d:43:ARG:O	12:d:47:LEU:HG	2.21	0.40
17:i:54:GLU:OE2	19:k:95:LEU:HB2	2.22	0.40
20:l:184:LEU:HD13	25:r:393:ILE:HG21	2.03	0.40
31:l:702:CDL:H201	31:l:702:CDL:H232	1.96	0.40
27:u:80:GLU:N	27:u:81:PRO:CD	2.84	0.40
29:w:165:SER:O	29:w:168:VAL:HG22	2.22	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%)	37 (97%)	1 (3%)	0	100	100
2	S	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
3	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
4	V	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	49
5	W	111/113 (98%)	109 (98%)	2 (2%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	Y	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
8	Z	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
9	a	138/140 (99%)	136 (99%)	1 (1%)	1 (1%)	18	49
10	b	99/126 (79%)	95 (96%)	4 (4%)	0	100	100
11	c	154/156 (99%)	145 (94%)	8 (5%)	1 (1%)	21	52
12	d	173/175 (99%)	172 (99%)	1 (1%)	0	100	100
13	e	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
14	f	40/42 (95%)	39 (98%)	1 (2%)	0	100	100
15	g	119/121 (98%)	114 (96%)	5 (4%)	0	100	100
16	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
17	i	345/347 (99%)	328 (95%)	15 (4%)	2 (1%)	21	52
18	j	95/113 (84%)	89 (94%)	6 (6%)	0	100	100
19	k	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
20	l	601/603 (100%)	575 (96%)	26 (4%)	0	100	100
21	m	125/175 (71%)	112 (90%)	13 (10%)	0	100	100
22	n	54/56 (96%)	54 (100%)	0	0	100	100
23	o	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
24	p	176/178 (99%)	163 (93%)	13 (7%)	0	100	100
25	r	457/459 (100%)	441 (96%)	16 (4%)	0	100	100
26	s	299/318 (94%)	286 (96%)	12 (4%)	1 (0%)	36	67
27	u	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
28	v	122/126 (97%)	115 (94%)	7 (6%)	0	100	100
29	w	318/320 (99%)	303 (95%)	15 (5%)	0	100	100
All	All	4586/4752 (96%)	4383 (96%)	197 (4%)	6 (0%)	49	78

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	i	93	VAL
11	c	81	ARG
9	a	95	GLU
17	i	92	PRO
4	V	46	PRO
26	s	90	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	34/34 (100%)	34 (100%)	0	100	100
2	S	58/58 (100%)	58 (100%)	0	100	100
3	U	69/69 (100%)	69 (100%)	0	100	100
4	V	100/101 (99%)	100 (100%)	0	100	100
5	W	98/99 (99%)	98 (100%)	0	100	100
6	X	77/81 (95%)	77 (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%)	120 (98%)	2 (2%)	55	75
10	b	98/119 (82%)	98 (100%)	0	100	100
11	c	141/141 (100%)	140 (99%)	1 (1%)	76	82
12	d	155/155 (100%)	155 (100%)	0	100	100
13	e	99/99 (100%)	99 (100%)	0	100	100
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%)	91 (98%)	2 (2%)	45	71
17	i	311/311 (100%)	311 (100%)	0	100	100
18	j	88/99 (89%)	87 (99%)	1 (1%)	65	78
19	k	85/85 (100%)	85 (100%)	0	100	100
20	l	537/537 (100%)	537 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	m	99/141 (70%)	99 (100%)	0	100	100
22	n	53/53 (100%)	53 (100%)	0	100	100
23	o	113/113 (100%)	113 (100%)	0	100	100
24	p	159/159 (100%)	159 (100%)	0	100	100
25	r	410/410 (100%)	410 (100%)	0	100	100
26	s	263/275 (96%)	262 (100%)	1 (0%)	84	86
27	u	153/153 (100%)	151 (99%)	2 (1%)	61	77
28	v	101/112 (90%)	101 (100%)	0	100	100
29	w	281/283 (99%)	279 (99%)	2 (1%)	76	82
All	All	4068/4176 (97%)	4057 (100%)	11 (0%)	84	87

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	a	78	THR
9	a	95	GLU
11	c	110	ASP
16	h	97	HIS
16	h	102	GLU
18	j	98	LEU
26	s	24	GLU
27	u	88	CYS
27	u	100	CYS
29	w	214	ILE
29	w	246	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	S	27	HIS
2	S	46	ASN
4	V	129	GLN
7	Y	83	HIS
9	a	170	GLN
9	a	181	HIS
11	c	164	ASN
15	g	119	HIS
17	i	49	ASN

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Mol	Chain	Res	Type
17	i	63	GLN
17	i	150	ASN
17	i	174	GLN
17	i	221	HIS
18	j	82	ASN
18	j	108	GLN
19	k	57	ASN
20	l	139	GLN
20	l	192	HIS
20	l	354	GLN
20	l	580	GLN
22	n	3	ASN
22	n	11	HIS
23	o	52	ASN
23	o	75	ASN
25	r	81	GLN
25	r	103	GLN
25	r	144	ASN
25	r	175	ASN
25	r	192	ASN
25	r	304	GLN
25	r	366	ASN
26	s	235	ASN
26	s	317	GLN
27	u	30	HIS
27	u	99	HIS
27	u	163	HIS
28	v	47	ASN
28	v	85	HIS
29	w	127	ASN
29	w	219	GLN
29	w	235	GLN
29	w	344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

23 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
31	CDL	g	202	-	96,96,99	1.11	8 (8%)	102,108,111	0.89	4 (3%)
32	8Q1	X	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.61	6 (15%)
33	PLX	a	202	-	51,51,51	0.60	0	53,59,59	0.70	0
33	PLX	r	502	-	51,51,51	1.20	5 (9%)	53,59,59	0.63	1 (1%)
34	UQ	s	403	-	28,28,63	3.30	7 (25%)	36,37,79	2.77	11 (30%)
31	CDL	a	201	-	90,90,99	0.97	4 (4%)	96,102,111	1.07	6 (6%)
31	CDL	u	201	-	77,77,99	1.02	4 (5%)	83,89,111	1.16	7 (8%)
33	PLX	j	201	-	51,51,51	1.21	4 (7%)	53,59,59	0.61	1 (1%)
31	CDL	o	201	-	67,67,99	1.11	4 (5%)	73,79,111	1.20	6 (8%)
31	CDL	i	401	-	65,65,99	1.14	4 (6%)	71,77,111	1.21	5 (7%)
30	PEE	i	402	-	46,46,50	1.22	6 (13%)	49,51,55	1.02	3 (6%)
31	CDL	l	701	-	98,98,99	0.92	4 (4%)	104,110,111	1.17	9 (8%)
30	PEE	s	401	-	40,40,50	1.16	5 (12%)	43,45,55	1.05	2 (4%)
33	PLX	g	201	-	51,51,51	1.18	3 (5%)	53,59,59	0.67	1 (1%)
31	CDL	l	702	-	99,99,99	1.11	8 (8%)	105,111,111	0.84	4 (3%)
30	PEE	s	402	-	50,50,50	1.18	6 (12%)	53,55,55	0.98	2 (3%)
30	PEE	U	101	-	50,50,50	1.17	6 (12%)	53,55,55	0.96	2 (3%)
31	CDL	V	202	-	93,93,99	0.95	4 (4%)	99,105,111	1.08	5 (5%)
30	PEE	l	703	-	45,45,50	1.24	6 (13%)	48,50,55	1.02	2 (4%)
30	PEE	b	201	-	45,45,50	1.24	6 (13%)	48,50,55	1.02	2 (4%)
35	ADP	w	401	-	28,29,29	3.16	9 (32%)	43,45,45	1.91	9 (20%)
30	PEE	r	501	-	50,50,50	1.17	6 (12%)	53,55,55	1.02	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PEE	V	201	-	39,39,50	1.33	6 (15%)	42,44,55	1.10	3 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CDL	g	202	-	-	63/107/107/110	-
32	8Q1	X	201	-	-	17/41/41/41	-
33	PLX	a	202	-	-	15/55/55/55	-
33	PLX	r	502	-	-	38/55/55/55	-
34	UQ	s	403	-	-	9/21/45/87	0/1/1/1
31	CDL	a	201	-	-	26/101/101/110	-
31	CDL	u	201	-	-	28/88/88/110	-
33	PLX	j	201	-	-	24/55/55/55	-
31	CDL	o	201	-	-	33/78/78/110	-
31	CDL	i	401	-	-	30/76/76/110	-
30	PEE	i	402	-	-	22/50/50/54	-
31	CDL	l	701	-	-	39/109/109/110	-
30	PEE	s	401	-	-	18/44/44/54	-
33	PLX	g	201	-	-	23/55/55/55	-
31	CDL	l	702	-	-	65/110/110/110	-
30	PEE	s	402	-	-	22/54/54/54	-
30	PEE	U	101	-	-	24/54/54/54	-
31	CDL	V	202	-	-	37/104/104/110	-
30	PEE	l	703	-	-	20/49/49/54	-
30	PEE	b	201	-	-	26/49/49/54	-
35	ADP	w	401	-	-	3/16/32/32	0/3/3/3
30	PEE	r	501	-	-	21/54/54/54	-
30	PEE	V	201	-	-	21/43/43/54	-

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	s	403	UQ	C13-C14	9.59	1.55	1.33
34	s	403	UQ	C8-C9	9.12	1.54	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	w	401	ADP	C3'-C4'	-8.95	1.30	1.53
34	s	403	UQ	C18-C19	7.94	1.56	1.32
35	w	401	ADP	O4'-C4'	7.65	1.62	1.45
35	w	401	ADP	PA-O3A	6.45	1.66	1.59
35	w	401	ADP	C6-N6	5.39	1.48	1.34
32	X	201	8Q1	C39-N41	5.05	1.45	1.33
32	X	201	8Q1	C34-N36	5.02	1.45	1.33
35	w	401	ADP	O4'-C1'	-4.59	1.31	1.42
31	i	401	CDL	OA8-CA7	4.30	1.45	1.33
31	o	201	CDL	OA8-CA7	4.29	1.45	1.33
31	a	201	CDL	OA8-CA7	4.29	1.45	1.33
31	i	401	CDL	OA6-CA5	4.28	1.46	1.34
31	l	701	CDL	OA8-CA7	4.27	1.45	1.33
31	V	202	CDL	OA8-CA7	4.27	1.45	1.33
31	i	401	CDL	OB8-CB7	4.26	1.45	1.33
31	u	201	CDL	OB8-CB7	4.26	1.45	1.33
31	V	202	CDL	OB8-CB7	4.25	1.45	1.33
31	o	201	CDL	OB8-CB7	4.24	1.45	1.33
31	l	701	CDL	OB8-CB7	4.21	1.45	1.33
31	V	202	CDL	OA6-CA5	4.19	1.46	1.34
31	a	201	CDL	OB8-CB7	4.19	1.45	1.33
31	i	401	CDL	OB6-CB5	4.16	1.46	1.34
31	a	201	CDL	OB6-CB5	4.15	1.46	1.34
31	u	201	CDL	OA8-CA7	4.13	1.45	1.33
31	V	202	CDL	OB6-CB5	4.12	1.45	1.34
31	o	201	CDL	OA6-CA5	4.11	1.45	1.34
31	a	201	CDL	OA6-CA5	4.07	1.45	1.34
31	u	201	CDL	OA6-CA5	4.01	1.45	1.34
31	l	701	CDL	OA6-CA5	3.98	1.45	1.34
31	o	201	CDL	OB6-CB5	3.98	1.45	1.34
31	l	701	CDL	OB6-CB5	3.98	1.45	1.34
31	u	201	CDL	OB6-CB5	3.90	1.45	1.34
30	s	401	PEE	C18-C19	3.84	1.53	1.31
30	V	201	PEE	C18-C19	3.82	1.53	1.31
30	s	402	PEE	C18-C19	3.82	1.53	1.31
30	r	501	PEE	C18-C19	3.81	1.53	1.31
30	l	703	PEE	C18-C19	3.80	1.53	1.31
30	b	201	PEE	C18-C19	3.80	1.53	1.31
30	i	402	PEE	C18-C19	3.79	1.53	1.31
30	U	101	PEE	C18-C19	3.75	1.53	1.31
30	r	501	PEE	C39-C38	3.74	1.52	1.31
30	l	703	PEE	C39-C38	3.73	1.52	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	i	402	PEE	C39-C38	3.73	1.52	1.31
30	V	201	PEE	C39-C38	3.72	1.52	1.31
30	b	201	PEE	C39-C38	3.72	1.52	1.31
30	U	101	PEE	C39-C38	3.70	1.52	1.31
30	s	402	PEE	C39-C38	3.70	1.52	1.31
31	l	702	CDL	OA8-CA7	3.47	1.43	1.33
35	w	401	ADP	C8-N9	-3.37	1.31	1.37
31	g	202	CDL	OA8-CA7	3.36	1.43	1.33
35	w	401	ADP	O2'-C2'	-3.09	1.35	1.43
35	w	401	ADP	O3'-C3'	3.07	1.50	1.43
31	g	202	CDL	OB6-CB5	3.06	1.42	1.34
31	l	702	CDL	OB6-CB5	3.00	1.42	1.34
31	l	702	CDL	OA6-CA5	2.98	1.42	1.34
31	l	702	CDL	OB8-CB7	2.97	1.42	1.33
31	g	202	CDL	OB8-CB7	2.93	1.41	1.33
33	r	502	PLX	O6-C4	-2.89	1.40	1.44
33	g	201	PLX	O6-C4	-2.86	1.40	1.44
31	g	202	CDL	OA6-CA5	2.79	1.42	1.34
30	s	402	PEE	O2-C2	-2.75	1.40	1.46
31	g	202	CDL	OA6-CA4	-2.72	1.40	1.46
33	j	201	PLX	O6-C4	-2.72	1.41	1.44
30	r	501	PEE	O2-C2	-2.67	1.40	1.46
30	l	703	PEE	O2-C2	-2.67	1.40	1.46
30	i	402	PEE	O2-C2	-2.66	1.40	1.46
30	U	101	PEE	O2-C2	-2.63	1.40	1.46
31	l	702	CDL	OA6-CA4	-2.62	1.40	1.46
34	s	403	UQ	C6-C1	2.60	1.53	1.46
30	b	201	PEE	O2-C2	-2.54	1.40	1.46
30	i	402	PEE	O3-C30	2.53	1.40	1.33
30	b	201	PEE	O3-C30	2.48	1.40	1.33
30	V	201	PEE	O3-C30	2.47	1.40	1.33
30	V	201	PEE	O2-C2	-2.44	1.40	1.46
30	s	401	PEE	O2-C2	-2.43	1.40	1.46
31	l	702	CDL	OB6-CB4	-2.42	1.40	1.46
30	s	402	PEE	O3-C30	2.41	1.40	1.33
30	U	101	PEE	O3-C30	2.41	1.40	1.33
35	w	401	ADP	C5-N7	-2.40	1.34	1.39
30	l	703	PEE	O3-C30	2.37	1.40	1.33
30	r	501	PEE	O3-C30	2.37	1.40	1.33
33	g	201	PLX	C7-C6	2.36	1.55	1.50
32	X	201	8Q1	O35-C34	-2.36	1.18	1.23
33	r	502	PLX	C7-C6	2.34	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	201	8Q1	O40-C39	-2.33	1.18	1.23
32	X	201	8Q1	C1-S44	2.32	1.81	1.76
30	s	401	PEE	O3-C30	2.32	1.40	1.33
30	b	201	PEE	O2-C10	2.30	1.40	1.34
30	s	401	PEE	O2-C10	2.29	1.40	1.34
30	V	201	PEE	O2-C10	2.28	1.40	1.34
30	s	401	PEE	O3-C3	-2.27	1.40	1.45
33	j	201	PLX	C7-C6	2.25	1.55	1.50
30	U	101	PEE	O2-C10	2.25	1.40	1.34
30	U	101	PEE	O3-C3	-2.24	1.40	1.45
33	j	201	PLX	P1-O4	2.23	1.68	1.59
31	l	702	CDL	PB2-OB2	2.23	1.68	1.59
30	r	501	PEE	O3-C3	-2.22	1.40	1.45
31	g	202	CDL	PB2-OB5	2.22	1.68	1.59
30	l	703	PEE	O3-C3	-2.21	1.40	1.45
31	g	202	CDL	PB2-OB2	2.20	1.68	1.59
34	s	403	UQ	O4-C4	-2.20	1.18	1.23
31	g	202	CDL	OB6-CB4	-2.19	1.41	1.46
30	l	703	PEE	O2-C10	2.18	1.40	1.34
31	l	702	CDL	PB2-OB5	2.18	1.67	1.59
30	b	201	PEE	O3-C3	-2.17	1.40	1.45
30	r	501	PEE	O2-C10	2.17	1.40	1.34
34	s	403	UQ	O3-CM3	-2.15	1.40	1.45
30	i	402	PEE	O2-C10	2.14	1.40	1.34
30	s	402	PEE	O3-C3	-2.14	1.40	1.45
33	r	502	PLX	P1-O4	2.14	1.67	1.59
32	X	201	8Q1	C6-C1	2.13	1.53	1.50
30	s	402	PEE	O2-C10	2.11	1.40	1.34
33	j	201	PLX	P1-O1	2.11	1.67	1.59
30	V	201	PEE	O3-C3	-2.10	1.40	1.45
34	s	403	UQ	O1-C1	-2.07	1.18	1.23
30	i	402	PEE	O3-C3	-2.06	1.40	1.45
33	g	201	PLX	P1-O4	2.05	1.67	1.59
33	r	502	PLX	C1-C2	2.02	1.57	1.51
33	r	502	PLX	P1-O1	2.01	1.67	1.59

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	403	UQ	C7-C8-C9	-9.66	110.19	126.83
34	s	403	UQ	C12-C13-C14	-6.19	113.45	127.62
32	X	201	8Q1	C6-C1-S44	5.98	120.53	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	w	401	ADP	C5-C4-N3	-5.45	119.21	126.72
31	l	701	CDL	OA6-CA5-C11	4.86	121.99	111.48
34	s	403	UQ	C10-C9-C8	-4.82	111.24	123.63
35	w	401	ADP	N3-C2-N1	-4.58	121.64	128.58
31	u	201	CDL	OA6-CA5-C11	4.40	121.00	111.48
34	s	403	UQ	C11-C9-C8	-4.39	111.31	121.17
31	i	401	CDL	OA6-CA5-C11	4.35	120.89	111.48
35	w	401	ADP	N3-C4-N9	4.25	134.40	127.17
30	r	501	PEE	O2-C10-C11	4.22	120.61	111.48
30	s	401	PEE	O2-C10-C11	4.21	120.58	111.48
31	o	201	CDL	OB6-CB5-C51	4.20	120.56	111.48
31	g	202	CDL	OB6-CB5-C51	4.11	120.37	111.48
30	l	703	PEE	O2-C10-C11	4.07	120.28	111.48
34	s	403	UQ	C17-C18-C19	-4.07	114.08	127.64
34	s	403	UQ	C15-C14-C13	-4.06	113.20	123.63
30	i	402	PEE	O2-C10-C11	4.01	120.16	111.48
30	b	201	PEE	O2-C10-C11	3.98	120.10	111.48
31	a	201	CDL	OB6-CB5-C51	3.97	120.07	111.48
31	V	202	CDL	OB6-CB5-C51	3.97	120.07	111.48
31	i	401	CDL	OB6-CB5-C51	3.92	119.96	111.48
31	l	701	CDL	CA4-OA6-CA5	-3.91	108.44	117.80
30	V	201	PEE	O2-C10-C11	3.88	119.87	111.48
31	o	201	CDL	OA6-CA5-C11	3.87	119.84	111.48
30	s	402	PEE	O2-C10-C11	3.86	119.83	111.48
31	l	702	CDL	OA6-CA5-C11	3.85	119.82	111.48
31	l	701	CDL	OB6-CB5-C51	3.85	119.81	111.48
31	g	202	CDL	OA6-CA5-C11	3.84	119.80	111.48
31	V	202	CDL	OA6-CA5-C11	3.78	119.66	111.48
30	U	101	PEE	O2-C10-C11	3.76	119.62	111.48
31	l	702	CDL	OB6-CB5-C51	3.76	119.61	111.48
31	a	201	CDL	OA6-CA5-C11	3.68	119.44	111.48
32	X	201	8Q1	O4-C1-C6	-3.60	119.83	123.98
35	w	401	ADP	C2-N3-C4	3.57	120.55	111.83
31	u	201	CDL	OB6-CB5-C51	3.57	119.20	111.48
34	s	403	UQ	C16-C14-C13	-3.53	113.25	121.17
35	w	401	ADP	N9-C8-N7	-3.50	108.97	113.94
32	X	201	8Q1	C37-C38-C39	3.36	117.99	112.39
35	w	401	ADP	C5-N7-C8	3.21	108.49	103.45
31	l	701	CDL	OB8-CB7-C71	3.17	121.50	111.83
34	s	403	UQ	C21-C19-C18	-3.16	113.16	122.66
35	w	401	ADP	C4-N9-C8	3.15	109.04	105.74
34	s	403	UQ	C7-C6-C5	-3.14	119.51	124.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	201	CDL	OB8-CB7-C71	3.12	121.34	111.83
31	V	202	CDL	OB8-CB7-C71	3.09	121.25	111.83
35	w	401	ADP	C4-C5-N7	-3.04	107.11	110.58
30	s	402	PEE	O3-C30-C31	3.03	121.07	111.83
31	a	201	CDL	OA8-CA7-C31	3.03	121.07	111.83
31	o	201	CDL	CB4-OB6-CB5	-3.02	110.58	117.80
31	i	401	CDL	OA8-CA7-C31	3.01	121.03	111.83
34	s	403	UQ	CM5-C5-C6	-3.00	119.52	124.45
30	r	501	PEE	O3-C30-C31	2.93	120.76	111.83
30	l	703	PEE	O3-C30-C31	2.88	120.61	111.83
31	o	201	CDL	OA8-CA7-C31	2.87	120.57	111.83
33	r	502	PLX	C1A-N1-C1	2.84	121.20	109.91
34	s	403	UQ	C20-C19-C18	-2.83	114.17	122.66
31	V	202	CDL	OA8-CA7-C31	2.82	120.43	111.83
31	V	202	CDL	CB4-OB6-CB5	-2.77	111.16	117.80
32	X	201	8Q1	C43-S44-C1	2.75	109.97	101.84
30	V	201	PEE	O3-C30-C31	2.74	120.19	111.83
31	u	201	CDL	OA8-CA7-C31	2.73	120.17	111.83
31	l	701	CDL	OA8-CA7-C31	2.71	120.11	111.83
30	b	201	PEE	O3-C30-C31	2.70	120.05	111.83
31	l	702	CDL	OA8-CA7-C31	2.69	120.04	111.83
31	g	202	CDL	OA8-CA7-C31	2.66	119.95	111.83
30	i	402	PEE	O3-C30-C31	2.66	119.95	111.83
30	s	401	PEE	O3-C30-C31	2.66	119.93	111.83
31	g	202	CDL	OB8-CB7-C71	2.64	119.88	111.83
30	U	101	PEE	O3-C30-C31	2.64	119.87	111.83
31	l	702	CDL	OB8-CB7-C71	2.62	119.83	111.83
31	u	201	CDL	OB8-CB7-C71	2.61	119.79	111.83
31	o	201	CDL	OB8-CB7-C71	2.59	119.75	111.83
31	i	401	CDL	OB8-CB7-C71	2.58	119.69	111.83
33	g	201	PLX	C1A-N1-C1	2.51	119.87	109.91
31	l	701	CDL	CB4-OB6-CB5	-2.49	111.83	117.80
33	j	201	PLX	C1A-N1-C1	2.44	119.62	109.91
31	l	701	CDL	OA6-CA5-OA7	-2.44	118.00	123.70
32	X	201	8Q1	O4-C1-S44	-2.39	119.64	122.68
30	V	201	PEE	C20-C19-C18	-2.37	112.14	126.42
31	i	401	CDL	CA4-OA6-CA5	-2.23	112.45	117.80
31	u	201	CDL	OA6-CA5-OA7	-2.23	118.49	123.70
31	u	201	CDL	CA4-OA6-CA5	-2.23	112.46	117.80
35	w	401	ADP	C4'-O4'-C1'	-2.22	104.56	109.47
31	l	701	CDL	OB8-CB7-OB9	-2.18	118.19	123.63
31	o	201	CDL	OB6-CB5-OB7	-2.11	118.78	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	201	CDL	OB8-CB7-OB9	-2.08	118.43	123.63
31	a	201	CDL	CB4-OB6-CB5	-2.07	112.84	117.80
32	X	201	8Q1	C38-C39-N41	2.04	120.05	116.34
31	u	201	CDL	CA6-CA4-CA3	-2.03	107.04	111.78
31	l	701	CDL	OB6-CB5-OB7	-2.02	118.97	123.70
30	i	402	PEE	C2-O2-C10	-2.02	112.96	117.80

There are no chirality outliers.

All (624) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	U	101	PEE	C1-O3P-P-O1P
30	U	101	PEE	C4-O4P-P-O3P
30	U	101	PEE	C4-O4P-P-O2P
30	U	101	PEE	C4-O4P-P-O1P
30	V	201	PEE	C11-C10-O2-C2
30	V	201	PEE	C1-O3P-P-O1P
30	V	201	PEE	C1-O3P-P-O4P
30	i	402	PEE	C4-O4P-P-O3P
30	i	402	PEE	C4-O4P-P-O2P
30	i	402	PEE	C4-O4P-P-O1P
30	l	703	PEE	C11-C10-O2-C2
30	l	703	PEE	O4-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	r	501	PEE	C11-C10-O2-C2
30	r	501	PEE	C4-O4P-P-O3P
30	r	501	PEE	C4-O4P-P-O2P
30	r	501	PEE	C4-O4P-P-O1P
30	s	401	PEE	C4-O4P-P-O3P
30	s	401	PEE	C4-O4P-P-O1P
31	V	202	CDL	CA3-OA5-PA1-OA2
31	V	202	CDL	CA3-OA5-PA1-OA4
31	V	202	CDL	CB2-OB2-PB2-OB3
31	V	202	CDL	CB2-OB2-PB2-OB4
31	V	202	CDL	CB2-OB2-PB2-OB5
31	V	202	CDL	CB3-OB5-PB2-OB2
31	V	202	CDL	CB3-OB5-PB2-OB3
31	V	202	CDL	CB3-OB5-PB2-OB4
31	a	201	CDL	CA2-OA2-PA1-OA3
31	a	201	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
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	g	202	CDL	CA2-OA2-PA1-OA3
31	g	202	CDL	CA2-OA2-PA1-OA4
31	g	202	CDL	CA2-OA2-PA1-OA5
31	g	202	CDL	OA6-CA4-CA6-OA8
31	g	202	CDL	CB3-OB5-PB2-OB2
31	g	202	CDL	C51-CB5-OB6-CB4
31	i	401	CDL	CB2-C1-CA2-OA2
31	i	401	CDL	CA2-OA2-PA1-OA4
31	i	401	CDL	CA2-OA2-PA1-OA5
31	i	401	CDL	CA3-OA5-PA1-OA2
31	i	401	CDL	CA3-OA5-PA1-OA4
31	i	401	CDL	CB2-OB2-PB2-OB3
31	i	401	CDL	CB3-OB5-PB2-OB2
31	i	401	CDL	CB3-OB5-PB2-OB3
31	l	701	CDL	CA2-OA2-PA1-OA5
31	l	701	CDL	CA3-OA5-PA1-OA3
31	l	701	CDL	CB3-OB5-PB2-OB2
31	l	701	CDL	CB3-OB5-PB2-OB4
31	l	702	CDL	O1-C1-CA2-OA2
31	l	702	CDL	CA2-OA2-PA1-OA3
31	l	702	CDL	CA2-OA2-PA1-OA4
31	l	702	CDL	CA2-OA2-PA1-OA5
31	l	702	CDL	CA3-OA5-PA1-OA2
31	l	702	CDL	CB2-OB2-PB2-OB4
31	l	702	CDL	CB2-OB2-PB2-OB5
31	l	702	CDL	OB6-CB4-CB6-OB8
31	o	201	CDL	CA2-OA2-PA1-OA4
31	o	201	CDL	CA2-OA2-PA1-OA5
31	o	201	CDL	CA3-OA5-PA1-OA2
31	o	201	CDL	CA3-OA5-PA1-OA3
31	o	201	CDL	CB2-OB2-PB2-OB3
31	o	201	CDL	CB2-OB2-PB2-OB4
31	o	201	CDL	CB2-OB2-PB2-OB5
31	o	201	CDL	CB3-OB5-PB2-OB2
31	o	201	CDL	CB3-OB5-PB2-OB3
31	u	201	CDL	CA2-OA2-PA1-OA4
31	u	201	CDL	CA2-OA2-PA1-OA5
31	u	201	CDL	CA3-OA5-PA1-OA2

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Mol	Chain	Res	Type	Atoms
31	u	201	CDL	CA3-OA5-PA1-OA3
31	u	201	CDL	CA3-OA5-PA1-OA4
31	u	201	CDL	CB2-OB2-PB2-OB4
31	u	201	CDL	CB2-OB2-PB2-OB5
31	u	201	CDL	CB3-OB5-PB2-OB3
32	X	201	8Q1	C1-C6-C7-C8
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	N36-C37-C38-C39
32	X	201	8Q1	C43-C42-N41-C39
33	a	202	PLX	O7-C6-O6-C4
33	a	202	PLX	C3-O4-P1-O1
33	a	202	PLX	C3-O4-P1-O3
33	a	202	PLX	O9-C24-O8-C5
33	g	201	PLX	O7-C6-O6-C4
33	g	201	PLX	C3-O4-P1-O1
33	g	201	PLX	C3-O4-P1-O2
33	g	201	PLX	C25-C24-O8-C5
33	j	201	PLX	O7-C6-C7-C8
33	j	201	PLX	O7-C6-O6-C4
33	r	502	PLX	O7-C6-O6-C4
33	r	502	PLX	C3-O4-P1-O1
33	r	502	PLX	C2-O1-P1-O4
33	r	502	PLX	C2-O1-P1-O2
33	r	502	PLX	C2-O1-P1-O3
33	r	502	PLX	O9-C24-C25-C26
34	s	403	UQ	C7-C8-C9-C10
34	s	403	UQ	C7-C8-C9-C11
34	s	403	UQ	C12-C13-C14-C16
35	w	401	ADP	C5'-O5'-PA-O2A
34	s	403	UQ	C17-C18-C19-C21
30	V	201	PEE	O4-C10-O2-C2
30	r	501	PEE	O4-C10-O2-C2
31	g	202	CDL	OB7-CB5-OB6-CB4
34	s	403	UQ	C12-C11-C9-C10
34	s	403	UQ	C13-C14-C16-C17
31	g	202	CDL	C71-CB7-OB8-CB6
31	l	701	CDL	C31-CA7-OA8-CA6
31	g	202	CDL	OB9-CB7-OB8-CB6
31	l	701	CDL	OA9-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
31	l	701	CDL	O1-C1-CA2-OA2
31	u	201	CDL	O1-C1-CA2-OA2
30	b	201	PEE	C31-C30-O3-C3
30	s	401	PEE	C31-C30-O3-C3
31	l	702	CDL	C71-CB7-OB8-CB6
31	l	702	CDL	C59-C60-C61-C62
30	U	101	PEE	C11-C10-O2-C2
30	i	402	PEE	C11-C10-O2-C2
31	o	201	CDL	C51-CB5-OB6-CB4
30	b	201	PEE	O5-C30-O3-C3
30	U	101	PEE	C19-C20-C21-C22
31	l	702	CDL	OB9-CB7-OB8-CB6
30	i	402	PEE	O4-C10-O2-C2
34	s	403	UQ	C14-C16-C17-C18
30	s	401	PEE	O5-C30-O3-C3
31	o	201	CDL	C31-CA7-OA8-CA6
31	l	702	CDL	C11-C12-C13-C14
30	U	101	PEE	C17-C18-C19-C20
30	b	201	PEE	C37-C38-C39-C40
31	V	202	CDL	C11-CA5-OA6-CA4
30	U	101	PEE	C30-C31-C32-C33
33	r	502	PLX	C30-C31-C32-C33
30	U	101	PEE	O4-C10-O2-C2
31	V	202	CDL	CA2-C1-CB2-OB2
31	g	202	CDL	CB2-C1-CA2-OA2
31	i	401	CDL	CA2-C1-CB2-OB2
31	i	401	CDL	C31-CA7-OA8-CA6
31	l	702	CDL	C35-C36-C37-C38
31	l	702	CDL	C54-C55-C56-C57
33	a	202	PLX	C11-C10-C9-C8
33	j	201	PLX	C28-C29-C30-C31
33	g	201	PLX	C7-C8-C9-C10
31	V	202	CDL	O1-C1-CB2-OB2
31	i	401	CDL	O1-C1-CA2-OA2
31	l	702	CDL	O1-C1-CB2-OB2
31	i	401	CDL	OA9-CA7-OA8-CA6
31	g	202	CDL	C36-C37-C38-C39
31	o	201	CDL	OB5-CB3-CB4-OB6
31	i	401	CDL	OB6-CB4-CB6-OB8
31	l	701	CDL	C58-C59-C60-C61
30	U	101	PEE	C32-C33-C34-C35
30	V	201	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	l	703	PEE	C37-C38-C39-C40
30	V	201	PEE	C10-C11-C12-C13
30	b	201	PEE	C10-C11-C12-C13
30	l	703	PEE	C31-C30-O3-C3
31	l	702	CDL	C39-C40-C41-C42
31	g	202	CDL	CB5-C51-C52-C53
31	o	201	CDL	C51-C52-C53-C54
31	a	201	CDL	C31-C32-C33-C34
33	r	502	PLX	C2-C1-N1-C1C
33	r	502	PLX	C2-C1-N1-C1A
31	g	202	CDL	CB7-C71-C72-C73
31	l	702	CDL	CB5-C51-C52-C53
30	r	501	PEE	C30-C31-C32-C33
31	g	202	CDL	CA5-C11-C12-C13
31	l	702	CDL	CB7-C71-C72-C73
33	r	502	PLX	C12-C13-C14-C15
30	V	201	PEE	C11-C12-C13-C14
31	V	202	CDL	C59-C60-C61-C62
31	g	202	CDL	C13-C14-C15-C16
31	g	202	CDL	O1-C1-CA2-OA2
31	i	401	CDL	O1-C1-CB2-OB2
31	V	202	CDL	OA7-CA5-OA6-CA4
31	o	201	CDL	OB7-CB5-OB6-CB4
30	s	402	PEE	C37-C38-C39-C40
31	o	201	CDL	OA9-CA7-OA8-CA6
30	l	703	PEE	O5-C30-O3-C3
31	l	701	CDL	CB2-C1-CA2-OA2
31	l	702	CDL	CB2-C1-CA2-OA2
31	o	201	CDL	C32-C33-C34-C35
31	o	201	CDL	C80-C81-C82-C83
31	l	701	CDL	C11-CA5-OA6-CA4
31	u	201	CDL	C11-CA5-OA6-CA4
31	V	202	CDL	CA6-CA4-OA6-CA5
33	j	201	PLX	C34-C35-C36-C37
31	u	201	CDL	OA7-CA5-OA6-CA4
30	r	501	PEE	C10-C11-C12-C13
31	g	202	CDL	C74-C75-C76-C77
31	g	202	CDL	CA7-C31-C32-C33
31	l	702	CDL	C57-C58-C59-C60
31	g	202	CDL	C73-C74-C75-C76
33	j	201	PLX	C12-C13-C14-C15
33	r	502	PLX	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	l	702	CDL	C72-C73-C74-C75
33	j	201	PLX	C10-C11-C12-C13
33	g	201	PLX	C27-C28-C29-C30
31	g	202	CDL	C71-C72-C73-C74
30	b	201	PEE	C11-C10-O2-C2
30	s	401	PEE	C11-C10-O2-C2
30	l	703	PEE	C31-C32-C33-C34
31	l	702	CDL	C53-C54-C55-C56
30	b	201	PEE	C2-C3-O3-C30
33	j	201	PLX	C13-C14-C15-C16
33	g	201	PLX	C33-C34-C35-C36
30	s	402	PEE	C31-C30-O3-C3
31	g	202	CDL	C55-C56-C57-C58
30	r	501	PEE	C12-C13-C14-C15
33	g	201	PLX	C28-C29-C30-C31
33	j	201	PLX	C25-C26-C27-C28
30	b	201	PEE	C13-C14-C15-C16
31	g	202	CDL	C41-C42-C43-C44
31	l	701	CDL	C52-C53-C54-C55
30	b	201	PEE	C22-C23-C24-C25
30	b	201	PEE	C31-C32-C33-C34
31	V	202	CDL	C52-C53-C54-C55
31	l	702	CDL	C33-C34-C35-C36
31	l	702	CDL	C58-C59-C60-C61
30	s	402	PEE	C35-C36-C37-C38
30	U	101	PEE	C31-C30-O3-C3
31	g	202	CDL	C75-C76-C77-C78
30	U	101	PEE	C41-C42-C43-C44
30	r	501	PEE	C20-C21-C22-C23
31	l	702	CDL	C56-C57-C58-C59
30	s	402	PEE	C33-C34-C35-C36
33	r	502	PLX	C31-C32-C33-C34
30	b	201	PEE	O4-C10-O2-C2
30	s	401	PEE	O4-C10-O2-C2
31	l	701	CDL	OA7-CA5-OA6-CA4
33	g	201	PLX	C11-C10-C9-C8
33	r	502	PLX	C11-C10-C9-C8
30	U	101	PEE	C22-C23-C24-C25
31	l	702	CDL	C14-C15-C16-C17
31	l	702	CDL	C60-C61-C62-C63
31	g	202	CDL	C35-C36-C37-C38
31	g	202	CDL	C62-C63-C64-C65

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Mol	Chain	Res	Type	Atoms
31	g	202	CDL	C17-C18-C19-C20
31	g	202	CDL	C43-C44-C45-C46
33	r	502	PLX	C15-C16-C17-C18
30	s	402	PEE	C21-C22-C23-C24
33	j	201	PLX	C27-C28-C29-C30
31	V	202	CDL	O1-C1-CA2-OA2
31	o	201	CDL	C11-CA5-OA6-CA4
31	u	201	CDL	C75-C76-C77-C78
33	r	502	PLX	C32-C33-C34-C35
31	l	702	CDL	CA7-C31-C32-C33
31	l	701	CDL	C51-C52-C53-C54
31	l	702	CDL	C52-C53-C54-C55
33	r	502	PLX	C2-C1-N1-C1B
30	s	401	PEE	C12-C13-C14-C15
30	s	402	PEE	O5-C30-O3-C3
30	i	402	PEE	C34-C35-C36-C37
31	l	702	CDL	C31-C32-C33-C34
30	b	201	PEE	C14-C15-C16-C17
33	g	201	PLX	C10-C11-C12-C13
30	U	101	PEE	O5-C30-O3-C3
31	a	201	CDL	CA7-C31-C32-C33
31	l	702	CDL	OA6-CA4-CA6-OA8
33	r	502	PLX	C14-C15-C16-C17
30	V	201	PEE	C31-C30-O3-C3
31	l	702	CDL	C55-C56-C57-C58
33	r	502	PLX	C28-C29-C30-C31
31	l	702	CDL	C74-C75-C76-C77
30	U	101	PEE	C36-C37-C38-C39
31	i	401	CDL	C11-C12-C13-C14
31	a	201	CDL	CB5-C51-C52-C53
31	l	702	CDL	C40-C41-C42-C43
31	l	702	CDL	C37-C38-C39-C40
33	g	201	PLX	C25-C26-C27-C28
30	V	201	PEE	C32-C33-C34-C35
30	l	703	PEE	C21-C22-C23-C24
33	j	201	PLX	C7-C8-C9-C10
30	s	401	PEE	C19-C20-C21-C22
30	b	201	PEE	C32-C33-C34-C35
30	i	402	PEE	C31-C32-C33-C34
33	g	201	PLX	C9-C10-C11-C12
30	r	501	PEE	C31-C30-O3-C3
31	g	202	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
30	r	501	PEE	C17-C18-C19-C20
30	b	201	PEE	C1-C2-C3-O3
31	g	202	CDL	CB3-CB4-CB6-OB8
31	l	702	CDL	CA3-CA4-CA6-OA8
31	l	702	CDL	CB3-CB4-CB6-OB8
31	u	201	CDL	CA3-CA4-CA6-OA8
33	j	201	PLX	C3-C4-C5-O8
33	r	502	PLX	C3-C4-C5-O8
30	l	703	PEE	C15-C16-C17-C18
30	s	402	PEE	C15-C16-C17-C18
30	s	402	PEE	C39-C40-C41-C42
33	j	201	PLX	C14-C15-C16-C17
30	i	402	PEE	C22-C23-C24-C25
30	r	501	PEE	C21-C22-C23-C24
30	V	201	PEE	O5-C30-O3-C3
31	V	202	CDL	C62-C63-C64-C65
31	l	702	CDL	C62-C63-C64-C65
32	X	201	8Q1	C9-C10-C11-C12
31	g	202	CDL	C11-C12-C13-C14
30	b	201	PEE	C33-C34-C35-C36
31	g	202	CDL	C63-C64-C65-C66
30	V	201	PEE	C35-C36-C37-C38
30	s	401	PEE	C22-C23-C24-C25
33	j	201	PLX	C30-C31-C32-C33
33	r	502	PLX	C7-C8-C9-C10
33	r	502	PLX	C25-C26-C27-C28
34	s	403	UQ	C12-C11-C9-C8
30	V	201	PEE	C33-C34-C35-C36
31	l	701	CDL	C35-C36-C37-C38
32	X	201	8Q1	C7-C8-C9-C10
30	s	401	PEE	O2-C2-C3-O3
31	V	202	CDL	OB6-CB4-CB6-OB8
31	g	202	CDL	OB6-CB4-CB6-OB8
31	i	401	CDL	OA6-CA4-CA6-OA8
32	X	201	8Q1	C31-C29-C32-O33
30	s	402	PEE	C14-C15-C16-C17
31	l	702	CDL	C64-C65-C66-C67
30	i	402	PEE	C24-C25-C26-C27
30	r	501	PEE	O5-C30-O3-C3
31	l	701	CDL	CB5-C51-C52-C53
31	a	201	CDL	C37-C38-C39-C40
30	s	401	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
30	s	402	PEE	C17-C18-C19-C20
33	r	502	PLX	C10-C11-C12-C13
31	i	401	CDL	C37-C38-C39-C40
31	u	201	CDL	C53-C54-C55-C56
33	a	202	PLX	C34-C35-C36-C37
30	s	402	PEE	C20-C21-C22-C23
31	g	202	CDL	C33-C34-C35-C36
31	g	202	CDL	C60-C61-C62-C63
31	g	202	CDL	OA9-CA7-OA8-CA6
31	g	202	CDL	C59-C60-C61-C62
31	l	701	CDL	C79-C80-C81-C82
31	o	201	CDL	C79-C80-C81-C82
30	i	402	PEE	O3P-C1-C2-C3
31	i	401	CDL	OB5-CB3-CB4-CB6
30	s	402	PEE	C11-C10-O2-C2
33	a	202	PLX	C7-C8-C9-C10
31	l	702	CDL	C81-C82-C83-C84
31	g	202	CDL	C64-C65-C66-C67
31	l	701	CDL	C37-C38-C39-C40
31	g	202	CDL	C51-C52-C53-C54
33	r	502	PLX	C13-C14-C15-C16
31	o	201	CDL	OA7-CA5-OA6-CA4
30	l	703	PEE	C13-C14-C15-C16
31	V	202	CDL	C37-C38-C39-C40
30	b	201	PEE	C23-C24-C25-C26
31	g	202	CDL	C37-C38-C39-C40
30	i	402	PEE	C1-C2-C3-O3
30	r	501	PEE	C44-C45-C46-C47
33	g	201	PLX	C32-C33-C34-C35
30	l	703	PEE	C30-C31-C32-C33
33	a	202	PLX	C14-C15-C16-C17
33	g	201	PLX	C13-C14-C15-C16
30	s	401	PEE	C33-C34-C35-C36
33	j	201	PLX	C33-C34-C35-C36
31	g	202	CDL	C57-C58-C59-C60
31	g	202	CDL	C76-C77-C78-C79
33	a	202	PLX	C10-C11-C12-C13
30	s	402	PEE	C34-C35-C36-C37
30	V	201	PEE	O3P-C1-C2-O2
31	V	202	CDL	OB5-CB3-CB4-OB6
31	a	201	CDL	OA5-CA3-CA4-OA6
31	i	401	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
31	l	701	CDL	OA5-CA3-CA4-OA6
31	l	702	CDL	OA5-CA3-CA4-OA6
30	l	703	PEE	C33-C34-C35-C36
31	l	701	CDL	CB7-C71-C72-C73
32	X	201	8Q1	O4-C1-S44-C43
31	l	702	CDL	C44-C45-C46-C47
30	b	201	PEE	C34-C35-C36-C37
31	l	702	CDL	C18-C19-C20-C21
33	r	502	PLX	C11-C12-C13-C14
31	l	701	CDL	C14-C15-C16-C17
30	r	501	PEE	C24-C25-C26-C27
30	s	401	PEE	C20-C21-C22-C23
30	r	501	PEE	C13-C14-C15-C16
31	g	202	CDL	C31-C32-C33-C34
30	U	101	PEE	C38-C39-C40-C41
30	b	201	PEE	C16-C17-C18-C19
30	r	501	PEE	C36-C37-C38-C39
32	X	201	8Q1	C6-C1-S44-C43
31	l	702	CDL	CA2-C1-CB2-OB2
31	u	201	CDL	CB2-C1-CA2-OA2
30	i	402	PEE	C11-C12-C13-C14
31	i	401	CDL	OA5-CA3-CA4-CA6
31	o	201	CDL	OB5-CB3-CB4-CB6
33	j	201	PLX	O4-C3-C4-C5
30	s	401	PEE	C13-C14-C15-C16
30	i	402	PEE	C18-C19-C20-C21
33	a	202	PLX	C25-C26-C27-C28
31	g	202	CDL	C80-C81-C82-C83
33	j	201	PLX	C24-C25-C26-C27
31	g	202	CDL	C78-C79-C80-C81
30	s	402	PEE	O4-C10-O2-C2
33	r	502	PLX	C16-C17-C18-C19
31	o	201	CDL	CA6-CA4-OA6-CA5
30	U	101	PEE	C44-C45-C46-C47
30	i	402	PEE	O3P-C1-C2-O2
31	i	401	CDL	OA5-CA3-CA4-OA6
30	s	402	PEE	C31-C32-C33-C34
31	l	701	CDL	C20-C21-C22-C23
31	o	201	CDL	C75-C76-C77-C78
31	g	202	CDL	CA3-CA4-CA6-OA8
31	i	401	CDL	CB3-CB4-CB6-OB8
34	s	403	UQ	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	V	202	CDL	C78-C79-C80-C81
30	V	201	PEE	C31-C32-C33-C34
31	g	202	CDL	C12-C13-C14-C15
31	i	401	CDL	C36-C37-C38-C39
31	l	701	CDL	C76-C77-C78-C79
30	b	201	PEE	C5-C4-O4P-P
31	a	201	CDL	C54-C55-C56-C57
30	b	201	PEE	O2-C2-C3-O3
31	u	201	CDL	OA6-CA4-CA6-OA8
33	r	502	PLX	O6-C4-C5-O8
30	i	402	PEE	C32-C33-C34-C35
33	r	502	PLX	C26-C27-C28-C29
30	U	101	PEE	C42-C43-C44-C45
31	o	201	CDL	C72-C73-C74-C75
31	l	702	CDL	C12-C13-C14-C15
31	l	701	CDL	CA4-CA3-OA5-PA1
33	a	202	PLX	N1-C1-C2-O1
31	o	201	CDL	C78-C79-C80-C81
30	i	402	PEE	C21-C22-C23-C24
33	r	502	PLX	O7-C6-C7-C8
30	r	501	PEE	C41-C42-C43-C44
33	j	201	PLX	C25-C24-O8-C5
33	r	502	PLX	C25-C24-O8-C5
31	l	702	CDL	C15-C16-C17-C18
31	l	702	CDL	C43-C44-C45-C46
31	V	202	CDL	C58-C59-C60-C61
31	g	202	CDL	OB5-CB3-CB4-CB6
32	X	201	8Q1	O27-C28-C29-C30
30	s	402	PEE	C23-C24-C25-C26
30	V	201	PEE	C38-C39-C40-C41
30	s	402	PEE	C22-C23-C24-C25
33	r	502	PLX	O8-C24-C25-C26
31	g	202	CDL	OB5-CB3-CB4-OB6
33	j	201	PLX	O4-C3-C4-O6
31	l	701	CDL	C51-CB5-OB6-CB4
30	b	201	PEE	C18-C19-C20-C21
30	l	703	PEE	C22-C23-C24-C25
30	i	402	PEE	O2-C2-C3-O3
33	j	201	PLX	O6-C4-C5-O8
30	s	401	PEE	C1-C2-C3-O3
31	V	202	CDL	CA3-CA4-CA6-OA8
31	V	202	CDL	CB3-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
30	U	101	PEE	C1-O3P-P-O2P
30	U	101	PEE	C1-O3P-P-O4P
30	V	201	PEE	C4-O4P-P-O1P
31	V	202	CDL	CA2-OA2-PA1-OA4
31	V	202	CDL	CA2-OA2-PA1-OA5
31	a	201	CDL	CB2-OB2-PB2-OB4
31	a	201	CDL	CB2-OB2-PB2-OB5
31	a	201	CDL	CB3-OB5-PB2-OB3
31	g	202	CDL	CB2-OB2-PB2-OB3
31	g	202	CDL	CB2-OB2-PB2-OB4
31	g	202	CDL	CB2-OB2-PB2-OB5
31	g	202	CDL	CB3-OB5-PB2-OB3
31	i	401	CDL	CB3-OB5-PB2-OB4
31	l	701	CDL	CA2-OA2-PA1-OA3
31	l	701	CDL	CA3-OA5-PA1-OA2
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	o	201	CDL	CA3-OA5-PA1-OA4
31	o	201	CDL	CB3-OB5-PB2-OB4
33	a	202	PLX	C2-O1-P1-O2
33	r	502	PLX	C3-C4-O6-C6
33	r	502	PLX	C5-C4-O6-C6
33	r	502	PLX	C3-O4-P1-O2
35	w	401	ADP	C5'-O5'-PA-O1A
35	w	401	ADP	C5'-O5'-PA-O3A
33	j	201	PLX	C9-C10-C11-C12
30	V	201	PEE	C2-C1-O3P-P
31	g	202	CDL	CB4-CB3-OB5-PB2
31	a	201	CDL	C71-C72-C73-C74
33	a	202	PLX	C15-C16-C17-C18
30	i	402	PEE	C38-C39-C40-C41
31	l	701	CDL	C24-C25-C26-C27
33	g	201	PLX	C16-C17-C18-C19
31	l	701	CDL	CA6-CA4-OA6-CA5
31	u	201	CDL	CA6-CA4-OA6-CA5
31	g	202	CDL	C44-C45-C46-C47
30	s	402	PEE	O3P-C1-C2-C3
31	a	201	CDL	OA5-CA3-CA4-CA6
31	l	701	CDL	OA5-CA3-CA4-CA6
31	l	702	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
30	s	402	PEE	O3P-C1-C2-O2
31	o	201	CDL	OA5-CA3-CA4-OA6
30	s	401	PEE	O3-C30-C31-C32
31	V	202	CDL	CA5-C11-C12-C13
33	r	502	PLX	C36-C37-C38-C39
33	g	201	PLX	C36-C37-C38-C39
31	l	701	CDL	C36-C37-C38-C39
31	l	701	CDL	OB7-CB5-OB6-CB4
31	l	702	CDL	C73-C74-C75-C76
31	i	401	CDL	CA3-CA4-CA6-OA8
31	V	202	CDL	C51-CB5-OB6-CB4
31	l	701	CDL	C56-C57-C58-C59
31	a	201	CDL	C75-C76-C77-C78
33	g	201	PLX	O8-C24-C25-C26
31	g	202	CDL	C20-C21-C22-C23
31	g	202	CDL	C56-C57-C58-C59
31	u	201	CDL	CB7-C71-C72-C73
31	a	201	CDL	C18-C19-C20-C21
30	i	402	PEE	C10-C11-C12-C13
31	l	702	CDL	C41-C42-C43-C44
31	l	702	CDL	C21-C22-C23-C24
31	i	401	CDL	C71-C72-C73-C74
33	r	502	PLX	C18-C19-C20-C21
31	a	201	CDL	C71-CB7-OB8-CB6
31	l	701	CDL	C83-C84-C85-C86
33	j	201	PLX	C15-C16-C17-C18
30	U	101	PEE	C23-C24-C25-C26
31	o	201	CDL	OA6-CA4-CA6-OA8
31	a	201	CDL	C39-C40-C41-C42
33	r	502	PLX	C24-C25-C26-C27
31	V	202	CDL	OB7-CB5-OB6-CB4
31	l	701	CDL	C82-C83-C84-C85
30	b	201	PEE	C38-C39-C40-C41
30	l	703	PEE	C2-C1-O3P-P
31	i	401	CDL	C33-C34-C35-C36
31	a	201	CDL	CA5-C11-C12-C13
33	g	201	PLX	C12-C13-C14-C15
30	l	703	PEE	C38-C39-C40-C41
30	l	703	PEE	C3-C2-O2-C10
31	a	201	CDL	CA6-CA4-OA6-CA5
31	i	401	CDL	CA6-CA4-OA6-CA5
31	o	201	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
31	o	201	CDL	C32-C31-CA7-OA8
33	j	201	PLX	C35-C36-C37-C38
33	g	201	PLX	C30-C31-C32-C33
30	r	501	PEE	O3P-C1-C2-O2
31	V	202	CDL	C1-CB2-OB2-PB2
31	o	201	CDL	OA5-CA3-CA4-CA6
30	b	201	PEE	C36-C37-C38-C39
33	a	202	PLX	C35-C36-C37-C38
30	i	402	PEE	C35-C36-C37-C38
33	r	502	PLX	C27-C28-C29-C30
33	j	201	PLX	O6-C6-C7-C8
31	g	202	CDL	C23-C24-C25-C26
30	i	402	PEE	C2-C1-O3P-P
31	V	202	CDL	C44-C45-C46-C47
30	l	703	PEE	C16-C17-C18-C19
33	a	202	PLX	O9-C24-C25-C26
31	u	201	CDL	OA5-CA3-CA4-OA6
31	i	401	CDL	C14-C15-C16-C17
31	i	401	CDL	C31-C32-C33-C34
31	l	701	CDL	C54-C55-C56-C57
30	s	401	PEE	C18-C19-C20-C21
31	a	201	CDL	OB9-CB7-OB8-CB6
31	l	702	CDL	C42-C43-C44-C45
30	V	201	PEE	O3P-C1-C2-C3
31	V	202	CDL	OB5-CB3-CB4-CB6
31	l	701	CDL	C39-C40-C41-C42
31	u	201	CDL	C58-C59-C60-C61
31	l	701	CDL	C55-C56-C57-C58
31	l	702	CDL	C17-C18-C19-C20
31	l	701	CDL	C81-C82-C83-C84
31	u	201	CDL	C77-C78-C79-C80
30	s	401	PEE	C16-C17-C18-C19
31	l	702	CDL	C34-C35-C36-C37
30	V	201	PEE	C37-C38-C39-C40
31	u	201	CDL	C19-C20-C21-C22
30	l	703	PEE	O3P-C1-C2-O2
31	u	201	CDL	C71-C72-C73-C74
30	U	101	PEE	C34-C35-C36-C37
30	V	201	PEE	C16-C17-C18-C19
30	i	402	PEE	C36-C37-C38-C39
30	s	402	PEE	C36-C37-C38-C39
32	X	201	8Q1	C31-C29-C32-C34

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Mol	Chain	Res	Type	Atoms
30	r	501	PEE	O3P-C1-C2-C3
31	g	202	CDL	OA5-CA3-CA4-CA6
31	l	702	CDL	C12-C11-CA5-OA6
31	g	202	CDL	C42-C43-C44-C45
31	u	201	CDL	C55-C56-C57-C58
30	b	201	PEE	O2-C10-C11-C12
31	u	201	CDL	C14-C15-C16-C17
33	j	201	PLX	C18-C19-C20-C21
31	a	201	CDL	C17-C18-C19-C20
30	r	501	PEE	C39-C40-C41-C42
31	l	702	CDL	OA9-CA7-OA8-CA6
30	s	402	PEE	C13-C14-C15-C16
31	l	702	CDL	C32-C31-CA7-OA8
30	V	201	PEE	C13-C14-C15-C16
32	X	201	8Q1	C13-C14-C15-C16
31	l	702	CDL	C51-C52-C53-C54
31	V	202	CDL	CB4-CB3-OB5-PB2
31	u	201	CDL	C54-C55-C56-C57
31	o	201	CDL	OB6-CB4-CB6-OB8
30	s	402	PEE	C42-C43-C44-C45
31	V	202	CDL	C41-C42-C43-C44
31	l	702	CDL	C31-CA7-OA8-CA6
30	b	201	PEE	O3-C30-C31-C32
31	g	202	CDL	C79-C80-C81-C82
31	a	201	CDL	C22-C23-C24-C25
32	X	201	8Q1	O27-C28-C29-C31
30	U	101	PEE	O2-C10-C11-C12
31	g	202	CDL	C32-C33-C34-C35
31	g	202	CDL	C72-C73-C74-C75
33	g	201	PLX	O6-C6-C7-C8
31	V	202	CDL	C72-C73-C74-C75
31	V	202	CDL	C35-C36-C37-C38
31	l	702	CDL	C12-C11-CA5-OA7
33	g	201	PLX	O9-C24-O8-C5
33	r	502	PLX	O9-C24-O8-C5
30	b	201	PEE	O4-C10-C11-C12
31	V	202	CDL	C39-C40-C41-C42
31	l	702	CDL	C32-C31-CA7-OA9
31	u	201	CDL	C12-C11-CA5-OA6
32	X	201	8Q1	O33-C32-C34-N36
30	U	101	PEE	O4-C10-C11-C12
31	g	202	CDL	C1-CA2-OA2-PA1

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Mol	Chain	Res	Type	Atoms
33	g	201	PLX	C6-C7-C8-C9
33	g	201	PLX	O4-C3-C4-C5
31	l	701	CDL	C23-C24-C25-C26
31	u	201	CDL	C22-C23-C24-C25
30	b	201	PEE	O5-C30-C31-C32

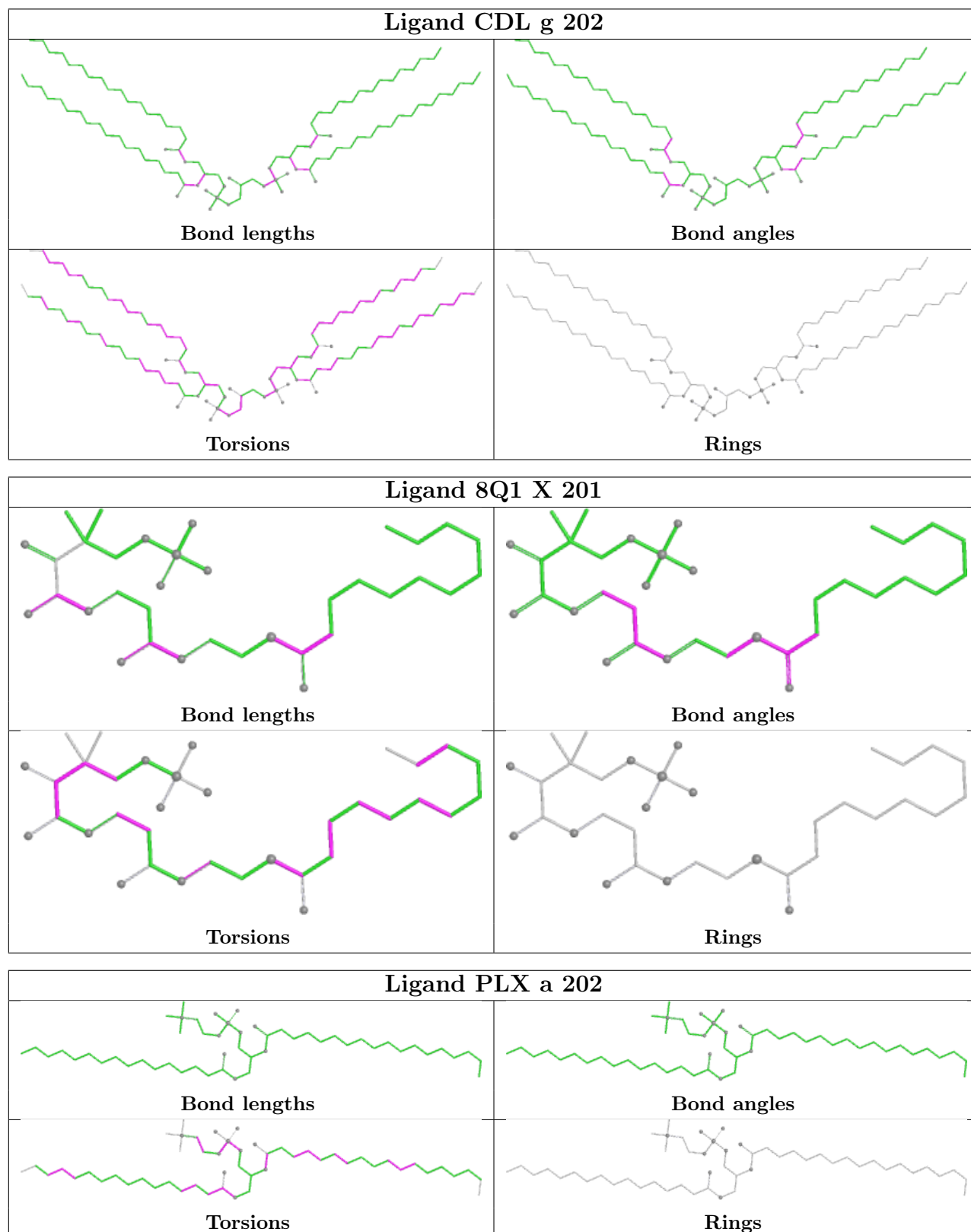
There are no ring outliers.

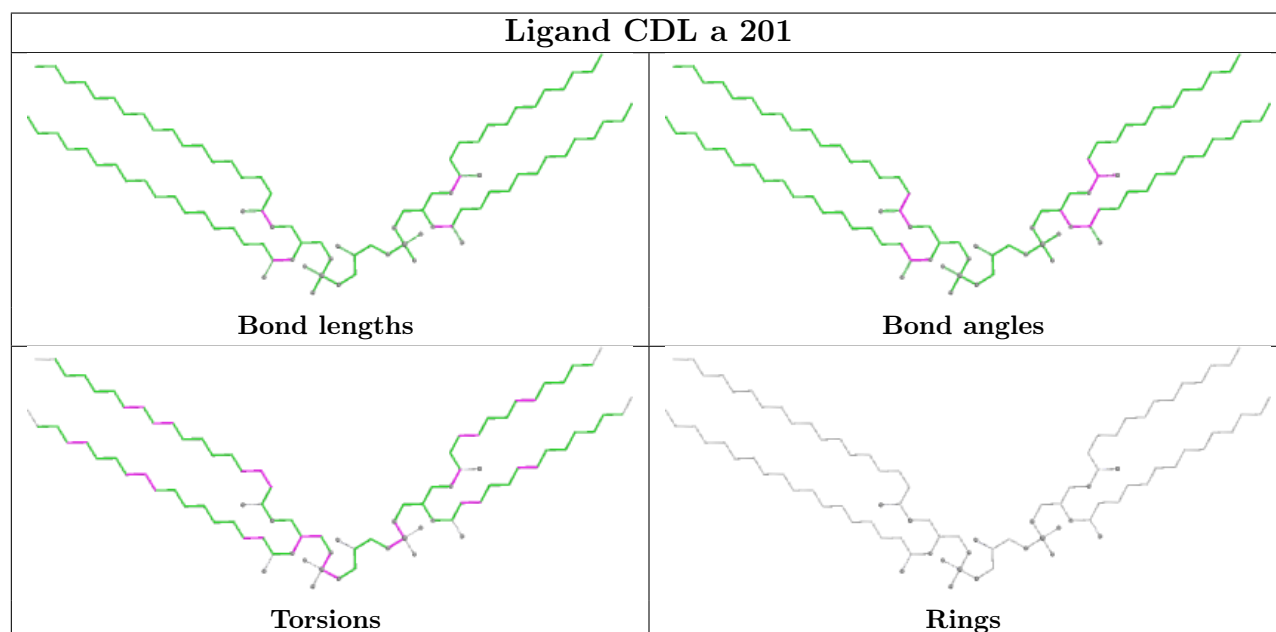
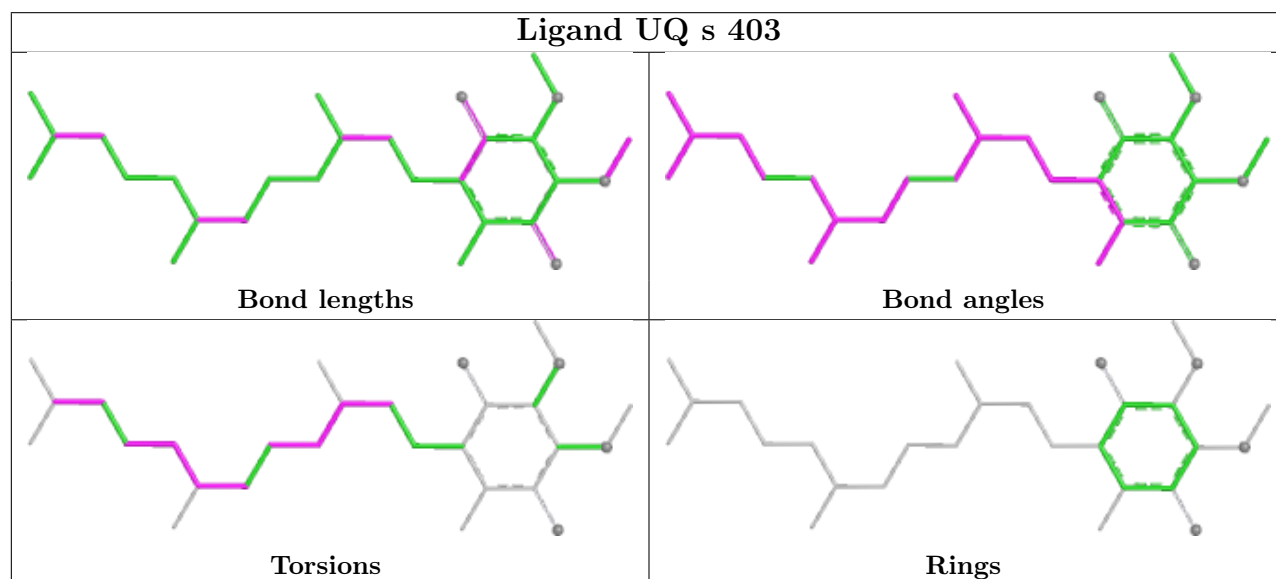
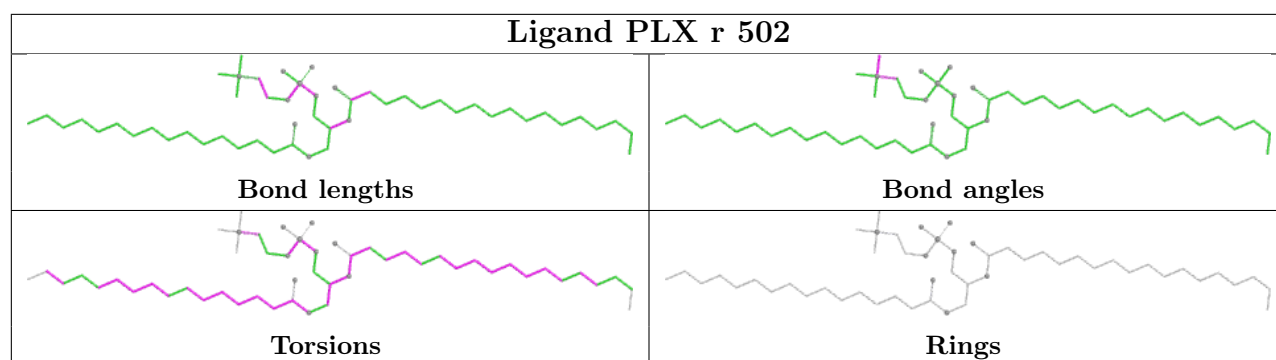
23 monomers are involved in 226 short contacts:

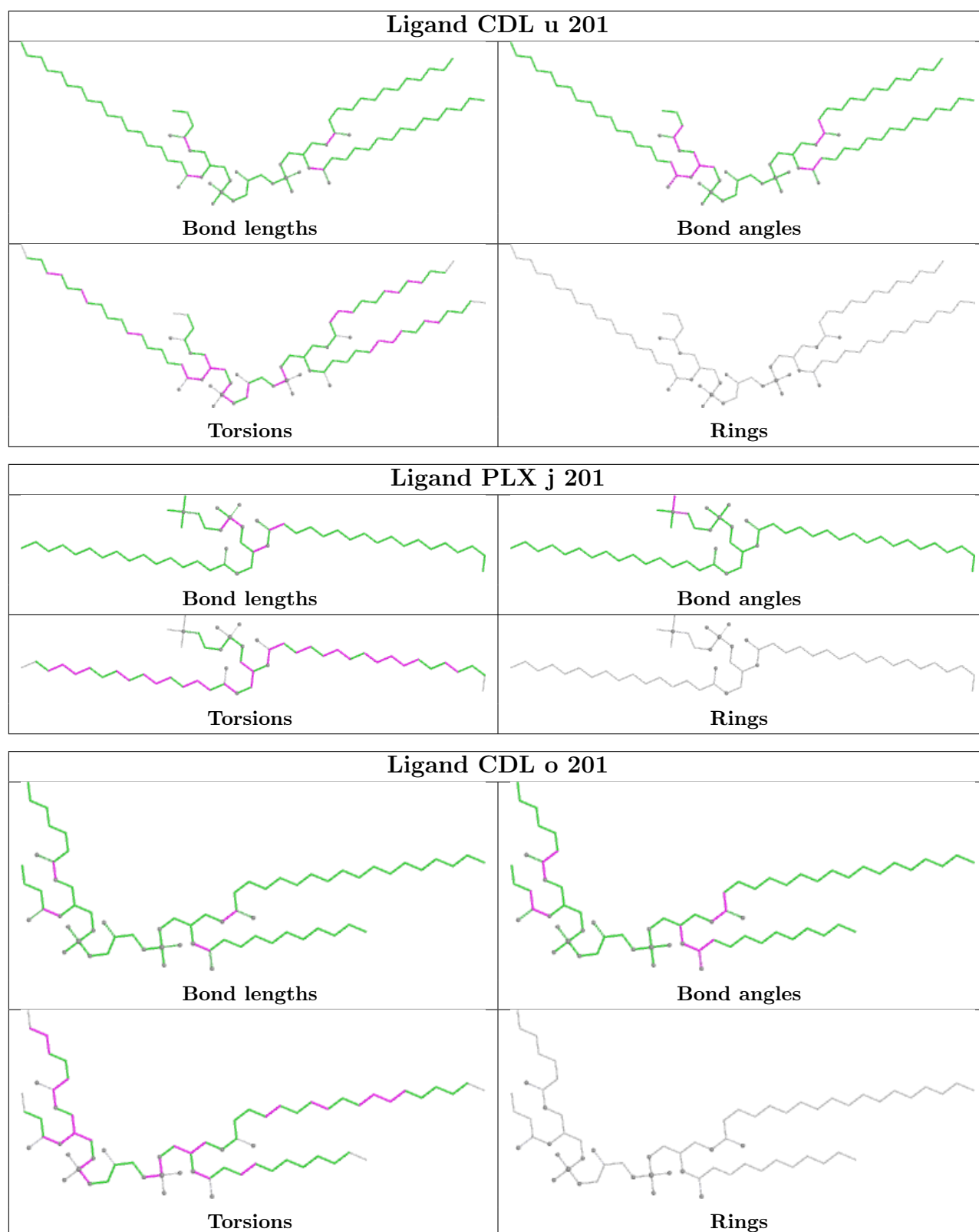
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	g	202	CDL	8	0
32	X	201	8Q1	2	0
33	a	202	PLX	9	0
33	r	502	PLX	7	0
34	s	403	UQ	5	0
31	a	201	CDL	16	0
31	u	201	CDL	13	0
33	j	201	PLX	2	0
31	o	201	CDL	14	0
31	i	401	CDL	16	0
30	i	402	PEE	10	0
31	l	701	CDL	39	0
30	s	401	PEE	8	0
33	g	201	PLX	1	0
31	l	702	CDL	7	0
30	s	402	PEE	2	0
30	U	101	PEE	6	0
31	V	202	CDL	19	0
30	l	703	PEE	8	0
30	b	201	PEE	18	0
35	w	401	ADP	4	0
30	r	501	PEE	21	0
30	V	201	PEE	6	0

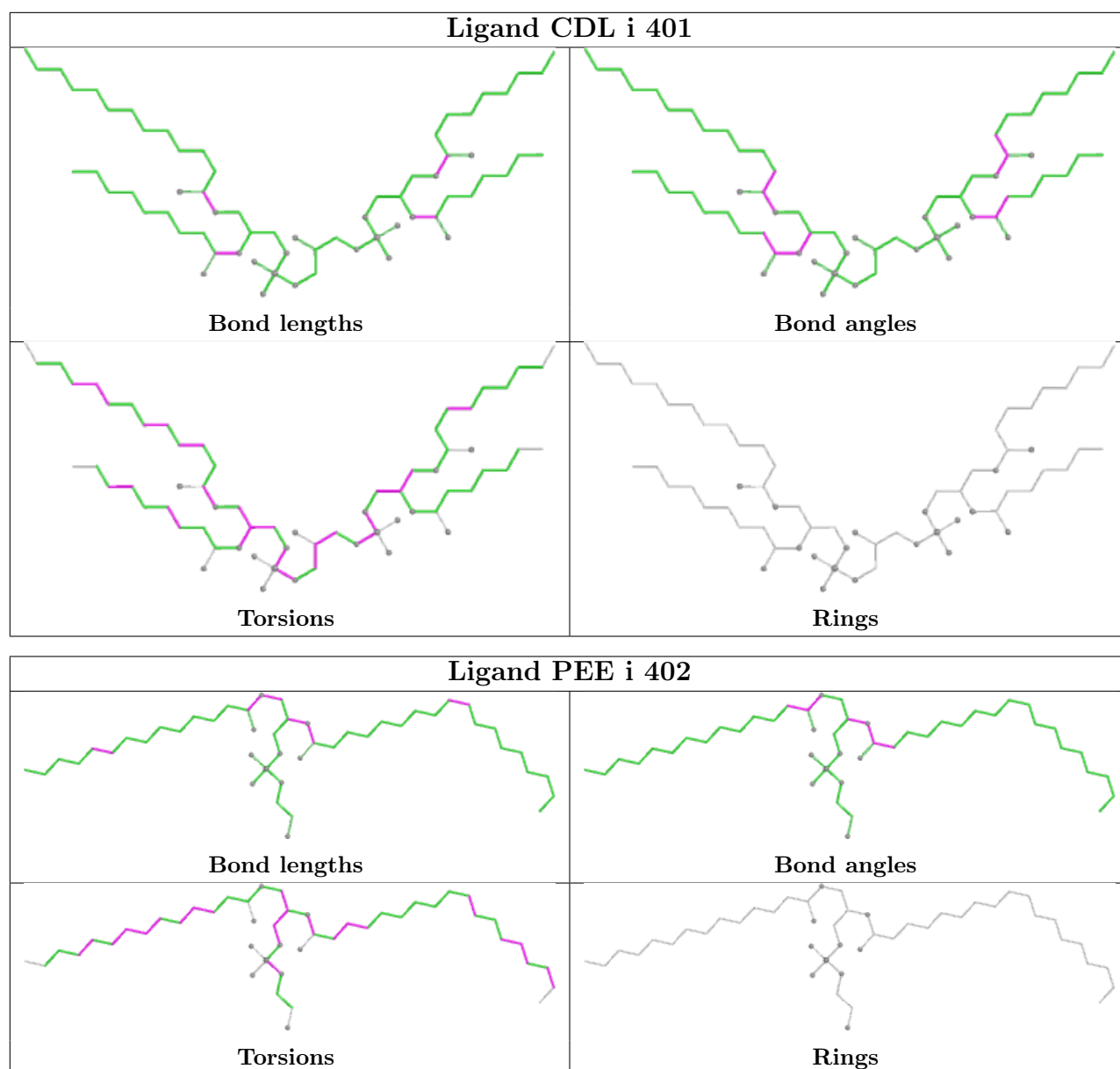
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

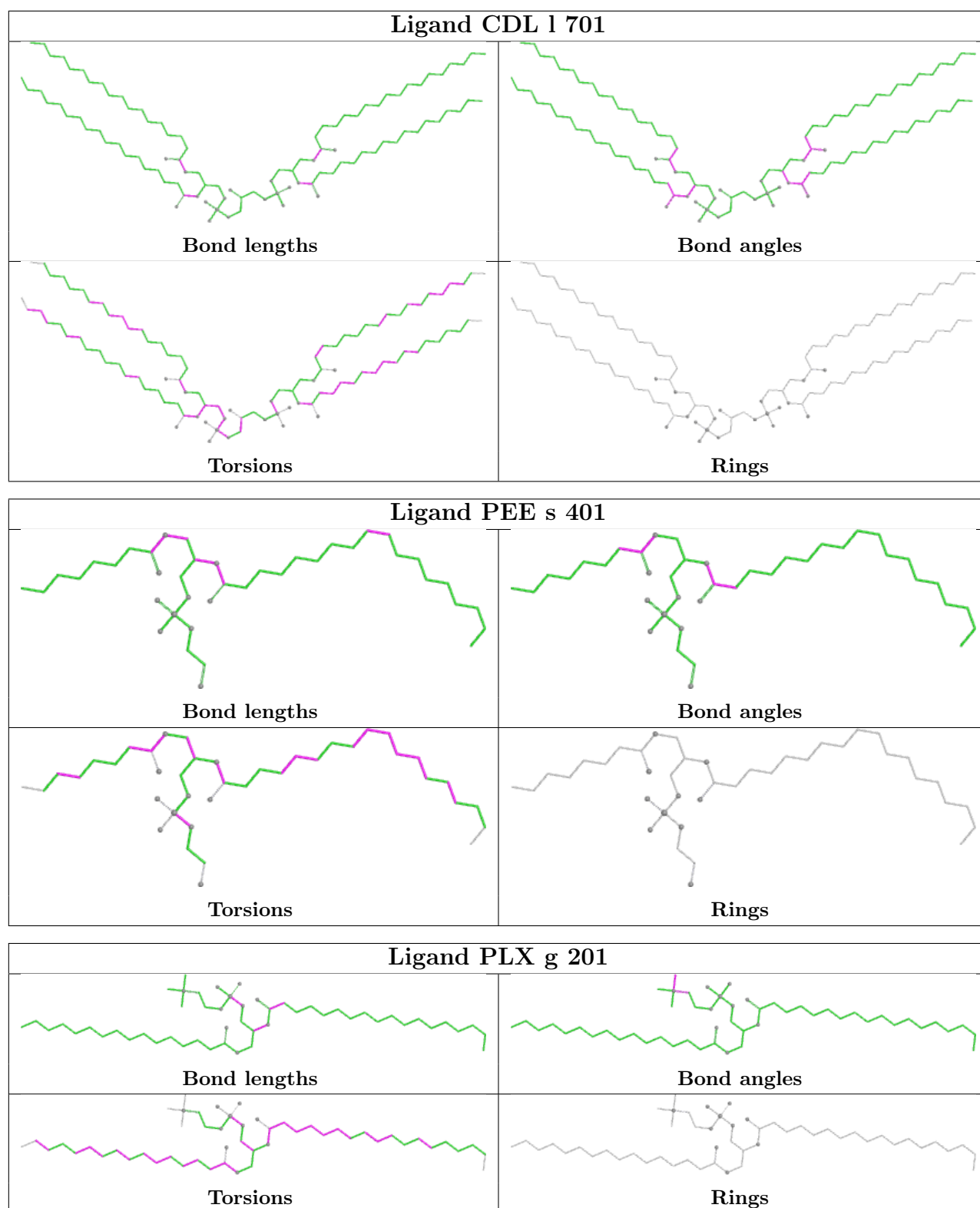
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

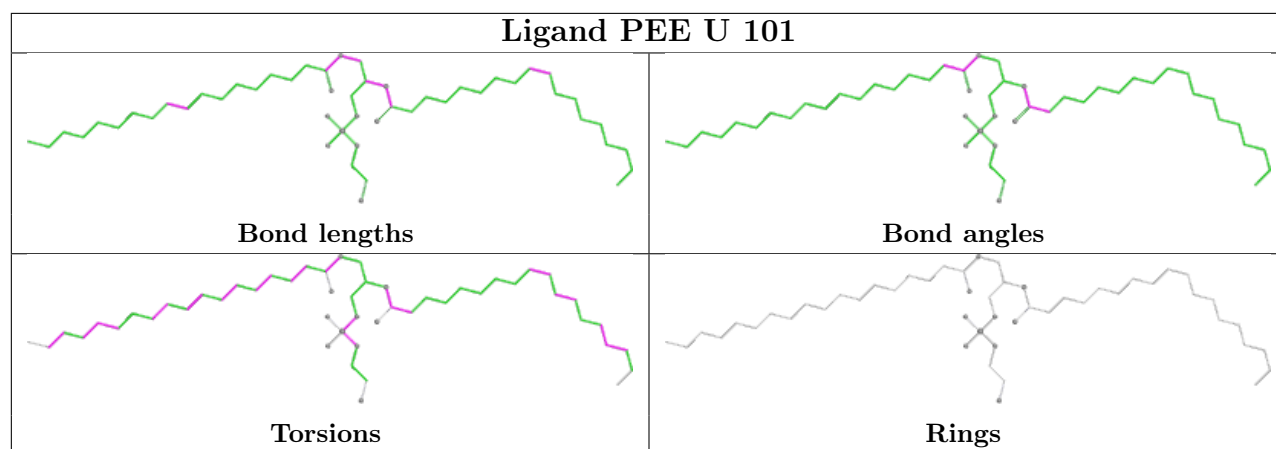
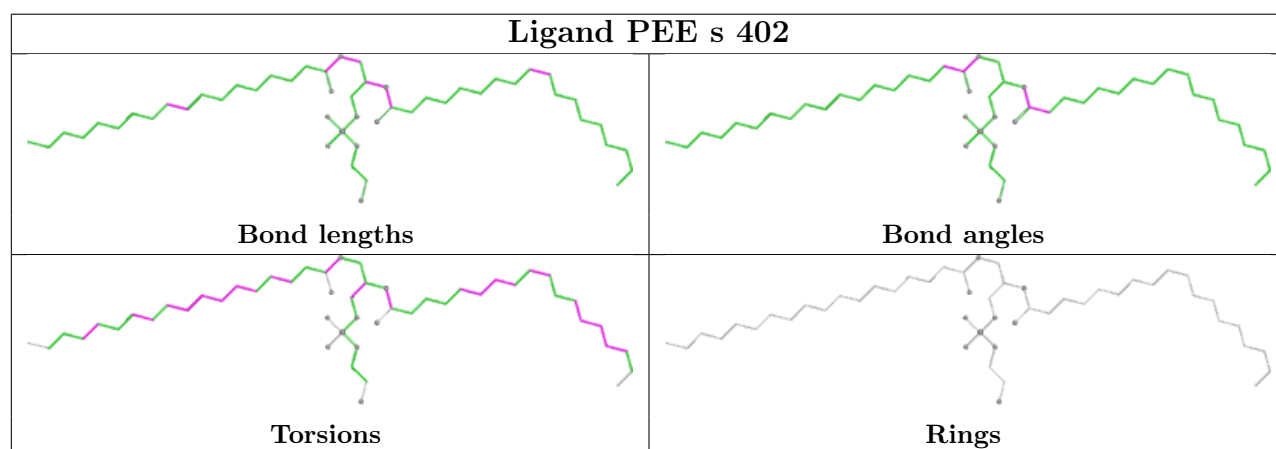
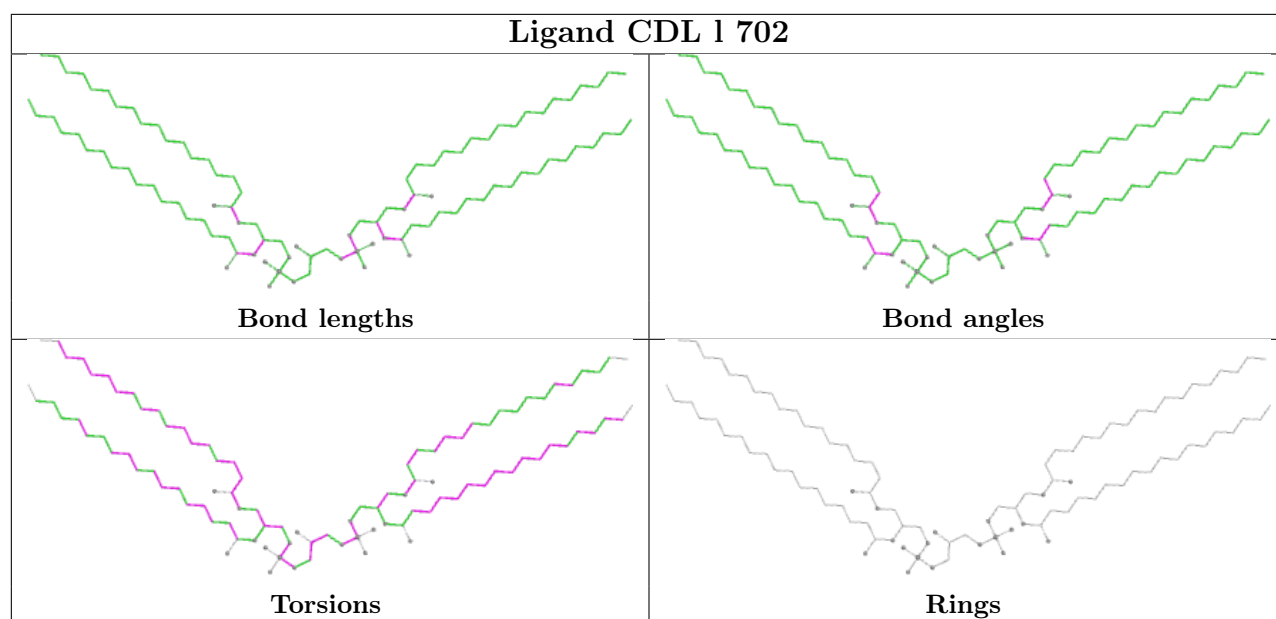


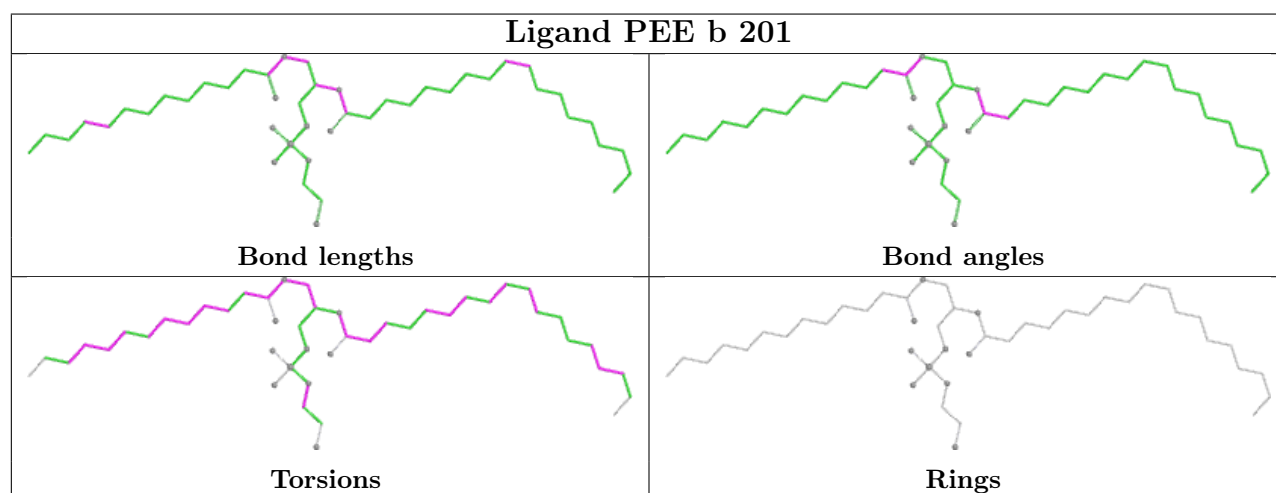
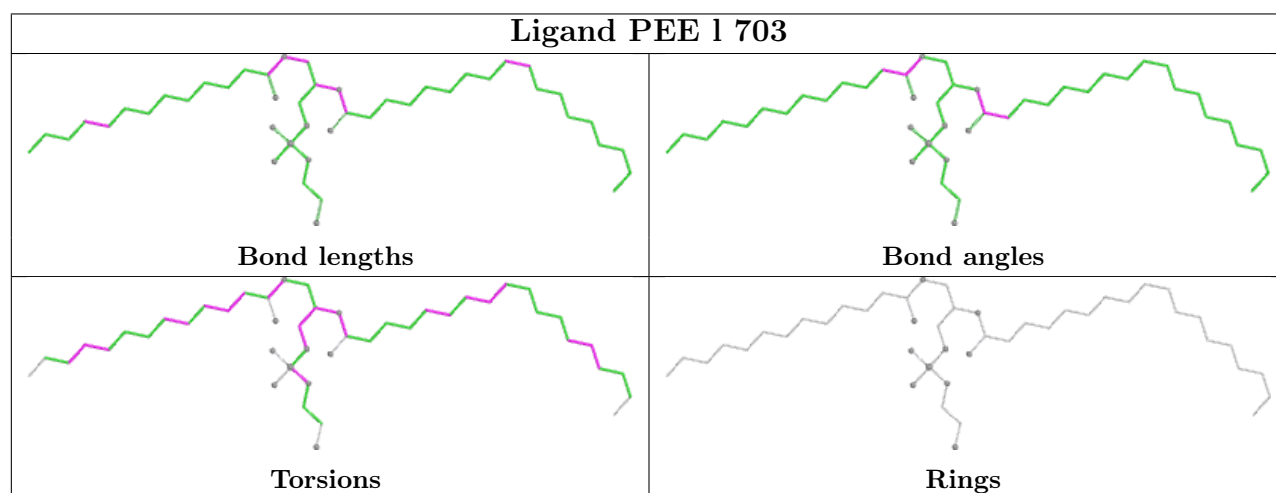
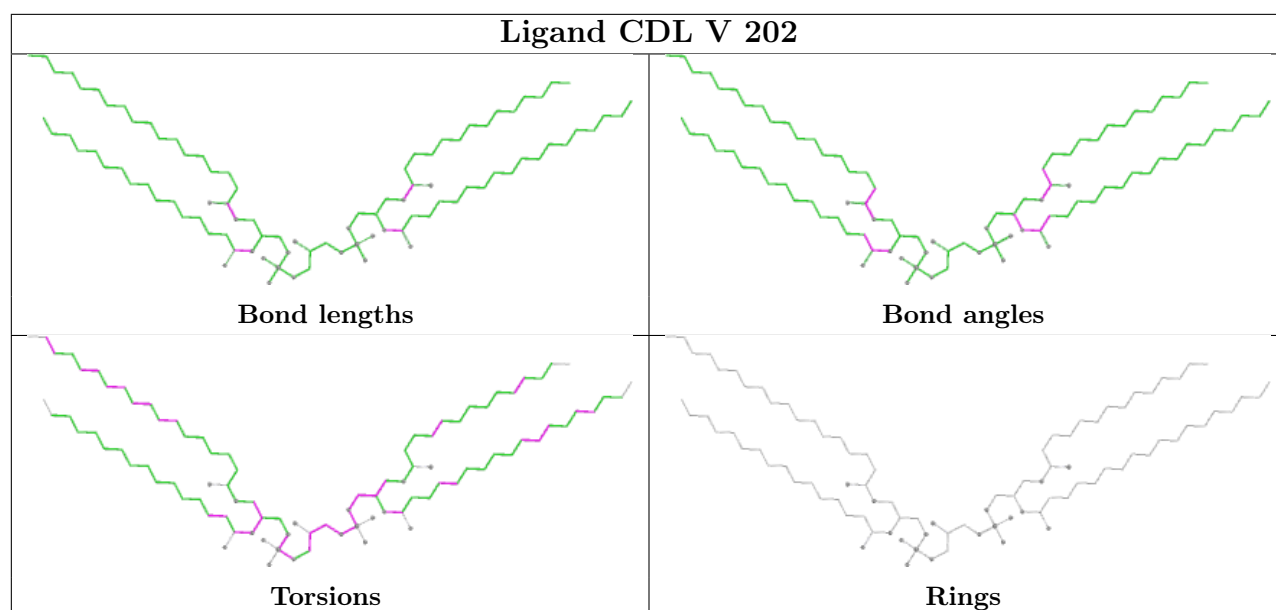


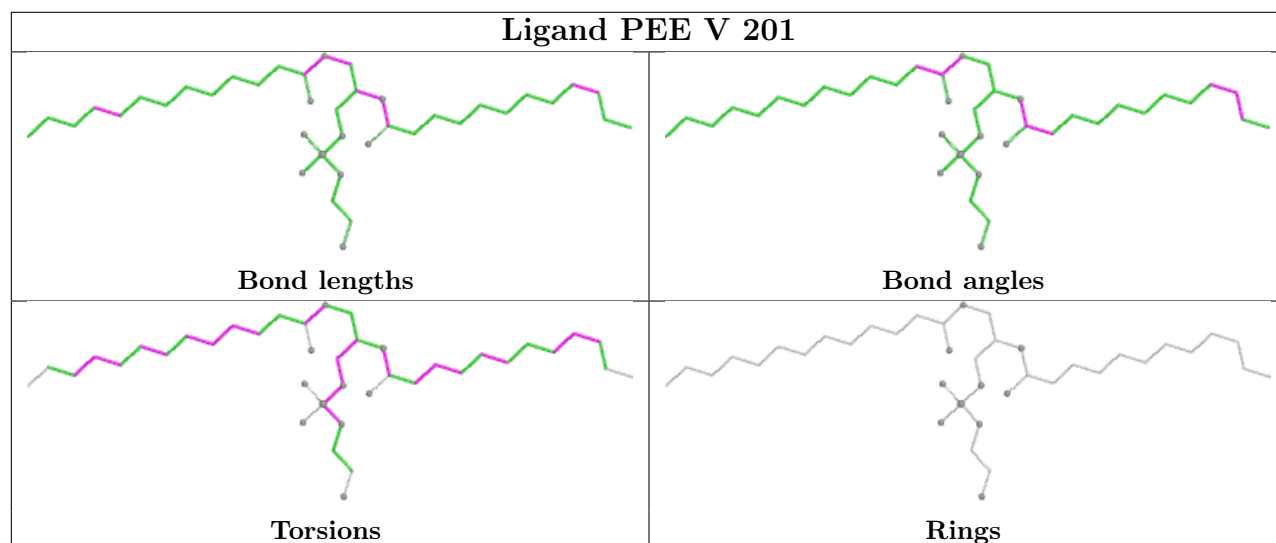
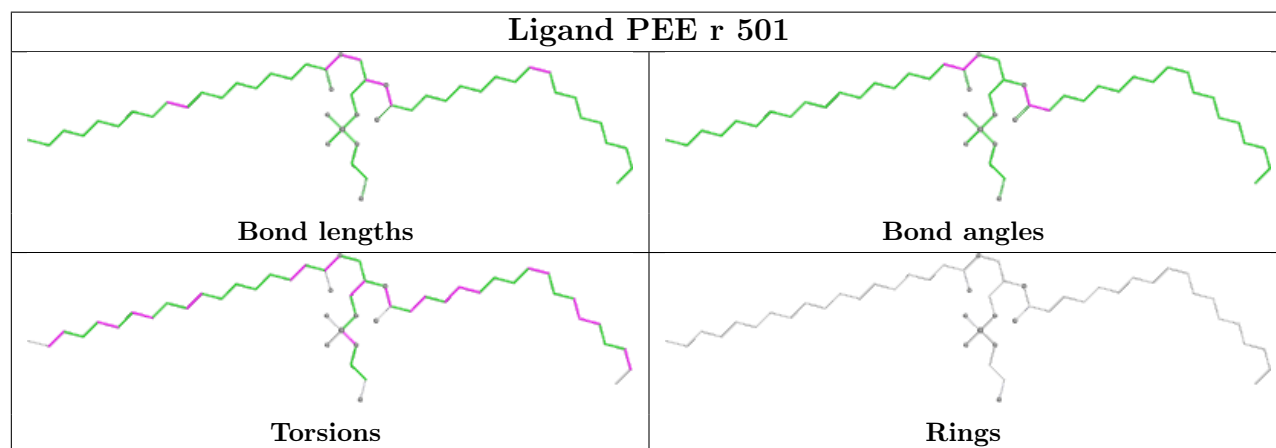
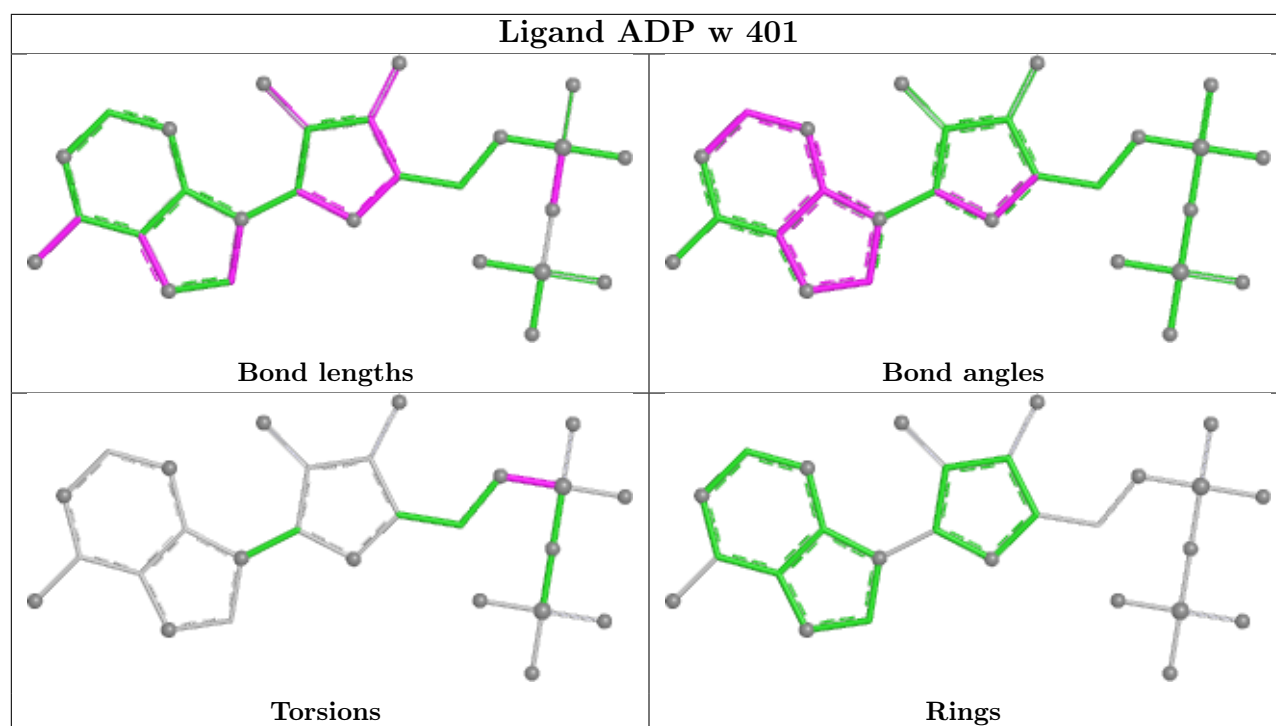












5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

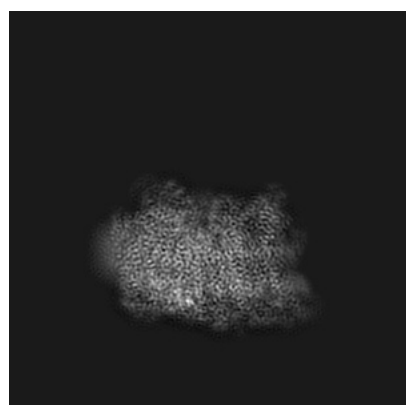
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32202. These allow visual inspection of the internal detail of the map and identification of artifacts.

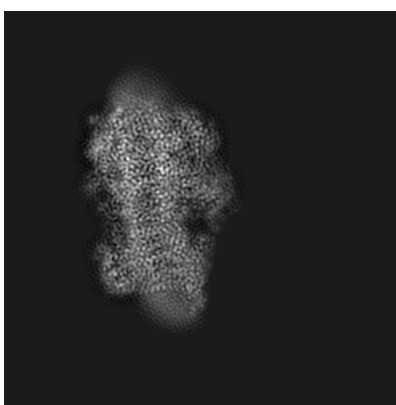
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

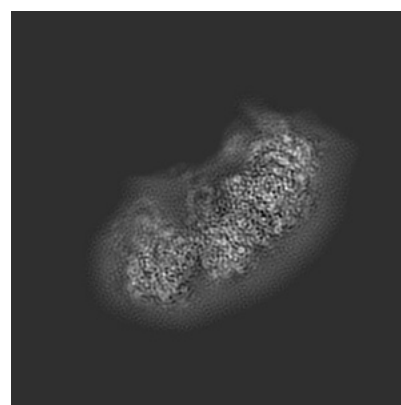
6.1.1 Primary map



X



Y

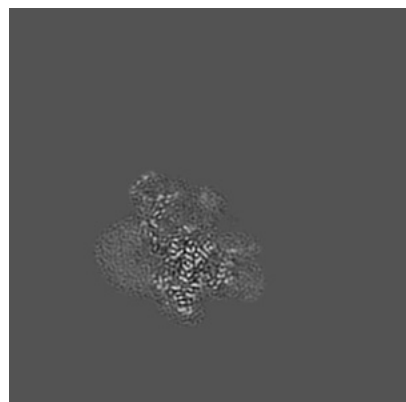


Z

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

6.2 Central slices [i](#)

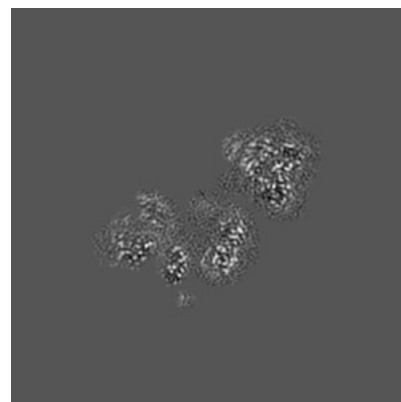
6.2.1 Primary map



X Index: 155



Y Index: 155

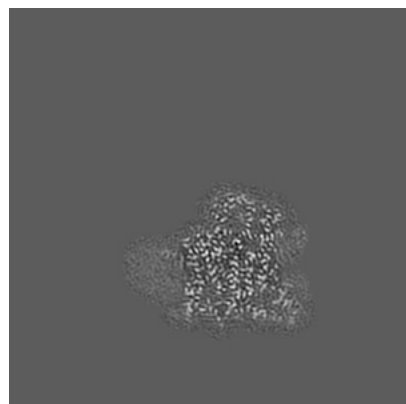


Z Index: 155

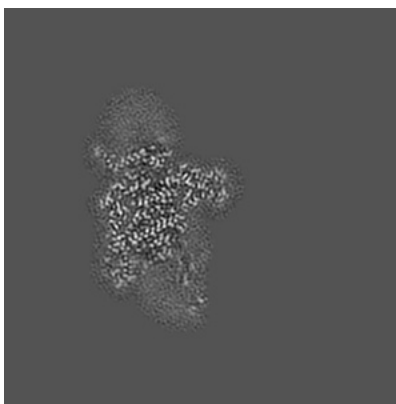
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

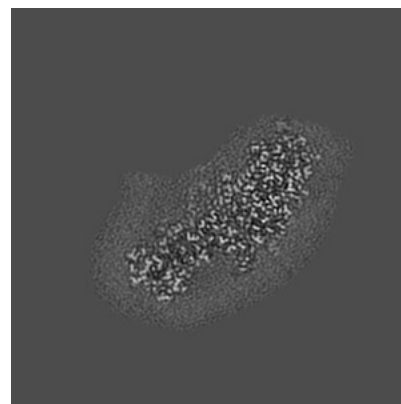
6.3.1 Primary map



X Index: 204



Y Index: 131

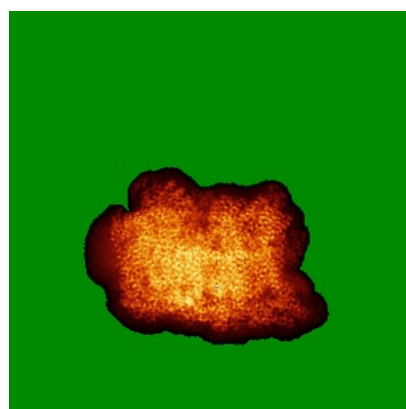


Z Index: 119

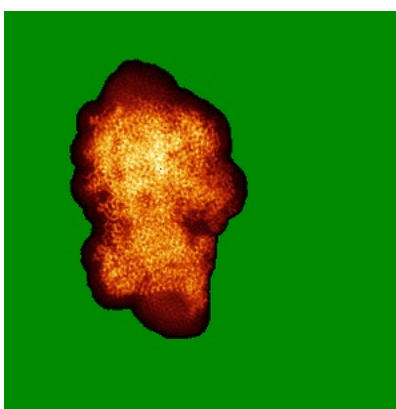
The images above show the largest variance slices of the map in three orthogonal directions.

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

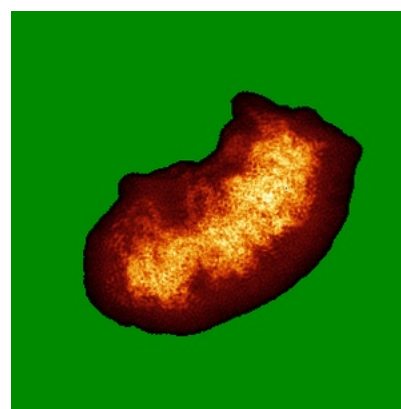
6.4.1 Primary map



X



Y

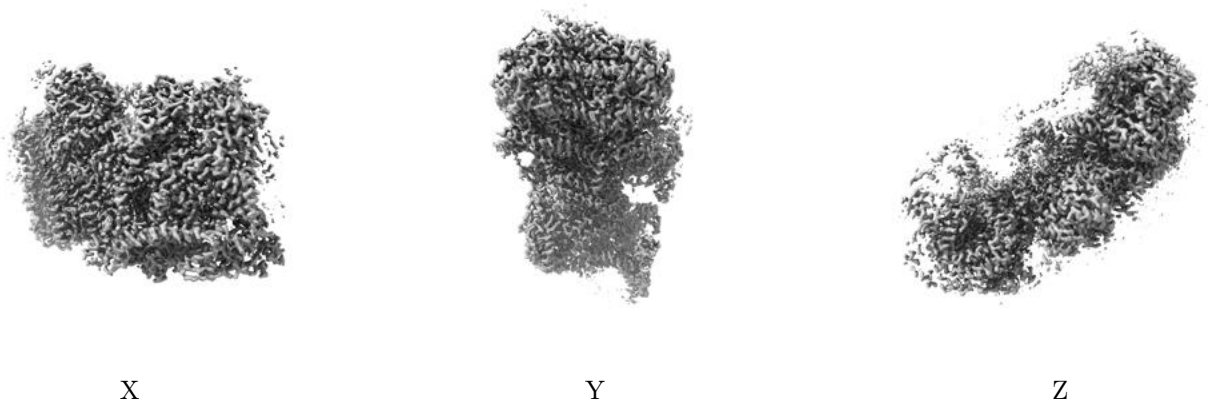


Z

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 0.0306. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

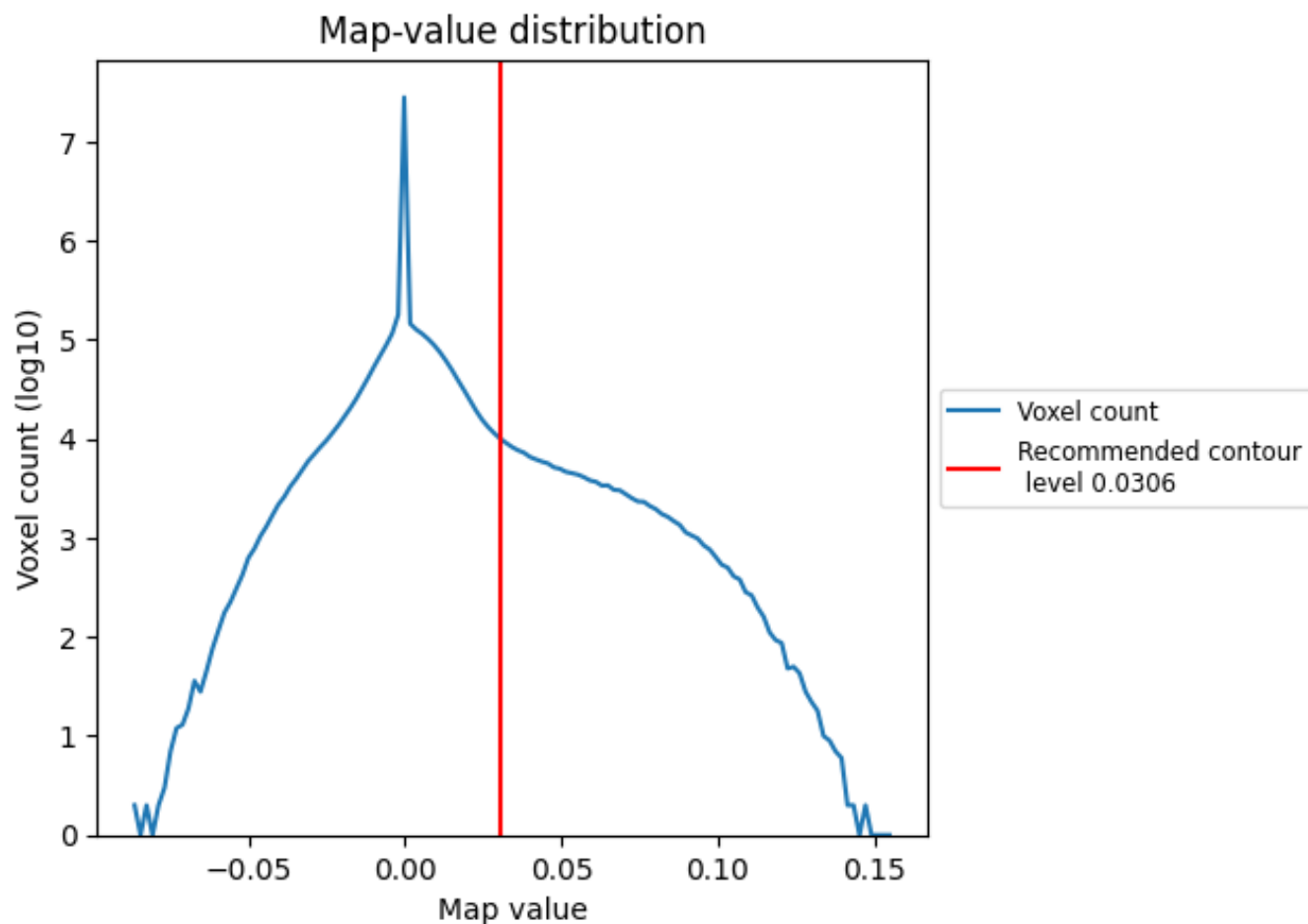
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

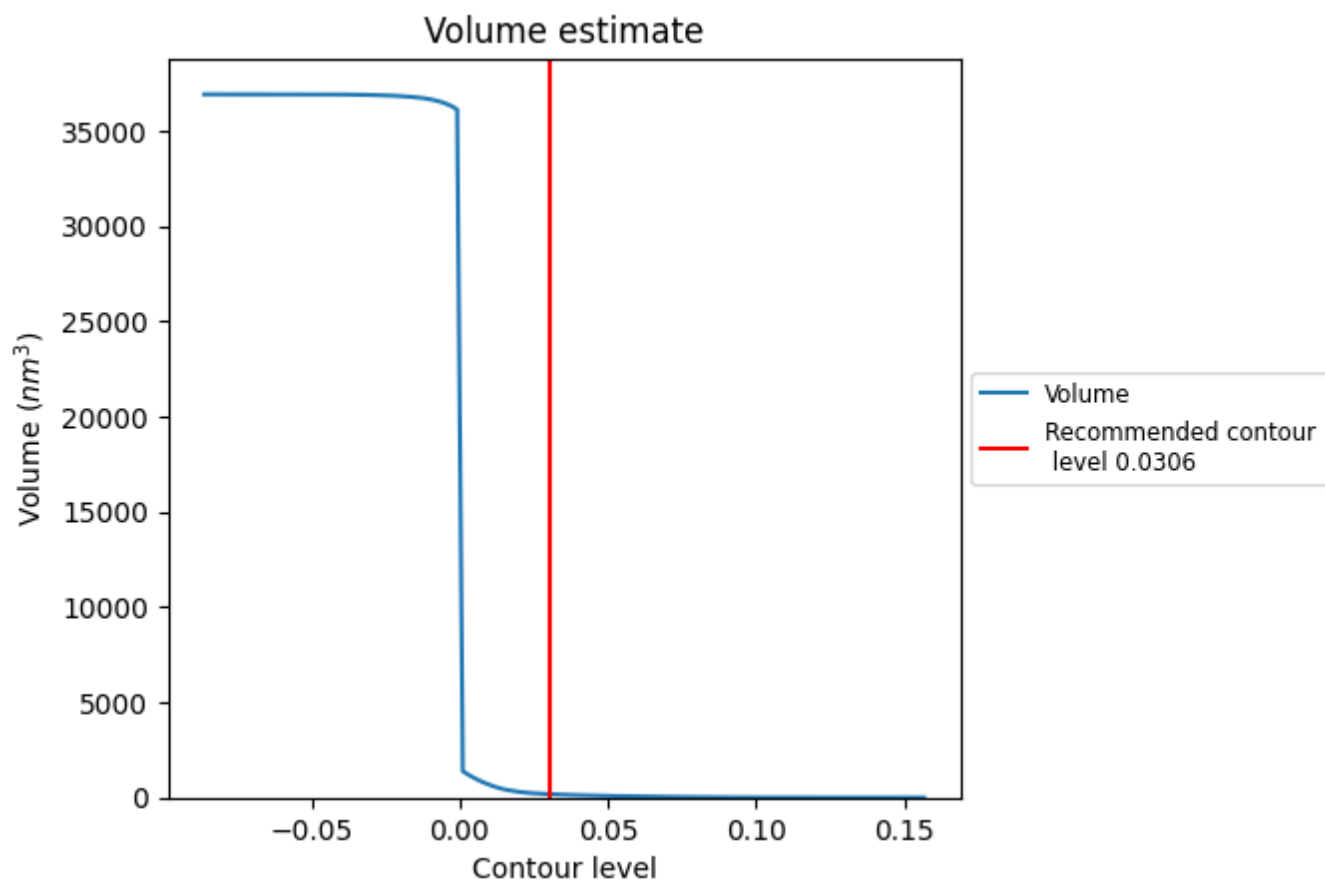
This section contains the results of statistical analysis of the map.

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.

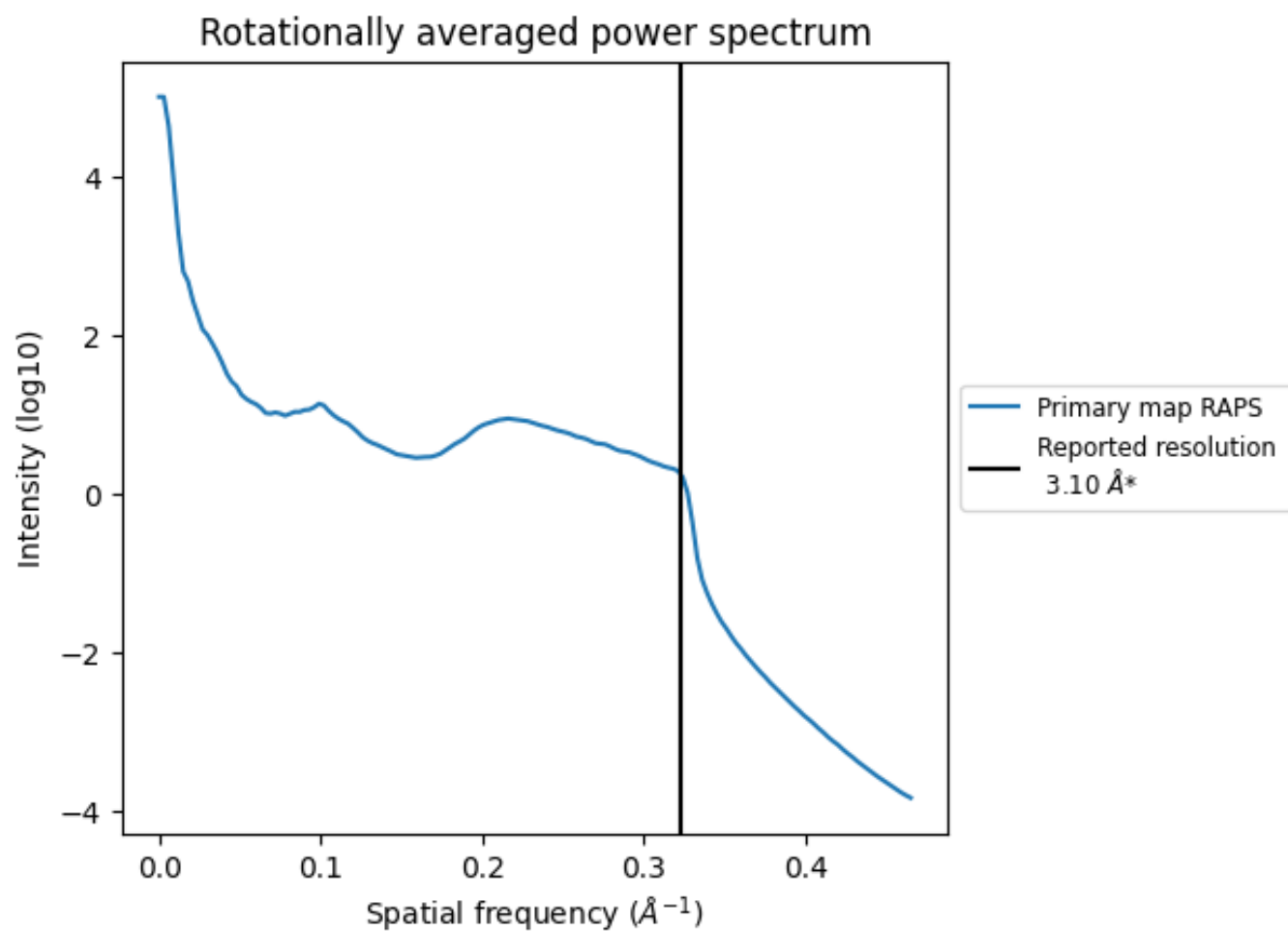
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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 0.323 Å⁻¹

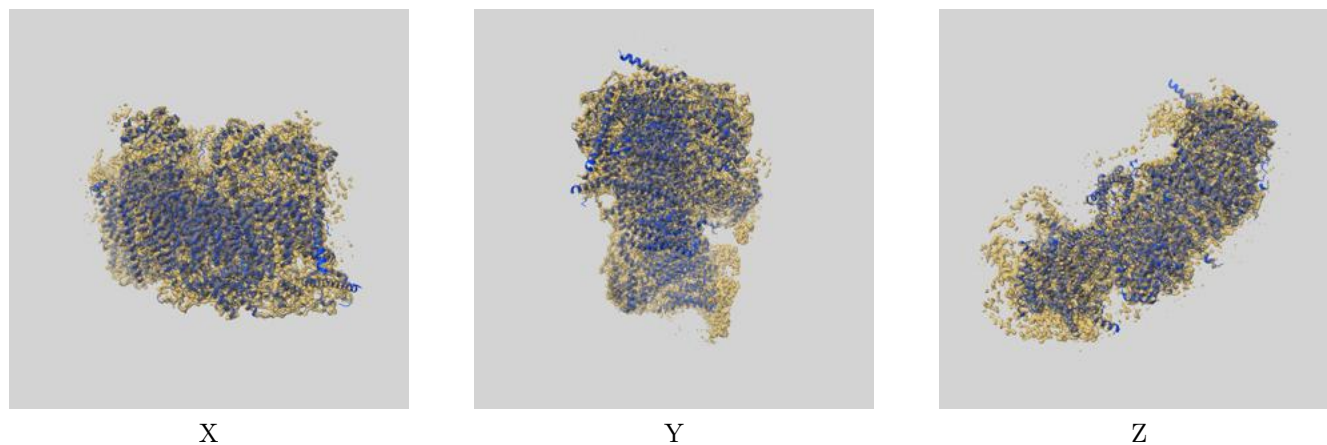
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

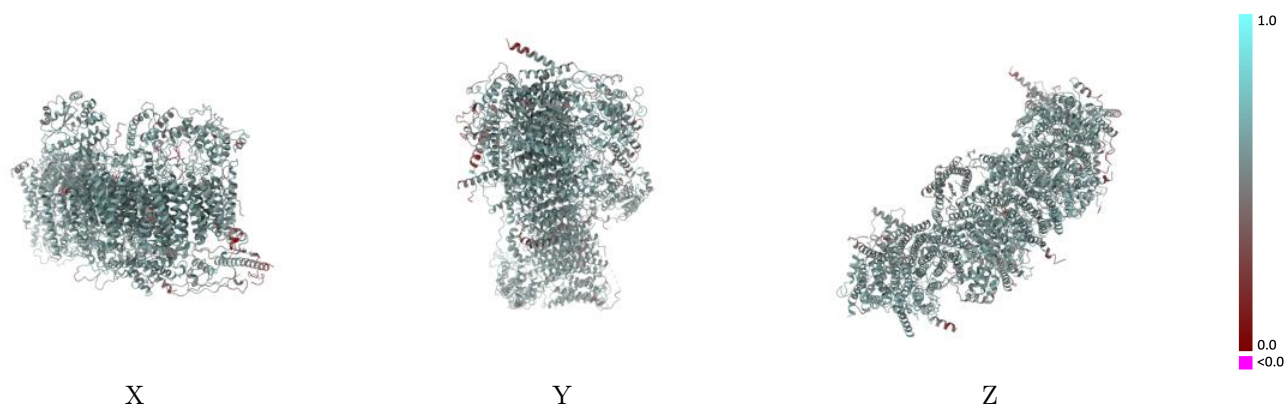
This section contains information regarding the fit between EMDB map EMD-32202 and PDB model 7VYE. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



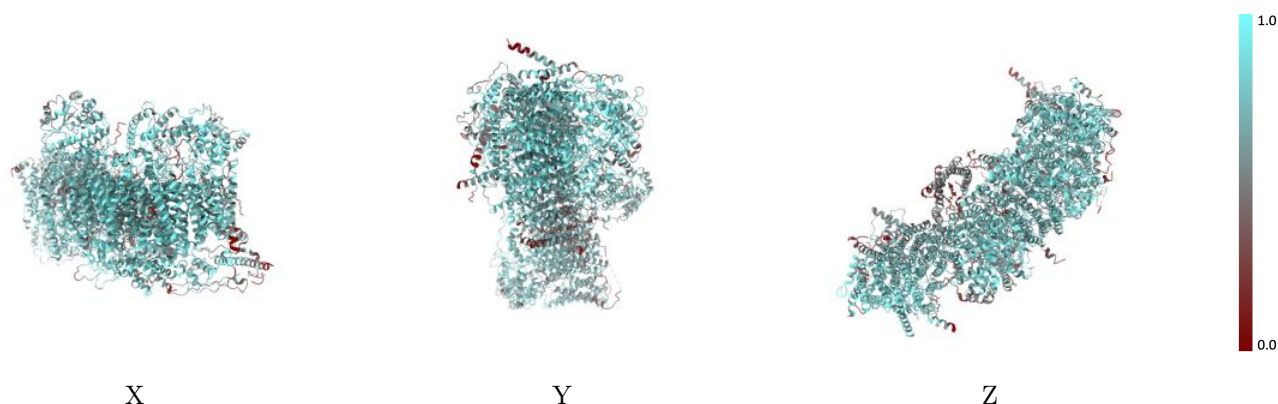
The images above show the 3D surface view of the map at the recommended contour level 0.0306 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



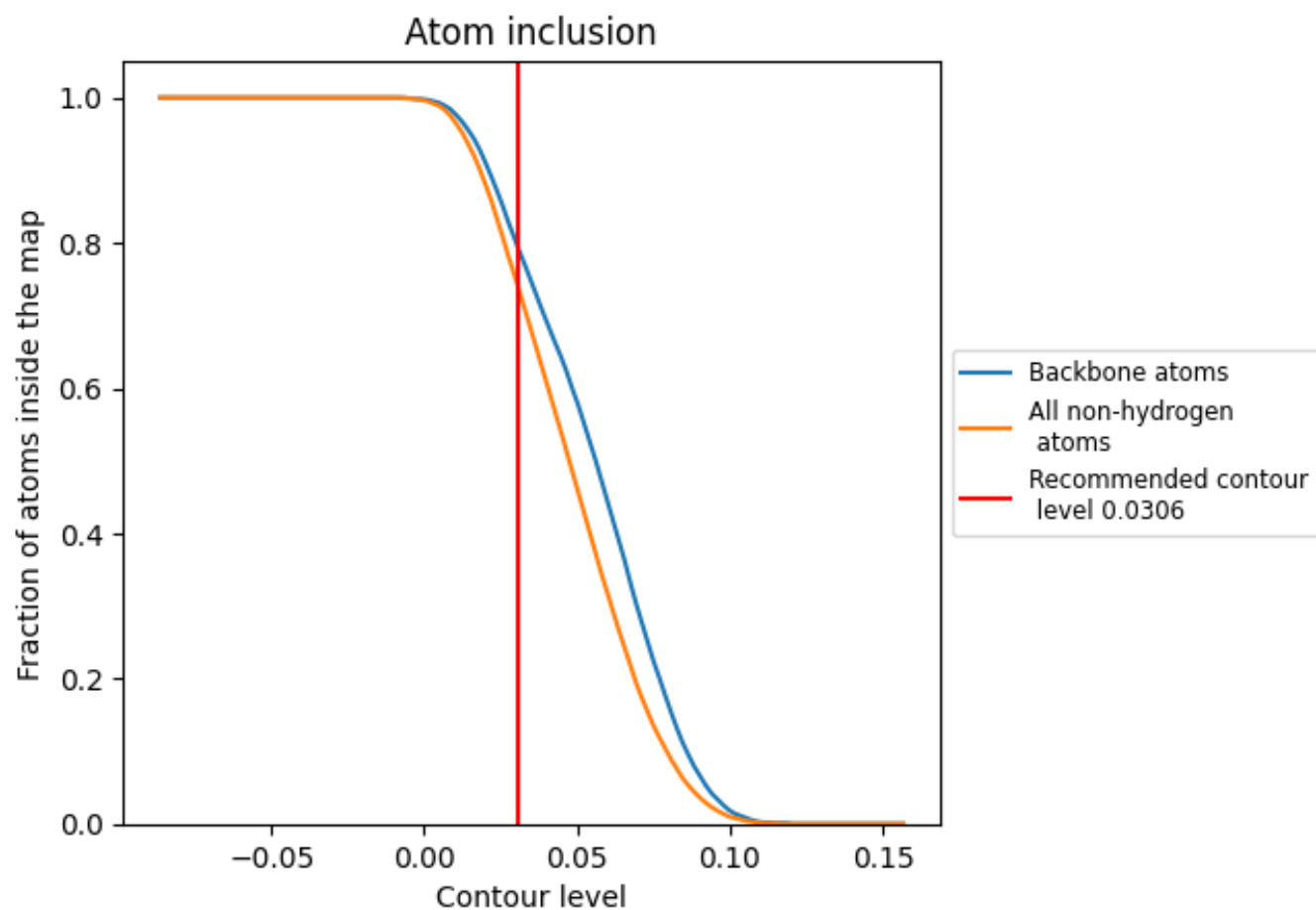
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0306).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0306) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7420	 0.5700
Q	 0.5950	 0.5550
S	 0.8170	 0.5770
U	 0.7120	 0.5550
V	 0.4550	 0.5080
W	 0.7870	 0.5860
X	 0.7270	 0.5500
Y	 0.6100	 0.5110
Z	 0.5610	 0.4790
a	 0.7680	 0.5850
b	 0.6630	 0.5280
c	 0.7610	 0.5690
d	 0.7390	 0.5590
e	 0.7010	 0.5560
f	 0.6650	 0.5450
g	 0.7750	 0.5850
h	 0.7670	 0.5780
i	 0.8250	 0.6030
j	 0.6210	 0.5370
k	 0.6970	 0.5690
l	 0.7830	 0.5870
m	 0.6940	 0.5530
n	 0.6490	 0.5300
o	 0.7070	 0.5660
p	 0.7810	 0.5720
r	 0.8480	 0.6060
s	 0.7630	 0.5800
u	 0.7450	 0.5760
v	 0.6430	 0.5080
w	 0.7230	 0.5640

