



## Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 06:45 PM UTC

PDB ID : 5XTC / pdb\_00005xtc  
EMDB ID : EMD-6772  
Title : Cryo-EM structure of human respiratory complex I transmembrane arm  
Authors : Gu, J.; Wu, M.; Yang, M.  
Deposited on : 2017-06-19  
Resolution : 3.70 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

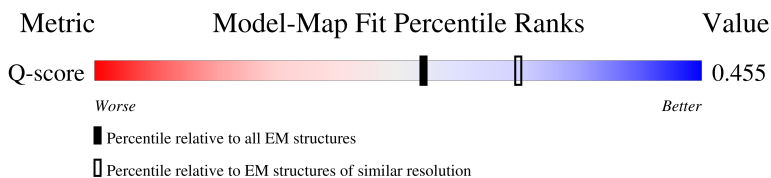
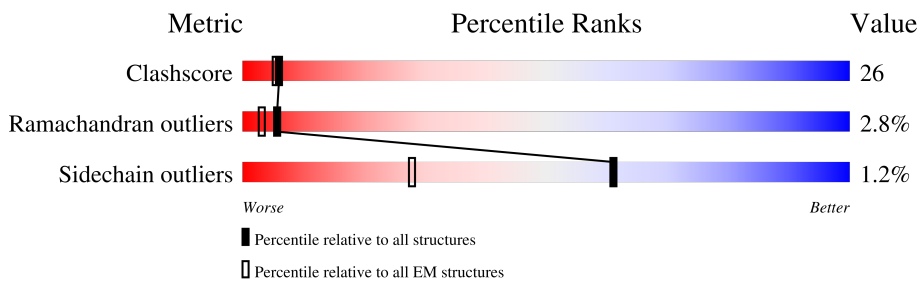
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 ( 3.20 - 4.20 )

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	46	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>89%</p> </div> <div style="text-align: center;"> <p>52%</p> </div> <div style="text-align: center;"> <p>43%</p> </div> </div>
2	S	70	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>13%</p> </div> <div style="text-align: center;"> <p>66%</p> </div> <div style="text-align: center;"> <p>31%</p> </div> </div>
3	U	83	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>16%</p> </div> <div style="text-align: center;"> <p>75%</p> </div> <div style="text-align: center;"> <p>25%</p> </div> </div>
4	V	140	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;"> <p>31%</p> </div> <div style="text-align: center;"> <p>64%</p> </div> <div style="text-align: center;"> <p>35%</p> </div> </div>

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Mol	Chain	Length	Quality of chain
5	W	116	8% 67% 31%
6	X	85	5% 53% 44%
7	Y	59	7% 31% 47% 19%
8	Z	80	15% 74% 26%
9	a	138	59% 36%
10	b	128	28% 42% 45% 9%
11	c	153	7% 50% 48%
12	d	171	6% 63% 33%
13	e	97	10% 71% 29%
14	f	47	30% 62% 34%
15	g	119	49% 49%
16	h	104	9% 48% 47% 5%
17	i	347	7% 51% 46%
18	j	115	50% 49% 48%
19	k	97	18% 47% 47%
20	l	603	9% 50% 44% 5%
21	m	174	26% 47% 49%
22	n	56	21% 59% 39%
23	o	128	5% 66% 33%
24	p	172	5% 58% 37% 5%
25	r	459	60% 39%
26	s	318	16% 49% 47%
27	u	169	62% 36%
28	v	122	18% 44% 44% 9%
29	w	320	57% 55% 42%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
30	PLX	b	201	-	-	X	-
32	PEE	V	202	-	-	X	-
32	PEE	l	701	-	-	X	-

## 2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 38835 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Q	46	381	247	65	68	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	S	70	568	367	101	96	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	U	83	647	427	105	113	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	V	140	1038	668	178	187	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	W	116	956	614	167	170	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	X	85	686	442	101	138	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	Y	59	533	354	87	91	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	Z	80	648	426	110	110	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	a	138	1174	771	199	202	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	b	124	1059	697	181	176	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	c	153	1236	795	208	222	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	d	171	1418	885	262	259	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	e	97	810	522	132	152	4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	f	47	405	269	69	67	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	g	119	1004	658	173	169	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	h	104	863	546	161	150	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	i	347	2735	1819	421	470	25	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	j	115	919	626	132	152	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	k	97	740	487	113	127	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	l	603	4717	3119	742	823	33	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	m	174	1313	879	194	229	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	n	56	473	305	85	80	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	o	128	1066	685	192	187	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	p	172	1495	961	265	261	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	r	459	3629	2411	569	619	30	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	s	318	2509	1678	380	435	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	u	169	1394	886	247	252	9	0	0

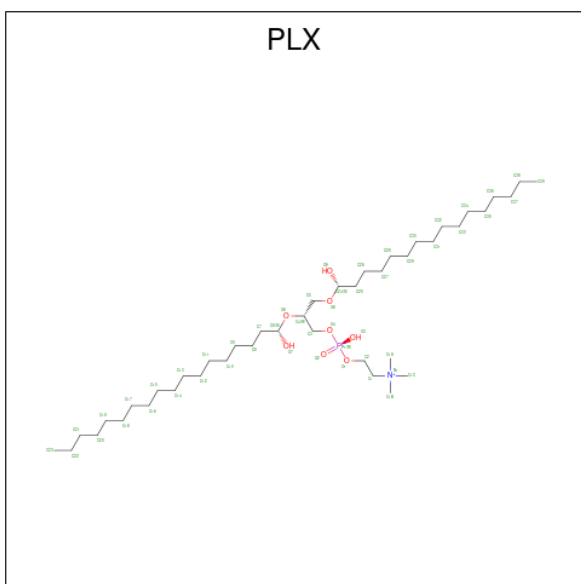
- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	v	111	921	569	187	156	9	0	0

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

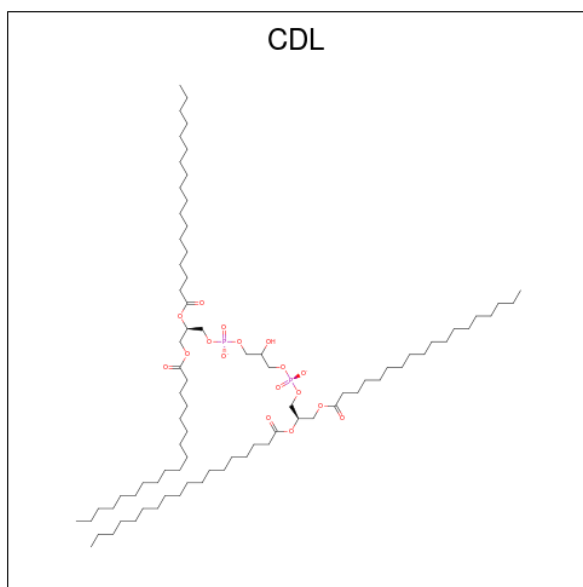
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	w	320	2474	1573	429	464	8	0	0

- Molecule 30 is (9R,11S)-9-({(1S)-1-HYDROXYHEXADECYL}OXY)METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,11-TRIOL (CCD ID: PLX) (formula: C<sub>42</sub>H<sub>89</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
30	U	1	52	42	1	8	1	0
30	V	1	52	42	1	8	1	0
30	b	1	52	42	1	8	1	0
30	g	1	52	42	1	8	1	0
30	g	1	52	42	1	8	1	0
30	g	1	52	42	1	8	1	0
30	r	1	52	42	1	8	1	0
30	r	1	52	42	1	8	1	0
30	s	1	52	42	1	8	1	0

- Molecule 31 is CARDIOLIPIN (CCD ID: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



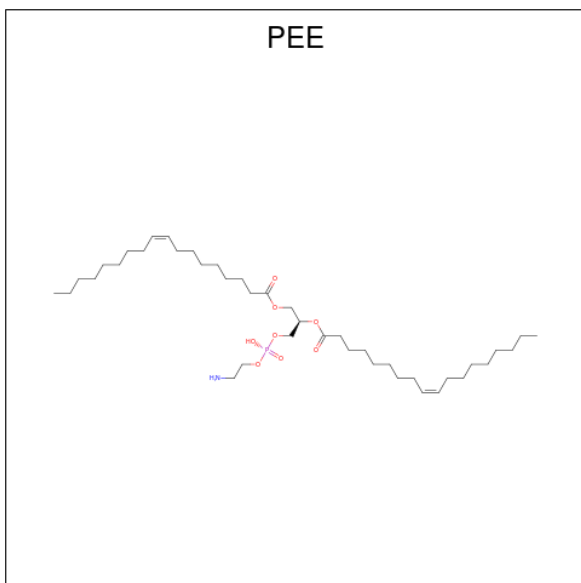
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
31	V	1	63	44	17	2	0
31	i	1	64	45	17	2	0
31	l	1	64	45	17	2	0

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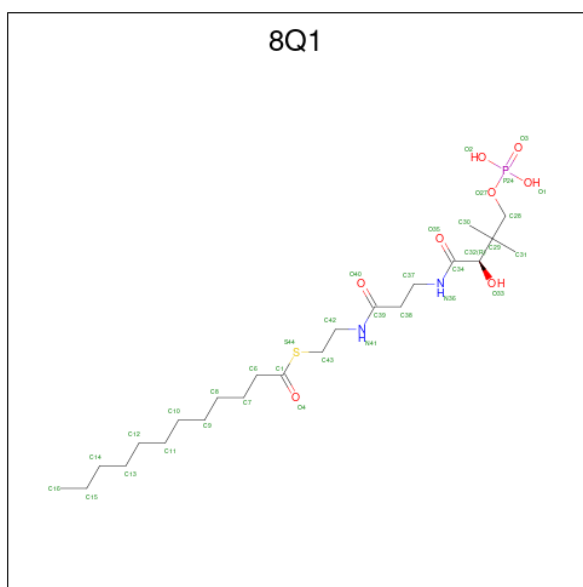
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
31	l	1	64	45	17	2	0
31	n	1	64	45	17	2	0

- Molecule 32 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:  $C_{41}H_{78}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
32	V	1	51	41	1	8	1	0
32	W	1	51	41	1	8	1	0
32	l	1	49	39	1	8	1	0
32	l	1	51	41	1	8	1	0

- Molecule 33 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula:  $C_{23}H_{45}N_2O_8PS$ ).

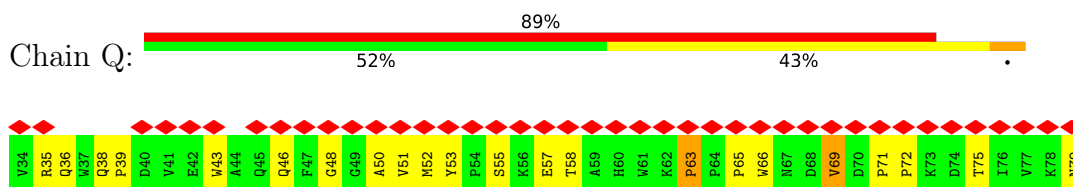


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
33	p	1	35	23	2	8	1	1	0

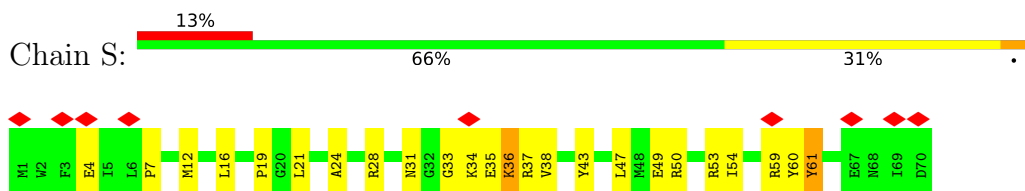
### 3 Residue-property plots [i](#)

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

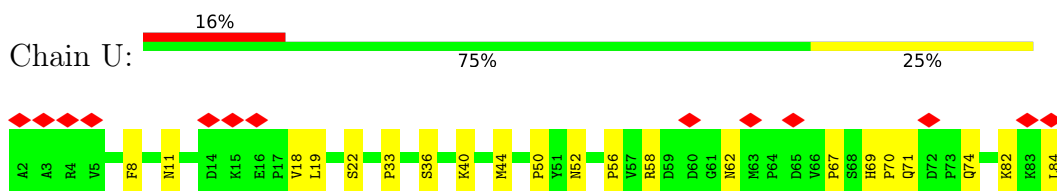
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



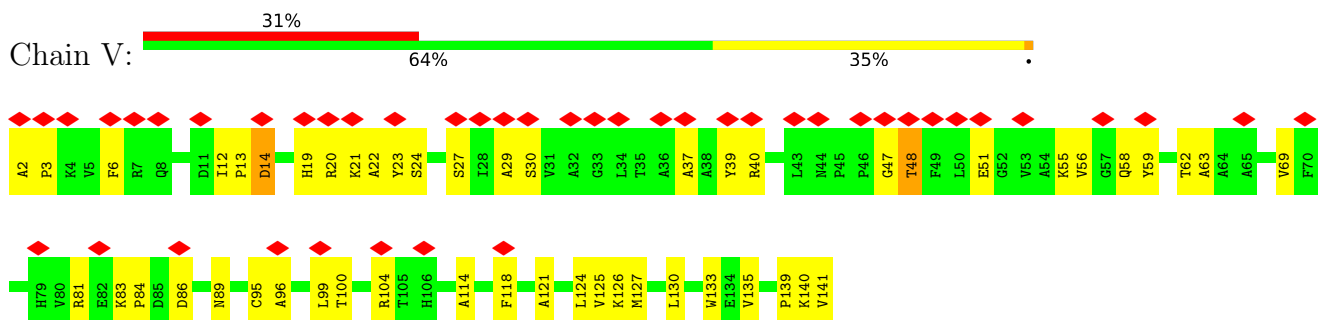
- Molecule 2: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



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



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

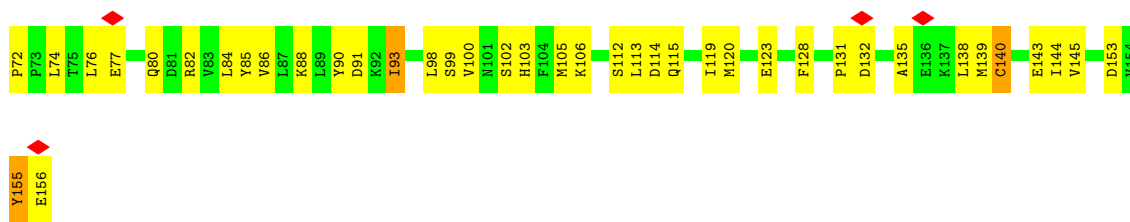


- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

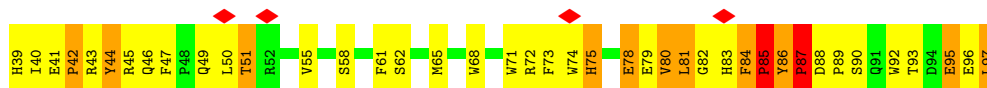




- Molecule 6: Acyl carrier protein, mitochondrial



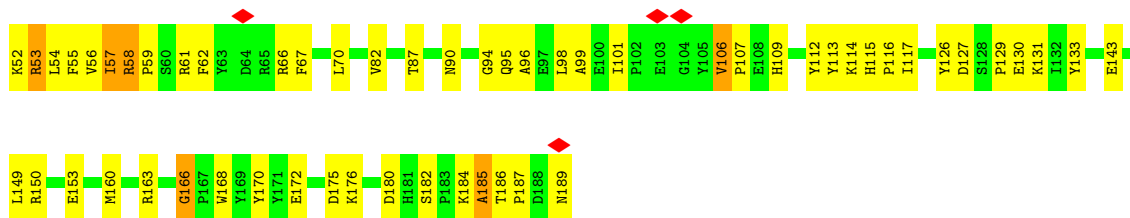
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial



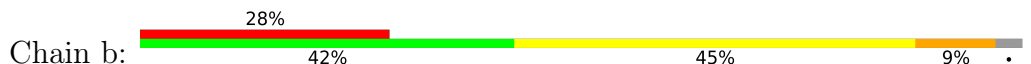
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

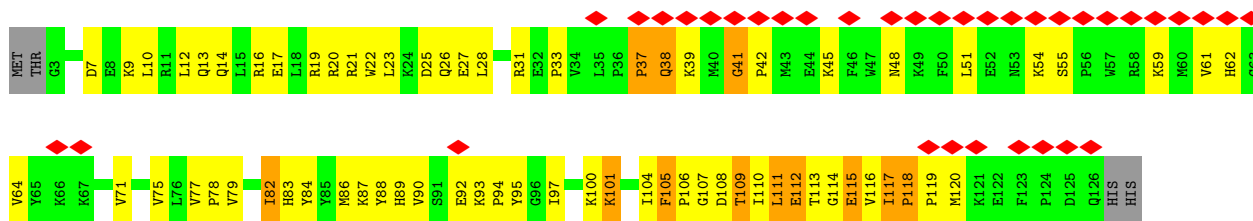


- Molecule 9: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

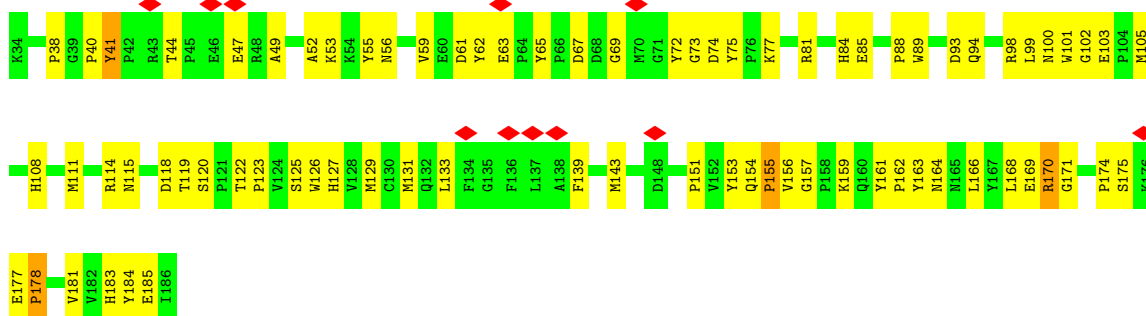


- Molecule 10: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

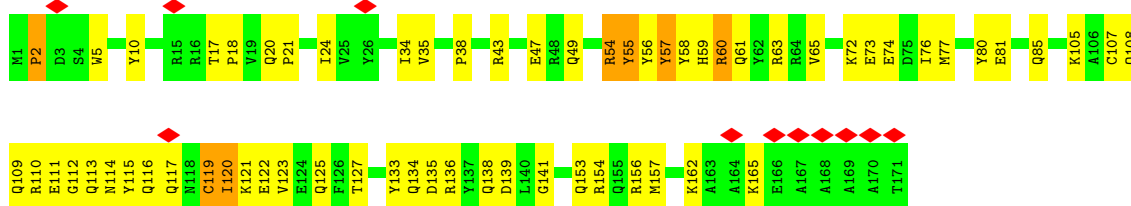




- Molecule 11: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



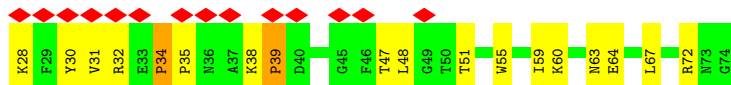
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



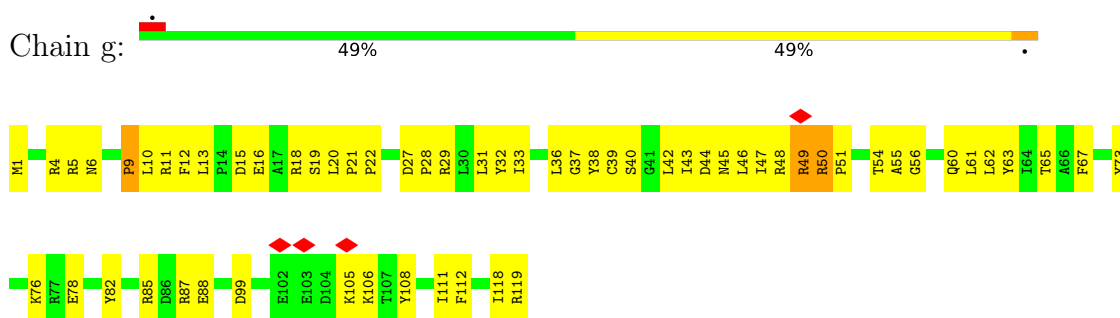
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



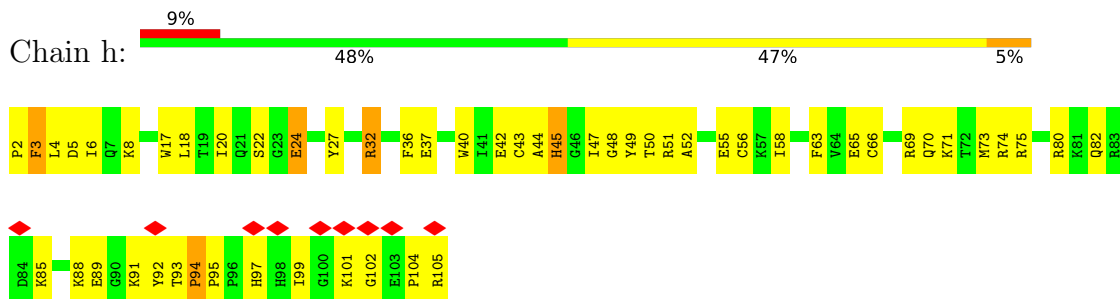
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



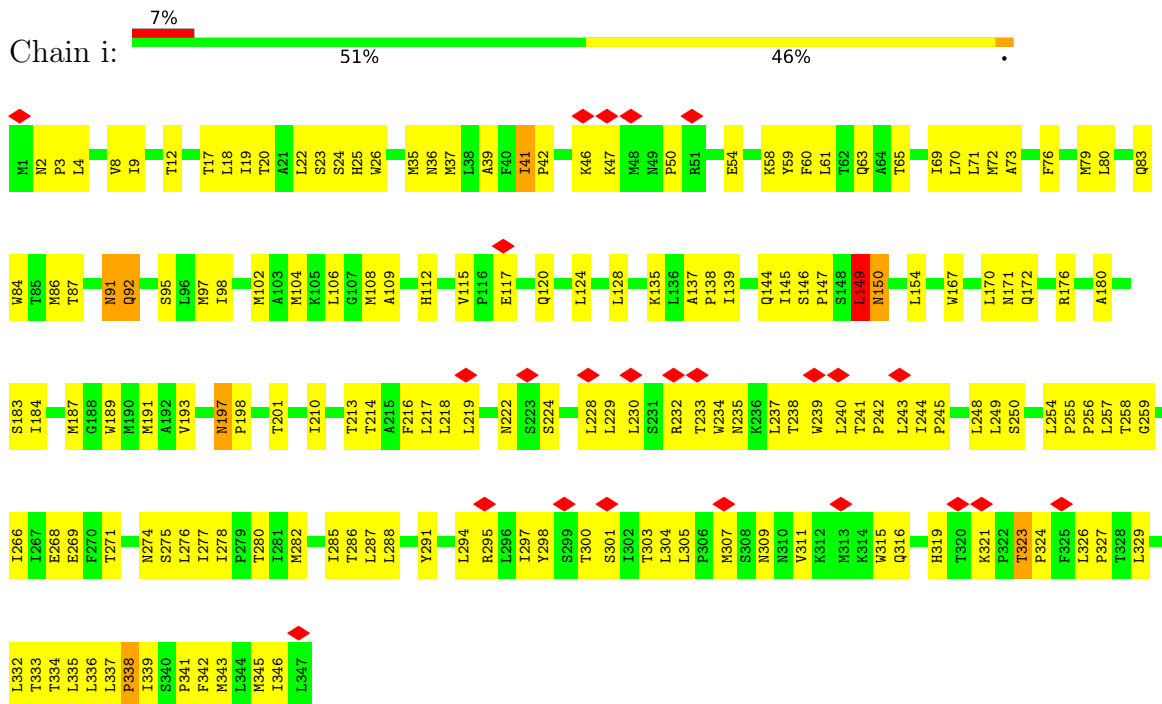
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

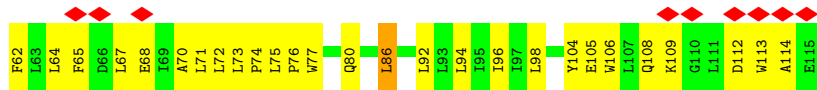
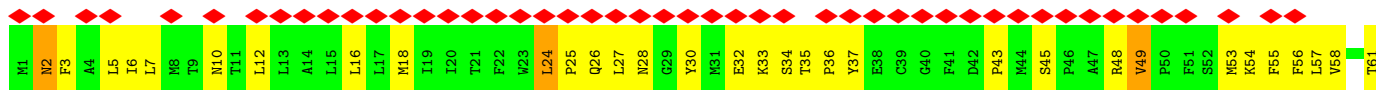


- Molecule 17: NADH-ubiquinone oxidoreductase chain 2

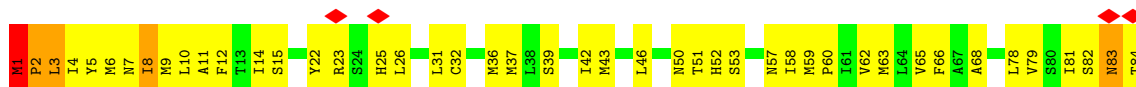


- Molecule 18: NADH-ubiquinone oxidoreductase chain 3

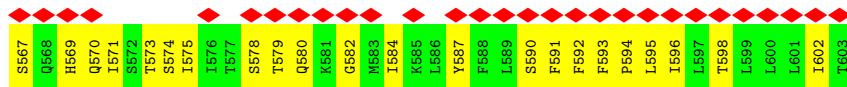
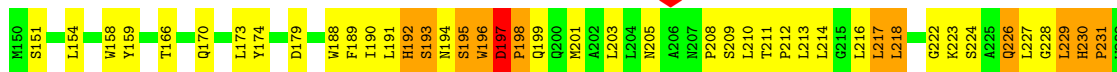
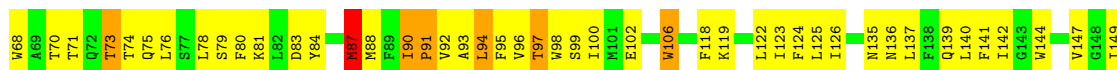




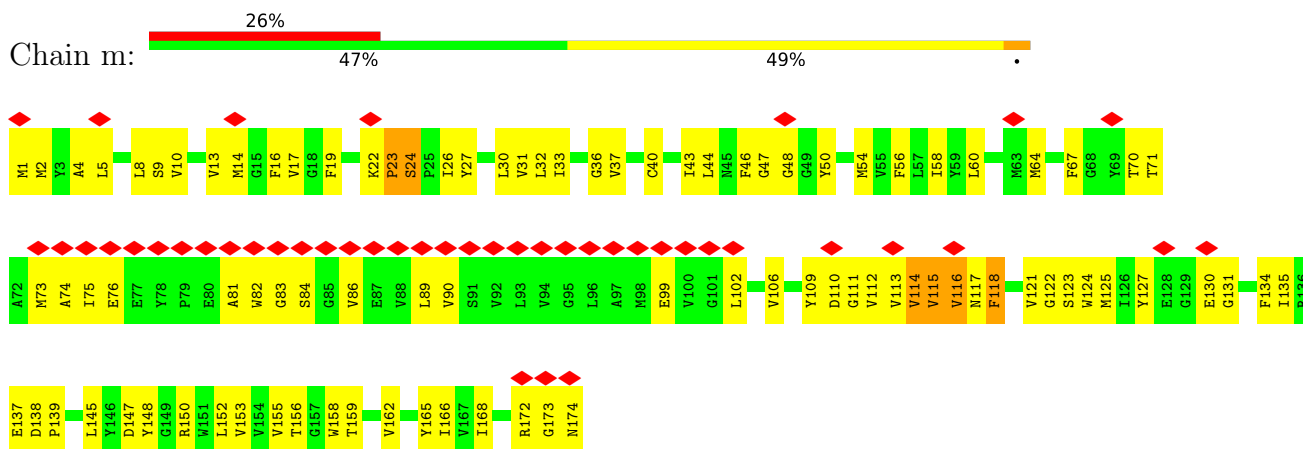
• Molecule 19: NADH-ubiquinone oxidoreductase chain 4L



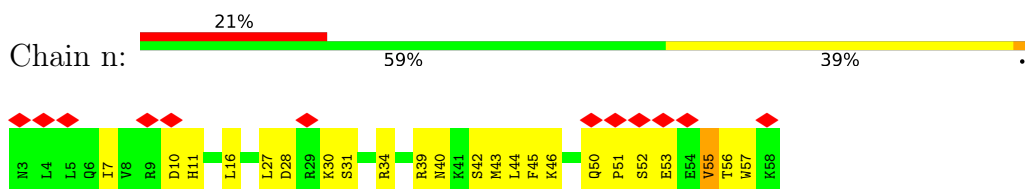
• Molecule 20: NADH-ubiquinone oxidoreductase chain 5



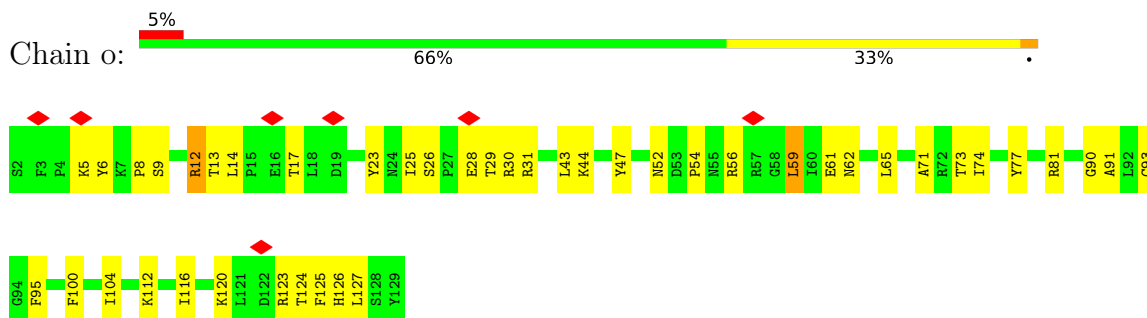
- Molecule 21: NADH-ubiquinone oxidoreductase chain 6



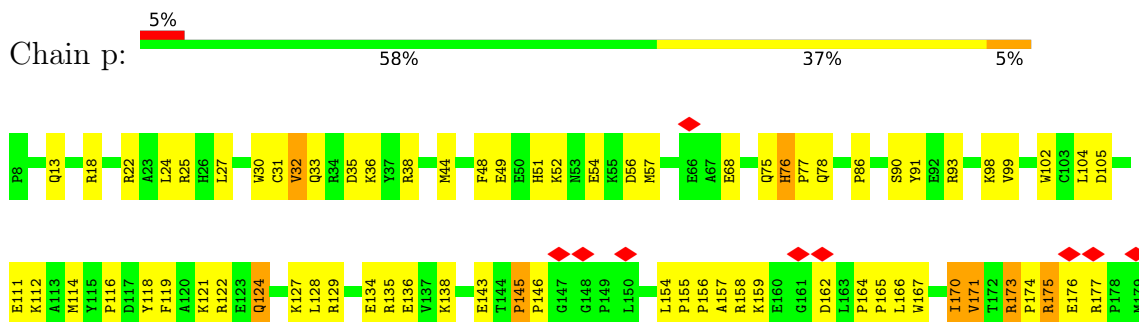
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



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

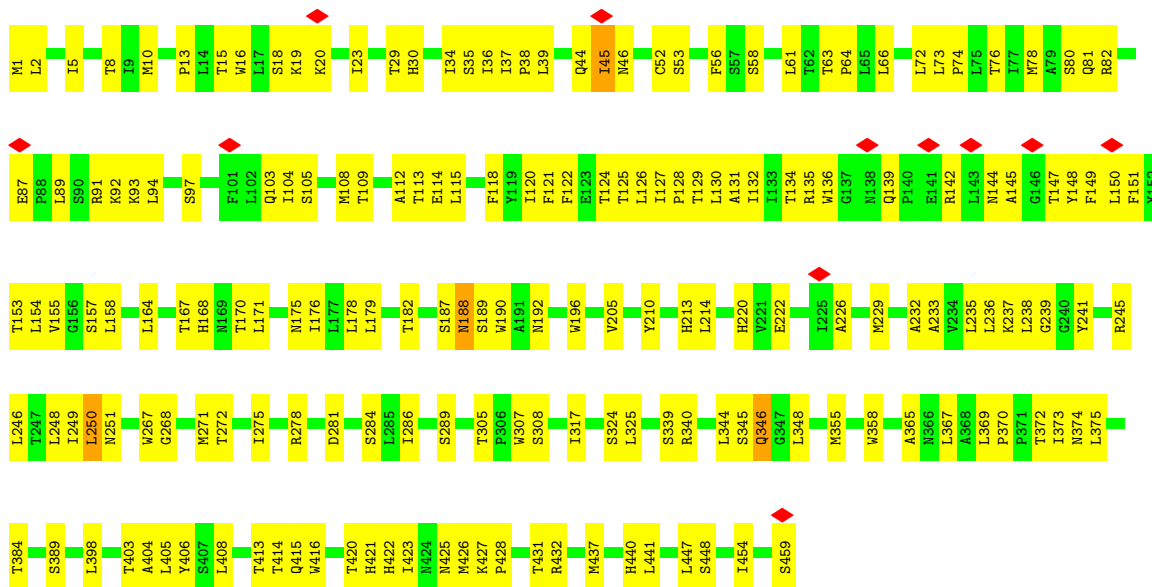


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

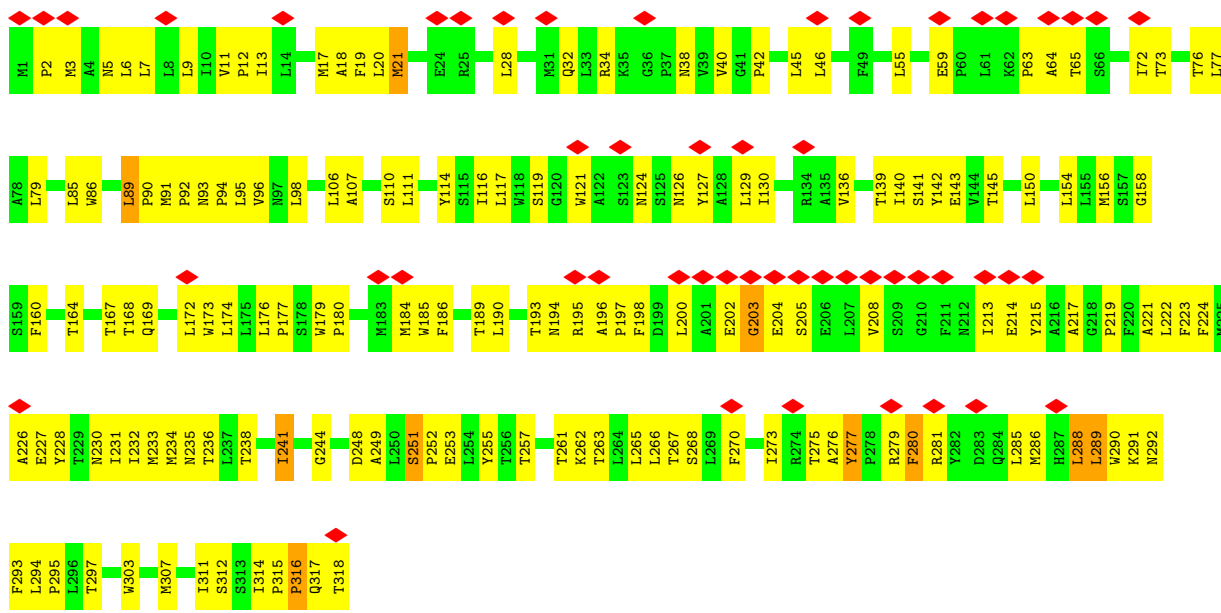


- Molecule 25: NADH-ubiquinone oxidoreductase chain 4

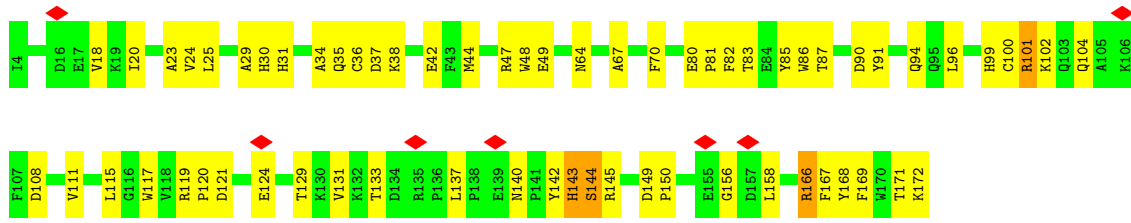




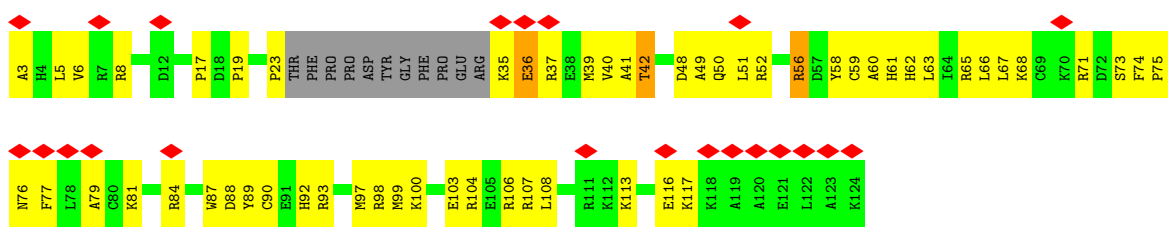
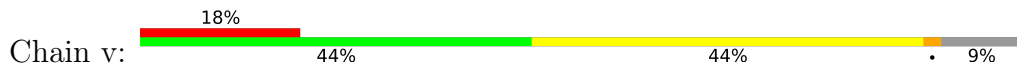
• Molecule 26: NADH-ubiquinone oxidoreductase chain 1



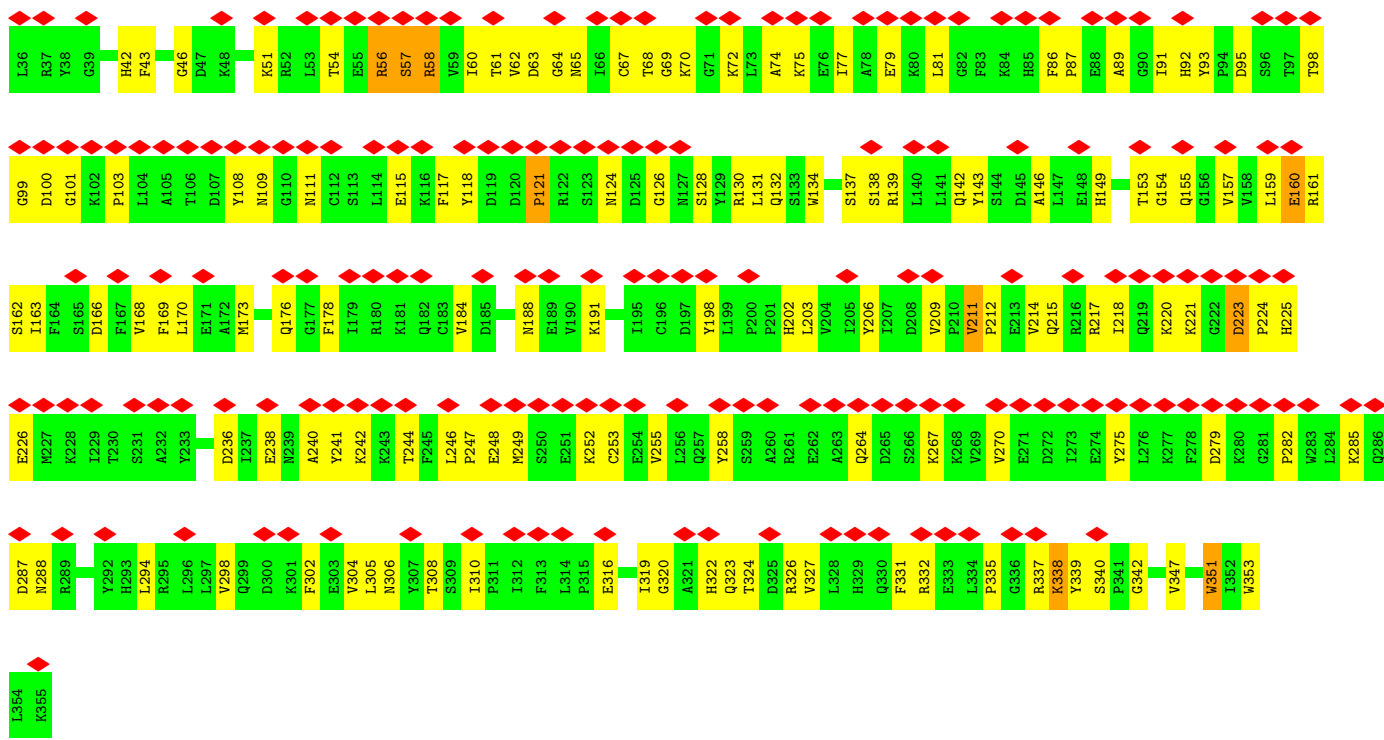
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



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



• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	167761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.305	Depositor
Minimum map value	-0.154	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0677	Depositor
Map size ( $\text{\AA}$ )	519.83997, 519.83997, 519.83997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.083, 1.083, 1.083	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.48	0/398	1.01	3/548 (0.5%)
2	S	0.81	0/583	0.94	1/785 (0.1%)
3	U	0.69	0/670	1.05	4/920 (0.4%)
4	V	0.64	0/1065	0.90	4/1450 (0.3%)
5	W	0.77	1/980 (0.1%)	0.95	3/1327 (0.2%)
6	X	0.71	0/698	0.89	0/942
7	Y	0.61	0/559	1.16	7/763 (0.9%)
8	Z	0.56	0/669	0.82	0/899
9	a	0.85	0/1209	0.99	6/1639 (0.4%)
10	b	0.71	3/1095 (0.3%)	1.08	6/1480 (0.4%)
11	c	0.69	0/1287	0.99	10/1761 (0.6%)
12	d	0.78	0/1445	0.98	3/1945 (0.2%)
13	e	0.76	0/835	0.95	0/1134
14	f	0.65	0/418	0.87	1/566 (0.2%)
15	g	0.78	0/1035	0.97	4/1398 (0.3%)
16	h	0.79	0/884	0.98	3/1182 (0.3%)
17	i	0.92	1/2808 (0.0%)	1.08	11/3843 (0.3%)
18	j	0.76	0/945	1.01	3/1292 (0.2%)
19	k	0.95	1/751 (0.1%)	1.04	3/1019 (0.3%)
20	l	0.84	6/4840 (0.1%)	1.03	29/6611 (0.4%)
21	m	0.82	0/1346	0.99	5/1832 (0.3%)
22	n	0.63	0/484	0.99	0/652
23	o	0.71	0/1093	0.89	0/1479
24	p	0.70	0/1549	1.00	11/2098 (0.5%)
25	r	0.96	1/3723 (0.0%)	1.02	2/5089 (0.0%)
26	s	0.83	0/2580	1.09	15/3539 (0.4%)
27	u	0.70	0/1433	0.96	2/1937 (0.1%)
28	v	0.63	0/934	1.00	4/1241 (0.3%)
29	w	0.53	1/2533 (0.0%)	0.91	7/3440 (0.2%)
All	All	0.78	14/38849 (0.0%)	1.00	147/52811 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
29	w	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	i	278	ILE	CA-CB	-7.69	1.50	1.54
10	b	117	ILE	C-N	6.55	1.41	1.33
5	W	117	VAL	CA-CB	-6.13	1.49	1.54
25	r	37	ILE	CA-CB	-5.94	1.51	1.54
10	b	105	PHE	C-N	5.77	1.41	1.33
29	w	211	VAL	CA-CB	5.58	1.57	1.54
10	b	118	PRO	N-CD	5.21	1.55	1.47
19	k	2	PRO	N-CD	5.21	1.55	1.47
20	l	90	ILE	C-N	5.18	1.41	1.34
20	l	231	PRO	N-CD	5.11	1.54	1.47
20	l	230	HIS	C-N	5.09	1.41	1.34
20	l	91	PRO	N-CD	5.08	1.54	1.47
20	l	198	PRO	N-CD	5.04	1.54	1.47
20	l	552	LEU	CA-C	-5.03	1.50	1.52

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	s	314	ILE	CA-C-N	9.73	126.77	119.66
26	s	314	ILE	C-N-CA	9.73	126.77	119.66
17	i	323	THR	CA-C-N	8.50	147.40	127.00
17	i	323	THR	C-N-CA	8.50	147.40	127.00
7	Y	86	TYR	C-N-CD	8.43	139.15	120.60
7	Y	92	TRP	N-CA-C	-8.39	92.15	107.75
7	Y	47	PHE	CA-C-N	8.23	128.26	119.78
7	Y	47	PHE	C-N-CA	8.23	128.26	119.78
12	d	119	CYS	N-CA-C	8.02	120.03	111.28
17	i	255	PRO	N-CA-C	7.81	120.23	110.70
12	d	2	PRO	N-CA-CB	7.77	111.41	103.25
28	v	17	PRO	N-CA-CB	7.48	110.40	103.15
28	v	42	THR	CB-CA-C	-7.42	108.03	116.63
26	s	89	LEU	CA-C-N	7.41	129.10	119.84
26	s	89	LEU	C-N-CA	7.41	129.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	i	323	THR	C-N-CD	-7.37	104.39	120.60
10	b	117	ILE	CA-C-N	-7.34	112.82	120.38
10	b	117	ILE	C-N-CA	-7.34	112.82	120.38
3	U	33	PRO	N-CA-C	7.31	119.62	110.70
26	s	277	TYR	CA-C-N	7.14	127.06	119.85
26	s	277	TYR	C-N-CA	7.14	127.06	119.85
15	g	21	PRO	CA-C-N	7.13	124.79	119.66
15	g	21	PRO	C-N-CA	7.13	124.79	119.66
24	p	173	ARG	CA-C-N	7.11	127.10	119.28
24	p	173	ARG	C-N-CA	7.11	127.10	119.28
20	l	515	SER	CA-C-N	7.10	127.09	119.78
20	l	515	SER	C-N-CA	7.10	127.09	119.78
20	l	537	ILE	CA-C-N	-7.03	111.54	119.28
20	l	537	ILE	C-N-CA	-7.03	111.54	119.28
24	p	171	VAL	N-CA-C	7.00	117.78	110.72
17	i	197	ASN	CA-C-N	6.98	126.95	119.28
17	i	197	ASN	C-N-CA	6.98	126.95	119.28
7	Y	93	THR	N-CA-C	6.90	120.00	108.20
16	h	94	PRO	CA-C-N	-6.84	113.34	120.38
16	h	94	PRO	C-N-CA	-6.84	113.34	120.38
20	l	24	VAL	CA-C-N	-6.80	115.37	122.85
20	l	24	VAL	C-N-CA	-6.80	115.37	122.85
11	c	157	GLY	CA-C-N	6.75	126.73	119.78
11	c	157	GLY	C-N-CA	6.75	126.73	119.78
10	b	105	PHE	CA-C-N	-6.72	112.83	119.76
10	b	105	PHE	C-N-CA	-6.72	112.83	119.76
28	v	23	PRO	N-CA-CB	6.71	110.38	103.00
11	c	72	TYR	N-CA-C	-6.68	100.14	110.10
2	S	61	TYR	N-CA-C	-6.62	104.07	111.28
20	l	562	LEU	CA-C-N	-6.58	111.61	119.84
20	l	562	LEU	C-N-CA	-6.58	111.61	119.84
7	Y	87	PRO	CA-N-CD	-6.58	102.30	111.50
1	Q	63	PRO	CA-C-N	6.51	124.41	119.66
1	Q	63	PRO	C-N-CA	6.51	124.41	119.66
21	m	135	ILE	N-CA-C	6.50	117.48	108.12
20	l	548	LEU	CA-C-N	-6.49	111.73	119.84
20	l	548	LEU	C-N-CA	-6.49	111.73	119.84
14	f	34	PRO	N-CA-C	6.36	118.46	110.70
29	w	211	VAL	CA-C-N	-6.35	112.00	119.05
29	w	211	VAL	C-N-CA	-6.35	112.00	119.05
26	s	179	TRP	CA-C-N	-6.27	112.38	119.28
26	s	179	TRP	C-N-CA	-6.27	112.38	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	78	GLN	CA-C-N	6.25	126.22	119.78
24	p	78	GLN	C-N-CA	6.25	126.22	119.78
4	V	14	ASP	N-CA-C	6.22	117.73	111.07
16	h	94	PRO	N-CA-C	6.20	118.27	110.70
28	v	19	PRO	N-CA-CB	6.19	110.08	103.39
29	w	56	ARG	N-CA-C	-6.15	105.71	112.72
20	l	447	ASN	N-CA-C	6.14	116.03	108.11
11	c	155	PRO	CA-C-N	-6.12	116.90	123.08
11	c	155	PRO	C-N-CA	-6.12	116.90	123.08
29	w	253	CYS	CB-CA-C	-6.08	109.55	116.54
5	W	31	SER	N-CA-C	-6.01	105.70	113.16
26	s	251	SER	CA-C-N	6.00	125.87	119.28
26	s	251	SER	C-N-CA	6.00	125.87	119.28
9	a	106	VAL	CA-C-N	5.96	125.88	119.85
9	a	106	VAL	C-N-CA	5.96	125.88	119.85
20	l	404	THR	N-CA-C	5.95	116.28	108.07
20	l	106	TRP	N-CA-C	5.93	117.82	111.36
24	p	155	PRO	CA-C-N	5.89	125.80	119.85
24	p	155	PRO	C-N-CA	5.89	125.80	119.85
26	s	158	GLY	N-CA-C	5.89	121.70	114.69
29	w	340	SER	N-CA-C	5.88	117.11	109.64
5	W	118	PRO	CA-C-N	5.84	125.75	119.85
5	W	118	PRO	C-N-CA	5.84	125.75	119.85
26	s	315	PRO	CA-C-N	5.84	127.14	119.84
26	s	315	PRO	C-N-CA	5.84	127.14	119.84
20	l	90	ILE	O-C-N	5.83	124.21	120.07
4	V	22	ALA	N-CA-C	-5.79	105.05	111.36
10	b	37	PRO	CA-N-CD	-5.78	103.92	112.00
7	Y	85	PRO	N-CA-C	5.75	124.31	112.47
20	l	87	MET	N-CA-C	5.71	117.31	111.14
20	l	197	ASP	CA-C-N	-5.70	112.73	119.05
20	l	197	ASP	C-N-CA	-5.70	112.73	119.05
25	r	427	LYS	CA-C-N	5.69	125.64	119.78
25	r	427	LYS	C-N-CA	5.69	125.64	119.78
26	s	21	MET	N-CA-C	-5.68	106.20	113.01
27	u	166	ARG	N-CA-C	-5.67	106.59	112.93
18	j	49	VAL	N-CA-C	5.66	114.50	108.95
26	s	280	PHE	N-CA-C	5.65	118.38	111.82
18	j	45	SER	CA-C-N	5.65	125.56	119.85
18	j	45	SER	C-N-CA	5.65	125.56	119.85
10	b	9	LYS	N-CA-C	-5.64	105.04	111.07
20	l	90	ILE	CA-C-N	-5.61	112.83	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	l	90	ILE	C-N-CA	-5.61	112.83	119.05
9	a	56	VAL	N-CA-C	5.60	117.82	111.88
20	l	450	LEU	N-CA-C	5.59	122.72	110.80
15	g	36	LEU	N-CA-C	-5.59	105.28	111.71
11	c	120	SER	CA-C-N	5.57	125.52	119.78
11	c	120	SER	C-N-CA	5.57	125.52	119.78
17	i	149	LEU	N-CA-C	5.55	120.05	113.28
20	l	25	ASN	N-CA-C	5.55	118.18	108.75
9	a	166	GLY	CA-C-N	5.51	125.34	119.28
9	a	166	GLY	C-N-CA	5.51	125.34	119.28
27	u	171	THR	N-CA-C	-5.50	106.62	113.38
21	m	127	TYR	CB-CA-C	-5.49	110.23	116.54
24	p	154	LEU	CA-C-N	5.44	123.58	119.66
24	p	154	LEU	C-N-CA	5.44	123.58	119.66
11	c	161	TYR	CA-C-N	5.43	125.37	119.78
11	c	161	TYR	C-N-CA	5.43	125.37	119.78
15	g	22	PRO	O-C-N	5.42	123.70	121.15
19	k	89	TYR	CB-CA-C	-5.40	109.37	115.79
11	c	126	TRP	N-CA-C	5.36	116.81	110.97
20	l	192	HIS	N-CA-C	5.35	117.19	111.36
20	l	270	ASN	CA-C-N	5.33	125.14	119.28
20	l	270	ASN	C-N-CA	5.33	125.14	119.28
1	Q	71	PRO	N-CA-C	5.32	117.19	110.70
17	i	172	GLN	N-CA-C	5.29	117.51	110.53
20	l	230	HIS	CA-C-N	-5.27	113.20	119.05
20	l	230	HIS	C-N-CA	-5.27	113.20	119.05
20	l	16	ILE	CB-CA-C	-5.26	108.78	114.35
24	p	145	PRO	CA-C-N	5.25	125.06	119.28
24	p	145	PRO	C-N-CA	5.25	125.06	119.28
21	m	137	GLU	N-CA-C	5.16	116.71	111.14
19	k	1	MET	CA-C-N	-5.15	113.33	119.05
19	k	1	MET	C-N-CA	-5.15	113.33	119.05
20	l	437	PHE	CA-C-N	5.14	125.08	119.78
20	l	437	PHE	C-N-CA	5.14	125.08	119.78
3	U	36	SER	CA-C-N	5.14	124.94	119.28
3	U	36	SER	C-N-CA	5.14	124.94	119.28
17	i	321	LYS	CA-C-N	5.13	124.92	119.28
17	i	321	LYS	C-N-CA	5.13	124.92	119.28
29	w	223	ASP	CA-C-N	5.12	124.91	119.28
29	w	223	ASP	C-N-CA	5.12	124.91	119.28
12	d	120	ILE	N-CA-C	5.11	115.83	110.62
21	m	114	VAL	CA-C-N	5.11	131.16	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	m	114	VAL	C-N-CA	5.11	131.16	121.97
3	U	62	ASN	CB-CA-C	-5.08	109.23	116.34
17	i	41	ILE	CB-CA-C	-5.05	107.38	114.00
9	a	106	VAL	N-CA-C	5.05	112.55	107.55
4	V	86	ASP	CA-C-N	5.04	124.70	119.56
4	V	86	ASP	C-N-CA	5.04	124.70	119.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	w	338	LYS	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	381	0	355	29	0
2	S	568	0	567	37	0
3	U	647	0	653	16	0
4	V	1038	0	1027	36	0
5	W	956	0	949	41	0
6	X	686	0	676	33	0
7	Y	533	0	475	97	0
8	Z	648	0	627	18	0
9	a	1174	0	1177	104	0
10	b	1059	0	1079	125	0
11	c	1236	0	1092	81	0
12	d	1418	0	1375	121	0
13	e	810	0	772	32	0
14	f	405	0	407	19	0
15	g	1004	0	1008	63	0
16	h	863	0	861	66	0
17	i	2735	0	2893	185	0
18	j	919	0	968	58	0
19	k	740	0	792	90	0
20	l	4717	0	4893	399	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	m	1313	0	1330	121	0
22	n	473	0	480	30	0
23	o	1066	0	1086	51	0
24	p	1495	0	1440	93	0
25	r	3629	0	3825	164	0
26	s	2509	0	2617	134	0
27	u	1394	0	1367	59	0
28	v	921	0	892	90	0
29	w	2474	0	2304	117	0
30	U	52	0	88	3	0
30	V	52	0	88	5	0
30	b	52	0	88	38	0
30	g	156	0	264	13	0
30	r	104	0	176	22	0
30	s	52	0	88	2	0
31	V	63	0	68	8	0
31	i	64	0	72	3	0
31	l	128	0	144	5	0
31	n	64	0	72	10	0
32	V	51	0	82	21	0
32	W	51	0	82	18	0
32	l	100	0	157	68	0
33	p	35	0	0	12	0
All	All	38835	0	39456	2064	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 26.

All (2064) 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:55:PHE:CE2	24:p:118:TYR:CE2	1.82	1.65
20:l:533:MET:CE	32:l:702:PEE:H36	1.25	1.58
20:l:37:LYS:HE2	20:l:98:TRP:CD1	1.40	1.57
9:a:55:PHE:HE2	24:p:118:TYR:CE2	1.17	1.56
9:a:55:PHE:CE2	24:p:118:TYR:CD2	1.91	1.55
9:a:98:LEU:HB3	12:d:57:TYR:CE1	1.45	1.52
17:i:288:LEU:CD2	32:l:701:PEE:H58	1.37	1.52
20:l:533:MET:HE1	32:l:702:PEE:C22	1.41	1.50
20:l:571:ILE:CD1	32:l:701:PEE:O5	1.64	1.43
20:l:84:TYR:CD1	20:l:88:MET:HE2	1.54	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:84:TYR:CE1	20:l:88:MET:CE	2.05	1.40
9:a:55:PHE:HE2	24:p:118:TYR:CD2	1.32	1.35
20:l:84:TYR:CE1	20:l:88:MET:HE2	1.64	1.31
17:i:288:LEU:HD23	32:l:701:PEE:C36	1.61	1.30
9:a:98:LEU:CB	12:d:57:TYR:HE1	1.46	1.28
9:a:55:PHE:CD2	24:p:118:TYR:CE2	2.22	1.27
20:l:188:TRP:CE2	20:l:192:HIS:HD2	1.54	1.26
20:l:447:ASN:OD1	20:l:448:PRO:HD2	1.30	1.24
7:Y:84:PHE:CE2	20:l:483:PRO:HG3	1.74	1.20
20:l:37:LYS:CE	20:l:98:TRP:CD1	2.24	1.20
7:Y:87:PRO:HB3	28:v:103:GLU:OE2	1.38	1.19
9:a:55:PHE:CD2	24:p:118:TYR:CZ	2.30	1.19
7:Y:72:ARG:NH1	20:l:390:TYR:OH	1.76	1.19
20:l:226:GLN:HE21	20:l:314:MET:CE	1.56	1.18
10:b:110:ILE:HG23	10:b:111:LEU:HG	1.24	1.17
32:V:202:PEE:C42	32:l:701:PEE:C45	2.23	1.17
9:a:55:PHE:HD2	24:p:118:TYR:CZ	1.62	1.16
32:V:202:PEE:H70	32:l:701:PEE:C45	1.74	1.16
32:W:201:PEE:H75	26:s:77:LEU:CD2	1.75	1.16
20:l:188:TRP:CE2	20:l:192:HIS:CD2	2.33	1.15
20:l:533:MET:SD	32:l:702:PEE:H36	1.86	1.14
17:i:291:TYR:CE2	32:l:701:PEE:C31	2.29	1.14
24:p:167:TRP:O	24:p:171:VAL:HG23	1.47	1.14
7:Y:84:PHE:CD1	7:Y:85:PRO:HD3	1.84	1.13
20:l:84:TYR:CE1	20:l:88:MET:HE3	1.74	1.12
12:d:59:HIS:CE1	13:e:120:ARG:HB3	1.84	1.12
19:k:4:ILE:HD11	21:m:125:MET:SD	1.91	1.11
32:W:201:PEE:H75	26:s:77:LEU:HD21	1.19	1.11
20:l:54:PHE:CE1	20:l:58:ASP:OD1	2.06	1.08
7:Y:71:TRP:CH2	7:Y:75:HIS:CD2	2.42	1.08
7:Y:84:PHE:CZ	20:l:483:PRO:HG3	1.88	1.08
9:a:98:LEU:CB	12:d:57:TYR:CE1	2.25	1.07
20:l:97:THR:HG21	20:l:125:LEU:HD12	1.35	1.07
11:c:181:VAL:CB	28:v:37:ARG:HH21	1.66	1.07
9:a:114:LYS:HB2	12:d:57:TYR:CE2	1.87	1.07
20:l:84:TYR:HE1	20:l:88:MET:CE	1.50	1.07
20:l:54:PHE:CZ	20:l:58:ASP:OD1	2.07	1.06
9:a:55:PHE:HD2	24:p:118:TYR:CE1	1.75	1.05
20:l:227:LEU:O	20:l:230:HIS:ND1	1.88	1.05
12:d:81:GLU:OE1	22:n:43:MET:HE3	1.57	1.05
29:w:332:ARG:O	29:w:338:LYS:HA	1.55	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:105:LYS:CE	20:l:197:ASP:OD2	2.04	1.05
7:Y:71:TRP:CH2	7:Y:75:HIS:HD2	1.76	1.04
19:k:1:MET:N	19:k:1:MET:SD	2.30	1.04
6:X:112:SER:CA	33:p:201:8Q1:O2	2.05	1.04
19:k:7:ASN:HD21	21:m:9:SER:C	1.65	1.04
20:l:84:TYR:CD1	20:l:88:MET:CE	2.30	1.03
17:i:285:ILE:HG12	32:l:701:PEE:H75	1.35	1.03
20:l:571:ILE:HD11	32:l:701:PEE:C30	1.89	1.03
9:a:96:ALA:HB3	12:d:55:TYR:HB2	1.33	1.02
9:a:96:ALA:CB	12:d:55:TYR:HB2	1.90	1.02
20:l:37:LYS:CE	20:l:98:TRP:HD1	1.65	1.02
20:l:59:GLN:HA	20:l:59:GLN:HE21	1.23	1.02
30:r:502:PLX:H332	30:r:502:PLX:H372	1.37	1.02
20:l:25:ASN:ND2	20:l:25:ASN:O	1.91	1.02
20:l:571:ILE:HD11	32:l:701:PEE:O5	0.84	1.01
12:d:105:LYS:NZ	20:l:197:ASP:OD2	1.91	1.01
20:l:222:GLY:CA	20:l:229:LEU:HD12	1.91	1.01
20:l:226:GLN:HG3	20:l:280:LEU:CD2	1.91	1.01
20:l:534:HIS:ND1	32:l:702:PEE:H14	1.74	1.01
24:p:170:ILE:H	24:p:170:ILE:HD12	1.24	1.01
17:i:291:TYR:CZ	32:l:701:PEE:H49	1.97	1.00
32:l:701:PEE:H37	25:r:155:VAL:HB	1.42	1.00
24:p:48:PHE:HE1	33:p:201:8Q1:C8	1.73	1.00
17:i:291:TYR:CE2	32:l:701:PEE:H48	1.95	1.00
20:l:193:SER:OG	20:l:205:ASN:ND2	1.95	1.00
20:l:533:MET:CE	32:l:702:PEE:C22	2.16	1.00
32:V:202:PEE:C25	32:V:202:PEE:H60	1.92	0.99
20:l:533:MET:HE1	32:l:702:PEE:H35	1.44	0.99
19:k:7:ASN:HD22	21:m:9:SER:CB	1.75	0.99
1:Q:53:TYR:HE1	32:l:701:PEE:O1P	1.44	0.98
10:b:107:GLY:N	10:b:115:GLU:OE1	1.95	0.98
20:l:84:TYR:HE1	20:l:88:MET:HE3	1.08	0.98
19:k:4:ILE:CD1	21:m:125:MET:SD	2.52	0.98
20:l:51:THR:HG21	20:l:91:PRO:HG2	1.42	0.98
20:l:231:PRO:O	20:l:234:PRO:HD2	1.64	0.98
32:l:701:PEE:C22	25:r:155:VAL:HG11	1.94	0.97
32:l:701:PEE:H36	25:r:155:VAL:HG11	1.44	0.97
10:b:93:LYS:HE3	20:l:65:ASN:O	1.64	0.97
20:l:226:GLN:NE2	20:l:314:MET:CE	2.27	0.97
24:p:44:MET:HE1	33:p:201:8Q1:C10	1.94	0.97
32:l:701:PEE:H37	25:r:155:VAL:CB	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:V:202:PEE:H14	17:i:276:LEU:CD1	1.96	0.96
24:p:48:PHE:CE1	33:p:201:8Q1:C8	2.48	0.96
20:l:84:TYR:HD1	20:l:88:MET:HE2	1.20	0.95
20:l:74:THR:CG2	20:l:194:ASN:OD1	2.14	0.95
32:V:202:PEE:H14	17:i:276:LEU:HD12	1.47	0.95
19:k:1:MET:HB3	21:m:125:MET:HB2	1.43	0.95
9:a:55:PHE:CD2	24:p:118:TYR:CD2	2.49	0.95
9:a:176:LYS:HE2	16:h:42:GLU:HG2	1.49	0.95
7:Y:86:TYR:OH	28:v:100:LYS:CE	2.15	0.94
30:b:201:PLX:O9	30:r:502:PLX:H1C3	1.67	0.94
10:b:88:TYR:CD1	30:b:201:PLX:H1C1	2.02	0.94
11:c:122:THR:OG1	23:o:12:ARG:NH1	1.99	0.94
20:l:226:GLN:CG	20:l:280:LEU:HD21	1.98	0.94
19:k:7:ASN:ND2	21:m:9:SER:CB	2.31	0.93
17:i:291:TYR:CE2	32:l:701:PEE:H49	2.00	0.93
10:b:118:PRO:O	10:b:120:MET:HG2	1.68	0.93
17:i:167:TRP:CZ3	20:l:573:THR:CB	2.52	0.93
7:Y:87:PRO:CB	28:v:103:GLU:OE2	2.17	0.92
12:d:59:HIS:HE1	13:e:120:ARG:HB3	1.24	0.92
19:k:3:LEU:CD2	21:m:117:ASN:HD21	1.83	0.92
12:d:59:HIS:CE1	13:e:120:ARG:CB	2.53	0.92
7:Y:83:HIS:O	7:Y:84:PHE:HB2	1.67	0.91
10:b:110:ILE:HG23	10:b:111:LEU:CG	1.99	0.91
30:b:201:PLX:H1C3	30:b:201:PLX:C3	2.01	0.90
7:Y:79:GLU:O	20:l:487:LYS:HE3	1.70	0.90
12:d:60:ARG:HG2	12:d:60:ARG:HH11	1.36	0.90
20:l:226:GLN:CG	20:l:280:LEU:CD2	2.49	0.89
20:l:227:LEU:HD12	20:l:230:HIS:ND1	1.85	0.89
12:d:105:LYS:HE2	20:l:197:ASP:OD2	1.70	0.89
19:k:7:ASN:ND2	21:m:9:SER:HB2	1.86	0.89
17:i:291:TYR:HE2	32:l:701:PEE:H48	1.32	0.89
20:l:51:THR:HG21	20:l:91:PRO:CG	2.02	0.89
25:r:78:MET:O	25:r:432:ARG:NH1	2.05	0.89
7:Y:96:GLU:OE2	11:c:185:GLU:O	1.89	0.89
10:b:110:ILE:C	10:b:111:LEU:HD23	1.98	0.89
20:l:78:LEU:HD21	20:l:80:PHE:CE1	2.07	0.89
9:a:114:LYS:HB2	12:d:57:TYR:HE2	1.31	0.89
12:d:108:GLN:HG2	20:l:199:GLN:HB3	1.54	0.89
12:d:110:ARG:HG2	12:d:110:ARG:HH11	1.38	0.89
20:l:37:LYS:HE3	20:l:102:GLU:HG3	1.53	0.88
32:l:701:PEE:H37	25:r:155:VAL:CG1	2.02	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:193:SER:HB2	20:l:195:SER:OG	1.74	0.88
11:c:169:GLU:OE2	28:v:56:ARG:NH2	2.05	0.88
20:l:88:MET:O	20:l:91:PRO:HD2	1.74	0.88
20:l:226:GLN:HG3	20:l:280:LEU:HD21	1.53	0.88
28:v:66:LEU:HD11	28:v:84:ARG:HD2	1.55	0.88
19:k:23:ARG:H	21:m:22:LYS:HE2	1.39	0.88
18:j:105:GLU:HG2	21:m:168:ILE:HD11	1.56	0.88
26:s:185:TRP:HE1	26:s:238:THR:HG22	1.39	0.88
9:a:87:THR:HG22	30:b:201:PLX:C13	2.03	0.88
17:i:167:TRP:HZ3	20:l:570:GLN:HA	1.37	0.88
19:k:2:PRO:HG2	21:m:115:VAL:HG21	1.56	0.88
7:Y:86:TYR:OH	28:v:100:LYS:CG	2.22	0.87
17:i:288:LEU:CD2	32:l:701:PEE:C36	2.32	0.87
7:Y:84:PHE:CG	7:Y:85:PRO:CD	2.57	0.87
30:b:201:PLX:H102	30:b:201:PLX:H6	1.56	0.87
17:i:224:SER:HB2	17:i:229:LEU:HB3	1.56	0.87
19:k:1:MET:HB2	19:k:4:ILE:CD1	2.04	0.87
20:l:78:LEU:HD21	20:l:80:PHE:HE1	1.39	0.87
11:c:181:VAL:CB	28:v:37:ARG:NH2	2.37	0.87
20:l:533:MET:SD	32:l:702:PEE:C22	2.62	0.87
20:l:447:ASN:OD1	20:l:448:PRO:CD	2.19	0.87
32:V:202:PEE:C43	32:l:701:PEE:C45	2.53	0.87
12:d:59:HIS:CE1	13:e:120:ARG:CG	2.58	0.87
29:w:99:GLY:HA3	29:w:337:ARG:HH12	1.40	0.86
10:b:110:ILE:O	10:b:111:LEU:HD23	1.75	0.86
20:l:533:MET:SD	32:l:702:PEE:H37	2.14	0.86
7:Y:84:PHE:CD1	7:Y:85:PRO:CD	2.58	0.86
32:W:201:PEE:O2P	32:W:201:PEE:N	2.08	0.85
9:a:96:ALA:HB3	12:d:55:TYR:CB	2.05	0.85
12:d:114:ASN:O	12:d:114:ASN:ND2	2.09	0.85
19:k:2:PRO:HG2	21:m:115:VAL:CG2	2.05	0.85
24:p:167:TRP:HE3	24:p:171:VAL:HG21	1.40	0.85
29:w:332:ARG:O	29:w:338:LYS:HG2	1.76	0.85
12:d:111:GLU:OE2	12:d:119:CYS:N	2.09	0.85
17:i:54:GLU:OE2	17:i:58:LYS:NZ	2.10	0.84
9:a:53:ARG:HD2	10:b:28:LEU:HD11	1.57	0.84
1:Q:53:TYR:CE1	32:l:701:PEE:O1P	2.30	0.84
32:V:202:PEE:H74	32:l:701:PEE:C45	2.08	0.84
15:g:1:MET:HE2	15:g:85:ARG:HD3	1.57	0.84
4:V:84:PRO:O	4:V:89:ASN:ND2	2.10	0.84
11:c:122:THR:HG1	23:o:12:ARG:HH12	1.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:12:THR:HG21	21:m:162:VAL:HG21	1.60	0.83
20:l:188:TRP:NE1	20:l:192:HIS:CD2	2.45	0.83
9:a:90:ASN:HD22	30:b:201:PLX:H122	1.43	0.83
15:g:62:LEU:HD22	30:g:203:PLX:H91	1.61	0.83
29:w:160:GLU:HG2	29:w:161:ARG:H	1.43	0.83
9:a:143:GLU:OE1	25:r:175:ASN:ND2	2.11	0.82
26:s:17:MET:HE1	26:s:232:ILE:HD12	1.61	0.82
12:d:59:HIS:CE1	13:e:120:ARG:HG2	2.14	0.82
9:a:54:LEU:HD22	10:b:26:GLN:C	2.05	0.82
18:j:6:ILE:O	18:j:10:ASN:ND2	2.12	0.82
17:i:235:ASN:ND2	17:i:307:MET:SD	2.53	0.82
9:a:87:THR:HG22	30:b:201:PLX:H132	1.60	0.82
11:c:93:ASP:OD1	23:o:44:LYS:NZ	2.13	0.82
24:p:124:GLN:O	24:p:128:LEU:HG	1.79	0.82
6:X:112:SER:N	33:p:201:8Q1:O2	2.14	0.81
7:Y:72:ARG:HH11	20:l:466:PHE:HD1	1.29	0.81
20:l:533:MET:HE1	32:l:702:PEE:H36	0.83	0.81
25:r:365:ALA:O	25:r:374:ASN:ND2	2.12	0.81
11:c:159:LYS:HA	28:v:98:ARG:HH22	1.46	0.81
15:g:49:ARG:HD3	29:w:339:TYR:HA	1.60	0.81
6:X:99:SER:HG	6:X:102:SER:HG	1.26	0.81
16:h:88:LYS:HG3	16:h:89:GLU:HG3	1.63	0.81
17:i:167:TRP:CZ3	20:l:570:GLN:HA	2.14	0.81
28:v:8:ARG:HH11	28:v:106:ARG:HH22	1.29	0.81
20:l:188:TRP:NE1	20:l:192:HIS:HD2	1.79	0.80
1:Q:58:THR:HG23	20:l:580:GLN:HE21	1.46	0.80
32:W:201:PEE:C44	26:s:77:LEU:HD21	2.09	0.80
7:Y:74:TRP:HZ3	7:Y:75:HIS:HD1	1.29	0.80
20:l:188:TRP:CZ2	20:l:192:HIS:CD2	2.69	0.80
20:l:222:GLY:HA2	20:l:229:LEU:HD12	1.63	0.80
30:r:502:PLX:H372	30:r:502:PLX:C33	2.09	0.80
20:l:227:LEU:O	20:l:227:LEU:HD12	1.82	0.80
32:l:701:PEE:C23	25:r:155:VAL:HG11	2.11	0.80
19:k:7:ASN:ND2	21:m:9:SER:C	2.38	0.80
29:w:332:ARG:O	29:w:338:LYS:CA	2.29	0.80
17:i:91:ASN:OD1	17:i:92:GLN:N	2.13	0.80
19:k:1:MET:HB2	19:k:4:ILE:HD12	1.63	0.80
20:l:226:GLN:NE2	20:l:314:MET:SD	2.54	0.79
7:Y:74:TRP:CE3	7:Y:75:HIS:HA	2.16	0.79
20:l:224:SER:OG	20:l:256:GLY:HA3	1.81	0.79
30:r:502:PLX:H52	30:r:502:PLX:O3	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:86:TYR:OH	28:v:100:LYS:HE2	1.82	0.79
17:i:12:THR:HG22	21:m:158:TRP:HE1	1.47	0.79
20:l:142:ILE:HG12	25:r:370:PRO:HB2	1.65	0.79
24:p:105:ASP:OD1	24:p:122:ARG:NH1	2.16	0.79
10:b:110:ILE:CG2	10:b:111:LEU:HG	2.11	0.79
20:l:4:HIS:CE1	20:l:87:MET:CE	2.65	0.79
11:c:166:LEU:HD21	28:v:56:ARG:HG3	1.65	0.79
10:b:86:MET:O	10:b:90:VAL:HG23	1.83	0.79
12:d:111:GLU:OE1	12:d:115:TYR:HB2	1.82	0.79
17:i:339:ILE:HG22	17:i:342:PHE:HB3	1.64	0.79
18:j:108:GLN:O	21:m:172:ARG:NH2	2.16	0.79
17:i:50:PRO:HB3	19:k:84:THR:HG21	1.65	0.78
24:p:143:GLU:OE2	24:p:158:ARG:NH2	2.15	0.78
7:Y:90:SER:HA	28:v:107:ARG:NH1	1.98	0.78
25:r:355:MET:HE1	25:r:437:MET:HE3	1.65	0.78
24:p:13:GLN:NE2	33:p:201:8Q1:O3	2.15	0.78
17:i:167:TRP:CH2	20:l:570:GLN:HG3	2.19	0.78
22:n:55:VAL:HG12	22:n:56:THR:H	1.48	0.78
24:p:167:TRP:O	24:p:171:VAL:CG2	2.28	0.78
7:Y:83:HIS:O	7:Y:84:PHE:CB	2.31	0.78
11:c:155:PRO:HB3	28:v:5:LEU:HD22	1.67	0.78
19:k:3:LEU:HD23	21:m:117:ASN:HD21	1.48	0.78
19:k:97:GLN:HB2	20:l:579:THR:HG21	1.66	0.78
21:m:111:GLY:HA2	21:m:116:VAL:HA	1.65	0.78
7:Y:86:TYR:OH	28:v:100:LYS:HG2	1.84	0.77
7:Y:84:PHE:CG	7:Y:85:PRO:HD2	2.19	0.77
30:b:201:PLX:H6	30:b:201:PLX:C10	2.13	0.77
7:Y:81:LEU:HD22	28:v:92:HIS:CD2	2.18	0.77
30:b:201:PLX:C6	30:b:201:PLX:H111	2.14	0.77
19:k:23:ARG:N	21:m:22:LYS:HE2	2.00	0.77
12:d:63:ARG:NH1	22:n:44:LEU:O	2.18	0.77
9:a:54:LEU:CD2	10:b:27:GLU:HA	2.14	0.77
7:Y:96:GLU:O	7:Y:97:LEU:HD23	1.84	0.77
29:w:64:GLY:O	29:w:161:ARG:NH2	2.17	0.77
17:i:288:LEU:HD23	32:l:701:PEE:H58	0.77	0.77
20:l:74:THR:HG22	20:l:194:ASN:OD1	1.83	0.77
20:l:90:ILE:O	20:l:94:LEU:HD22	1.84	0.77
20:l:226:GLN:NE2	20:l:314:MET:HE3	1.99	0.77
20:l:226:GLN:HE21	20:l:314:MET:HE1	1.48	0.76
29:w:56:ARG:NH1	29:w:81:LEU:O	2.18	0.76
29:w:60:ILE:HG13	29:w:203:LEU:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:190:ILE:H	20:l:190:ILE:HD12	1.49	0.76
21:m:115:VAL:O	21:m:117:ASN:N	2.18	0.76
24:p:54:GLU:OE2	33:p:201:8Q1:C38	2.34	0.75
9:a:55:PHE:CD2	24:p:118:TYR:CE1	2.64	0.75
3:U:82:LYS:NZ	27:u:121:ASP:OD1	2.18	0.75
20:l:54:PHE:CD1	20:l:58:ASP:HA	2.21	0.75
20:l:190:ILE:HD11	20:l:196:TRP:NE1	2.02	0.75
20:l:228:GLY:C	20:l:229:LEU:HD23	2.11	0.75
4:V:40:ARG:HH22	4:V:55:LYS:HD3	1.50	0.75
9:a:189:ASN:ND2	27:u:142:TYR:OH	2.20	0.75
7:Y:84:PHE:CZ	20:l:483:PRO:CG	2.68	0.75
12:d:81:GLU:CD	22:n:43:MET:HE3	2.11	0.75
7:Y:89:PRO:O	28:v:107:ARG:NH2	2.20	0.74
20:l:533:MET:SD	32:l:702:PEE:C23	2.75	0.74
7:Y:45:ARG:HH21	20:l:439:THR:HG21	1.52	0.74
7:Y:71:TRP:CZ2	7:Y:75:HIS:CD2	2.74	0.74
30:b:201:PLX:H1C3	30:b:201:PLX:H32	1.68	0.74
7:Y:84:PHE:CG	7:Y:85:PRO:HD3	2.22	0.74
29:w:319:ILE:HG23	29:w:323:GLN:HE21	1.53	0.74
32:V:202:PEE:H60	32:V:202:PEE:H41	1.67	0.74
9:a:163:ARG:NH2	15:g:99:ASP:OD2	2.20	0.74
9:a:168:TRP:NE1	15:g:88:GLU:OE1	2.20	0.74
12:d:154:ARG:NH2	15:g:108:TYR:O	2.19	0.74
20:l:78:LEU:HG	20:l:139:GLN:NE2	2.02	0.74
29:w:98:THR:O	29:w:337:ARG:NH2	2.18	0.74
7:Y:86:TYR:HH	28:v:100:LYS:HE2	1.52	0.74
18:j:6:ILE:HG13	26:s:6:LEU:HD11	1.67	0.74
24:p:170:ILE:HD12	24:p:170:ILE:N	2.02	0.74
20:l:135:ASN:OD1	20:l:198:PRO:HG3	1.88	0.74
25:r:114:GLU:HG3	27:u:169:PHE:HB3	1.68	0.74
11:c:123:PRO:HG3	24:p:75:GLN:HE21	1.52	0.73
24:p:27:LEU:HD11	24:p:44:MET:HG3	1.67	0.73
26:s:289:LEU:HA	26:s:293:PHE:HB3	1.70	0.73
32:V:202:PEE:C44	32:l:701:PEE:C45	2.66	0.73
20:l:4:HIS:NE2	20:l:87:MET:HE1	2.02	0.73
32:V:202:PEE:H39	32:V:202:PEE:H32	1.70	0.73
29:w:209:VAL:HG13	29:w:214:VAL:HG21	1.70	0.73
16:h:70:GLN:HG2	21:m:115:VAL:HG12	1.71	0.73
12:d:154:ARG:NH1	15:g:111:ILE:O	2.22	0.72
20:l:571:ILE:CG1	32:l:701:PEE:O5	2.36	0.72
20:l:227:LEU:HD12	20:l:230:HIS:CE1	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:3:LEU:HD22	21:m:117:ASN:HD21	1.53	0.72
9:a:54:LEU:HD22	10:b:26:GLN:O	1.90	0.72
20:l:451:LEU:H	20:l:453:PRO:HD2	1.54	0.72
18:j:25:PRO:O	18:j:27:LEU:N	2.23	0.72
20:l:384:PRO:O	20:l:389:PHE:HB2	1.89	0.72
10:b:109:THR:HB	10:b:113:THR:HA	1.70	0.72
12:d:73:GLU:HG2	15:g:111:ILE:HD11	1.72	0.72
20:l:170:GLN:NE2	32:l:702:PEE:O2P	2.22	0.72
20:l:59:GLN:HA	20:l:59:GLN:NE2	2.00	0.72
17:i:167:TRP:CE3	20:l:573:THR:CB	2.72	0.72
7:Y:43:ARG:HG3	7:Y:46:GLN:HB2	1.72	0.72
20:l:450:LEU:C	20:l:450:LEU:HD22	2.15	0.72
9:a:55:PHE:CE2	24:p:118:TYR:HE2	1.96	0.71
32:V:202:PEE:H60	32:V:202:PEE:H42	1.73	0.71
7:Y:86:TYR:HB3	7:Y:87:PRO:CA	2.19	0.71
20:l:78:LEU:CD2	20:l:80:PHE:HE1	2.02	0.71
5:W:115:ARG:HH11	16:h:36:PHE:HD1	1.36	0.71
12:d:136:ARG:NH2	13:e:138:GLU:O	2.23	0.71
20:l:341:MET:HE2	20:l:457:LEU:HD12	1.72	0.71
20:l:379:ALA:HA	20:l:386:LEU:HD11	1.73	0.71
30:r:502:PLX:H31	30:r:502:PLX:H72	1.73	0.71
20:l:567:SER:O	20:l:571:ILE:CD1	2.39	0.71
10:b:10:LEU:HD22	24:p:156:PRO:HB2	1.71	0.71
10:b:106:PRO:HA	10:b:115:GLU:OE2	1.89	0.71
19:k:7:ASN:HD22	21:m:9:SER:HB2	1.47	0.71
20:l:10:LEU:HD22	20:l:46:ILE:HG21	1.72	0.70
24:p:104:LEU:HD21	24:p:119:PHE:HE1	1.56	0.70
24:p:170:ILE:H	24:p:170:ILE:CD1	2.02	0.70
17:i:298:TYR:O	17:i:303:THR:OG1	2.08	0.70
18:j:67:LEU:HD21	19:k:68:ALA:HB3	1.72	0.70
20:l:71:THR:HG21	25:r:307:TRP:HE1	1.54	0.70
20:l:78:LEU:HG	20:l:139:GLN:HE22	1.55	0.70
7:Y:86:TYR:OH	28:v:100:LYS:HE3	1.89	0.70
20:l:135:ASN:HD21	20:l:199:GLN:HE22	1.40	0.70
7:Y:81:LEU:HD23	7:Y:81:LEU:C	2.15	0.70
25:r:44:GLN:O	25:r:46:ASN:N	2.24	0.70
20:l:338:MET:HE3	20:l:372:SER:HB2	1.74	0.70
32:l:701:PEE:H46	25:r:155:VAL:HG12	1.71	0.70
6:X:91:ASP:OD1	8:Z:47:ARG:NH1	2.24	0.70
20:l:190:ILE:HG13	20:l:196:TRP:CD1	2.27	0.70
1:Q:48:GLY:HA2	17:i:228:LEU:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:108:GLU:OE2	16:h:75:ARG:NH1	2.24	0.70
12:d:59:HIS:HE1	13:e:120:ARG:CB	1.97	0.70
12:d:65:VAL:H	12:d:85:GLN:NE2	1.89	0.70
20:l:78:LEU:CD2	20:l:80:PHE:CE1	2.74	0.70
10:b:105:PHE:CE2	28:v:68:LYS:HA	2.26	0.70
20:l:100:ILE:HD12	20:l:246:LEU:HG	1.72	0.70
20:l:567:SER:O	20:l:571:ILE:HD12	1.92	0.70
20:l:546:GLN:OE1	25:r:278:ARG:NE	2.22	0.70
23:o:23:TYR:OH	24:p:68:GLU:OE1	2.09	0.70
5:W:134:LEU:HD11	21:m:2:MET:HB2	1.72	0.69
7:Y:86:TYR:CB	7:Y:87:PRO:HA	2.22	0.69
19:k:66:PHE:HE1	21:m:159:THR:HG21	1.57	0.69
6:X:84:LEU:HD22	6:X:98:LEU:HD21	1.74	0.69
15:g:15:ASP:HB2	15:g:18:ARG:HH21	1.57	0.69
26:s:235:ASN:HD22	26:s:267:THR:HG22	1.55	0.69
19:k:2:PRO:CG	21:m:115:VAL:HG21	2.21	0.69
29:w:67:CYS:N	29:w:70:LYS:HD3	2.07	0.69
10:b:16:ARG:O	10:b:20:ARG:HG2	1.93	0.69
30:b:201:PLX:O3	30:b:201:PLX:O7	2.05	0.69
10:b:14:GLN:HE22	24:p:157:ALA:HB3	1.56	0.69
13:e:129:ARG:NH1	13:e:136:ILE:O	2.24	0.69
20:l:226:GLN:HG3	20:l:280:LEU:HD23	1.74	0.69
32:W:201:PEE:H24	32:W:201:PEE:H53	1.74	0.69
10:b:54:LYS:HG3	10:b:55:SER:H	1.58	0.69
13:e:76:TYR:O	25:r:82:ARG:NH1	2.21	0.69
20:l:141:PHE:HE2	25:r:375:LEU:HD21	1.58	0.69
20:l:4:HIS:CE1	20:l:87:MET:HE3	2.28	0.69
20:l:4:HIS:HE1	20:l:87:MET:HE3	1.57	0.69
29:w:176:GLN:NE2	29:w:236:ASP:OD2	2.24	0.69
9:a:98:LEU:HA	12:d:57:TYR:CD1	2.28	0.69
20:l:4:HIS:CE1	20:l:87:MET:HE1	2.28	0.69
10:b:94:PRO:HB3	12:d:5:TRP:HA	1.73	0.68
10:b:120:MET:SD	28:v:65:ARG:NH2	2.66	0.68
32:l:701:PEE:H37	25:r:155:VAL:HG11	1.70	0.68
18:j:30:TYR:HB2	18:j:33:LYS:HD2	1.75	0.68
32:l:701:PEE:H36	25:r:155:VAL:CG1	2.21	0.68
21:m:121:VAL:O	21:m:123:SER:N	2.26	0.68
29:w:63:ASP:OD2	29:w:241:TYR:OH	2.11	0.68
10:b:12:LEU:HB3	10:b:16:ARG:HH12	1.58	0.68
20:l:396:ILE:O	20:l:400:ASN:ND2	2.26	0.68
4:V:81:ARG:HG2	4:V:83:LYS:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:144:ASN:O	25:r:147:THR:OG1	2.10	0.68
9:a:55:PHE:CD2	24:p:118:TYR:CG	2.82	0.68
17:i:180:ALA:O	17:i:183:SER:OG	2.08	0.68
7:Y:86:TYR:HB3	7:Y:87:PRO:HA	1.75	0.68
20:l:222:GLY:HA3	20:l:229:LEU:HD12	1.74	0.68
30:b:201:PLX:H6	30:b:201:PLX:C11	2.24	0.68
20:l:447:ASN:CG	20:l:448:PRO:HD2	2.16	0.68
26:s:85:LEU:HB3	26:s:233:MET:SD	2.34	0.68
32:W:201:PEE:H36	18:j:7:LEU:HD22	1.77	0.67
30:b:201:PLX:H6	30:b:201:PLX:H111	1.75	0.67
9:a:98:LEU:HA	12:d:57:TYR:HD1	1.60	0.67
24:p:48:PHE:HE1	33:p:201:8Q1:C7	2.06	0.67
27:u:34:ALA:HB2	27:u:120:PRO:HD3	1.75	0.67
10:b:88:TYR:O	10:b:92:GLU:CB	2.42	0.67
11:c:122:THR:O	23:o:12:ARG:NH2	2.27	0.67
20:l:188:TRP:CD2	20:l:192:HIS:HD2	2.09	0.67
11:c:62:TYR:OH	11:c:74:ASP:O	2.11	0.67
7:Y:81:LEU:CD2	28:v:92:HIS:CD2	2.78	0.67
9:a:98:LEU:CB	12:d:57:TYR:CD1	2.77	0.67
19:k:25:HIS:HA	19:k:90:VAL:HG13	1.77	0.67
19:k:83:ASN:ND2	21:m:173:GLY:O	2.27	0.67
20:l:444:ASN:OD1	20:l:445:GLU:N	2.26	0.67
29:w:132:GLN:HE22	29:w:169:PHE:HD2	1.41	0.67
7:Y:84:PHE:CD2	7:Y:85:PRO:HD2	2.30	0.67
12:d:49:GLN:OE1	12:d:49:GLN:N	2.27	0.67
18:j:3:PHE:HA	18:j:6:ILE:HD13	1.77	0.67
26:s:265:LEU:O	26:s:268:SER:OG	2.10	0.67
10:b:51:LEU:HD11	10:b:62:HIS:CD2	2.30	0.67
17:i:170:LEU:HD12	20:l:574:SER:HB3	1.77	0.67
18:j:5:LEU:HD13	26:s:3:MET:HE1	1.77	0.67
25:r:15:THR:O	25:r:93:LYS:NZ	2.24	0.67
10:b:93:LYS:CE	20:l:65:ASN:O	2.41	0.67
10:b:115:GLU:HG2	10:b:116:VAL:N	2.10	0.67
18:j:36:PRO:HG2	18:j:43:PRO:HG3	1.77	0.67
19:k:3:LEU:HD23	21:m:117:ASN:ND2	2.09	0.67
6:X:120:MET:HE1	24:p:24:LEU:HB2	1.77	0.67
10:b:38:GLN:OE1	10:b:39:LYS:N	2.28	0.67
11:c:184:TYR:CB	28:v:37:ARG:HG3	2.25	0.67
12:d:108:GLN:NE2	20:l:199:GLN:O	2.29	0.66
20:l:190:ILE:HG12	20:l:196:TRP:CE2	2.31	0.66
25:r:150:LEU:O	25:r:153:THR:OG1	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:369:LEU:O	25:r:372:THR:OG1	2.12	0.66
5:W:86:MET:SD	5:W:128:ARG:NH1	2.66	0.66
26:s:169:GLN:HE21	26:s:174:LEU:H	1.42	0.66
12:d:108:GLN:NE2	20:l:203:LEU:HG	2.10	0.66
19:k:51:THR:O	19:k:53:SER:N	2.27	0.66
7:Y:90:SER:HA	28:v:107:ARG:HH12	1.59	0.66
26:s:200:LEU:HD12	26:s:285:LEU:HD11	1.77	0.66
20:l:226:GLN:HG2	20:l:280:LEU:CD2	2.25	0.66
20:l:359:MET:O	20:l:436:ARG:NH2	2.29	0.66
20:l:332:HIS:HE1	20:l:336:LYS:HZ1	1.44	0.66
25:r:305:THR:O	25:r:308:SER:OG	2.12	0.66
10:b:114:GLY:O	10:b:115:GLU:HB3	1.95	0.66
9:a:58:ARG:HH21	9:a:61:ARG:HD2	1.60	0.66
10:b:105:PHE:CZ	28:v:67:LEU:HB2	2.31	0.66
19:k:26:LEU:HD11	19:k:78:LEU:HD21	1.78	0.66
7:Y:85:PRO:HG2	28:v:99:MET:HE2	1.78	0.66
26:s:202:GLU:O	26:s:204:GLU:N	2.29	0.66
20:l:453:PRO:HA	20:l:456:ARG:NH2	2.11	0.65
17:i:12:THR:HG22	21:m:158:TRP:NE1	2.10	0.65
28:v:74:PHE:O	28:v:76:ASN:ND2	2.29	0.65
7:Y:81:LEU:HD12	28:v:88:ASP:HB3	1.78	0.65
29:w:58:ARG:NH1	29:w:279:ASP:O	2.28	0.65
19:k:11:ALA:HB1	21:m:16:PHE:CD2	2.31	0.65
26:s:185:TRP:NE1	26:s:238:THR:HG22	2.12	0.65
32:W:201:PEE:H1	26:s:98:LEU:HD22	1.79	0.65
29:w:188:ASN:HA	29:w:191:LYS:HE2	1.78	0.65
10:b:110:ILE:HG23	10:b:111:LEU:CD2	2.26	0.65
21:m:147:ASP:OD1	21:m:148:TYR:N	2.30	0.65
26:s:20:LEU:HD13	26:s:232:ILE:HD11	1.78	0.65
29:w:249:MET:HB3	29:w:255:VAL:HG11	1.79	0.65
2:S:53:ARG:NH2	16:h:105:ARG:HD3	2.12	0.65
30:U:101:PLX:HO9	18:j:106:TRP:CD1	2.13	0.65
17:i:42:PRO:HG3	21:m:166:ILE:HG23	1.78	0.65
19:k:1:MET:HB2	19:k:4:ILE:HD13	1.77	0.65
19:k:4:ILE:HD13	21:m:125:MET:SD	2.34	0.65
15:g:27:ASP:OD2	15:g:29:ARG:NH1	2.29	0.65
20:l:227:LEU:HD12	20:l:230:HIS:HD1	1.60	0.65
29:w:332:ARG:O	29:w:338:LYS:CG	2.45	0.65
5:W:68:ARG:HD3	21:m:134:PHE:CZ	2.32	0.64
12:d:110:ARG:HG2	12:d:110:ARG:NH1	2.11	0.64
5:W:68:ARG:HD3	21:m:134:PHE:CE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:79:GLU:O	7:Y:80:VAL:HG13	1.96	0.64
9:a:94:GLY:O	9:a:96:ALA:N	2.30	0.64
13:e:76:TYR:H	25:r:432:ARG:HD2	1.61	0.64
32:l:701:PEE:C22	25:r:155:VAL:HG21	2.27	0.64
27:u:31:HIS:CE1	27:u:119:ARG:HB3	2.33	0.64
1:Q:35:ARG:NH1	13:e:60:GLU:OE2	2.28	0.64
16:h:91:LYS:HG3	16:h:92:TYR:H	1.62	0.64
20:l:226:GLN:OE1	20:l:226:GLN:HA	1.97	0.64
20:l:307:SER:HA	20:l:310:LEU:HD12	1.80	0.64
32:l:701:PEE:H36	25:r:155:VAL:HG21	1.79	0.64
26:s:228:TYR:HD1	26:s:231:ILE:HD12	1.63	0.64
5:W:39:GLY:O	5:W:42:THR:OG1	2.15	0.64
10:b:112:GLU:N	10:b:112:GLU:OE2	2.31	0.64
20:l:97:THR:HG21	20:l:125:LEU:CD1	2.20	0.64
17:i:291:TYR:CD2	32:l:701:PEE:H51	2.32	0.64
11:c:159:LYS:HA	28:v:98:ARG:HH12	1.62	0.64
20:l:67:HIS:CE1	20:l:75:GLN:HG3	2.33	0.64
20:l:405:ASN:OD1	20:l:406:ALA:N	2.31	0.64
10:b:108:ASP:O	10:b:113:THR:HA	1.98	0.64
17:i:197:ASN:HB3	17:i:269:GLU:OE1	1.98	0.64
17:i:288:LEU:HD21	32:l:701:PEE:H64	1.80	0.64
27:u:140:ASN:ND2	27:u:143:HIS:O	2.31	0.64
16:h:5:ASP:HB3	16:h:8:LYS:HB3	1.80	0.64
20:l:88:MET:O	20:l:92:VAL:HG23	1.98	0.64
25:r:112:ALA:O	25:r:113:THR:OG1	2.14	0.64
9:a:95:GLN:HA	9:a:116:PRO:HD3	1.79	0.64
9:a:96:ALA:CB	12:d:55:TYR:CB	2.70	0.64
9:a:127:ASP:HB3	9:a:131:LYS:HD3	1.80	0.64
20:l:501:ALA:O	20:l:505:ASN:ND2	2.29	0.64
26:s:280:PHE:HE2	26:s:288:LEU:HD11	1.63	0.64
32:W:201:PEE:H75	26:s:77:LEU:HD23	1.75	0.63
20:l:537:ILE:HD11	32:l:702:PEE:H38	1.80	0.63
4:V:27:SER:O	4:V:30:SER:OG	2.14	0.63
20:l:190:ILE:HD11	20:l:196:TRP:HE1	1.61	0.63
12:d:112:GLY:O	12:d:115:TYR:HB3	1.99	0.63
14:f:38:LYS:HB2	14:f:39:PRO:HD3	1.81	0.63
21:m:116:VAL:O	21:m:118:PHE:N	2.31	0.63
29:w:89:ALA:N	29:w:160:GLU:OE1	2.27	0.63
32:V:202:PEE:H32	32:V:202:PEE:C24	2.25	0.63
18:j:77:TRP:NE1	26:s:318:THR:O	2.31	0.63
7:Y:74:TRP:HE3	7:Y:75:HIS:HA	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:32:ILE:HD12	24:p:35:ASP:OD1	1.98	0.63
9:a:87:THR:HG22	30:b:201:PLX:H131	1.81	0.63
19:k:92:ASN:ND2	20:l:582:GLY:O	2.31	0.63
23:o:56:ARG:HH12	23:o:59:LEU:C	2.06	0.63
27:u:24:VAL:HG22	27:u:86:TRP:NE1	2.12	0.63
10:b:105:PHE:CE2	28:v:68:LYS:CA	2.81	0.63
17:i:271:THR:HG22	17:i:276:LEU:HD22	1.81	0.63
25:r:373:ILE:HG23	25:r:448:SER:HA	1.81	0.63
7:Y:73:PHE:HA	20:l:385:PHE:CE2	2.33	0.63
10:b:88:TYR:CD1	30:b:201:PLX:C1C	2.79	0.63
17:i:72:MET:HE1	19:k:9:MET:HG2	1.81	0.63
20:l:534:HIS:ND1	32:l:702:PEE:C11	2.59	0.63
25:r:210:TYR:O	25:r:213:HIS:ND1	2.31	0.63
26:s:107:ALA:O	26:s:110:SER:OG	2.11	0.63
26:s:169:GLN:NE2	26:s:244:GLY:H	1.96	0.63
11:c:159:LYS:HA	28:v:98:ARG:NH2	2.13	0.63
28:v:40:VAL:HB	28:v:61:HIS:CE1	2.34	0.63
19:k:82:SER:HB3	19:k:87:LEU:HD23	1.80	0.62
21:m:56:PHE:HD2	26:s:107:ALA:HB1	1.64	0.62
29:w:117:PHE:HB2	29:w:131:LEU:HD21	1.80	0.62
30:b:201:PLX:O4	30:b:201:PLX:H11	1.99	0.62
20:l:124:PHE:HE1	20:l:147:VAL:HG13	1.64	0.62
20:l:229:LEU:HD23	20:l:229:LEU:N	2.13	0.62
10:b:7:ASP:HB2	24:p:156:PRO:HG3	1.79	0.62
17:i:245:PRO:HB3	17:i:297:ILE:HG12	1.80	0.62
20:l:450:LEU:O	20:l:450:LEU:HD13	2.00	0.62
29:w:149:HIS:O	29:w:153:THR:OG1	2.16	0.62
8:Z:24:ILE:HD11	8:Z:47:ARG:HG2	1.80	0.62
28:v:52:ARG:O	28:v:56:ARG:NH1	2.33	0.62
27:u:30:HIS:CE1	27:u:119:ARG:HH11	2.17	0.62
7:Y:96:GLU:O	7:Y:97:LEU:HB2	1.98	0.62
20:l:54:PHE:HD2	20:l:55:MET:HE2	1.65	0.62
17:i:37:MET:HE1	17:i:60:PHE:HA	1.82	0.62
29:w:60:ILE:O	29:w:159:LEU:N	2.33	0.62
21:m:56:PHE:CD2	26:s:107:ALA:HB1	2.35	0.62
30:r:502:PLX:H31	30:r:502:PLX:C7	2.30	0.62
20:l:37:LYS:NZ	20:l:98:TRP:NE1	2.47	0.62
32:l:701:PEE:H32	25:r:155:VAL:HG21	1.80	0.62
23:o:26:SER:O	23:o:29:THR:OG1	2.15	0.62
2:S:53:ARG:HB2	16:h:105:ARG:HH12	1.64	0.61
19:k:10:LEU:HD12	21:m:102:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:4:HIS:HE1	20:l:87:MET:CE	2.10	0.61
20:l:216:LEU:HD22	20:l:259:LEU:HD21	1.80	0.61
20:l:303:ALA:O	20:l:306:THR:OG1	2.17	0.61
21:m:118:PHE:CD1	21:m:121:VAL:HB	2.34	0.61
9:a:55:PHE:CD2	24:p:118:TYR:CD1	2.88	0.61
12:d:107:CYS:SG	12:d:119:CYS:HA	2.39	0.61
20:l:450:LEU:HD22	20:l:450:LEU:O	2.00	0.61
1:Q:51:VAL:HG13	17:i:171:ASN:OD1	2.00	0.61
25:r:61:LEU:HD22	25:r:241:TYR:HD1	1.64	0.61
12:d:60:ARG:HG2	12:d:60:ARG:NH1	2.12	0.61
26:s:186:PHE:O	26:s:189:THR:OG1	2.16	0.61
7:Y:81:LEU:HD23	7:Y:82:GLY:N	2.14	0.61
10:b:42:PRO:HA	10:b:45:LYS:HB2	1.81	0.61
20:l:37:LYS:NZ	20:l:98:TRP:CD1	2.69	0.61
1:Q:38:GLN:HE21	17:i:304:LEU:HB2	1.64	0.61
6:X:138:LEU:HD21	6:X:144:ILE:HG12	1.83	0.61
20:l:194:ASN:HB2	23:o:125:PHE:O	2.01	0.61
21:m:118:PHE:HE1	21:m:124:TRP:HE1	1.47	0.61
25:r:150:LEU:HD21	25:r:154:LEU:HD12	1.79	0.61
1:Q:53:TYR:HE1	32:l:701:PEE:P	2.22	0.61
10:b:12:LEU:HB3	10:b:16:ARG:NH1	2.16	0.61
18:j:32:GLU:O	18:j:37:TYR:OH	2.18	0.61
29:w:67:CYS:H	29:w:70:LYS:HD3	1.65	0.61
10:b:14:GLN:NE2	24:p:164:PRO:HD3	2.15	0.61
16:h:37:GLU:HB2	16:h:63:PHE:CE1	2.35	0.61
29:w:160:GLU:HG2	29:w:161:ARG:N	2.13	0.61
31:V:201:CDL:OA7	31:V:201:CDL:O1	2.15	0.61
7:Y:73:PHE:O	7:Y:73:PHE:HD1	1.84	0.61
20:l:552:LEU:HD13	23:o:90:GLY:HA2	1.83	0.61
2:S:50:ARG:HA	16:h:105:ARG:CZ	2.30	0.61
17:i:58:LYS:HE3	20:l:584:ILE:HG12	1.82	0.61
26:s:280:PHE:CE2	26:s:288:LEU:HD11	2.36	0.61
12:d:59:HIS:NE2	13:e:121:GLU:HG2	2.16	0.60
20:l:37:LYS:HE2	20:l:98:TRP:HD1	0.69	0.60
26:s:28:LEU:O	26:s:32:GLN:HB2	2.01	0.60
20:l:427:ILE:HG23	20:l:431:LEU:HD12	1.82	0.60
25:r:447:LEU:HD13	25:r:454:ILE:HD11	1.83	0.60
25:r:447:LEU:HD11	30:r:502:PLX:H382	1.82	0.60
14:f:55:TRP:O	14:f:59:ILE:HG12	2.00	0.60
15:g:9:PRO:O	15:g:11:ARG:N	2.32	0.60
18:j:55:PHE:O	18:j:58:VAL:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:3:LEU:CD2	21:m:117:ASN:ND2	2.60	0.60
5:W:111:PHE:HE2	5:W:117:VAL:HG11	1.66	0.60
10:b:88:TYR:HD1	10:b:92:GLU:OE2	1.82	0.60
28:v:8:ARG:HH11	28:v:106:ARG:NH2	1.97	0.60
6:X:72:PRO:HG3	20:l:442:ASN:HD22	1.65	0.60
10:b:100:LYS:O	10:b:101:LYS:HG2	2.01	0.60
22:n:50:GLN:HG3	22:n:51:PRO:HD2	1.83	0.60
32:W:201:PEE:C44	26:s:77:LEU:CD2	2.67	0.60
15:g:32:TYR:OH	17:i:335:LEU:O	2.13	0.60
16:h:49:TYR:HA	16:h:52:ALA:HB3	1.82	0.60
10:b:115:GLU:HG2	10:b:116:VAL:H	1.65	0.60
11:c:84:HIS:CE1	11:c:114:ARG:HA	2.37	0.60
20:l:575:ILE:O	20:l:578:SER:OG	2.16	0.60
22:n:10:ASP:HB3	25:r:19:LYS:HZ3	1.65	0.60
12:d:54:ARG:HD3	12:d:56:TYR:CE1	2.37	0.60
17:i:291:TYR:CE2	32:l:701:PEE:C32	2.85	0.60
25:r:190:TRP:NE1	30:r:501:PLX:H1A2	2.17	0.60
29:w:65:ASN:HD22	29:w:209:VAL:HG21	1.67	0.60
30:U:101:PLX:H252	18:j:106:TRP:CD1	2.36	0.60
11:c:105:MET:HE2	23:o:65:LEU:HA	1.83	0.60
12:d:108:GLN:HG2	20:l:199:GLN:CB	2.31	0.60
26:s:172:LEU:HD21	26:s:176:LEU:HB2	1.84	0.59
9:a:176:LYS:HB2	16:h:45:HIS:CD2	2.36	0.59
20:l:149:ILE:HD12	25:r:369:LEU:HD21	1.84	0.59
24:p:121:LYS:O	24:p:124:GLN:HG2	2.02	0.59
11:c:169:GLU:O	11:c:169:GLU:HG2	2.02	0.59
17:i:8:VAL:HG11	21:m:165:TYR:CE2	2.37	0.59
19:k:97:GLN:HG2	20:l:582:GLY:HA2	1.84	0.59
7:Y:45:ARG:HG3	8:Z:52:ARG:HB2	1.84	0.59
12:d:54:ARG:HD3	12:d:56:TYR:CZ	2.37	0.59
17:i:193:VAL:HG21	17:i:266:ILE:HG12	1.82	0.59
20:l:367:PRO:O	20:l:370:SER:OG	2.17	0.59
21:m:83:GLY:HA2	21:m:89:LEU:HD21	1.83	0.59
4:V:40:ARG:HA	31:V:201:CDL:OB3	2.02	0.59
8:Z:66:VAL:HG22	20:l:363:LEU:HD22	1.85	0.59
17:i:24:SER:O	17:i:86:MET:HG2	2.02	0.59
5:W:81:ARG:HH22	27:u:64:ASN:ND2	2.00	0.59
10:b:79:VAL:HG11	12:d:35:VAL:HG11	1.84	0.59
16:h:94:PRO:HG2	16:h:95:PRO:HD3	1.85	0.59
22:n:31:SER:O	22:n:34:ARG:HG2	2.02	0.59
25:r:30:HIS:O	25:r:34:ILE:HD12	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:w:304:VAL:HG23	29:w:305:LEU:HG	1.84	0.59
32:V:202:PEE:H71	32:l:701:PEE:C45	2.27	0.59
10:b:88:TYR:CG	30:b:201:PLX:C1C	2.86	0.59
10:b:100:LYS:HB2	20:l:60:GLU:HB2	1.84	0.59
18:j:54:LYS:HE3	18:j:113:TRP:CD1	2.38	0.59
20:l:174:TYR:OH	32:l:702:PEE:H19	2.02	0.59
20:l:227:LEU:HB2	20:l:284:THR:HG22	1.84	0.59
20:l:247:LEU:O	20:l:252:MET:HB3	2.03	0.59
10:b:51:LEU:HD21	10:b:62:HIS:HB2	1.83	0.59
16:h:44:ALA:HA	16:h:47:ILE:HD12	1.85	0.59
16:h:51:ARG:NH1	16:h:55:GLU:OE2	2.36	0.59
24:p:112:LYS:HA	24:p:119:PHE:CE2	2.38	0.59
29:w:132:GLN:HG2	29:w:170:LEU:HD12	1.85	0.59
2:S:53:ARG:HB2	16:h:105:ARG:NH1	2.18	0.59
32:V:202:PEE:C11	17:i:276:LEU:HD12	2.28	0.59
8:Z:25:GLU:HA	8:Z:30:GLU:HG3	1.84	0.59
11:c:93:ASP:OD2	11:c:101:TRP:N	2.36	0.59
11:c:94:GLN:O	11:c:98:ARG:N	2.30	0.59
12:d:134:GLN:NE2	23:o:123:ARG:O	2.35	0.59
18:j:2:ASN:O	18:j:5:LEU:HG	2.03	0.59
20:l:37:LYS:CE	20:l:98:TRP:NE1	2.65	0.59
10:b:88:TYR:O	10:b:92:GLU:HB2	2.03	0.58
10:b:105:PHE:HE2	28:v:68:LYS:N	2.01	0.58
18:j:7:LEU:HA	18:j:10:ASN:HD22	1.67	0.58
20:l:456:ARG:CB	20:l:456:ARG:HH21	2.16	0.58
23:o:25:ILE:HD12	23:o:30:ARG:HD3	1.85	0.58
30:b:201:PLX:P1	30:b:201:PLX:H72	2.43	0.58
18:j:32:GLU:HA	18:j:35:THR:HG23	1.84	0.58
24:p:98:LYS:HE2	24:p:176:GLU:HA	1.83	0.58
29:w:170:LEU:HD21	29:w:184:VAL:HG22	1.84	0.58
32:W:201:PEE:H8	26:s:98:LEU:HD22	1.84	0.58
9:a:53:ARG:HH21	10:b:28:LEU:HD11	1.66	0.58
9:a:67:PHE:HD1	25:r:431:THR:HG23	1.68	0.58
17:i:145:ILE:HD12	17:i:149:LEU:HD11	1.84	0.58
27:u:38:LYS:O	27:u:42:GLU:HB2	2.03	0.58
5:W:61:GLN:HE22	26:s:317:GLN:HA	1.68	0.58
17:i:249:LEU:HB3	17:i:254:LEU:HD12	1.84	0.58
26:s:294:LEU:O	26:s:297:THR:OG1	2.15	0.58
27:u:96:LEU:HD11	27:u:99:HIS:CD2	2.38	0.58
12:d:153:GLN:O	12:d:157:MET:HG2	2.03	0.58
18:j:72:LEU:HD21	18:j:94:LEU:HD22	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:37:MET:HE1	19:k:63:MET:HB3	1.86	0.58
20:l:88:MET:C	20:l:91:PRO:HD2	2.28	0.58
20:l:227:LEU:CD1	20:l:230:HIS:CE1	2.86	0.58
17:i:277:ILE:O	17:i:280:THR:OG1	2.21	0.58
22:n:10:ASP:HB3	25:r:19:LYS:NZ	2.18	0.58
6:X:84:LEU:O	6:X:88:LYS:HG2	2.03	0.58
12:d:21:PRO:HG2	12:d:24:ILE:HD12	1.85	0.58
20:l:96:VAL:O	20:l:100:ILE:HG13	2.04	0.58
9:a:52:LYS:O	9:a:53:ARG:HG2	2.02	0.58
2:S:49:GLU:O	16:h:105:ARG:NH2	2.37	0.58
12:d:135:ASP:HB3	12:d:156:ARG:NH2	2.19	0.58
32:l:701:PEE:C23	25:r:155:VAL:CB	2.77	0.58
25:r:126:LEU:O	25:r:129:THR:OG1	2.19	0.58
26:s:85:LEU:HD13	26:s:233:MET:HE1	1.85	0.58
27:u:124:GLU:OE1	27:u:124:GLU:N	2.37	0.58
29:w:332:ARG:O	29:w:338:LYS:CB	2.52	0.58
3:U:67:PRO:HB3	3:U:74:GLN:HB2	1.86	0.57
17:i:245:PRO:HA	17:i:248:LEU:HD12	1.85	0.57
20:l:310:LEU:HA	20:l:313:MET:HE3	1.86	0.57
28:v:113:LYS:HE2	28:v:117:LYS:HE3	1.84	0.57
20:l:286:LEU:HD12	20:l:411:ILE:HG23	1.86	0.57
23:o:54:PRO:HA	24:p:129:ARG:HH21	1.67	0.57
26:s:169:GLN:NE2	26:s:174:LEU:H	2.03	0.57
7:Y:72:ARG:NH1	20:l:466:PHE:HD1	2.02	0.57
10:b:105:PHE:CD2	28:v:68:LYS:HA	2.39	0.57
17:i:120:GLN:O	17:i:176:ARG:NH2	2.37	0.57
4:V:40:ARG:HD3	4:V:59:TYR:HE2	1.68	0.57
5:W:78:GLU:HB3	16:h:105:ARG:HB3	1.86	0.57
32:W:201:PEE:H1	26:s:98:LEU:CD2	2.34	0.57
20:l:27:ASN:HB3	20:l:29:LYS:HG2	1.84	0.57
20:l:453:PRO:HA	20:l:456:ARG:HH22	1.69	0.57
20:l:556:THR:OG1	20:l:557:TRP:N	2.37	0.57
30:r:502:PLX:H72	30:r:502:PLX:C3	2.31	0.57
5:W:47:HIS:CE1	26:s:307:MET:HE1	2.40	0.57
10:b:88:TYR:CG	30:b:201:PLX:H1C1	2.38	0.57
11:c:156:VAL:O	28:v:98:ARG:HG2	2.05	0.57
17:i:258:THR:HG22	17:i:336:LEU:HB3	1.87	0.57
19:k:2:PRO:HG2	21:m:115:VAL:HG23	1.86	0.57
19:k:8:ILE:HG21	19:k:43:MET:HB2	1.87	0.57
22:n:56:THR:HG1	22:n:57:TRP:CD1	2.22	0.57
24:p:176:GLU:HG2	24:p:177:ARG:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:39:HIS:ND1	7:Y:40:ILE:HG13	2.20	0.57
7:Y:44:TYR:CD1	20:l:440:LEU:HB2	2.40	0.57
15:g:1:MET:SD	17:i:345:MET:HE1	2.45	0.57
17:i:58:LYS:NZ	19:k:92:ASN:OD1	2.35	0.57
20:l:272:LEU:O	20:l:275:THR:OG1	2.18	0.57
7:Y:73:PHE:HA	20:l:385:PHE:HE2	1.70	0.57
5:W:111:PHE:HE1	16:h:65:GLU:OE1	1.88	0.57
18:j:57:LEU:O	18:j:61:THR:HG23	2.04	0.57
20:l:35:TYR:CZ	20:l:39:ILE:HD11	2.40	0.57
29:w:124:ASN:HB3	29:w:316:GLU:HG2	1.85	0.57
10:b:88:TYR:CD1	10:b:92:GLU:OE2	2.57	0.57
10:b:111:LEU:O	10:b:112:GLU:HB2	2.04	0.57
6:X:132:ASP:OD2	24:p:18:ARG:HG2	2.05	0.57
9:a:114:LYS:CB	12:d:57:TYR:CE2	2.76	0.57
30:g:203:PLX:H251	17:i:324:PRO:HB2	1.85	0.57
17:i:316:GLN:NE2	29:w:95:ASP:OD1	2.33	0.57
20:l:37:LYS:HZ3	20:l:98:TRP:NE1	2.02	0.57
4:V:139:PRO:O	4:V:141:VAL:N	2.38	0.56
32:V:202:PEE:H57	32:V:202:PEE:H40	1.87	0.56
9:a:53:ARG:O	9:a:54:LEU:HD23	2.04	0.56
25:r:178:LEU:O	25:r:182:THR:OG1	2.16	0.56
14:f:72:ARG:HH11	15:g:19:SER:HB3	1.70	0.56
18:j:114:ALA:HB1	26:s:286:MET:HB2	1.87	0.56
20:l:332:HIS:HE1	20:l:336:LYS:NZ	2.02	0.56
25:r:210:TYR:HB2	25:r:268:GLY:HA3	1.85	0.56
7:Y:86:TYR:OH	28:v:100:LYS:HG3	2.03	0.56
11:c:153:TYR:HB3	20:l:403:TYR:HD1	1.70	0.56
17:i:237:LEU:HD13	17:i:240:LEU:HD12	1.86	0.56
20:l:51:THR:HG21	20:l:91:PRO:HG3	1.86	0.56
20:l:452:ASN:HB2	20:l:453:PRO:HD3	1.87	0.56
20:l:564:LYS:O	20:l:567:SER:OG	2.22	0.56
29:w:115:GLU:OE2	29:w:225:HIS:ND1	2.39	0.56
2:S:59:ARG:O	2:S:61:TYR:N	2.36	0.56
4:V:40:ARG:NH2	4:V:55:LYS:HD3	2.20	0.56
8:Z:51:TRP:O	8:Z:53:TYR:N	2.37	0.56
10:b:88:TYR:O	10:b:92:GLU:HB3	2.05	0.56
10:b:110:ILE:HG13	10:b:111:LEU:HD21	1.87	0.56
11:c:127:HIS:O	11:c:131:MET:HG2	2.04	0.56
17:i:230:LEU:HD11	17:i:244:ILE:HG21	1.86	0.56
19:k:7:ASN:ND2	21:m:9:SER:OG	2.31	0.56
17:i:250:SER:O	17:i:259:GLY:HA3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:452:ASN:N	20:l:453:PRO:CD	2.68	0.56
32:l:702:PEE:O4	32:l:702:PEE:H7	2.05	0.56
26:s:156:MET:HE1	26:s:177:PRO:HB2	1.88	0.56
26:s:280:PHE:O	26:s:281:ARG:HB3	2.05	0.56
4:V:62:THR:HG22	4:V:104:ARG:HE	1.69	0.56
8:Z:22:TRP:CE3	8:Z:51:TRP:HA	2.41	0.56
10:b:105:PHE:HE2	28:v:68:LYS:HA	1.70	0.56
12:d:59:HIS:ND1	13:e:120:ARG:HG2	2.21	0.56
12:d:107:CYS:HG	12:d:119:CYS:HA	1.70	0.56
24:p:30:TRP:CE2	24:p:76:HIS:HB2	2.40	0.56
26:s:190:LEU:HD22	26:s:195:ARG:HG2	1.86	0.56
27:u:35:GLN:O	27:u:37:ASP:N	2.34	0.56
6:X:99:SER:OG	6:X:102:SER:OG	2.11	0.56
7:Y:85:PRO:CG	28:v:99:MET:HE2	2.36	0.56
30:g:203:PLX:H1A2	30:g:203:PLX:H72	1.87	0.56
21:m:156:THR:O	21:m:159:THR:OG1	2.22	0.56
23:o:8:PRO:HB3	23:o:14:LEU:HG	1.88	0.56
9:a:98:LEU:CA	12:d:57:TYR:CE1	2.89	0.56
16:h:70:GLN:HG2	21:m:115:VAL:CG1	2.36	0.56
21:m:16:PHE:HA	21:m:19:PHE:CE1	2.40	0.56
24:p:56:ASP:OD1	24:p:57:MET:N	2.38	0.56
10:b:105:PHE:CE2	28:v:68:LYS:N	2.74	0.56
12:d:60:ARG:HH11	12:d:60:ARG:CG	2.12	0.56
20:l:73:THR:OG1	20:l:74:THR:N	2.39	0.56
20:l:407:TRP:NE1	20:l:411:ILE:HD11	2.21	0.56
21:m:81:ALA:HB3	21:m:84:SER:HB3	1.88	0.56
25:r:346:GLN:HB2	25:r:420:THR:HG23	1.88	0.56
27:u:44:MET:HE3	27:u:48:TRP:CZ3	2.41	0.56
28:v:40:VAL:H	28:v:61:HIS:HE1	1.53	0.56
4:V:3:PRO:HA	4:V:6:PHE:HB3	1.88	0.56
29:w:287:ASP:OD1	29:w:288:ASN:N	2.34	0.56
17:i:106:LEU:HD21	17:i:138:PRO:HB2	1.87	0.55
2:S:50:ARG:HA	16:h:105:ARG:NE	2.21	0.55
4:V:47:GLY:O	4:V:48:THR:OG1	2.25	0.55
10:b:75:VAL:O	10:b:79:VAL:HG23	2.06	0.55
30:g:201:PLX:H261	17:i:346:ILE:HG23	1.87	0.55
16:h:2:PRO:O	16:h:4:LEU:N	2.39	0.55
17:i:287:LEU:HD21	25:r:158:LEU:HD11	1.87	0.55
20:l:508:THR:O	24:p:36:LYS:NZ	2.30	0.55
25:r:164:LEU:O	25:r:167:THR:OG1	2.18	0.55
5:W:122:GLY:HA3	21:m:124:TRP:CE3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:84:TYR:HE1	12:d:43:ARG:HD3	1.71	0.55
15:g:47:ILE:HD12	17:i:327:PRO:HG3	1.88	0.55
15:g:51:PRO:HG2	15:g:55:ALA:HB2	1.87	0.55
24:p:86:PRO:HA	24:p:91:TYR:CD1	2.41	0.55
24:p:102:TRP:HZ2	25:r:422:HIS:HA	1.70	0.55
25:r:232:ALA:O	25:r:237:LYS:NZ	2.39	0.55
27:u:115:LEU:HB3	27:u:117:TRP:CZ3	2.42	0.55
1:Q:66:TRP:NE1	29:w:310:ILE:HD11	2.20	0.55
32:V:202:PEE:H60	32:V:202:PEE:C24	2.36	0.55
16:h:74:ARG:HA	21:m:116:VAL:HG21	1.89	0.55
17:i:124:LEU:HD23	17:i:176:ARG:HD3	1.88	0.55
18:j:80:GLN:NE2	26:s:316:PRO:O	2.39	0.55
20:l:456:ARG:NH2	20:l:456:ARG:HB2	2.21	0.55
21:m:16:PHE:CD1	21:m:19:PHE:HE1	2.25	0.55
4:V:40:ARG:HD3	4:V:59:TYR:CE2	2.41	0.55
18:j:92:LEU:O	18:j:96:ILE:HG12	2.06	0.55
27:u:100:CYS:SG	27:u:101:ARG:N	2.78	0.55
3:U:67:PRO:HA	3:U:74:GLN:OE1	2.07	0.55
7:Y:74:TRP:HE3	7:Y:75:HIS:CA	2.19	0.55
7:Y:81:LEU:CD1	28:v:88:ASP:HB3	2.37	0.55
9:a:59:PRO:HD3	24:p:99:VAL:HG21	1.89	0.55
10:b:83:HIS:CD2	20:l:6:THR:HG21	2.42	0.55
11:c:56:ASN:ND2	23:o:43:LEU:HD11	2.22	0.55
19:k:57:ASN:O	19:k:60:PRO:HD2	2.06	0.55
12:d:109:GLN:HG2	20:l:62:ILE:HD13	1.88	0.55
22:n:30:LYS:NZ	31:n:101:CDL:HA31	2.22	0.55
23:o:28:GLU:HA	23:o:31:ARG:HD3	1.88	0.55
26:s:117:LEU:HD12	26:s:136:VAL:HG21	1.88	0.55
21:m:138:ASP:HB2	21:m:139:PRO:HD3	1.88	0.55
25:r:403:THR:HA	25:r:406:TYR:CE2	2.42	0.55
10:b:87:LYS:HE3	12:d:43:ARG:HG2	1.89	0.55
10:b:110:ILE:HG13	10:b:111:LEU:CD2	2.37	0.55
11:c:184:TYR:O	28:v:35:LYS:O	2.25	0.55
12:d:81:GLU:OE1	22:n:43:MET:CE	2.43	0.55
12:d:134:GLN:O	12:d:138:GLN:HB2	2.06	0.55
20:l:546:GLN:O	20:l:550:LEU:HB2	2.07	0.55
25:r:73:LEU:HD12	25:r:103:GLN:HG2	1.89	0.55
7:Y:74:TRP:CE3	7:Y:74:TRP:C	2.85	0.55
17:i:288:LEU:HD21	32:l:701:PEE:H58	1.70	0.55
18:j:24:LEU:H	18:j:25:PRO:HD2	1.72	0.55
19:k:1:MET:CB	19:k:4:ILE:HD13	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:102:GLU:OE1	20:l:453:PRO:HG3	2.07	0.55
25:r:1:MET:HG3	25:r:2:LEU:H	1.71	0.55
10:b:45:LYS:HA	10:b:48:ASN:HB2	1.87	0.54
20:l:3:MET:O	20:l:7:MET:HG2	2.08	0.54
22:n:7:ILE:O	22:n:11:HIS:N	2.37	0.54
1:Q:72:PRO:O	1:Q:75:THR:OG1	2.18	0.54
10:b:105:PHE:HE2	28:v:67:LEU:C	2.15	0.54
15:g:44:ASP:OD2	15:g:63:TYR:OH	2.16	0.54
20:l:238:GLU:N	20:l:238:GLU:OE1	2.40	0.54
20:l:452:ASN:N	20:l:452:ASN:OD1	2.36	0.54
21:m:48:GLY:HA2	21:m:138:ASP:OD2	2.08	0.54
25:r:91:ARG:HG2	25:r:136:TRP:HH2	1.72	0.54
12:d:114:ASN:OD1	28:v:50:GLN:HG2	2.07	0.54
17:i:17:THR:OG1	17:i:36:ASN:ND2	2.39	0.54
17:i:167:TRP:HH2	20:l:570:GLN:HG3	1.70	0.54
25:r:358:TRP:CE3	25:r:441:LEU:HD12	2.42	0.54
6:X:84:LEU:HD11	6:X:100:VAL:HG22	1.87	0.54
12:d:115:TYR:CD1	12:d:115:TYR:C	2.85	0.54
20:l:190:ILE:O	20:l:194:ASN:HA	2.08	0.54
15:g:46:LEU:HD11	17:i:239:TRP:HB3	1.88	0.54
21:m:155:VAL:O	21:m:159:THR:HG23	2.08	0.54
25:r:236:LEU:O	25:r:239:GLY:N	2.40	0.54
25:r:317:ILE:HD12	25:r:454:ILE:HG23	1.88	0.54
7:Y:96:GLU:O	7:Y:97:LEU:CB	2.55	0.54
7:Y:96:GLU:O	7:Y:97:LEU:CD2	2.54	0.54
20:l:293:LEU:HD23	20:l:422:TYR:HB3	1.90	0.54
26:s:145:THR:HG21	26:s:289:LEU:HD22	1.90	0.54
7:Y:81:LEU:HD22	28:v:92:HIS:HD2	1.70	0.54
9:a:133:TYR:OH	12:d:81:GLU:HG2	2.08	0.54
21:m:32:LEU:HD13	21:m:64:MET:HE1	1.88	0.54
29:w:206:TYR:OH	29:w:238:GLU:OE2	2.25	0.54
5:W:81:ARG:HH2	27:u:64:ASN:HD21	1.56	0.54
19:k:87:LEU:HD11	21:m:73:MET:O	2.08	0.54
20:l:95:PHE:CD1	20:l:95:PHE:C	2.86	0.54
20:l:197:ASP:O	20:l:201:MET:HG3	2.08	0.54
21:m:16:PHE:HD1	21:m:19:PHE:HE1	1.54	0.54
29:w:128:SER:O	29:w:131:LEU:HG	2.08	0.54
2:S:12:MET:HE1	26:s:20:LEU:HD12	1.90	0.54
9:a:54:LEU:HD23	10:b:27:GLU:HA	1.89	0.54
20:l:98:TRP:CD1	20:l:98:TRP:C	2.86	0.54
29:w:61:THR:HG22	29:w:159:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:69:VAL:HG12	1:Q:72:PRO:HD2	1.90	0.53
13:e:74:HIS:ND1	13:e:87:MET:HG3	2.23	0.53
1:Q:43:TRP:HZ3	17:i:305:LEU:HD21	1.74	0.53
17:i:217:LEU:HB3	17:i:326:LEU:HD12	1.89	0.53
18:j:104:TYR:CG	21:m:165:TYR:HE1	2.26	0.53
9:a:98:LEU:HB3	12:d:57:TYR:HE1	0.54	0.53
11:c:84:HIS:CD2	11:c:118:ASP:HB3	2.43	0.53
24:p:102:TRP:NE1	25:r:426:MET:HE1	2.23	0.53
26:s:127:TYR:HA	26:s:130:ILE:HD12	1.89	0.53
32:W:201:PEE:C3	26:s:98:LEU:HD22	2.38	0.53
8:Z:24:ILE:HG22	8:Z:30:GLU:HB2	1.90	0.53
10:b:78:PRO:O	10:b:82:ILE:HD12	2.08	0.53
16:h:48:GLY:O	16:h:50:THR:N	2.37	0.53
20:l:525:MET:HE2	24:p:77:PRO:HB3	1.90	0.53
25:r:414:THR:O	25:r:415:GLN:NE2	2.41	0.53
2:S:28:ARG:NH1	27:u:91:TYR:OH	2.42	0.53
32:V:202:PEE:C24	32:V:202:PEE:H57	2.39	0.53
9:a:98:LEU:CA	12:d:57:TYR:CD1	2.91	0.53
19:k:66:PHE:CE1	21:m:159:THR:HG21	2.40	0.53
20:l:51:THR:CG2	20:l:91:PRO:HG2	2.30	0.53
20:l:282:ALA:O	20:l:285:THR:OG1	2.27	0.53
27:u:83:THR:O	27:u:86:TRP:HB3	2.08	0.53
29:w:138:SER:O	29:w:142:GLN:HG2	2.07	0.53
29:w:149:HIS:CE1	29:w:155:GLN:HB3	2.43	0.53
9:a:112:TYR:HD1	12:d:58:TYR:O	1.92	0.53
26:s:32:GLN:HB3	26:s:34:ARG:HG2	1.91	0.53
26:s:126:ASN:HA	26:s:129:LEU:HD12	1.91	0.53
26:s:195:ARG:NH1	26:s:270:PHE:HB3	2.24	0.53
6:X:93:ILE:HG21	6:X:98:LEU:HD12	1.91	0.53
10:b:110:ILE:N	12:d:17:THR:O	2.41	0.53
17:i:311:VAL:HG12	17:i:315:TRP:HE1	1.74	0.53
29:w:137:SER:O	29:w:139:ARG:N	2.37	0.53
10:b:95:TYR:HE2	12:d:10:TYR:CD1	2.27	0.53
16:h:99:ILE:HD12	16:h:101:LYS:HD2	1.91	0.53
17:i:291:TYR:HB2	25:r:151:PHE:CZ	2.44	0.53
19:k:11:ALA:HB1	21:m:16:PHE:HD2	1.71	0.53
20:l:293:LEU:HD11	20:l:418:LEU:HD22	1.90	0.53
25:r:73:LEU:O	25:r:76:THR:OG1	2.18	0.53
25:r:272:THR:HA	25:r:275:ILE:HD12	1.90	0.53
3:U:69:HIS:ND1	3:U:70:PRO:HA	2.24	0.53
7:Y:84:PHE:CE2	20:l:483:PRO:CG	2.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:105:PHE:HE2	28:v:68:LYS:CA	2.19	0.53
25:r:286:ILE:O	25:r:289:SER:OG	2.23	0.53
7:Y:71:TRP:CE3	7:Y:71:TRP:C	2.87	0.53
16:h:40:TRP:HH2	17:i:83:GLN:HE21	1.57	0.53
17:i:300:THR:OG1	17:i:301:SER:N	2.38	0.53
19:k:62:VAL:HG21	21:m:152:LEU:HD21	1.91	0.53
21:m:19:PHE:CZ	21:m:32:LEU:HD21	2.43	0.53
2:S:54:ILE:HG13	16:h:105:ARG:HH11	1.72	0.52
10:b:105:PHE:HD2	28:v:68:LYS:HG3	1.74	0.52
17:i:229:LEU:HD22	17:i:232:ARG:NH1	2.24	0.52
19:k:7:ASN:OD1	21:m:13:VAL:CG2	2.57	0.52
19:k:15:SER:OG	19:k:36:MET:HG2	2.08	0.52
12:d:57:TYR:HD1	12:d:57:TYR:O	1.91	0.52
12:d:73:GLU:HG3	15:g:106:LYS:O	2.08	0.52
19:k:58:ILE:HG23	21:m:145:LEU:HD12	1.92	0.52
21:m:23:PRO:O	21:m:24:SER:OG	2.23	0.52
30:r:501:PLX:H262	30:r:501:PLX:H6	1.91	0.52
28:v:56:ARG:O	28:v:60:ALA:HB2	2.10	0.52
2:S:12:MET:CE	26:s:20:LEU:HD12	2.39	0.52
11:c:101:TRP:NE1	23:o:61:GLU:O	2.43	0.52
18:j:24:LEU:H	18:j:25:PRO:CD	2.22	0.52
20:l:144:TRP:NE1	20:l:179:ASP:OD1	2.42	0.52
9:a:90:ASN:ND2	30:b:201:PLX:H122	2.19	0.52
12:d:57:TYR:CD1	12:d:57:TYR:C	2.85	0.52
19:k:4:ILE:O	19:k:8:ILE:HD13	2.09	0.52
20:l:106:TRP:HB2	20:l:449:THR:OG1	2.09	0.52
20:l:195:SER:O	20:l:196:TRP:HB2	2.08	0.52
20:l:566:ILE:HA	20:l:569:HIS:HD2	1.73	0.52
22:n:40:ASN:ND2	22:n:56:THR:HG23	2.25	0.52
25:r:131:ALA:O	25:r:135:ARG:HB3	2.09	0.52
29:w:58:ARG:HB3	29:w:202:HIS:CE1	2.44	0.52
4:V:124:LEU:HD23	4:V:127:MET:HE3	1.91	0.52
7:Y:61:PHE:CE2	20:l:455:LYS:HG2	2.44	0.52
15:g:27:ASP:OD1	27:u:172:LYS:NZ	2.42	0.52
17:i:239:TRP:HA	31:i:401:CDL:HB32	1.91	0.52
20:l:194:ASN:HD22	23:o:127:LEU:HD12	1.74	0.52
21:m:36:GLY:HA3	21:m:60:LEU:HD21	1.90	0.52
21:m:50:TYR:O	21:m:54:MET:HG2	2.10	0.52
21:m:106:VAL:HG11	21:m:117:ASN:HD22	1.75	0.52
27:u:24:VAL:HG13	27:u:86:TRP:CD1	2.45	0.52
1:Q:66:TRP:CE2	29:w:310:ILE:HD11	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:b:22:TRP:O	10:b:25:ASP:HB3	2.10	0.52
10:b:105:PHE:CD2	28:v:68:LYS:CB	2.93	0.52
12:d:110:ARG:NH1	12:d:110:ARG:CG	2.73	0.52
17:i:285:ILE:CG1	32:l:701:PEE:H75	2.25	0.52
20:l:59:GLN:HE21	20:l:59:GLN:CA	2.09	0.52
26:s:13:ILE:HG23	26:s:17:MET:HE3	1.92	0.52
26:s:139:THR:O	26:s:143:GLU:HG3	2.09	0.52
27:u:111:VAL:HG12	27:u:117:TRP:O	2.09	0.52
29:w:294:LEU:O	29:w:298:VAL:HG23	2.09	0.52
1:Q:39:PRO:HB3	1:Q:43:TRP:CE3	2.45	0.52
5:W:33:TYR:CG	5:W:34:SER:N	2.77	0.52
5:W:35:MET:HA	5:W:38:ILE:HD12	1.91	0.52
7:Y:73:PHE:CD1	7:Y:73:PHE:C	2.88	0.52
21:m:130:GLU:HG2	21:m:131:GLY:O	2.10	0.52
25:r:187:SER:O	25:r:192:ASN:ND2	2.43	0.52
2:S:37:ARG:O	5:W:143:TYR:OH	2.27	0.52
4:V:58:GLN:O	4:V:62:THR:HG23	2.10	0.52
9:a:129:PRO:HG2	12:d:60:ARG:HH22	1.74	0.52
11:c:69:GLY:CA	23:o:81:ARG:H	2.23	0.52
17:i:222:ASN:HD21	17:i:233:THR:HG22	1.75	0.52
25:r:20:LYS:HA	25:r:89:LEU:HD13	1.92	0.52
29:w:198:TYR:OH	29:w:304:VAL:HG12	2.10	0.52
1:Q:55:SER:OG	20:l:580:GLN:NE2	2.42	0.52
2:S:34:LYS:NZ	27:u:90:ASP:HB3	2.25	0.52
10:b:39:LYS:HG3	10:b:41:GLY:H	1.74	0.52
10:b:105:PHE:CD2	28:v:68:LYS:HB2	2.45	0.52
12:d:110:ARG:HH11	12:d:110:ARG:CG	2.14	0.52
18:j:18:MET:SD	26:s:72:ILE:HA	2.50	0.52
20:l:190:ILE:CG1	20:l:196:TRP:CD1	2.93	0.52
20:l:190:ILE:CG1	20:l:196:TRP:NE1	2.73	0.52
9:a:153:GLU:OE2	27:u:166:ARG:NH1	2.33	0.52
17:i:336:LEU:HD21	17:i:343:MET:SD	2.50	0.52
20:l:244:SER:HA	20:l:248:HIS:HD2	1.73	0.52
20:l:371:THR:O	20:l:374:THR:OG1	2.28	0.52
25:r:5:ILE:O	25:r:8:THR:OG1	2.26	0.52
25:r:130:LEU:HD11	25:r:150:LEU:HD12	1.92	0.52
26:s:173:TRP:CZ3	26:s:262:LYS:HE2	2.45	0.52
27:u:31:HIS:CE1	27:u:111:VAL:HG11	2.44	0.52
3:U:84:LEU:O	5:W:59:ARG:NH1	2.41	0.51
18:j:70:ALA:HB1	21:m:58:ILE:HD11	1.92	0.51
30:r:502:PLX:C7	30:r:502:PLX:C3	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:17:MET:CE	26:s:232:ILE:HD12	2.38	0.51
9:a:87:THR:CG2	30:b:201:PLX:H131	2.40	0.51
10:b:105:PHE:HZ	28:v:67:LEU:CB	2.23	0.51
30:b:201:PLX:O3	30:b:201:PLX:H72	2.10	0.51
12:d:135:ASP:C	12:d:156:ARG:HH21	2.18	0.51
4:V:12:ILE:HG22	4:V:13:PRO:O	2.11	0.51
11:c:159:LYS:HA	28:v:98:ARG:NH1	2.24	0.51
17:i:137:ALA:HB3	17:i:138:PRO:HD3	1.93	0.51
20:l:135:ASN:OD1	20:l:198:PRO:CG	2.57	0.51
20:l:332:HIS:CE1	20:l:336:LYS:HG3	2.46	0.51
20:l:592:PHE:CE2	20:l:596:ILE:HD11	2.45	0.51
29:w:98:THR:HG23	29:w:337:ARG:NH2	2.25	0.51
19:k:7:ASN:OD1	21:m:13:VAL:HG23	2.10	0.51
20:l:226:GLN:HG2	20:l:280:LEU:HD21	1.85	0.51
20:l:567:SER:O	20:l:571:ILE:HD13	2.09	0.51
21:m:27:TYR:HB3	21:m:82:TRP:CZ2	2.45	0.51
25:r:145:ALA:HA	25:r:148:TYR:HB3	1.91	0.51
12:d:76:ILE:O	12:d:80:TYR:N	2.40	0.51
17:i:37:MET:HE3	17:i:41:ILE:HD11	1.93	0.51
20:l:227:LEU:HD12	20:l:227:LEU:C	2.35	0.51
20:l:419:THR:HA	20:l:422:TYR:CE2	2.45	0.51
21:m:114:VAL:O	21:m:115:VAL:HG13	2.11	0.51
6:X:77:GLU:HB2	8:Z:13:LYS:HE2	1.93	0.51
9:a:160:MET:HE2	9:a:168:TRP:HB2	1.92	0.51
10:b:108:ASP:O	10:b:109:THR:HB	2.10	0.51
13:e:87:MET:HE1	25:r:431:THR:HG21	1.92	0.51
20:l:119:LYS:O	20:l:123:ILE:HG12	2.11	0.51
20:l:485:TYR:O	20:l:489:THR:HG23	2.10	0.51
20:l:563:PRO:HG3	25:r:148:TYR:OH	2.10	0.51
25:r:281:ASP:HB2	25:r:284:SER:OG	2.10	0.51
27:u:142:TYR:O	27:u:144:SER:N	2.44	0.51
29:w:54:THR:C	29:w:56:ARG:H	2.19	0.51
29:w:115:GLU:HA	29:w:118:TYR:HD2	1.76	0.51
1:Q:72:PRO:HB2	17:i:50:PRO:HG3	1.91	0.51
17:i:128:LEU:HD11	17:i:213:THR:HG22	1.92	0.51
20:l:87:MET:O	20:l:91:PRO:HD3	2.11	0.51
23:o:17:THR:O	23:o:23:TYR:OH	2.21	0.51
29:w:128:SER:OG	29:w:173:MET:SD	2.69	0.51
6:X:155:TYR:CD1	10:b:23:LEU:HB3	2.46	0.51
13:e:56:GLN:HG2	29:w:320:GLY:HA3	1.93	0.51
19:k:8:ILE:CD1	19:k:8:ILE:N	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:343:SER:O	20:l:347:ILE:HD12	2.11	0.51
20:l:593:PHE:HB2	20:l:594:PRO:HD3	1.93	0.51
26:s:154:LEU:HD13	26:s:160:PHE:CD1	2.46	0.51
7:Y:86:TYR:HB3	7:Y:87:PRO:HB3	1.93	0.51
10:b:19:ARG:NH2	24:p:173:ARG:HB2	2.26	0.51
10:b:86:MET:HA	10:b:89:HIS:HB3	1.92	0.51
12:d:111:GLU:HB3	12:d:115:TYR:CB	2.41	0.51
30:g:202:PLX:H1C2	30:g:202:PLX:H31	1.93	0.51
25:r:104:ILE:O	25:r:108:MET:HG2	2.10	0.51
26:s:223:PHE:O	26:s:227:GLU:HG3	2.11	0.51
3:U:58:ARG:NH2	27:u:49:GLU:OE1	2.43	0.51
6:X:85:TYR:HE2	7:Y:45:ARG:NH1	2.09	0.51
10:b:92:GLU:HG2	10:b:93:LYS:HG3	1.93	0.51
10:b:113:THR:OG1	10:b:114:GLY:N	2.44	0.51
16:h:99:ILE:HD12	16:h:101:LYS:HB2	1.93	0.51
17:i:234:TRP:O	17:i:238:THR:HG22	2.11	0.51
17:i:243:LEU:HD21	31:i:401:CDL:H752	1.92	0.51
17:i:268:GLU:OE2	27:u:168:TYR:OH	2.24	0.51
18:j:65:PHE:HA	18:j:68:GLU:HB2	1.93	0.51
24:p:104:LEU:HD21	24:p:119:PHE:CE1	2.41	0.51
25:r:271:MET:O	25:r:275:ILE:HG13	2.11	0.51
29:w:121:PRO:HG2	29:w:178:PHE:HB3	1.93	0.51
2:S:24:ALA:HA	26:s:93:ASN:HD22	1.76	0.50
30:V:203:PLX:H151	23:o:91:ALA:HB2	1.93	0.50
30:b:201:PLX:H21	12:d:43:ARG:HH22	1.77	0.50
15:g:29:ARG:HH21	27:u:172:LYS:HB3	1.76	0.50
16:h:80:ARG:NH1	21:m:121:VAL:HG22	2.26	0.50
17:i:139:ILE:HD11	17:i:187:MET:HE1	1.92	0.50
20:l:42:SER:O	20:l:46:ILE:HG12	2.12	0.50
21:m:67:PHE:O	21:m:71:THR:HG23	2.11	0.50
25:r:144:ASN:OD1	25:r:145:ALA:N	2.45	0.50
14:f:55:TRP:CE2	15:g:65:THR:HG22	2.46	0.50
16:h:6:ILE:HB	17:i:22:LEU:HD22	1.93	0.50
19:k:81:ILE:HG22	19:k:87:LEU:HA	1.92	0.50
25:r:120:ILE:O	25:r:124:THR:HG23	2.11	0.50
29:w:218:ILE:HD11	29:w:226:GLU:HB3	1.93	0.50
8:Z:29:LEU:HD23	24:p:35:ASP:OD1	2.12	0.50
9:a:184:LYS:O	9:a:186:THR:N	2.45	0.50
12:d:156:ARG:NH1	13:e:139:SER:O	2.37	0.50
20:l:15:LEU:O	20:l:18:PRO:HD2	2.11	0.50
20:l:428:LEU:HD23	20:l:432:THR:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:r:134:THR:O	25:r:142:ARG:NE	2.33	0.50
25:r:423:ILE:HD12	25:r:425:ASN:H	1.76	0.50
7:Y:51:THR:HG21	20:l:446:ASN:HD21	1.76	0.50
14:f:47:THR:HG22	30:g:203:PLX:H1A1	1.94	0.50
17:i:150:ASN:HD21	20:l:602:ILE:HD13	1.77	0.50
20:l:68:TRP:HB2	20:l:76:LEU:CD1	2.41	0.50
22:n:50:GLN:OE1	22:n:51:PRO:HD2	2.11	0.50
30:r:502:PLX:C33	30:r:502:PLX:C37	2.85	0.50
26:s:303:TRP:NE1	26:s:307:MET:SD	2.85	0.50
28:v:5:LEU:O	28:v:8:ARG:HG2	2.11	0.50
29:w:139:ARG:HD2	29:w:166:ASP:OD2	2.12	0.50
30:V:203:PLX:H201	23:o:95:PHE:CZ	2.47	0.50
9:a:54:LEU:CD2	10:b:27:GLU:CA	2.89	0.50
13:e:112:TYR:O	25:r:45:ILE:HG23	2.11	0.50
16:h:101:LYS:C	16:h:104:PRO:HD2	2.37	0.50
17:i:98:ILE:O	17:i:102:MET:HG2	2.12	0.50
17:i:315:TRP:HZ3	29:w:327:VAL:HG12	1.76	0.50
20:l:136:ASN:OD1	20:l:137:LEU:N	2.44	0.50
20:l:594:PRO:O	20:l:598:THR:HG23	2.12	0.50
24:p:170:ILE:O	24:p:173:ARG:HG3	2.11	0.50
26:s:230:ASN:O	26:s:234:MET:HG2	2.11	0.50
6:X:88:LYS:HZ1	6:X:98:LEU:HD22	1.76	0.50
7:Y:86:TYR:HB3	7:Y:87:PRO:CB	2.40	0.50
12:d:60:ARG:NH1	12:d:60:ARG:CG	2.73	0.50
14:f:30:TYR:HD2	29:w:98:THR:HA	1.77	0.50
17:i:244:ILE:HB	17:i:245:PRO:HD3	1.93	0.50
17:i:309:ASN:OD1	29:w:319:ILE:HD11	2.11	0.50
23:o:6:TYR:OH	23:o:12:ARG:HG2	2.12	0.50
25:r:355:MET:HA	25:r:358:TRP:HD1	1.77	0.50
29:w:248:GLU:OE1	29:w:252:LYS:NZ	2.45	0.50
29:w:331:PHE:CZ	29:w:337:ARG:HB3	2.46	0.50
10:b:89:HIS:C	10:b:89:HIS:CD2	2.90	0.50
20:l:44:PHE:O	20:l:47:SER:OG	2.24	0.50
20:l:49:PHE:O	20:l:52:THR:OG1	2.22	0.50
20:l:306:THR:HA	20:l:336:LYS:NZ	2.27	0.50
26:s:180:PRO:O	26:s:184:MET:HG2	2.11	0.50
1:Q:65:PRO:HG2	1:Q:69:VAL:HG22	1.94	0.50
20:l:190:ILE:CD1	20:l:196:TRP:NE1	2.73	0.50
25:r:220:HIS:HE1	25:r:232:ALA:HB2	1.77	0.50
6:X:103:HIS:HB2	6:X:106:LYS:HB3	1.94	0.50
11:c:69:GLY:HA3	23:o:81:ARG:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:l:70:THR:HG23	20:l:75:GLN:HB3	1.94	0.50
20:l:74:THR:HG23	20:l:194:ASN:OD1	2.08	0.50
31:n:101:CDL:HB62	27:u:172:LYS:HB2	1.93	0.50
26:s:167:THR:C	26:s:169:GLN:H	2.18	0.50
26:s:203:GLY:O	26:s:205:SER:N	2.43	0.50
28:v:39:MET:SD	28:v:58:TYR:HD1	2.34	0.50
9:a:99:ALA:O	12:d:58:TYR:HD1	1.95	0.49
10:b:77:VAL:HB	10:b:78:PRO:HD3	1.94	0.49
11:c:55:TYR:OH	11:c:74:ASP:OD2	2.24	0.49
15:g:38:TYR:CE2	15:g:42:LEU:HD11	2.47	0.49
20:l:188:TRP:CD2	20:l:212:PRO:HG3	2.47	0.49
20:l:332:HIS:HA	20:l:335:PHE:CE2	2.46	0.49
20:l:566:ILE:HA	20:l:569:HIS:CD2	2.47	0.49
26:s:9:LEU:HD13	26:s:95:LEU:HD12	1.94	0.49
26:s:195:ARG:HG3	26:s:197:PRO:HD2	1.93	0.49
29:w:57:SER:OG	29:w:154:GLY:O	2.28	0.49
32:V:202:PEE:H40	32:V:202:PEE:C35	2.42	0.49
10:b:33:PRO:HD2	24:p:114:MET:O	2.12	0.49
10:b:61:VAL:HA	10:b:64:VAL:HG12	1.93	0.49
15:g:4:ARG:NH1	15:g:6:ASN:HB3	2.28	0.49
18:j:109:LYS:HA	18:j:112:ASP:HB2	1.94	0.49
21:m:33:ILE:HA	21:m:60:LEU:HD22	1.94	0.49
29:w:149:HIS:HE1	29:w:155:GLN:HB3	1.76	0.49
29:w:335:PRO:HA	29:w:338:LYS:HG3	1.94	0.49
11:c:111:MET:HG3	25:r:278:ARG:HH12	1.77	0.49
17:i:9:ILE:O	17:i:12:THR:OG1	2.30	0.49
17:i:329:LEU:O	17:i:333:THR:HG23	2.11	0.49
1:Q:79:ASN:ND2	19:k:82:SER:O	2.45	0.49
9:a:115:HIS:HE1	9:a:117:ILE:HD12	1.77	0.49
15:g:27:ASP:OD1	15:g:28:PRO:HD2	2.13	0.49
17:i:234:TRP:C	17:i:238:THR:HG22	2.37	0.49
18:j:28:ASN:HB2	18:j:30:TYR:CZ	2.47	0.49
20:l:450:LEU:C	20:l:450:LEU:CD2	2.85	0.49
23:o:8:PRO:HD3	23:o:14:LEU:HD21	1.95	0.49
24:p:167:TRP:CE3	24:p:171:VAL:HG21	2.32	0.49
29:w:305:LEU:O	29:w:308:THR:HG22	2.12	0.49
10:b:13:GLN:O	10:b:17:GLU:HG2	2.12	0.49
20:l:189:PHE:CD1	20:l:201:MET:HE3	2.48	0.49
4:V:62:THR:HG22	4:V:104:ARG:NE	2.27	0.49
5:W:101:VAL:HG21	16:h:82:GLN:NE2	2.28	0.49
6:X:90:TYR:HD2	6:X:93:ILE:HD12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:108:HIS:HE1	20:l:546:GLN:HG2	1.77	0.49
17:i:232:ARG:NH2	29:w:306:ASN:OD1	2.29	0.49
19:k:60:PRO:O	19:k:63:MET:HB2	2.12	0.49
32:l:701:PEE:C23	25:r:155:VAL:HB	2.29	0.49
21:m:130:GLU:OE1	21:m:130:GLU:N	2.39	0.49
26:s:141:SER:HB2	26:s:290:TRP:HE1	1.77	0.49
26:s:228:TYR:CD1	26:s:231:ILE:HD12	2.43	0.49
27:u:131:VAL:HG12	27:u:133:THR:HG23	1.95	0.49
4:V:39:TYR:HD2	31:V:201:CDL:H721	1.76	0.49
7:Y:78:GLU:HG2	20:l:385:PHE:HE1	1.78	0.49
7:Y:86:TYR:HH	28:v:100:LYS:HG2	1.78	0.49
9:a:101:ILE:HG13	12:d:58:TYR:HB3	1.94	0.49
11:c:52:ALA:CB	11:c:59:VAL:HA	2.42	0.49
15:g:29:ARG:NH2	27:u:172:LYS:HD2	2.28	0.49
20:l:75:GLN:HG2	20:l:75:GLN:O	2.13	0.49
20:l:286:LEU:HB2	20:l:411:ILE:HG23	1.95	0.49
21:m:22:LYS:N	21:m:23:PRO:HD3	2.28	0.49
24:p:136:GLU:HG2	24:p:165:PRO:HA	1.94	0.49
26:s:79:LEU:HD11	26:s:222:LEU:HD22	1.94	0.49
7:Y:44:TYR:HD1	20:l:440:LEU:HB2	1.78	0.49
17:i:41:ILE:HD11	17:i:60:PHE:HD1	1.78	0.49
20:l:100:ILE:HD12	20:l:246:LEU:CG	2.39	0.49
21:m:118:PHE:HZ	21:m:124:TRP:HZ2	1.61	0.49
25:r:113:THR:O	25:r:176:ILE:HG13	2.12	0.49
32:V:202:PEE:H41	32:V:202:PEE:C37	2.40	0.49
6:X:76:LEU:HD12	6:X:156:GLU:HB2	1.94	0.49
11:c:111:MET:HG3	25:r:278:ARG:NH1	2.27	0.49
20:l:47:SER:O	20:l:50:PRO:HD2	2.12	0.49
20:l:51:THR:CG2	20:l:91:PRO:CG	2.84	0.49
20:l:386:LEU:HD12	20:l:387:THR:N	2.28	0.49
25:r:220:HIS:CE1	25:r:232:ALA:HB2	2.47	0.49
28:v:113:LYS:HA	28:v:116:GLU:OE1	2.13	0.49
29:w:217:ARG:HA	29:w:220:LYS:HD2	1.95	0.49
17:i:334:THR:OG1	17:i:335:LEU:N	2.45	0.49
17:i:337:LEU:O	17:i:339:ILE:N	2.46	0.49
20:l:119:LYS:HD2	31:l:703:CDL:HB32	1.95	0.49
4:V:62:THR:HG22	4:V:104:ARG:HD3	1.95	0.48
15:g:38:TYR:O	15:g:42:LEU:HG	2.13	0.48
16:h:32:ARG:NH2	19:k:50:ASN:O	2.42	0.48
19:k:81:ILE:CG2	19:k:87:LEU:HA	2.43	0.48
25:r:18:SER:OG	25:r:23:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:r:502:PLX:H52	30:r:502:PLX:P1	2.53	0.48
26:s:73:THR:O	26:s:76:THR:OG1	2.20	0.48
28:v:41:ALA:O	28:v:42:THR:OG1	2.31	0.48
29:w:242:LYS:HA	29:w:246:LEU:HG	1.95	0.48
29:w:323:GLN:O	29:w:326:ARG:HB3	2.13	0.48
8:Z:28:PRO:O	8:Z:31:THR:OG1	2.22	0.48
17:i:18:LEU:O	17:i:22:LEU:HG	2.14	0.48
20:l:347:ILE:HG12	20:l:354:GLN:HG2	1.95	0.48
20:l:383:MET:SD	20:l:384:PRO:HD2	2.52	0.48
22:n:55:VAL:HG12	22:n:56:THR:N	2.24	0.48
26:s:106:LEU:HD21	26:s:150:LEU:HD12	1.94	0.48
2:S:50:ARG:CZ	2:S:54:ILE:HD11	2.43	0.48
3:U:58:ARG:HH12	27:u:137:LEU:N	2.10	0.48
5:W:141:MET:SD	21:m:47:GLY:HA2	2.53	0.48
9:a:54:LEU:HD21	10:b:27:GLU:HA	1.91	0.48
9:a:114:LYS:CA	12:d:57:TYR:CD2	2.97	0.48
10:b:39:LYS:O	10:b:42:PRO:HD2	2.13	0.48
15:g:119:ARG:HD3	23:o:116:ILE:HD13	1.96	0.48
17:i:59:TYR:CZ	17:i:63:GLN:OE1	2.67	0.48
17:i:115:VAL:HG12	17:i:180:ALA:HB1	1.95	0.48
31:l:704:CDL:OA9	31:l:704:CDL:O1	2.19	0.48
29:w:109:ASN:HD21	29:w:111:ASN:HD22	1.61	0.48
4:V:29:ALA:O	4:V:63:ALA:HB1	2.14	0.48
5:W:47:HIS:O	5:W:51:MET:HG3	2.13	0.48
13:e:107:ALA:O	30:r:502:PLX:H1B3	2.13	0.48
17:i:326:LEU:HB3	17:i:327:PRO:HD3	1.95	0.48
20:l:37:LYS:HZ3	20:l:98:TRP:CD1	2.31	0.48
20:l:173:LEU:HD21	25:r:405:LEU:HD21	1.96	0.48
2:S:28:ARG:O	2:S:33:GLY:N	2.47	0.48
2:S:53:ARG:HH21	16:h:105:ARG:HD3	1.77	0.48
20:l:224:SER:OG	20:l:256:GLY:CA	2.59	0.48
25:r:61:LEU:HD22	25:r:241:TYR:CD1	2.45	0.48
25:r:188:ASN:CG	25:r:189:SER:H	2.21	0.48
26:s:226:ALA:O	26:s:230:ASN:ND2	2.40	0.48
29:w:139:ARG:HH12	29:w:160:GLU:CD	2.21	0.48
29:w:335:PRO:HA	29:w:338:LYS:NZ	2.29	0.48
9:a:55:PHE:CE2	24:p:118:TYR:CG	2.82	0.48
9:a:160:MET:HE3	9:a:166:GLY:HA3	1.96	0.48
17:i:117:GLU:OE1	17:i:117:GLU:N	2.41	0.48
17:i:282:MET:O	17:i:286:THR:HG23	2.14	0.48
20:l:302:VAL:O	20:l:305:SER:OG	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:34:ILE:HG13	12:d:35:VAL:HG13	1.95	0.48
17:i:106:LEU:HB3	17:i:187:MET:HE2	1.95	0.48
17:i:128:LEU:HD13	17:i:216:PHE:HD2	1.78	0.48
18:j:54:LYS:HB3	18:j:113:TRP:NE1	2.29	0.48
5:W:30:LEU:HB2	5:W:32:GLY:H	1.78	0.48
17:i:37:MET:CE	17:i:60:PHE:HA	2.44	0.48
20:l:591:PHE:O	20:l:594:PRO:HD2	2.13	0.48
25:r:1:MET:HG3	25:r:2:LEU:N	2.29	0.48
25:r:127:ILE:HB	25:r:128:PRO:HD3	1.94	0.48
27:u:24:VAL:HG22	27:u:86:TRP:HE1	1.76	0.48
3:U:52:ASN:HD21	16:h:27:TYR:C	2.20	0.48
6:X:102:SER:O	6:X:140:CYS:HA	2.14	0.48
9:a:95:GLN:OE1	9:a:114:LYS:NZ	2.46	0.48
10:b:108:ASP:CG	10:b:109:THR:H	2.20	0.48
7:Y:41:GLU:HG2	20:l:442:ASN:HB2	1.96	0.48
16:h:91:LYS:HG3	16:h:92:TYR:N	2.28	0.48
17:i:288:LEU:HD22	32:l:701:PEE:H58	1.69	0.48
20:l:213:LEU:HB3	20:l:273:ILE:HD13	1.96	0.48
23:o:73:THR:OG1	23:o:74:ILE:N	2.47	0.48
25:r:94:LEU:O	25:r:97:SER:OG	2.21	0.48
26:s:42:PRO:HD2	26:s:45:LEU:HD12	1.95	0.48
26:s:205:SER:OG	26:s:279:ARG:NH1	2.47	0.48
29:w:258:TYR:CE1	29:w:267:LYS:HA	2.49	0.48
32:W:201:PEE:N	32:W:201:PEE:P	2.87	0.47
10:b:109:THR:HG22	10:b:111:LEU:H	1.79	0.47
30:b:201:PLX:H111	30:b:201:PLX:C7	2.43	0.47
17:i:149:LEU:HD23	17:i:154:LEU:HD13	1.96	0.47
17:i:237:LEU:HD22	17:i:240:LEU:HD12	1.96	0.47
18:j:67:LEU:HD23	19:k:65:VAL:HG13	1.95	0.47
19:k:97:GLN:HG2	20:l:587:TYR:OH	2.13	0.47
20:l:19:ILE:HD11	20:l:126:ILE:HD11	1.96	0.47
25:r:44:GLN:O	25:r:46:ASN:ND2	2.47	0.47
25:r:132:ILE:O	25:r:136:TRP:HB2	2.14	0.47
27:u:85:TYR:OH	27:u:104:GLN:NE2	2.44	0.47
4:V:37:ALA:HB1	4:V:56:VAL:HG22	1.95	0.47
4:V:40:ARG:HG3	31:V:201:CDL:HB22	1.97	0.47
31:V:201:CDL:H552	31:V:201:CDL:H522	1.70	0.47
9:a:114:LYS:N	12:d:57:TYR:HD2	2.12	0.47
30:b:201:PLX:O7	30:b:201:PLX:H31	2.13	0.47
15:g:20:LEU:HD21	27:u:158:LEU:HB3	1.96	0.47
17:i:198:PRO:O	17:i:201:THR:OG1	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:l:701:PEE:H65	32:l:701:PEE:H71	1.79	0.47
24:p:157:ALA:HB2	24:p:164:PRO:N	2.30	0.47
2:S:21:LEU:HD21	26:s:253:GLU:HA	1.96	0.47
2:S:53:ARG:HB2	16:h:105:ARG:NH2	2.30	0.47
6:X:80:GLN:HG3	6:X:145:VAL:HG11	1.95	0.47
9:a:126:TYR:OH	13:e:109:LEU:HD22	2.14	0.47
10:b:105:PHE:CZ	28:v:67:LEU:CB	2.96	0.47
30:b:201:PLX:H171	30:b:201:PLX:H141	1.68	0.47
11:c:38:PRO:HG2	23:o:71:ALA:HB2	1.95	0.47
12:d:18:PRO:HG2	28:v:71:ARG:NH1	2.29	0.47
12:d:20:GLN:OE1	28:v:71:ARG:NH1	2.48	0.47
13:e:89:LEU:HD13	25:r:29:THR:HG21	1.95	0.47
17:i:17:THR:HG23	17:i:137:ALA:HB2	1.96	0.47
17:i:135:LYS:O	17:i:139:ILE:HG12	2.14	0.47
20:l:233:LEU:HB3	20:l:234:PRO:HD3	1.96	0.47
20:l:360:GLY:HA3	20:l:435:PRO:HA	1.96	0.47
20:l:549:PRO:HG3	25:r:271:MET:HE3	1.96	0.47
29:w:332:ARG:HA	29:w:332:ARG:HD3	1.61	0.47
4:V:96:ALA:HA	4:V:99:LEU:HD12	1.95	0.47
7:Y:50:LEU:O	7:Y:51:THR:OG1	2.27	0.47
10:b:42:PRO:HA	10:b:45:LYS:HD2	1.97	0.47
14:f:31:VAL:O	14:f:34:PRO:HD2	2.15	0.47
15:g:67:PHE:CE1	30:g:203:PLX:H172	2.49	0.47
16:h:22:SER:HB3	16:h:37:GLU:OE1	2.13	0.47
17:i:319:HIS:CE1	29:w:302:PHE:HD2	2.32	0.47
20:l:95:PHE:C	20:l:95:PHE:HD1	2.23	0.47
31:n:101:CDL:H312	31:n:101:CDL:H341	1.56	0.47
26:s:65:THR:O	26:s:124:ASN:ND2	2.46	0.47
26:s:126:ASN:O	26:s:130:ILE:HG13	2.13	0.47
26:s:253:GLU:O	26:s:257:THR:HG23	2.13	0.47
2:S:50:ARG:HD3	16:h:105:ARG:HG2	1.97	0.47
32:W:201:PEE:H28	32:W:201:PEE:H22	1.50	0.47
9:a:113:TYR:C	12:d:57:TYR:HD2	2.23	0.47
11:c:156:VAL:HG12	28:v:98:ARG:CD	2.44	0.47
16:h:18:LEU:HD21	19:k:59:MET:HE3	1.96	0.47
17:i:256:PRO:HG2	17:i:257:LEU:HG	1.96	0.47
19:k:83:ASN:HD21	21:m:174:ASN:HA	1.78	0.47
20:l:159:TYR:HB2	25:r:416:TRP:CG	2.49	0.47
24:p:54:GLU:OE2	33:p:201:8Q1:C37	2.61	0.47
9:a:114:LYS:HA	12:d:57:TYR:CD2	2.50	0.47
9:a:182:SER:O	9:a:184:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:c:184:TYR:HA	28:v:36:GLU:C	2.39	0.47
30:g:203:PLX:H72	30:g:203:PLX:H11	1.96	0.47
17:i:319:HIS:CE1	29:w:302:PHE:CD2	3.02	0.47
20:l:194:ASN:ND2	23:o:127:LEU:HB2	2.29	0.47
1:Q:57:GLU:HB2	20:l:580:GLN:CD	2.39	0.47
4:V:14:ASP:O	4:V:21:LYS:NZ	2.45	0.47
5:W:101:VAL:HG13	5:W:102:PRO:HD2	1.96	0.47
9:a:168:TRP:HZ2	15:g:85:ARG:HG3	1.80	0.47
11:c:159:LYS:CA	28:v:98:ARG:HH12	2.27	0.47
13:e:71:PRO:O	13:e:72:ASP:HB2	2.15	0.47
14:f:60:LYS:O	14:f:64:GLU:HG3	2.15	0.47
17:i:241:THR:OG1	17:i:242:PRO:HD3	2.15	0.47
20:l:95:PHE:CZ	20:l:456:ARG:HG2	2.50	0.47
20:l:190:ILE:CG1	20:l:196:TRP:CE2	2.96	0.47
20:l:315:VAL:O	20:l:318:GLY:N	2.47	0.47
25:r:61:LEU:O	25:r:64:PRO:HD2	2.15	0.47
26:s:142:TYR:CE1	26:s:289:LEU:HD21	2.49	0.47
26:s:231:ILE:HG23	26:s:270:PHE:HD2	1.79	0.47
26:s:280:PHE:HZ	30:s:401:PLX:H272	1.79	0.47
1:Q:57:GLU:HB2	20:l:580:GLN:NE2	2.29	0.47
2:S:35:GLU:HG2	2:S:35:GLU:O	2.14	0.47
5:W:48:TRP:O	5:W:51:MET:HB2	2.15	0.47
7:Y:88:ASP:N	7:Y:89:PRO:CD	2.78	0.47
30:b:201:PLX:H72	30:b:201:PLX:O2	2.14	0.47
12:d:141:GLY:HA3	15:g:118:ILE:HD12	1.97	0.47
9:a:82:VAL:HG11	13:e:104:THR:HG21	1.96	0.47
10:b:108:ASP:CG	10:b:109:THR:N	2.73	0.47
14:f:28:LYS:HB3	14:f:31:VAL:HB	1.96	0.47
14:f:28:LYS:HE2	29:w:100:ASP:HA	1.97	0.47
17:i:274:ASN:O	17:i:275:SER:OG	2.30	0.47
20:l:189:PHE:CG	20:l:201:MET:HE3	2.50	0.47
20:l:548:LEU:HB2	20:l:549:PRO:HD3	1.95	0.47
25:r:66:LEU:HA	25:r:66:LEU:HD23	1.76	0.47
25:r:130:LEU:O	25:r:134:THR:OG1	2.25	0.47
29:w:46:GLY:HA2	29:w:51:LYS:HE3	1.97	0.47
1:Q:46:GLN:NE2	32:l:701:PEE:H11	2.29	0.47
20:l:527:GLY:C	20:l:529:TYR:H	2.22	0.47
25:r:58:SER:HB2	25:r:63:THR:HG22	1.97	0.47
25:r:80:SER:HB3	25:r:226:ALA:HB2	1.97	0.47
26:s:236:THR:HG22	26:s:263:THR:HG21	1.96	0.47
2:S:4:GLU:O	2:S:7:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:53:ARG:HB2	16:h:105:ARG:HH22	1.80	0.46
7:Y:74:TRP:CE3	7:Y:75:HIS:CA	2.91	0.46
10:b:106:PRO:HG2	10:b:118:PRO:HD3	1.96	0.46
30:b:201:PLX:C3	30:b:201:PLX:C1C	2.86	0.46
11:c:163:TYR:OH	28:v:42:THR:O	2.11	0.46
20:l:140:LEU:O	20:l:144:TRP:HB2	2.15	0.46
28:v:104:ARG:O	28:v:108:LEU:HG	2.15	0.46
5:W:77:ALA:O	5:W:80:ASP:HB3	2.16	0.46
6:X:82:ARG:O	6:X:86:VAL:HG23	2.15	0.46
12:d:120:ILE:O	12:d:123:VAL:N	2.48	0.46
15:g:33:ILE:HG22	15:g:67:PHE:HB3	1.97	0.46
17:i:332:LEU:HD22	17:i:336:LEU:HD12	1.97	0.46
18:j:3:PHE:O	18:j:6:ILE:HB	2.14	0.46
19:k:12:PHE:O	19:k:15:SER:OG	2.25	0.46
20:l:508:THR:HG22	20:l:514:LYS:HE3	1.96	0.46
10:b:111:LEU:HB2	10:b:112:GLU:OE1	2.14	0.46
18:j:56:PHE:CE1	21:m:70:THR:HG21	2.51	0.46
20:l:559:GLU:O	20:l:564:LYS:HG2	2.15	0.46
22:n:34:ARG:CZ	31:n:101:CDL:HB22	2.45	0.46
22:n:42:SER:O	22:n:46:LYS:HB2	2.16	0.46
25:r:35:SER:O	25:r:38:PRO:HD2	2.15	0.46
25:r:63:THR:OG1	25:r:64:PRO:HD3	2.15	0.46
2:S:47:LEU:HA	2:S:50:ARG:HB3	1.98	0.46
4:V:121:ALA:O	4:V:125:VAL:HG23	2.15	0.46
9:a:168:TRP:CZ2	15:g:85:ARG:HG3	2.50	0.46
10:b:105:PHE:CD2	28:v:68:LYS:CA	2.98	0.46
12:d:120:ILE:O	12:d:121:LYS:C	2.56	0.46
12:d:121:LYS:O	12:d:125:GLN:HG3	2.15	0.46
12:d:133:TYR:O	12:d:136:ARG:N	2.48	0.46
20:l:100:ILE:CD1	20:l:246:LEU:HG	2.40	0.46
25:r:73:LEU:HB3	25:r:74:PRO:HD3	1.97	0.46
26:s:294:LEU:HB3	26:s:295:PRO:HD3	1.97	0.46
29:w:270:VAL:O	29:w:275:TYR:N	2.47	0.46
9:a:66:ARG:NH1	13:e:74:HIS:NE2	2.63	0.46
9:a:170:TYR:HE2	9:a:172:GLU:HG2	1.80	0.46
10:b:38:GLN:OE1	10:b:38:GLN:HA	2.14	0.46
14:f:55:TRP:CZ2	15:g:65:THR:HG22	2.51	0.46
15:g:32:TYR:HB2	31:n:101:CDL:H732	1.97	0.46
18:j:62:PHE:CG	26:s:140:ILE:HG23	2.50	0.46
19:k:2:PRO:CG	21:m:115:VAL:CG2	2.84	0.46
21:m:10:VAL:O	21:m:14:MET:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:n:101:CDL:H342	31:n:101:CDL:HA62	1.97	0.46
23:o:52:ASN:HD22	24:p:166:LEU:HG	1.81	0.46
12:d:65:VAL:HG11	12:d:81:GLU:HB3	1.96	0.46
30:g:202:PLX:H101	30:g:202:PLX:H132	1.45	0.46
20:l:32:TYR:HB3	20:l:33:PRO:HD3	1.96	0.46
20:l:211:THR:HG21	31:l:704:CDL:HA4	1.96	0.46
21:m:19:PHE:HB3	21:m:31:VAL:HB	1.98	0.46
22:n:34:ARG:HH22	31:n:101:CDL:PA1	2.38	0.46
23:o:52:ASN:O	24:p:129:ARG:NH2	2.49	0.46
25:r:367:LEU:HD13	25:r:404:ALA:HA	1.97	0.46
29:w:137:SER:C	29:w:139:ARG:H	2.18	0.46
10:b:89:HIS:CE1	10:b:97:ILE:HG13	2.51	0.46
10:b:104:ILE:HB	28:v:48:ASP:HB3	1.98	0.46
10:b:111:LEU:HB2	10:b:112:GLU:CD	2.41	0.46
11:c:44:THR:HB	11:c:47:GLU:HG2	1.97	0.46
11:c:123:PRO:HG3	24:p:75:GLN:NE2	2.25	0.46
11:c:168:LEU:HD12	11:c:169:GLU:HB3	1.98	0.46
17:i:39:ALA:O	17:i:42:PRO:HD2	2.16	0.46
19:k:37:MET:HE1	19:k:63:MET:HE3	1.97	0.46
20:l:79:SER:OG	20:l:135:ASN:HB3	2.16	0.46
20:l:370:SER:O	20:l:374:THR:HG23	2.16	0.46
25:r:1:MET:HE1	25:r:53:SER:HB3	1.98	0.46
25:r:267:TRP:O	25:r:271:MET:HG2	2.15	0.46
26:s:248:ASP:OD1	26:s:249:ALA:N	2.49	0.46
29:w:86:PHE:CE2	29:w:157:VAL:HG11	2.50	0.46
29:w:91:ILE:HG23	29:w:134:TRP:CD1	2.51	0.46
29:w:212:PRO:O	29:w:215:GLN:HB2	2.14	0.46
2:S:43:TYR:CZ	5:W:68:ARG:HD2	2.51	0.46
5:W:115:ARG:NH1	16:h:36:PHE:HD1	2.08	0.46
7:Y:89:PRO:O	28:v:107:ARG:NH1	2.49	0.46
8:Z:49:GLU:OE2	24:p:38:ARG:NH2	2.33	0.46
9:a:187:PRO:HB3	27:u:47:ARG:HG3	1.96	0.46
10:b:112:GLU:N	10:b:112:GLU:CD	2.74	0.46
13:e:113:ARG:HH21	25:r:459:SER:HB2	1.80	0.46
30:g:202:PLX:H1B3	30:g:202:PLX:H22	1.58	0.46
17:i:146:SER:O	17:i:149:LEU:HD13	2.16	0.46
17:i:335:LEU:O	17:i:338:PRO:HD2	2.16	0.46
20:l:367:PRO:O	20:l:371:THR:HG23	2.16	0.46
20:l:369:THR:O	20:l:372:SER:OG	2.27	0.46
26:s:7:LEU:HD23	26:s:7:LEU:HA	1.78	0.46
2:S:38:VAL:HG21	27:u:94:GLN:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:V:203:PLX:H221	23:o:95:PHE:CE1	2.51	0.46
10:b:106:PRO:HA	10:b:115:GLU:CD	2.41	0.46
10:b:109:THR:HA	12:d:18:PRO:HA	1.97	0.46
11:c:101:TRP:CD1	23:o:62:ASN:ND2	2.84	0.46
17:i:92:GLN:O	17:i:95:SER:OG	2.21	0.46
17:i:339:ILE:HG22	17:i:342:PHE:CB	2.42	0.46
20:l:587:TYR:O	20:l:590:SER:OG	2.27	0.46
24:p:51:HIS:O	33:p:201:8Q1:C38	2.64	0.46
7:Y:42:PRO:HD2	8:Z:14:MET:HG3	1.98	0.46
8:Z:31:THR:O	8:Z:34:LYS:HB3	2.16	0.46
11:c:41:TYR:CE1	11:c:67:ASP:HB3	2.51	0.46
11:c:153:TYR:HB3	20:l:403:TYR:CD1	2.48	0.46
14:f:47:THR:O	14:f:51:THR:HG23	2.16	0.46
18:j:86:LEU:HD21	21:m:150:ARG:HD3	1.96	0.46
20:l:302:VAL:O	20:l:306:THR:HG23	2.16	0.46
20:l:306:THR:HA	20:l:336:LYS:HZ3	1.79	0.46
20:l:319:ILE:HG22	20:l:319:ILE:O	2.16	0.46
21:m:109:TYR:O	21:m:112:VAL:HG23	2.16	0.46
21:m:118:PHE:HD1	21:m:121:VAL:HB	1.79	0.46
22:n:50:GLN:CG	22:n:51:PRO:HD2	2.46	0.46
6:X:140:CYS:HB2	6:X:143:GLU:CD	2.41	0.45
12:d:20:GLN:NE2	20:l:57:LEU:HD21	2.30	0.45
14:f:47:THR:OG1	14:f:48:LEU:N	2.48	0.45
15:g:48:ARG:O	15:g:50:ARG:HG3	2.16	0.45
16:h:80:ARG:NH1	21:m:1:MET:SD	2.89	0.45
17:i:46:LYS:O	17:i:47:LYS:HB2	2.16	0.45
17:i:291:TYR:CZ	32:l:701:PEE:C31	2.71	0.45
32:l:701:PEE:H33	32:l:701:PEE:H27	1.62	0.45
25:r:339:SER:O	25:r:340:ARG:HB2	2.17	0.45
27:u:25:LEU:O	27:u:29:ALA:HB2	2.16	0.45
28:v:60:ALA:O	28:v:61:HIS:C	2.59	0.45
29:w:124:ASN:O	29:w:126:GLY:N	2.41	0.45
2:S:54:ILE:HG13	16:h:105:ARG:NH1	2.32	0.45
6:X:132:ASP:HA	6:X:135:ALA:HB3	1.98	0.45
10:b:88:TYR:CG	30:b:201:PLX:H1C2	2.51	0.45
11:c:174:PRO:O	11:c:175:SER:OG	2.26	0.45
12:d:43:ARG:O	12:d:47:GLU:HG2	2.16	0.45
14:f:32:ARG:O	14:f:35:PRO:HD2	2.16	0.45
17:i:25:HIS:CE1	17:i:84:TRP:CE3	3.04	0.45
17:i:102:MET:HE3	17:i:138:PRO:HB3	1.98	0.45
25:r:405:LEU:HA	25:r:405:LEU:HD23	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:23:ALA:HB1	27:u:90:ASP:OD1	2.16	0.45
28:v:62:HIS:CD2	28:v:90:CYS:HG	2.33	0.45
2:S:53:ARG:HB3	16:h:102:GLY:HA2	1.98	0.45
5:W:57:ARG:CZ	26:s:168:THR:HG22	2.47	0.45
5:W:111:PHE:CD2	5:W:117:VAL:HG21	2.51	0.45
14:f:34:PRO:O	14:f:38:LYS:HG3	2.16	0.45
15:g:32:TYR:CD2	17:i:339:ILE:HD11	2.51	0.45
23:o:17:THR:HG21	24:p:22:ARG:HH12	1.82	0.45
29:w:79:GLU:OE1	29:w:79:GLU:N	2.43	0.45
29:w:139:ARG:O	29:w:142:GLN:HB2	2.16	0.45
29:w:168:VAL:HG11	29:w:241:TYR:HA	1.97	0.45
2:S:16:LEU:O	2:S:19:PRO:HD2	2.16	0.45
9:a:175:ASP:OD1	9:a:176:LYS:N	2.50	0.45
11:c:69:GLY:HA2	23:o:81:ARG:H	1.80	0.45
12:d:59:HIS:HD2	13:e:121:GLU:OE2	1.99	0.45
15:g:39:CYS:O	15:g:43:ILE:HG13	2.17	0.45
17:i:58:LYS:HZ1	19:k:92:ASN:CG	2.22	0.45
20:l:173:LEU:HA	20:l:173:LEU:HD23	1.73	0.45
20:l:286:LEU:O	20:l:290:VAL:HG23	2.17	0.45
21:m:32:LEU:HB3	21:m:64:MET:HE3	1.99	0.45
21:m:118:PHE:HZ	21:m:124:TRP:CZ2	2.34	0.45
22:n:7:ILE:HG23	22:n:11:HIS:HB2	1.98	0.45
26:s:89:LEU:HA	26:s:90:PRO:HD3	1.65	0.45
30:g:203:PLX:H101	30:g:203:PLX:H291	1.98	0.45
16:h:36:PHE:HD2	16:h:66:CYS:HB2	1.82	0.45
17:i:337:LEU:C	17:i:339:ILE:H	2.23	0.45
19:k:22:TYR:CG	19:k:22:TYR:O	2.70	0.45
20:l:166:THR:CG2	32:l:702:PEE:H2	2.46	0.45
20:l:558:LEU:HD23	20:l:558:LEU:HA	1.71	0.45
21:m:13:VAL:HG11	21:m:99:GLU:HG2	1.99	0.45
25:r:13:PRO:HA	25:r:16:TRP:HB2	1.98	0.45
29:w:108:TYR:HD1	29:w:327:VAL:HG13	1.82	0.45
29:w:211:VAL:HG13	29:w:212:PRO:HD3	1.98	0.45
3:U:18:VAL:HG11	26:s:292:ASN:O	2.16	0.45
11:c:56:ASN:HD21	23:o:43:LEU:HD11	1.81	0.45
17:i:2:ASN:HD21	17:i:4:LEU:HB2	1.81	0.45
20:l:30:ASN:O	20:l:33:PRO:HD2	2.17	0.45
20:l:533:MET:HE3	32:l:702:PEE:H32	1.97	0.45
20:l:595:LEU:O	20:l:598:THR:OG1	2.31	0.45
10:b:90:VAL:HG22	10:b:97:ILE:HD12	1.98	0.45
30:b:201:PLX:H1C3	30:b:201:PLX:H31	1.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:324:PRO:C	17:i:326:LEU:H	2.24	0.45
20:l:18:PRO:HG3	20:l:39:ILE:HD12	1.99	0.45
20:l:194:ASN:ND2	23:o:127:LEU:HD12	2.32	0.45
20:l:304:PHE:HZ	20:l:526:LEU:HD22	1.81	0.45
23:o:6:TYR:HE1	23:o:12:ARG:NH2	2.15	0.45
25:r:56:PHE:HZ	25:r:108:MET:HE1	1.82	0.45
26:s:288:LEU:O	26:s:293:PHE:N	2.50	0.45
4:V:2:ALA:O	4:V:6:PHE:N	2.45	0.45
31:V:201:CDL:H541	31:V:201:CDL:H572	1.46	0.45
7:Y:73:PHE:HD1	7:Y:73:PHE:C	2.24	0.45
7:Y:78:GLU:CG	20:l:385:PHE:HE1	2.30	0.45
9:a:55:PHE:HE2	24:p:118:TYR:HE2	1.27	0.45
10:b:116:VAL:HG12	10:b:117:ILE:N	2.32	0.45
11:c:177:GLU:O	11:c:178:PRO:C	2.59	0.45
18:j:75:LEU:N	18:j:76:PRO:HD2	2.32	0.45
20:l:33:PRO:HA	20:l:118:PHE:HD2	1.82	0.45
20:l:434:GLN:HB3	20:l:435:PRO:HD2	1.99	0.45
25:r:145:ALA:HB3	25:r:222:GLU:OE2	2.17	0.45
7:Y:74:TRP:HE3	7:Y:75:HIS:N	2.15	0.45
17:i:4:LEU:HG	29:w:43:PHE:HE2	1.82	0.45
17:i:20:THR:O	17:i:23:SER:OG	2.34	0.45
17:i:146:SER:OG	17:i:147:PRO:HD3	2.17	0.45
19:k:42:ILE:O	19:k:46:LEU:HG	2.17	0.45
20:l:481:THR:HG22	28:v:92:HIS:CD2	2.52	0.45
26:s:234:MET:O	26:s:238:THR:HG23	2.17	0.45
27:u:82:PHE:CE2	27:u:86:TRP:HD1	2.35	0.45
29:w:58:ARG:HB3	29:w:202:HIS:HE1	1.82	0.45
29:w:92:HIS:HB3	29:w:103:PRO:HB3	1.99	0.45
6:X:138:LEU:CD2	6:X:144:ILE:HG12	2.47	0.45
19:k:31:LEU:HD23	19:k:31:LEU:HA	1.75	0.45
20:l:399:ALA:O	20:l:402:SER:OG	2.33	0.45
30:r:501:PLX:H101	30:r:501:PLX:H132	1.58	0.45
29:w:351:TRP:HA	29:w:353:TRP:CZ3	2.52	0.45
32:V:202:PEE:H60	32:V:202:PEE:H40	1.99	0.44
7:Y:81:LEU:HD11	28:v:89:TYR:HA	1.98	0.44
11:c:52:ALA:HB2	11:c:62:TYR:HB2	1.99	0.44
17:i:291:TYR:CE2	32:l:701:PEE:H51	2.52	0.44
26:s:40:VAL:CG1	26:s:46:LEU:HB2	2.47	0.44
2:S:31:ASN:HD21	2:S:36:LYS:HD3	1.83	0.44
4:V:69:VAL:HG21	4:V:100:THR:HG21	1.98	0.44
7:Y:72:ARG:NH1	20:l:390:TYR:CZ	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:81:LEU:HD12	28:v:88:ASP:CB	2.45	0.44
19:k:59:MET:HB2	19:k:60:PRO:HD3	1.99	0.44
26:s:257:THR:O	26:s:261:THR:HG23	2.16	0.44
27:u:100:CYS:O	27:u:102:LYS:N	2.49	0.44
5:W:111:PHE:CE2	5:W:117:VAL:HG11	2.49	0.44
7:Y:55:VAL:O	7:Y:58:SER:OG	2.33	0.44
7:Y:85:PRO:O	7:Y:86:TYR:CD1	2.70	0.44
11:c:166:LEU:HB2	11:c:170:ARG:NH2	2.32	0.44
15:g:78:GLU:OE1	17:i:342:PHE:HD1	2.01	0.44
16:h:3:PHE:HB2	17:i:144:GLN:HE21	1.82	0.44
17:i:2:ASN:HA	17:i:3:PRO:HD2	1.87	0.44
32:l:701:PEE:H51	32:l:701:PEE:H56	1.56	0.44
25:r:246:LEU:HD23	25:r:246:LEU:HA	1.80	0.44
26:s:266:LEU:HA	26:s:266:LEU:HD23	1.72	0.44
28:v:49:ALA:O	28:v:51:LEU:N	2.46	0.44
29:w:238:GLU:O	29:w:242:LYS:HG3	2.17	0.44
4:V:40:ARG:HE	31:V:201:CDL:CA2	2.30	0.44
7:Y:65:MET:SD	20:l:375:ILE:HG12	2.58	0.44
11:c:63:GLU:O	11:c:77:LYS:N	2.43	0.44
12:d:107:CYS:HG	12:d:119:CYS:CA	2.31	0.44
15:g:45:ASN:HD21	15:g:60:GLN:HE21	1.65	0.44
20:l:37:LYS:HE3	20:l:102:GLU:CG	2.37	0.44
23:o:6:TYR:CD2	23:o:14:LEU:HD23	2.53	0.44
25:r:109:THR:HG22	25:r:121:PHE:HB2	2.00	0.44
25:r:325:LEU:HD12	25:r:440:HIS:HB3	1.98	0.44
26:s:142:TYR:CD2	26:s:289:LEU:HD11	2.52	0.44
32:W:201:PEE:H51	32:W:201:PEE:H56	1.33	0.44
10:b:105:PHE:HZ	28:v:67:LEU:HB2	1.75	0.44
11:c:101:TRP:CD1	23:o:47:TYR:CD1	3.06	0.44
14:f:32:ARG:C	14:f:35:PRO:HD2	2.42	0.44
18:j:34:SER:HB2	26:s:63:PRO:HA	1.99	0.44
18:j:48:ARG:HD2	18:j:49:VAL:H	1.83	0.44
20:l:98:TRP:CD1	20:l:98:TRP:O	2.71	0.44
20:l:567:SER:C	20:l:571:ILE:HD13	2.42	0.44
25:r:36:ILE:O	25:r:39:LEU:HB3	2.18	0.44
25:r:339:SER:HB2	25:r:344:LEU:HD12	2.00	0.44
30:r:502:PLX:H192	30:r:502:PLX:H162	1.44	0.44
26:s:89:LEU:HD12	26:s:91:MET:HE2	1.98	0.44
26:s:215:TYR:HD1	26:s:219:PRO:HB2	1.83	0.44
17:i:8:VAL:O	17:i:12:THR:HG23	2.18	0.44
18:j:30:TYR:HB2	18:j:33:LYS:CD	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:k:46:LEU:HD22	21:m:46:PHE:CD2	2.53	0.44
22:n:27:LEU:HD12	25:r:2:LEU:HD21	1.98	0.44
29:w:246:LEU:HB2	29:w:247:PRO:HD3	1.99	0.44
5:W:120:LEU:HG	16:h:69:ARG:NH1	2.32	0.44
32:W:201:PEE:C2	26:s:98:LEU:HD22	2.47	0.44
13:e:54:PRO:O	13:e:56:GLN:HG3	2.18	0.44
17:i:197:ASN:HA	17:i:198:PRO:HD3	1.79	0.44
30:r:502:PLX:H151	30:r:502:PLX:H122	1.83	0.44
28:v:63:LEU:O	28:v:67:LEU:HG	2.18	0.44
1:Q:55:SER:N	1:Q:58:THR:OG1	2.51	0.44
20:l:122:LEU:HD23	20:l:122:LEU:HA	1.85	0.44
21:m:2:MET:N	21:m:123:SER:OG	2.50	0.44
23:o:100:PHE:CZ	23:o:104:ILE:HD11	2.53	0.44
24:p:173:ARG:HA	24:p:174:PRO:HD3	1.83	0.44
25:r:72:LEU:O	25:r:76:THR:HG23	2.18	0.44
26:s:92:PRO:HB3	26:s:255:TYR:CD2	2.53	0.44
27:u:104:GLN:O	27:u:108:ASP:N	2.41	0.44
29:w:86:PHE:HD2	29:w:159:LEU:HD13	1.83	0.44
2:S:12:MET:HE1	26:s:19:PHE:C	2.43	0.44
11:c:108:HIS:CE1	20:l:546:GLN:HG2	2.53	0.44
11:c:139:PHE:O	11:c:143:MET:HG2	2.18	0.44
15:g:87:ARG:HD2	27:u:156:GLY:C	2.42	0.44
30:g:201:PLX:H1B1	16:h:2:PRO:HG2	1.99	0.44
17:i:79:MET:SD	19:k:43:MET:HE1	2.58	0.44
9:a:150:ARG:NH1	25:r:168:HIS:CE1	2.86	0.43
10:b:79:VAL:HG22	20:l:10:LEU:CD1	2.48	0.43
10:b:111:LEU:C	10:b:112:GLU:CD	2.85	0.43
12:d:111:GLU:OE1	12:d:119:CYS:HB2	2.18	0.43
17:i:309:ASN:HD21	29:w:130:ARG:HD3	1.82	0.43
20:l:356:ILE:CG2	20:l:429:LEU:HB3	2.48	0.43
24:p:25:ARG:HA	24:p:25:ARG:HD3	1.80	0.43
25:r:237:LYS:HD2	25:r:237:LYS:N	2.33	0.43
26:s:224:PHE:CZ	26:s:228:TYR:HE2	2.36	0.43
3:U:52:ASN:ND2	16:h:27:TYR:O	2.42	0.43
4:V:51:GLU:HB3	4:V:55:LYS:NZ	2.34	0.43
13:e:115:LYS:O	13:e:118:SER:OG	2.30	0.43
16:h:56:CYS:HA	27:u:145:ARG:NH1	2.33	0.43
16:h:82:GLN:HA	16:h:85:LYS:HE3	1.99	0.43
17:i:237:LEU:HB3	17:i:240:LEU:HB2	2.00	0.43
18:j:34:SER:HB2	26:s:64:ALA:H	1.82	0.43
23:o:9:SER:OG	23:o:12:ARG:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:p:30:TRP:O	24:p:32:VAL:HG23	2.18	0.43
25:r:345:SER:O	25:r:348:LEU:HG	2.18	0.43
30:r:501:PLX:H211	30:r:501:PLX:H182	1.67	0.43
27:u:121:ASP:HB3	27:u:124:GLU:OE2	2.18	0.43
28:v:93:ARG:O	28:v:97:MET:HG2	2.18	0.43
2:S:43:TYR:CE2	5:W:68:ARG:HD2	2.53	0.43
9:a:150:ARG:NH1	25:r:168:HIS:HE1	2.16	0.43
11:c:41:TYR:CZ	11:c:67:ASP:HB3	2.54	0.43
17:i:232:ARG:NH1	29:w:306:ASN:O	2.50	0.43
18:j:49:VAL:HG12	21:m:75:ILE:H	1.82	0.43
19:k:8:ILE:N	19:k:8:ILE:HD12	2.33	0.43
20:l:81:LYS:HD3	20:l:83:ASP:OD2	2.18	0.43
20:l:151:SER:HA	20:l:247:LEU:HD13	2.01	0.43
20:l:208:PRO:HG2	20:l:266:LEU:HB3	1.99	0.43
20:l:210:LEU:HD21	20:l:214:LEU:HD13	2.00	0.43
20:l:533:MET:CE	32:l:702:PEE:H32	2.48	0.43
25:r:115:LEU:O	25:r:118:PHE:HB3	2.19	0.43
25:r:408:LEU:HD23	25:r:408:LEU:HA	1.70	0.43
26:s:59:GLU:OE1	26:s:59:GLU:N	2.52	0.43
29:w:217:ARG:O	29:w:221:LYS:HG2	2.18	0.43
2:S:53:ARG:HH21	16:h:105:ARG:HA	1.83	0.43
5:W:110:VAL:HG11	16:h:71:LYS:HB2	2.01	0.43
6:X:123:GLU:HB2	6:X:128:PHE:O	2.18	0.43
8:Z:65:ASP:O	8:Z:69:LYS:HB2	2.19	0.43
12:d:57:TYR:CD1	12:d:57:TYR:O	2.70	0.43
13:e:57:GLU:HB2	29:w:323:GLN:HB3	1.99	0.43
24:p:54:GLU:OE1	24:p:54:GLU:N	2.51	0.43
27:u:18:VAL:HG12	27:u:20:ILE:H	1.83	0.43
28:v:50:GLN:O	28:v:56:ARG:NH1	2.41	0.43
10:b:71:VAL:O	10:b:75:VAL:HB	2.18	0.43
10:b:115:GLU:CG	10:b:116:VAL:N	2.81	0.43
15:g:15:ASP:OD1	15:g:16:GLU:N	2.52	0.43
19:k:32:CYS:O	19:k:36:MET:HG3	2.18	0.43
19:k:87:LEU:HD13	21:m:74:ALA:HB2	2.00	0.43
20:l:222:GLY:HA2	20:l:229:LEU:CD1	2.43	0.43
20:l:222:GLY:N	20:l:229:LEU:HD12	2.31	0.43
20:l:227:LEU:HA	20:l:230:HIS:HB3	2.00	0.43
26:s:289:LEU:HA	26:s:289:LEU:HD23	1.82	0.43
7:Y:58:SER:HB2	20:l:371:THR:HG21	2.01	0.43
15:g:82:TYR:OH	17:i:341:PRO:O	2.35	0.43
17:i:218:LEU:HD23	17:i:218:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:j:53:MET:HG3	19:k:79:VAL:HG13	1.99	0.43
18:j:64:LEU:O	18:j:68:GLU:HG2	2.18	0.43
25:r:87:GLU:O	25:r:92:LYS:HE3	2.18	0.43
25:r:105:SER:O	25:r:109:THR:HG23	2.18	0.43
26:s:142:TYR:CE2	26:s:289:LEU:HD11	2.54	0.43
27:u:80:GLU:N	27:u:81:PRO:HD2	2.33	0.43
27:u:149:ASP:HA	27:u:150:PRO:HD3	1.88	0.43
30:V:203:PLX:H332	30:V:203:PLX:H141	2.01	0.43
18:j:68:GLU:HG3	18:j:98:LEU:HD21	2.01	0.43
20:l:209:SER:O	20:l:212:PRO:HD2	2.18	0.43
4:V:19:HIS:CD2	4:V:20:ARG:HG3	2.54	0.43
9:a:66:ARG:O	9:a:70:LEU:HG	2.19	0.43
9:a:185:ALA:O	27:u:48:TRP:HZ2	2.01	0.43
11:c:154:GLN:C	11:c:156:VAL:HG23	2.44	0.43
14:f:28:LYS:HE3	29:w:101:GLY:H	1.83	0.43
17:i:71:LEU:HA	17:i:71:LEU:HD23	1.73	0.43
17:i:76:PHE:CZ	17:i:80:LEU:HD11	2.54	0.43
18:j:106:TRP:HZ3	26:s:291:LYS:HA	1.84	0.43
20:l:67:HIS:ND1	20:l:75:GLN:HG3	2.33	0.43
20:l:217:LEU:O	20:l:217:LEU:HD23	2.19	0.43
22:n:39:ARG:HB2	22:n:57:TRP:CZ2	2.53	0.43
24:p:104:LEU:HD22	24:p:122:ARG:NH2	2.33	0.43
25:r:45:ILE:O	25:r:45:ILE:HG22	2.19	0.43
26:s:251:SER:HA	26:s:252:PRO:HD2	1.86	0.43
1:Q:69:VAL:HG12	1:Q:72:PRO:CD	2.48	0.43
5:W:33:TYR:O	5:W:34:SER:OG	2.27	0.43
9:a:170:TYR:CD1	15:g:5:ARG:HD3	2.54	0.43
16:h:73:MET:HG2	21:m:124:TRP:CH2	2.54	0.43
19:k:39:SER:HB3	21:m:16:PHE:HE2	1.84	0.43
19:k:97:GLN:CD	20:l:587:TYR:HE1	2.27	0.43
20:l:68:TRP:HB2	20:l:76:LEU:HD12	2.01	0.43
20:l:280:LEU:O	20:l:284:THR:HG23	2.19	0.43
21:m:56:PHE:CZ	26:s:111:LEU:HD11	2.54	0.43
24:p:49:GLU:O	24:p:52:LYS:HG2	2.19	0.43
25:r:122:PHE:CE1	25:r:238:LEU:HD21	2.54	0.43
26:s:55:LEU:HD13	26:s:221:ALA:HB2	2.01	0.43
29:w:163:ILE:HD12	29:w:166:ASP:OD2	2.19	0.43
7:Y:74:TRP:C	7:Y:74:TRP:CD2	2.97	0.43
30:b:201:PLX:C2	12:d:43:ARG:HH22	2.31	0.43
11:c:44:THR:HB	11:c:47:GLU:CG	2.49	0.43
15:g:51:PRO:HG2	15:g:55:ALA:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:i:214:THR:HG22	17:i:329:LEU:HB3	2.01	0.43
17:i:258:THR:CG2	17:i:336:LEU:HB3	2.48	0.43
18:j:64:LEU:HD23	18:j:64:LEU:HA	1.81	0.43
20:l:227:LEU:HD22	20:l:283:ILE:HG22	2.00	0.43
20:l:548:LEU:O	20:l:552:LEU:HB2	2.18	0.43
32:l:701:PEE:H36	25:r:155:VAL:CG2	2.46	0.43
21:m:26:ILE:HD13	26:s:121:TRP:CE2	2.54	0.43
31:n:101:CDL:H741	31:n:101:CDL:H711	1.60	0.43
24:p:48:PHE:CZ	33:p:201:8Q1:C8	2.99	0.43
26:s:150:LEU:O	26:s:154:LEU:HG	2.19	0.43
4:V:62:THR:HG22	4:V:104:ARG:CD	2.49	0.42
4:V:95:CYS:O	4:V:99:LEU:HG	2.19	0.42
11:c:61:ASP:O	11:c:63:GLU:HG3	2.19	0.42
15:g:32:TYR:CE2	17:i:339:ILE:HD11	2.54	0.42
19:k:7:ASN:ND2	21:m:9:SER:CA	2.82	0.42
20:l:95:PHE:HZ	20:l:456:ARG:HG2	1.83	0.42
20:l:548:LEU:HD22	23:o:93:CYS:HB3	2.01	0.42
20:l:550:LEU:HA	20:l:554:ASP:HB3	2.01	0.42
21:m:86:VAL:O	21:m:90:VAL:HG23	2.19	0.42
26:s:195:ARG:O	26:s:198:PHE:N	2.52	0.42
4:V:133:TRP:CG	32:V:202:PEE:H7	2.54	0.42
9:a:87:THR:CG2	30:b:201:PLX:C13	2.87	0.42
15:g:51:PRO:HB2	15:g:54:THR:OG1	2.19	0.42
17:i:234:TRP:HH2	17:i:305:LEU:HB2	1.83	0.42
17:i:298:TYR:HE2	25:r:147:THR:HG23	1.83	0.42
20:l:149:ILE:HD12	25:r:369:LEU:HD11	2.01	0.42
21:m:43:ILE:HG22	21:m:48:GLY:HA3	2.00	0.42
25:r:179:LEU:O	25:r:248:LEU:HD13	2.19	0.42
25:r:308:SER:HB3	25:r:384:THR:HG21	2.01	0.42
26:s:169:GLN:NE2	26:s:241:ILE:O	2.42	0.42
1:Q:39:PRO:HD2	17:i:304:LEU:O	2.19	0.42
7:Y:40:ILE:HD11	20:l:446:ASN:ND2	2.34	0.42
8:Z:18:ASP:OD1	8:Z:19:TYR:N	2.52	0.42
11:c:102:GLY:HA3	23:o:43:LEU:HD13	2.00	0.42
15:g:15:ASP:HB2	15:g:18:ARG:NH2	2.29	0.42
15:g:61:LEU:O	15:g:65:THR:HG23	2.19	0.42
15:g:87:ARG:HD2	27:u:156:GLY:O	2.19	0.42
16:h:58:ILE:HD12	27:u:145:ARG:NH2	2.34	0.42
18:j:49:VAL:CG1	21:m:75:ILE:H	2.32	0.42
21:m:27:TYR:HA	21:m:30:LEU:HD12	2.01	0.42
24:p:90:SER:HB2	24:p:93:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:u:67:ALA:O	27:u:70:PHE:HB3	2.19	0.42
2:S:53:ARG:HB2	16:h:105:ARG:CZ	2.49	0.42
5:W:72:LEU:HD23	5:W:72:LEU:HA	1.84	0.42
6:X:105:MET:HE2	6:X:139:MET:HE3	2.00	0.42
13:e:87:MET:HE3	13:e:87:MET:HB3	1.77	0.42
16:h:17:TRP:CZ3	16:h:18:LEU:HB2	2.55	0.42
22:n:40:ASN:HD22	22:n:56:THR:HG23	1.82	0.42
22:n:51:PRO:O	22:n:53:GLU:HG3	2.20	0.42
31:n:101:CDL:H712	31:n:101:CDL:H512	2.01	0.42
25:r:398:LEU:HA	25:r:398:LEU:HD23	1.81	0.42
26:s:18:ALA:O	26:s:21:MET:HG2	2.19	0.42
28:v:5:LEU:HG	28:v:6:VAL:N	2.34	0.42
3:U:40:LYS:O	3:U:44:MET:HG2	2.18	0.42
9:a:54:LEU:CD2	10:b:26:GLN:C	2.87	0.42
9:a:101:ILE:HG13	12:d:58:TYR:CB	2.49	0.42
10:b:51:LEU:HD22	10:b:59:LYS:HA	2.01	0.42
15:g:37:GLY:O	15:g:40:SER:OG	2.28	0.42
17:i:26:TRP:HD1	17:i:84:TRP:O	2.02	0.42
17:i:109:ALA:CB	17:i:112:HIS:HD2	2.33	0.42
20:l:14:SER:O	20:l:17:PRO:HD2	2.20	0.42
25:r:10:MET:O	25:r:13:PRO:HD2	2.20	0.42
26:s:231:ILE:HG23	26:s:270:PHE:CD2	2.54	0.42
30:b:201:PLX:C6	30:b:201:PLX:C11	2.85	0.42
11:c:101:TRP:CD1	23:o:62:ASN:HD22	2.38	0.42
11:c:119:THR:HB	23:o:13:THR:HG23	2.02	0.42
16:h:94:PRO:O	16:h:97:HIS:N	2.52	0.42
20:l:93:ALA:O	20:l:97:THR:OG1	2.38	0.42
24:p:48:PHE:HE1	33:p:201:8Q1:C6	2.33	0.42
30:r:502:PLX:H311	30:r:502:PLX:H282	1.76	0.42
26:s:90:PRO:HB2	26:s:92:PRO:O	2.18	0.42
28:v:79:ALA:C	28:v:81:LYS:H	2.26	0.42
29:w:143:TYR:OH	29:w:162:SER:HB2	2.20	0.42
3:U:69:HIS:CE1	3:U:70:PRO:HA	2.54	0.42
32:W:201:PEE:H36	18:j:7:LEU:CD2	2.47	0.42
6:X:155:TYR:CD2	6:X:155:TYR:O	2.73	0.42
9:a:57:ILE:HA	24:p:104:LEU:HD12	2.01	0.42
10:b:117:ILE:CG2	10:b:118:PRO:HD2	2.50	0.42
10:b:117:ILE:HG23	10:b:118:PRO:HD2	2.01	0.42
11:c:94:GLN:OE1	11:c:99:LEU:HB2	2.20	0.42
11:c:125:SER:O	11:c:129:MET:HG3	2.20	0.42
11:c:183:HIS:CB	28:v:37:ARG:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:d:24:ILE:HD11	20:l:56:CYS:HB3	2.02	0.42
16:h:74:ARG:HG2	21:m:116:VAL:HG13	2.02	0.42
17:i:79:MET:HE3	19:k:5:TYR:CD2	2.55	0.42
20:l:158:TRP:CH2	20:l:240:PRO:HB3	2.55	0.42
22:n:50:GLN:HG3	22:n:51:PRO:CD	2.50	0.42
24:p:31:CYS:HB3	24:p:36:LYS:HD2	2.02	0.42
25:r:374:ASN:OD1	25:r:374:ASN:N	2.52	0.42
26:s:11:VAL:N	26:s:12:PRO:HD2	2.34	0.42
30:b:201:PLX:C10	30:b:201:PLX:C6	2.85	0.42
11:c:81:ARG:HD3	11:c:85:GLU:OE1	2.20	0.42
12:d:134:GLN:OE1	23:o:124:THR:HA	2.20	0.42
12:d:162:LYS:O	12:d:165:LYS:HB3	2.20	0.42
17:i:294:LEU:HD23	17:i:294:LEU:HA	1.74	0.42
20:l:154:LEU:HD23	20:l:154:LEU:HA	1.85	0.42
20:l:404:THR:HB	20:l:405:ASN:H	1.66	0.42
21:m:40:CYS:O	21:m:44:LEU:HG	2.19	0.42
2:S:53:ARG:CZ	16:h:105:ARG:NH2	2.83	0.42
5:W:57:ARG:NH2	26:s:316:PRO:HG3	2.35	0.42
9:a:98:LEU:HB2	12:d:57:TYR:CE1	2.39	0.42
11:c:100:ASN:HB2	11:c:103:GLU:HG3	2.02	0.42
11:c:133:LEU:HD13	20:l:532:ILE:HD12	2.00	0.42
17:i:120:GLN:HA	17:i:176:ARG:HE	1.85	0.42
17:i:217:LEU:HD23	17:i:217:LEU:HA	1.86	0.42
18:j:12:LEU:O	18:j:16:LEU:HB2	2.20	0.42
18:j:71:LEU:O	18:j:74:PRO:HD2	2.20	0.42
20:l:336:LYS:HD3	20:l:336:LYS:HA	1.90	0.42
20:l:558:LEU:HB3	25:r:214:LEU:HD11	2.02	0.42
21:m:33:ILE:HD11	26:s:114:TYR:CE1	2.55	0.42
22:n:16:LEU:HD21	25:r:10:MET:HE3	2.02	0.42
24:p:174:PRO:O	24:p:175:ARG:HB3	2.19	0.42
25:r:344:LEU:O	25:r:420:THR:HG21	2.20	0.42
28:v:59:CYS:O	28:v:87:TRP:HZ3	2.03	0.42
32:W:201:PEE:H60	21:m:56:PHE:HZ	1.84	0.42
7:Y:95:GLU:CD	7:Y:95:GLU:N	2.77	0.42
9:a:180:ASP:HB3	16:h:24:GLU:HG3	2.02	0.42
15:g:44:ASP:OD1	17:i:327:PRO:HG2	2.20	0.42
17:i:2:ASN:ND2	17:i:4:LEU:HB2	2.35	0.42
20:l:7:MET:O	20:l:11:THR:HG23	2.20	0.42
20:l:310:LEU:HD23	20:l:313:MET:HE3	2.01	0.42
20:l:414:ILE:O	20:l:417:SER:OG	2.29	0.42
20:l:536:THR:O	20:l:539:TYR:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:19:LEU:O	3:U:22:SER:OG	2.29	0.41
9:a:129:PRO:CG	12:d:60:ARG:HH22	2.33	0.41
20:l:106:TRP:CZ2	20:l:348:HIS:HD2	2.38	0.41
20:l:305:SER:O	20:l:309:GLN:HG2	2.20	0.41
22:n:28:ASP:OD1	25:r:2:LEU:HB3	2.19	0.41
25:r:245:ARG:HA	25:r:245:ARG:HD3	1.86	0.41
25:r:248:LEU:HD12	25:r:249:ILE:N	2.35	0.41
29:w:223:ASP:HA	29:w:224:PRO:HD3	1.85	0.41
4:V:23:TYR:O	4:V:24:SER:HB2	2.20	0.41
4:V:126:LYS:HE3	4:V:130:LEU:HD11	2.02	0.41
30:b:201:PLX:P1	30:b:201:PLX:O6	2.79	0.41
11:c:49:ALA:O	11:c:53:LYS:HG2	2.21	0.41
12:d:74:GLU:HB2	15:g:105:LYS:HD2	2.01	0.41
30:g:203:PLX:H22	30:g:203:PLX:H1B3	1.74	0.41
16:h:56:CYS:HA	27:u:145:ARG:HH12	1.84	0.41
22:n:43:MET:HE3	22:n:43:MET:HB2	1.87	0.41
27:u:104:GLN:HB3	27:u:108:ASP:OD2	2.20	0.41
29:w:93:TYR:CZ	29:w:142:GLN:OE1	2.73	0.41
7:Y:81:LEU:HB3	20:l:480:THR:OG1	2.20	0.41
10:b:118:PRO:HA	10:b:119:PRO:HD3	1.94	0.41
17:i:108:MET:SD	17:i:191:MET:HG3	2.60	0.41
17:i:307:MET:O	29:w:319:ILE:HD12	2.20	0.41
20:l:37:LYS:NZ	20:l:98:TRP:HE1	2.18	0.41
25:r:188:ASN:O	25:r:189:SER:OG	2.21	0.41
30:r:501:PLX:H282	30:r:501:PLX:H251	1.77	0.41
26:s:275:THR:OG1	26:s:276:ALA:N	2.53	0.41
29:w:62:VAL:HG21	29:w:74:ALA:HB2	2.02	0.41
29:w:77:ILE:HG23	29:w:81:LEU:HD13	2.03	0.41
29:w:240:ALA:O	29:w:244:THR:OG1	2.14	0.41
6:X:105:MET:CE	6:X:139:MET:HG3	2.50	0.41
6:X:115:GLN:HE21	6:X:119:ILE:HD11	1.84	0.41
9:a:149:LEU:HD23	9:a:149:LEU:HA	1.79	0.41
10:b:119:PRO:HB2	28:v:40:VAL:HG13	2.02	0.41
15:g:46:LEU:CD1	17:i:239:TRP:HB3	2.49	0.41
15:g:51:PRO:HG2	15:g:55:ALA:CB	2.50	0.41
17:i:69:ILE:HD12	17:i:104:MET:HE1	2.01	0.41
18:j:70:ALA:HA	18:j:73:LEU:HD13	2.01	0.41
19:k:10:LEU:O	19:k:14:ILE:HG13	2.20	0.41
20:l:174:TYR:OH	20:l:534:HIS:HE1	2.03	0.41
20:l:188:TRP:O	20:l:192:HIS:HB2	2.20	0.41
31:l:703:CDL:HA61	31:l:703:CDL:H1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:173:TRP:HZ3	26:s:262:LYS:HE2	1.86	0.41
6:X:131:PRO:HG3	11:c:89:TRP:CE3	2.55	0.41
10:b:111:LEU:C	10:b:113:THR:N	2.78	0.41
11:c:151:PRO:O	11:c:153:TYR:HD1	2.03	0.41
11:c:163:TYR:HB3	11:c:168:LEU:HD21	2.02	0.41
15:g:73:TYR:O	15:g:76:LYS:HB3	2.21	0.41
18:j:94:LEU:HD12	21:m:153:VAL:HG13	2.03	0.41
20:l:452:ASN:CB	20:l:453:PRO:HD3	2.51	0.41
20:l:562:LEU:O	20:l:566:ILE:HD12	2.21	0.41
21:m:5:LEU:HD23	21:m:8:LEU:HD12	2.02	0.41
24:p:76:HIS:HA	24:p:77:PRO:HD3	1.86	0.41
24:p:135:ARG:HD3	24:p:162:ASP:OD1	2.21	0.41
25:r:121:PHE:O	25:r:125:THR:HG23	2.20	0.41
27:u:83:THR:O	27:u:87:THR:HG23	2.21	0.41
29:w:86:PHE:HE2	29:w:146:ALA:HB2	1.86	0.41
8:Z:53:TYR:HA	20:l:435:PRO:HG2	2.02	0.41
9:a:106:VAL:HA	9:a:107:PRO:HD2	1.82	0.41
15:g:27:ASP:O	15:g:31:LEU:HG	2.19	0.41
17:i:167:TRP:HZ3	20:l:570:GLN:CA	2.20	0.41
17:i:256:PRO:HB3	25:r:124:THR:HG22	2.01	0.41
20:l:197:ASP:O	20:l:201:MET:CG	2.69	0.41
21:m:33:ILE:O	21:m:37:VAL:HG23	2.19	0.41
24:p:124:GLN:HA	24:p:127:LYS:NZ	2.36	0.41
25:r:355:MET:HA	25:r:358:TRP:CD1	2.54	0.41
26:s:154:LEU:HA	26:s:154:LEU:HD23	1.73	0.41
2:S:34:LYS:HZ1	27:u:90:ASP:HB3	1.85	0.41
9:a:62:PHE:HB2	24:p:111:GLU:OE2	2.19	0.41
30:b:201:PLX:C6	30:b:201:PLX:P1	3.08	0.41
11:c:65:TYR:CE2	11:c:77:LYS:HG3	2.55	0.41
11:c:159:LYS:HA	28:v:98:ARG:CZ	2.50	0.41
11:c:162:PRO:O	11:c:166:LEU:HD12	2.21	0.41
12:d:76:ILE:HG22	12:d:77:MET:HE2	2.02	0.41
12:d:123:VAL:O	12:d:127:THR:HG23	2.21	0.41
16:h:6:ILE:HD12	17:i:22:LEU:HD21	2.02	0.41
17:i:210:ILE:O	17:i:214:THR:HG23	2.20	0.41
18:j:36:PRO:HA	26:s:214:GLU:OE2	2.21	0.41
18:j:54:LYS:HB3	18:j:113:TRP:HE1	1.85	0.41
26:s:150:LEU:HD23	26:s:150:LEU:HA	1.88	0.41
26:s:164:THR:O	26:s:167:THR:OG1	2.38	0.41
27:u:24:VAL:CG2	27:u:86:TRP:HE1	2.34	0.41
1:Q:35:ARG:HH21	29:w:322:HIS:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:56:PRO:HB3	27:u:129:THR:OG1	2.20	0.41
31:V:201:CDL:H722	31:V:201:CDL:H752	1.75	0.41
5:W:86:MET:HG2	5:W:128:ARG:HH22	1.86	0.41
9:a:130:GLU:HA	22:n:45:PHE:CD2	2.56	0.41
11:c:73:GLY:C	11:c:75:TYR:H	2.28	0.41
19:k:3:LEU:O	19:k:3:LEU:HD13	2.20	0.41
20:l:452:ASN:N	20:l:453:PRO:HD2	2.35	0.41
20:l:536:THR:OG1	20:l:537:ILE:N	2.53	0.41
24:p:134:GLU:O	24:p:138:LYS:HG3	2.21	0.41
24:p:145:PRO:HA	24:p:146:PRO:HD3	1.84	0.41
25:r:153:THR:O	25:r:157:SER:N	2.54	0.41
25:r:229:MET:HE2	25:r:229:MET:HB3	1.90	0.41
29:w:42:HIS:O	29:w:46:GLY:N	2.54	0.41
29:w:335:PRO:HA	29:w:338:LYS:HZ3	1.84	0.41
4:V:114:ALA:HB1	4:V:118:PHE:CE2	2.56	0.41
9:a:115:HIS:CG	9:a:116:PRO:HD2	2.56	0.41
10:b:111:LEU:C	10:b:113:THR:H	2.27	0.41
11:c:88:PRO:HB2	24:p:86:PRO:HG2	2.03	0.41
11:c:154:GLN:HE22	28:v:3:ALA:HB2	1.86	0.41
12:d:35:VAL:C	12:d:38:PRO:HD2	2.46	0.41
13:e:150:PRO:HD3	15:g:112:PHE:CD1	2.56	0.41
14:f:34:PRO:HG3	29:w:342:GLY:HA2	2.03	0.41
15:g:45:ASN:HD21	15:g:60:GLN:NE2	2.19	0.41
17:i:19:ILE:HD12	17:i:35:MET:HE1	2.02	0.41
17:i:112:HIS:HB2	17:i:184:ILE:HD13	2.03	0.41
19:k:10:LEU:CD1	21:m:102:LEU:HD12	2.49	0.41
19:k:14:ILE:HD13	21:m:17:VAL:HG22	2.02	0.41
20:l:311:GLY:O	20:l:315:VAL:HG23	2.21	0.41
20:l:396:ILE:HG22	20:l:400:ASN:HD21	1.85	0.41
20:l:493:VAL:O	20:l:496:LEU:HB3	2.21	0.41
21:m:114:VAL:O	21:m:115:VAL:HG22	2.20	0.41
23:o:112:LYS:NZ	25:r:389:SER:HA	2.36	0.41
23:o:124:THR:C	23:o:126:HIS:H	2.29	0.41
24:p:31:CYS:O	24:p:33:GLN:N	2.54	0.41
24:p:158:ARG:O	24:p:162:ASP:HB2	2.21	0.41
25:r:130:LEU:HD21	25:r:149:PHE:HD2	1.86	0.41
26:s:86:TRP:HH2	26:s:232:ILE:HG22	1.85	0.41
30:s:401:PLX:H332	30:s:401:PLX:H301	1.80	0.41
2:S:47:LEU:O	2:S:50:ARG:HB3	2.20	0.41
6:X:113:LEU:HD12	6:X:114:ASP:N	2.36	0.41
7:Y:62:SER:O	7:Y:65:MET:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:a:96:ALA:CB	12:d:55:TYR:H	2.34	0.41
9:a:112:TYR:CD1	12:d:58:TYR:O	2.72	0.41
19:k:3:LEU:C	19:k:3:LEU:CD1	2.94	0.41
20:l:100:ILE:HD12	20:l:246:LEU:CD2	2.51	0.41
20:l:218:LEU:C	20:l:218:LEU:CD2	2.94	0.41
20:l:244:SER:HA	20:l:248:HIS:CD2	2.56	0.41
20:l:272:LEU:HD11	31:l:704:CDL:HB61	2.02	0.41
21:m:106:VAL:HG11	21:m:117:ASN:ND2	2.34	0.41
25:r:170:THR:OG1	25:r:171:LEU:N	2.53	0.41
30:r:502:PLX:H392	30:r:502:PLX:H361	1.64	0.41
26:s:195:ARG:HG3	26:s:196:ALA:N	2.36	0.41
1:Q:52:MET:HE2	17:i:295:ARG:HH21	1.86	0.40
1:Q:65:PRO:CG	1:Q:69:VAL:HG22	2.51	0.40
30:V:203:PLX:H371	30:V:203:PLX:H342	1.76	0.40
7:Y:45:ARG:O	7:Y:45:ARG:HG2	2.22	0.40
9:a:109:HIS:O	9:a:112:TYR:HD2	2.03	0.40
12:d:56:TYR:HD1	12:d:56:TYR:HA	1.78	0.40
13:e:67:TYR:CE2	25:r:428:PRO:HG2	2.56	0.40
15:g:37:GLY:HA2	15:g:67:PHE:CE2	2.56	0.40
17:i:189:TRP:HE1	17:i:286:THR:HG21	1.85	0.40
19:k:31:LEU:HD21	21:m:67:PHE:CE2	2.56	0.40
20:l:362:LEU:HA	20:l:365:THR:OG1	2.22	0.40
20:l:522:PHE:HA	20:l:528:PHE:CE2	2.56	0.40
23:o:6:TYR:HE2	23:o:14:LEU:HA	1.85	0.40
25:r:196:TRP:NE1	25:r:250:LEU:HD13	2.36	0.40
25:r:375:LEU:HD12	25:r:375:LEU:HA	1.85	0.40
26:s:2:PRO:O	26:s:5:ASN:HB2	2.20	0.40
26:s:311:ILE:O	26:s:312:SER:OG	2.28	0.40
30:U:101:PLX:H22	30:U:101:PLX:H1B3	1.86	0.40
7:Y:43:ARG:HH11	7:Y:49:GLN:HG2	1.86	0.40
7:Y:74:TRP:CZ3	7:Y:75:HIS:HA	2.53	0.40
10:b:105:PHE:HD2	28:v:68:LYS:CB	2.34	0.40
17:i:61:LEU:O	17:i:65:THR:HG23	2.21	0.40
31:i:401:CDL:H311	31:i:401:CDL:H341	1.83	0.40
20:l:70:THR:HA	20:l:75:GLN:HB2	2.04	0.40
20:l:84:TYR:HD1	20:l:88:MET:CE	2.01	0.40
20:l:550:LEU:HD23	20:l:554:ASP:OD2	2.22	0.40
22:n:30:LYS:HZ2	31:n:101:CDL:HA31	1.86	0.40
25:r:89:LEU:O	25:r:93:LYS:HG3	2.20	0.40
29:w:72:LYS:HD2	29:w:75:LYS:HD2	2.03	0.40
3:U:50:PRO:HB2	5:W:69:ILE:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:111:PHE:CE2	5:W:117:VAL:HG21	2.56	0.40
7:Y:68:TRP:CZ3	20:l:386:LEU:HA	2.56	0.40
12:d:138:GLN:HG2	12:d:139:ASP:OD1	2.22	0.40
17:i:124:LEU:HD13	17:i:219:LEU:HG	2.02	0.40
17:i:342:PHE:CD2	17:i:343:MET:HE2	2.57	0.40
19:k:46:LEU:HD22	21:m:46:PHE:CE2	2.56	0.40
19:k:97:GLN:N	20:l:579:THR:OG1	2.41	0.40
20:l:39:ILE:O	20:l:43:THR:HG23	2.22	0.40
24:p:30:TRP:NE1	24:p:76:HIS:HB2	2.36	0.40
25:r:233:ALA:HB2	25:r:324:SER:HB3	2.04	0.40
25:r:235:LEU:O	25:r:238:LEU:HB3	2.22	0.40
26:s:116:ILE:O	26:s:119:SER:OG	2.34	0.40
26:s:193:THR:O	26:s:194:ASN:HB2	2.20	0.40
26:s:273:ILE:HG23	26:s:277:TYR:HD2	1.86	0.40
28:v:75:PRO:O	28:v:77:PHE:N	2.43	0.40
29:w:68:THR:OG1	29:w:69:GLY:N	2.54	0.40
4:V:124:LEU:HA	4:V:127:MET:HE3	2.03	0.40
5:W:93:GLU:OE1	16:h:93:THR:HG21	2.21	0.40
9:a:54:LEU:HD23	9:a:54:LEU:HA	1.81	0.40
10:b:88:TYR:HB2	30:b:201:PLX:C1B	2.51	0.40
30:b:201:PLX:C11	30:b:201:PLX:C7	3.00	0.40
11:c:168:LEU:HD12	11:c:169:GLU:N	2.36	0.40
12:d:72:LYS:HE3	15:g:105:LYS:O	2.20	0.40
12:d:107:CYS:HB2	12:d:122:GLU:OE1	2.22	0.40
20:l:417:SER:HB3	20:l:493:VAL:CG1	2.51	0.40
20:l:564:LYS:HG3	23:o:77:TYR:OH	2.21	0.40
24:p:158:ARG:O	24:p:159:LYS:HB2	2.21	0.40
25:r:346:GLN:HA	25:r:413:THR:O	2.21	0.40
1:Q:50:ALA:HB2	1:Q:63:PRO:HB3	2.03	0.40
1:Q:69:VAL:O	1:Q:72:PRO:HD2	2.22	0.40
3:U:8:PHE:O	3:U:11:ASN:HB3	2.21	0.40
10:b:12:LEU:HD23	10:b:12:LEU:HA	1.90	0.40
10:b:31:ARG:HH12	24:p:116:PRO:HG2	1.85	0.40
14:f:63:ASN:O	14:f:67:LEU:HG	2.22	0.40
15:g:11:ARG:O	15:g:13:LEU:N	2.54	0.40
17:i:70:LEU:HD23	17:i:70:LEU:HA	1.76	0.40
17:i:73:ALA:HA	17:i:97:MET:HE3	2.03	0.40
17:i:86:MET:HE2	17:i:144:GLN:OE1	2.21	0.40
20:l:417:SER:O	20:l:420:SER:OG	2.27	0.40
25:r:80:SER:O	25:r:81:GLN:C	2.64	0.40
30:r:501:PLX:H301	30:r:501:PLX:H271	1.66	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:s:94:PRO:HB2	26:s:96:VAL:O	2.22	0.40
29:w:86:PHE:HA	29:w:87:PRO:HD2	1.85	0.40
29:w:246:LEU:O	29:w:249:MET:HB2	2.22	0.40
29:w:319:ILE:HG21	29:w:324:THR:HB	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	44/46 (96%)	40 (91%)	2 (4%)	2 (4%)	2	18
2	S	68/70 (97%)	61 (90%)	5 (7%)	2 (3%)	3	26
3	U	81/83 (98%)	76 (94%)	4 (5%)	1 (1%)	10	40
4	V	138/140 (99%)	129 (94%)	6 (4%)	3 (2%)	5	31
5	W	114/116 (98%)	109 (96%)	4 (4%)	1 (1%)	14	45
6	X	83/85 (98%)	73 (88%)	6 (7%)	4 (5%)	2	17
7	Y	57/59 (97%)	50 (88%)	1 (2%)	6 (10%)	0	5
8	Z	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
9	a	136/138 (99%)	121 (89%)	12 (9%)	3 (2%)	5	31
10	b	122/128 (95%)	107 (88%)	10 (8%)	5 (4%)	2	20
11	c	151/153 (99%)	129 (85%)	15 (10%)	7 (5%)	2	18
12	d	169/171 (99%)	165 (98%)	3 (2%)	1 (1%)	21	52
13	e	95/97 (98%)	84 (88%)	8 (8%)	3 (3%)	3	25
14	f	45/47 (96%)	43 (96%)	1 (2%)	1 (2%)	5	31
15	g	117/119 (98%)	105 (90%)	6 (5%)	6 (5%)	1	17
16	h	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	i	345/347 (99%)	324 (94%)	15 (4%)	6 (2%)	7	34
18	j	113/115 (98%)	103 (91%)	7 (6%)	3 (3%)	4	27
19	k	95/97 (98%)	88 (93%)	4 (4%)	3 (3%)	3	25
20	l	601/603 (100%)	551 (92%)	38 (6%)	12 (2%)	6	32
21	m	172/174 (99%)	150 (87%)	12 (7%)	10 (6%)	1	15
22	n	54/56 (96%)	50 (93%)	2 (4%)	2 (4%)	2	22
23	o	126/128 (98%)	113 (90%)	9 (7%)	4 (3%)	3	25
24	p	170/172 (99%)	157 (92%)	10 (6%)	3 (2%)	6	34
25	r	457/459 (100%)	420 (92%)	28 (6%)	9 (2%)	6	32
26	s	316/318 (99%)	286 (90%)	21 (7%)	9 (3%)	4	27
27	u	167/169 (99%)	152 (91%)	10 (6%)	5 (3%)	3	26
28	v	107/122 (88%)	90 (84%)	14 (13%)	3 (3%)	4	27
29	w	318/320 (99%)	281 (88%)	28 (9%)	9 (3%)	4	27
All	All	4641/4716 (98%)	4217 (91%)	295 (6%)	129 (3%)	6	27

All (129) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	S	60	TYR
3	U	71	GLN
5	W	34	SER
6	X	155	TYR
7	Y	84	PHE
9	a	58	ARG
11	c	115	ASN
11	c	178	PRO
12	d	2	PRO
16	h	20	ILE
17	i	91	ASN
17	i	323	THR
18	j	24	LEU
18	j	26	GLN
19	k	52	HIS
20	l	450	LEU
21	m	115	VAL
21	m	116	VAL
21	m	118	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	n	55	VAL
25	r	52	CYS
25	r	346	GLN
29	w	57	SER
29	w	264	GLN
29	w	282	PRO
29	w	347	VAL
4	V	135	VAL
4	V	140	LYS
7	Y	44	TYR
7	Y	51	THR
9	a	57	ILE
9	a	185	ALA
10	b	101	LYS
11	c	170	ARG
15	g	9	PRO
16	h	3	PHE
16	h	24	GLU
16	h	43	CYS
18	j	2	ASN
20	l	73	THR
20	l	512	LYS
21	m	122	GLY
22	n	52	SER
25	r	45	ILE
25	r	188	ASN
25	r	250	LEU
25	r	421	HIS
26	s	203	GLY
26	s	213	ILE
26	s	217	ALA
26	s	316	PRO
28	v	56	ARG
29	w	285	LYS
1	Q	36	GLN
6	X	140	CYS
7	Y	85	PRO
10	b	37	PRO
10	b	109	THR
11	c	164	ASN
13	e	61	PRO
13	e	111	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	g	10	LEU
15	g	12	PHE
15	g	50	ARG
17	i	87	THR
19	k	83	ASN
19	k	96	LEU
20	l	65	ASN
20	l	451	LEU
20	l	511	LEU
20	l	549	PRO
20	l	554	ASP
20	l	563	PRO
21	m	4	ALA
21	m	76	GLU
21	m	110	ASP
23	o	5	LYS
23	o	12	ARG
25	r	139	GLN
26	s	38	ASN
27	u	36	CYS
27	u	101	ARG
27	u	143	HIS
28	v	73	SER
29	w	351	TRP
2	S	36	LYS
6	X	74	LEU
7	Y	42	PRO
7	Y	87	PRO
10	b	115	GLU
11	c	40	PRO
11	c	41	TYR
15	g	49	ARG
15	g	56	GLY
16	h	32	ARG
16	h	45	HIS
17	i	150	ASN
20	l	249	SER
20	l	387	THR
20	l	562	LEU
23	o	59	LEU
23	o	120	LYS
24	p	76	HIS

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Mol	Chain	Res	Type
25	r	251	ASN
26	s	208	VAL
26	s	288	LEU
26	s	289	LEU
27	u	167	PHE
28	v	36	GLU
4	V	48	THR
6	X	153	ASP
11	c	171	GLY
17	i	92	GLN
21	m	113	VAL
24	p	175	ARG
27	u	144	SER
29	w	58	ARG
29	w	121	PRO
29	w	160	GLU
10	b	41	GLY
14	f	39	PRO
21	m	24	SER
24	p	32	VAL
25	r	205	VAL
26	s	241	ILE
21	m	23	PRO
1	Q	69	VAL
17	i	338	PRO
13	e	135	PRO

### 5.3.2 Protein sidechains [i](#)

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	41/41 (100%)	41 (100%)	0	100	100
2	S	59/59 (100%)	59 (100%)	0	100	100
3	U	72/72 (100%)	72 (100%)	0	100	100
4	V	102/102 (100%)	102 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	W	100/100 (100%)	100 (100%)	0	100	100
6	X	78/79 (99%)	77 (99%)	1 (1%)	61	71
7	Y	57/57 (100%)	50 (88%)	7 (12%)	4	22
8	Z	62/63 (98%)	62 (100%)	0	100	100
9	a	124/124 (100%)	123 (99%)	1 (1%)	73	76
10	b	118/122 (97%)	113 (96%)	5 (4%)	26	51
11	c	124/137 (90%)	124 (100%)	0	100	100
12	d	145/154 (94%)	137 (94%)	8 (6%)	19	46
13	e	90/90 (100%)	90 (100%)	0	100	100
14	f	43/43 (100%)	43 (100%)	0	100	100
15	g	105/105 (100%)	105 (100%)	0	100	100
16	h	90/90 (100%)	90 (100%)	0	100	100
17	i	314/314 (100%)	313 (100%)	1 (0%)	86	83
18	j	102/103 (99%)	101 (99%)	1 (1%)	68	74
19	k	85/85 (100%)	81 (95%)	4 (5%)	23	48
20	l	531/532 (100%)	512 (96%)	19 (4%)	31	54
21	m	137/137 (100%)	137 (100%)	0	100	100
22	n	53/53 (100%)	53 (100%)	0	100	100
23	o	114/114 (100%)	114 (100%)	0	100	100
24	p	157/157 (100%)	155 (99%)	2 (1%)	61	71
25	r	416/416 (100%)	416 (100%)	0	100	100
26	s	278/278 (100%)	278 (100%)	0	100	100
27	u	153/153 (100%)	153 (100%)	0	100	100
28	v	89/111 (80%)	89 (100%)	0	100	100
29	w	249/288 (86%)	249 (100%)	0	100	100
All	All	4088/4179 (98%)	4039 (99%)	49 (1%)	61	72

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	X	93	ILE
7	Y	75	HIS
7	Y	78	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	Y	80	VAL
7	Y	81	LEU
7	Y	87	PRO
7	Y	95	GLU
7	Y	97	LEU
9	a	53	ARG
10	b	21	ARG
10	b	38	GLN
10	b	82	ILE
10	b	111	LEU
10	b	112	GLU
12	d	54	ARG
12	d	55	TYR
12	d	57	TYR
12	d	60	ARG
12	d	61	GLN
12	d	113	GLN
12	d	116	GLN
12	d	117	GLN
17	i	149	LEU
18	j	86	LEU
19	k	1	MET
19	k	3	LEU
19	k	6	MET
19	k	8	ILE
20	l	25	ASN
20	l	59	GLN
20	l	87	MET
20	l	94	LEU
20	l	97	THR
20	l	99	SER
20	l	191	LEU
20	l	193	SER
20	l	195	SER
20	l	196	TRP
20	l	197	ASP
20	l	217	LEU
20	l	218	LEU
20	l	223	LYS
20	l	226	GLN
20	l	229	LEU
20	l	447	ASN

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Mol	Chain	Res	Type
20	l	450	LEU
20	l	452	ASN
24	p	124	GLN
24	p	170	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	38	GLN
2	S	44	HIS
4	V	44	ASN
5	W	61	GLN
5	W	112	HIS
5	W	135	HIS
6	X	142	GLN
7	Y	75	HIS
8	Z	33	GLN
9	a	90	ASN
9	a	109	HIS
9	a	115	HIS
9	a	189	ASN
10	b	14	GLN
10	b	83	HIS
10	b	89	HIS
11	c	56	ASN
11	c	84	HIS
11	c	127	HIS
11	c	154	GLN
11	c	165	ASN
12	d	59	HIS
12	d	61	GLN
12	d	85	GLN
12	d	108	GLN
12	d	113	GLN
12	d	116	GLN
12	d	117	GLN
13	e	140	ASN
15	g	45	ASN
15	g	58	HIS
15	g	96	HIS
17	i	83	GLN
17	i	112	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	i	150	ASN
17	i	186	HIS
17	i	222	ASN
18	j	10	ASN
19	k	7	ASN
19	k	94	ASN
20	l	4	HIS
20	l	59	GLN
20	l	113	ASN
20	l	139	GLN
20	l	192	HIS
20	l	199	GLN
20	l	205	ASN
20	l	226	GLN
20	l	248	HIS
20	l	274	GLN
20	l	296	ASN
20	l	323	HIS
20	l	332	HIS
20	l	348	HIS
20	l	394	HIS
20	l	400	ASN
20	l	442	ASN
20	l	446	ASN
20	l	534	HIS
20	l	569	HIS
20	l	580	GLN
21	m	117	ASN
22	n	40	ASN
23	o	52	ASN
23	o	62	ASN
23	o	126	HIS
24	p	26	HIS
24	p	75	GLN
25	r	21	HIS
25	r	46	ASN
25	r	168	HIS
25	r	390	ASN
25	r	415	GLN
25	r	425	ASN
26	s	93	ASN
26	s	97	ASN

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Mol	Chain	Res	Type
26	s	169	GLN
26	s	235	ASN
27	u	30	HIS
27	u	31	HIS
27	u	64	ASN
27	u	77	HIS
27	u	99	HIS
27	u	104	GLN
27	u	140	ASN
27	u	143	HIS
28	v	43	GLN
28	v	61	HIS
28	v	85	HIS
28	v	92	HIS
29	w	92	HIS
29	w	111	ASN
29	w	132	GLN
29	w	149	HIS
29	w	257	GLN
29	w	323	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	PLX	r	501	-	51,51,51	0.77	1 (1%)	53,59,59	0.67	1 (1%)
31	CDL	V	201	-	61,61,99	1.23	5 (8%)	64,71,111	0.95	3 (4%)
30	PLX	g	202	-	51,51,51	0.77	1 (1%)	53,59,59	0.62	1 (1%)
30	PLX	g	203	-	51,51,51	0.81	1 (1%)	53,59,59	0.59	1 (1%)
30	PLX	b	201	-	51,51,51	0.55	0	53,59,59	0.64	0
30	PLX	r	502	-	51,51,51	0.62	0	53,59,59	0.66	1 (1%)
30	PLX	U	101	-	51,51,51	0.76	1 (1%)	53,59,59	0.71	2 (3%)
31	CDL	n	101	-	63,63,99	1.25	5 (7%)	69,75,111	1.08	4 (5%)
33	8Q1	p	201	-	32,34,34	1.59	5 (15%)	39,43,43	1.59	6 (15%)
32	PEE	l	701	-	48,48,50	1.36	4 (8%)	51,53,55	0.98	2 (3%)
32	PEE	W	201	-	50,50,50	1.16	6 (12%)	53,55,55	0.99	2 (3%)
31	CDL	l	704	-	63,63,99	1.27	5 (7%)	69,75,111	1.02	4 (5%)
31	CDL	l	703	-	63,63,99	1.23	5 (7%)	69,75,111	1.08	4 (5%)
30	PLX	V	203	-	51,51,51	0.80	1 (1%)	53,59,59	0.60	1 (1%)
30	PLX	s	401	-	51,51,51	0.79	1 (1%)	53,59,59	0.69	1 (1%)
32	PEE	l	702	-	50,50,50	1.19	6 (12%)	53,55,55	1.00	2 (3%)
31	CDL	i	401	-	63,63,99	1.23	5 (7%)	69,75,111	1.06	5 (7%)
30	PLX	g	201	-	51,51,51	0.85	1 (1%)	53,59,59	0.70	1 (1%)
32	PEE	V	202	-	50,50,50	1.18	6 (12%)	53,55,55	0.92	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PLX	r	501	-	-	27/55/55/55	-
31	CDL	V	201	-	-	40/69/69/110	-
30	PLX	g	202	-	-	26/55/55/55	-
30	PLX	g	203	-	-	22/55/55/55	-
30	PLX	b	201	-	-	26/55/55/55	-
30	PLX	r	502	-	-	36/55/55/55	-
30	PLX	U	101	-	-	22/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CDL	n	101	-	-	32/74/74/110	-
33	8Q1	p	201	-	-	20/41/41/41	-
32	PEE	l	701	-	-	31/52/52/54	-
32	PEE	W	201	-	-	29/54/54/54	-
31	CDL	l	704	-	-	42/74/74/110	-
31	CDL	l	703	-	-	36/74/74/110	-
30	PLX	V	203	-	-	26/55/55/55	-
30	PLX	s	401	-	-	22/55/55/55	-
32	PEE	l	702	-	-	27/54/54/54	-
31	CDL	i	401	-	-	39/74/74/110	-
30	PLX	g	201	-	-	24/55/55/55	-
32	PEE	V	202	-	-	26/54/54/54	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	p	201	8Q1	C39-N41	5.06	1.45	1.33
33	p	201	8Q1	C34-N36	4.93	1.45	1.33
31	l	704	CDL	OB8-CB7	4.36	1.46	1.33
31	n	101	CDL	OA6-CA5	4.30	1.46	1.34
31	l	703	CDL	OA6-CA5	4.29	1.46	1.34
32	l	701	PEE	C39-C38	4.27	1.55	1.31
31	V	201	CDL	OA6-CA5	4.26	1.46	1.34
31	l	703	CDL	OB8-CB7	4.23	1.45	1.33
32	l	701	PEE	C18-C19	4.21	1.55	1.31
31	V	201	CDL	OB8-CB7	4.17	1.45	1.33
31	l	704	CDL	OA8-CA7	4.14	1.45	1.33
31	l	704	CDL	OA6-CA5	4.14	1.46	1.34
32	l	701	PEE	O3-C30	4.13	1.45	1.33
31	n	101	CDL	OB8-CB7	4.13	1.45	1.33
31	i	401	CDL	OB8-CB7	4.08	1.45	1.33
31	i	401	CDL	OA6-CA5	4.01	1.45	1.34
31	n	101	CDL	OA8-CA7	3.92	1.44	1.33
32	l	702	PEE	C18-C19	3.86	1.53	1.31
32	V	202	PEE	C18-C19	3.84	1.53	1.31
32	W	201	PEE	C18-C19	3.83	1.53	1.31
31	l	703	CDL	OA8-CA7	3.81	1.44	1.33
32	V	202	PEE	C39-C38	3.80	1.53	1.31
32	l	702	PEE	C39-C38	3.79	1.53	1.31
32	W	201	PEE	C39-C38	3.75	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	i	401	CDL	OA8-CA7	3.74	1.44	1.33
31	l	704	CDL	OB6-CB5	3.31	1.43	1.34
32	l	701	PEE	O2-C10	3.31	1.43	1.34
31	n	101	CDL	OB6-CB5	3.28	1.43	1.34
31	l	703	CDL	OB6-CB5	3.25	1.43	1.34
31	i	401	CDL	OB6-CB5	3.13	1.43	1.34
31	V	201	CDL	OB6-CB5	3.13	1.43	1.34
30	s	401	PLX	O6-C4	-3.07	1.40	1.44
31	V	201	CDL	OA8-CA7	3.06	1.45	1.33
30	g	203	PLX	O6-C4	-3.03	1.40	1.44
31	n	101	CDL	OB6-CB4	-2.92	1.39	1.46
30	g	201	PLX	O6-C4	-2.92	1.40	1.44
30	V	203	PLX	O6-C4	-2.89	1.40	1.44
31	V	201	CDL	OB6-CB4	-2.77	1.40	1.46
31	i	401	CDL	OB6-CB4	-2.70	1.40	1.46
30	U	101	PLX	O6-C4	-2.62	1.41	1.44
30	g	202	PLX	O6-C4	-2.57	1.41	1.44
33	p	201	8Q1	O35-C34	-2.53	1.18	1.23
31	l	703	CDL	OB6-CB4	-2.52	1.40	1.46
31	l	704	CDL	OB6-CB4	-2.50	1.40	1.46
30	r	501	PLX	O6-C4	-2.49	1.41	1.44
32	l	702	PEE	O2-C2	-2.42	1.40	1.46
32	l	702	PEE	O2-C10	2.40	1.41	1.34
32	V	202	PEE	O2-C10	2.40	1.41	1.34
32	V	202	PEE	O2-C2	-2.40	1.41	1.46
33	p	201	8Q1	O40-C39	-2.39	1.18	1.23
32	l	702	PEE	O3-C30	2.36	1.40	1.33
32	W	201	PEE	O2-C2	-2.35	1.41	1.46
32	V	202	PEE	O3-C3	-2.31	1.40	1.45
32	W	201	PEE	O2-C10	2.26	1.40	1.34
33	p	201	8Q1	C1-S44	2.25	1.81	1.76
32	V	202	PEE	O3-C30	2.25	1.39	1.33
32	l	702	PEE	O3-C3	-2.25	1.40	1.45
32	W	201	PEE	O3-C30	2.23	1.39	1.33
32	W	201	PEE	O3-C3	-2.19	1.40	1.45

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	p	201	8Q1	C6-C1-S44	5.93	120.47	113.40
32	l	702	PEE	O2-C10-C11	4.38	120.96	111.48
31	l	703	CDL	OA6-CA5-C11	4.17	120.51	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	i	401	CDL	OA6-CA5-C11	4.13	120.42	111.48
31	l	704	CDL	OA6-CA5-C11	4.11	120.36	111.48
31	V	201	CDL	OB6-CB5-C51	4.08	120.31	111.48
31	n	101	CDL	OB6-CB5-C51	4.07	120.29	111.48
32	l	701	PEE	O2-C10-C11	4.00	120.14	111.48
31	l	703	CDL	OB6-CB5-C51	3.94	120.00	111.48
31	l	704	CDL	OB6-CB5-C51	3.92	119.96	111.48
31	n	101	CDL	OA6-CA5-C11	3.90	119.91	111.48
33	p	201	8Q1	O4-C1-C6	-3.70	119.71	123.98
32	W	201	PEE	O2-C10-C11	3.67	119.43	111.48
32	V	202	PEE	O2-C10-C11	3.57	119.20	111.48
31	i	401	CDL	OB6-CB5-C51	3.52	119.09	111.48
31	V	201	CDL	OA6-CA5-C11	3.43	118.89	111.48
31	l	703	CDL	OA8-CA7-C31	3.10	121.28	111.83
32	V	202	PEE	O3-C30-C31	2.96	120.86	111.83
32	l	702	PEE	O3-C30-C31	2.95	120.83	111.83
33	p	201	8Q1	C43-S44-C1	2.86	110.30	101.84
31	i	401	CDL	OB8-CB7-C71	2.86	120.54	111.83
31	n	101	CDL	OA8-CA7-C31	2.84	120.50	111.83
31	l	704	CDL	OA8-CA7-C31	2.83	120.46	111.83
32	W	201	PEE	O3-C30-C31	2.81	120.41	111.83
31	n	101	CDL	OB8-CB7-C71	2.81	120.39	111.83
31	l	703	CDL	OB8-CB7-C71	2.79	120.35	111.83
31	l	704	CDL	OB8-CB7-C71	2.76	120.26	111.83
31	V	201	CDL	OB8-CB7-C71	2.62	119.83	111.83
31	i	401	CDL	OA8-CA7-C31	2.48	119.40	111.83
30	s	401	PLX	C1C-N1-C1	2.44	119.59	109.91
32	l	701	PEE	O3-C30-C31	2.40	119.14	111.83
33	p	201	8Q1	C38-C39-N41	2.39	120.71	116.34
30	V	203	PLX	C1C-N1-C1	2.39	119.41	109.91
30	U	101	PLX	C1C-N1-C1	2.36	119.31	109.91
30	g	203	PLX	C1C-N1-C1	2.33	119.15	109.91
30	g	201	PLX	C1C-N1-C1	2.27	118.92	109.91
30	g	202	PLX	C1C-N1-C1	2.26	118.91	109.91
33	p	201	8Q1	O4-C1-S44	-2.25	119.82	122.68
30	r	502	PLX	C2-C1-N1	-2.20	108.76	115.82
30	r	501	PLX	C1C-N1-C1	2.13	118.36	109.91
33	p	201	8Q1	C32-C34-N36	2.12	120.51	116.48
30	U	101	PLX	C5-C4-C3	-2.09	106.91	111.78
31	i	401	CDL	OA6-CA5-OA7	-2.08	118.84	123.70

There are no chirality outliers.

All (553) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	U	101	PLX	O7-C6-C7-C8
30	U	101	PLX	O7-C6-O6-C4
30	U	101	PLX	C3-O4-P1-O1
30	U	101	PLX	C3-O4-P1-O2
30	U	101	PLX	N1-C1-C2-O1
30	U	101	PLX	O9-C24-C25-C26
30	V	203	PLX	O7-C6-C7-C8
30	V	203	PLX	N1-C1-C2-O1
30	V	203	PLX	O9-C24-C25-C26
30	b	201	PLX	O7-C6-O6-C4
30	b	201	PLX	C3-O4-P1-O1
30	b	201	PLX	N1-C1-C2-O1
30	b	201	PLX	O9-C24-O8-C5
30	g	201	PLX	O7-C6-C7-C8
30	g	201	PLX	O7-C6-O6-C4
30	g	201	PLX	C3-C4-O6-C6
30	g	201	PLX	C3-O4-P1-O1
30	g	201	PLX	C3-O4-P1-O3
30	g	202	PLX	C2-O1-P1-O4
30	g	202	PLX	C2-O1-P1-O2
30	g	202	PLX	C2-O1-P1-O3
30	g	202	PLX	O9-C24-O8-C5
30	g	203	PLX	O7-C6-O6-C4
30	g	203	PLX	C2-O1-P1-O4
30	g	203	PLX	C2-O1-P1-O2
30	g	203	PLX	C25-C24-O8-C5
30	r	501	PLX	C3-O4-P1-O1
30	r	501	PLX	C3-O4-P1-O2
30	r	501	PLX	C3-O4-P1-O3
30	r	501	PLX	O8-C24-C25-C26
30	r	502	PLX	C7-C6-O6-C4
30	r	502	PLX	C3-O4-P1-O1
30	r	502	PLX	C3-O4-P1-O2
30	r	502	PLX	C3-O4-P1-O3
30	r	502	PLX	C2-O1-P1-O4
30	r	502	PLX	C2-O1-P1-O2
30	r	502	PLX	N1-C1-C2-O1
30	r	502	PLX	O9-C24-C25-C26
30	s	401	PLX	C2-O1-P1-O4
30	s	401	PLX	C2-O1-P1-O2
30	s	401	PLX	N1-C1-C2-O1
31	V	201	CDL	CB2-C1-CA2-OA2

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Mol	Chain	Res	Type	Atoms
31	V	201	CDL	CA2-OA2-PA1-OA3
31	V	201	CDL	CA2-OA2-PA1-OA4
31	V	201	CDL	CA2-OA2-PA1-OA5
31	V	201	CDL	CA3-OA5-PA1-OA2
31	V	201	CDL	CA3-OA5-PA1-OA3
31	V	201	CDL	CA3-OA5-PA1-OA4
31	V	201	CDL	OA9-CA7-OA8-CA6
31	V	201	CDL	CB3-OB5-PB2-OB2
31	V	201	CDL	CB3-OB5-PB2-OB4
31	V	201	CDL	C51-CB5-OB6-CB4
31	i	401	CDL	O1-C1-CA2-OA2
31	i	401	CDL	CB2-C1-CA2-OA2
31	i	401	CDL	CA2-OA2-PA1-OA3
31	i	401	CDL	CA2-OA2-PA1-OA4
31	i	401	CDL	CA2-OA2-PA1-OA5
31	i	401	CDL	CA3-OA5-PA1-OA2
31	i	401	CDL	CA3-OA5-PA1-OA3
31	i	401	CDL	CA3-OA5-PA1-OA4
31	i	401	CDL	OA6-CA4-CA6-OA8
31	i	401	CDL	CB2-OB2-PB2-OB4
31	i	401	CDL	CB2-OB2-PB2-OB5
31	i	401	CDL	CB3-OB5-PB2-OB3
31	i	401	CDL	CB3-OB5-PB2-OB4
31	l	703	CDL	CA2-OA2-PA1-OA3
31	l	703	CDL	CA2-OA2-PA1-OA5
31	l	703	CDL	CB3-OB5-PB2-OB2
31	l	703	CDL	CB3-OB5-PB2-OB4
31	l	704	CDL	CA2-OA2-PA1-OA3
31	l	704	CDL	CA2-OA2-PA1-OA4
31	l	704	CDL	CA2-OA2-PA1-OA5
31	l	704	CDL	CA3-OA5-PA1-OA2
31	l	704	CDL	CA3-OA5-PA1-OA4
31	l	704	CDL	C11-CA5-OA6-CA4
31	l	704	CDL	CB2-OB2-PB2-OB3
31	n	101	CDL	CA2-OA2-PA1-OA3
31	n	101	CDL	CA2-OA2-PA1-OA4
31	n	101	CDL	CA2-OA2-PA1-OA5
31	n	101	CDL	OA7-CA5-OA6-CA4
31	n	101	CDL	C11-CA5-OA6-CA4
31	n	101	CDL	CB2-OB2-PB2-OB3
31	n	101	CDL	CB2-OB2-PB2-OB4
31	n	101	CDL	CB2-OB2-PB2-OB5

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Mol	Chain	Res	Type	Atoms
31	n	101	CDL	C51-CB5-OB6-CB4
32	V	202	PEE	C2-C1-O3P-P
32	V	202	PEE	C1-O3P-P-O4P
32	V	202	PEE	O4P-C4-C5-N
32	W	201	PEE	C4-O4P-P-O3P
32	W	201	PEE	C4-O4P-P-O1P
32	l	701	PEE	C11-C10-O2-C2
32	l	701	PEE	C4-O4P-P-O2P
32	l	701	PEE	C4-O4P-P-O1P
33	p	201	8Q1	C1-C6-C7-C8
33	p	201	8Q1	O4-C1-S44-C43
33	p	201	8Q1	C6-C1-S44-C43
33	p	201	8Q1	C28-C29-C32-C34
33	p	201	8Q1	C28-C29-C32-O33
33	p	201	8Q1	C30-C29-C32-C34
33	p	201	8Q1	C31-C29-C32-C34
33	p	201	8Q1	C31-C29-C32-O33
33	p	201	8Q1	C28-O27-P24-O2
33	p	201	8Q1	C28-O27-P24-O1
31	l	704	CDL	OA9-CA7-OA8-CA6
31	l	704	CDL	OB9-CB7-OB8-CB6
31	n	101	CDL	OA9-CA7-OA8-CA6
31	V	201	CDL	OB7-CB5-OB6-CB4
31	l	703	CDL	OB7-CB5-OB6-CB4
31	l	704	CDL	OA7-CA5-OA6-CA4
31	n	101	CDL	OB7-CB5-OB6-CB4
32	l	701	PEE	O4-C10-O2-C2
31	l	704	CDL	C31-CA7-OA8-CA6
31	l	704	CDL	C71-CB7-OB8-CB6
31	n	101	CDL	C31-CA7-OA8-CA6
31	n	101	CDL	C71-CB7-OB8-CB6
31	l	703	CDL	C51-CB5-OB6-CB4
32	l	701	PEE	C37-C38-C39-C40
32	l	702	PEE	C37-C38-C39-C40
31	n	101	CDL	OB9-CB7-OB8-CB6
32	l	702	PEE	O5-C30-O3-C3
31	l	703	CDL	O1-C1-CA2-OA2
31	l	704	CDL	O1-C1-CA2-OA2
31	i	401	CDL	C11-CA5-OA6-CA4
32	l	702	PEE	C31-C30-O3-C3
30	b	201	PLX	C4-C3-O4-P1
32	W	201	PEE	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
32	l	701	PEE	C32-C33-C34-C35
31	l	703	CDL	CB2-C1-CA2-OA2
32	W	201	PEE	C31-C30-O3-C3
30	g	203	PLX	C26-C27-C28-C29
30	r	501	PLX	C10-C11-C12-C13
32	V	202	PEE	C20-C21-C22-C23
32	W	201	PEE	C21-C22-C23-C24
30	r	502	PLX	C16-C17-C18-C19
32	W	201	PEE	C32-C33-C34-C35
31	V	201	CDL	O1-C1-CA2-OA2
31	l	703	CDL	O1-C1-CB2-OB2
30	b	201	PLX	C14-C15-C16-C17
30	g	203	PLX	C30-C31-C32-C33
30	r	502	PLX	C30-C31-C32-C33
32	W	201	PEE	O5-C30-O3-C3
30	g	202	PLX	C10-C11-C12-C13
31	i	401	CDL	OA7-CA5-OA6-CA4
31	l	703	CDL	OB5-CB3-CB4-OB6
30	r	502	PLX	C12-C13-C14-C15
31	i	401	CDL	C31-C32-C33-C34
32	l	702	PEE	C17-C18-C19-C20
32	W	201	PEE	C15-C16-C17-C18
32	l	702	PEE	C10-C11-C12-C13
31	l	703	CDL	C73-C74-C75-C76
31	i	401	CDL	CA5-C11-C12-C13
31	l	704	CDL	CB5-C51-C52-C53
31	n	101	CDL	CA7-C31-C32-C33
32	V	202	PEE	C10-C11-C12-C13
31	V	201	CDL	C54-C55-C56-C57
32	W	201	PEE	C12-C13-C14-C15
32	l	701	PEE	C34-C35-C36-C37
30	r	501	PLX	C12-C13-C14-C15
31	i	401	CDL	C31-CA7-OA8-CA6
30	V	203	PLX	C13-C14-C15-C16
32	V	202	PEE	C17-C18-C19-C20
32	l	701	PEE	C17-C18-C19-C20
32	l	701	PEE	C30-C31-C32-C33
32	V	202	PEE	C31-C30-O3-C3
31	l	703	CDL	CA2-C1-CB2-OB2
31	l	703	CDL	C71-CB7-OB8-CB6
30	r	501	PLX	C27-C28-C29-C30
32	l	701	PEE	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
30	U	101	PLX	O6-C6-C7-C8
30	g	203	PLX	O8-C24-C25-C26
30	s	401	PLX	O6-C6-C7-C8
31	l	704	CDL	C51-CB5-OB6-CB4
31	l	704	CDL	OB7-CB5-OB6-CB4
31	n	101	CDL	C31-C32-C33-C34
30	g	201	PLX	C13-C14-C15-C16
30	g	201	PLX	C7-C8-C9-C10
30	g	202	PLX	C7-C8-C9-C10
30	g	203	PLX	C29-C30-C31-C32
30	s	401	PLX	C27-C28-C29-C30
31	n	101	CDL	C13-C14-C15-C16
32	l	701	PEE	C22-C23-C24-C25
32	W	201	PEE	C37-C38-C39-C40
30	g	203	PLX	C34-C35-C36-C37
31	n	101	CDL	C12-C13-C14-C15
32	W	201	PEE	C14-C15-C16-C17
32	V	202	PEE	O5-C30-O3-C3
30	g	203	PLX	O9-C24-C25-C26
30	r	501	PLX	O9-C24-C25-C26
30	s	401	PLX	O7-C6-C7-C8
31	l	704	CDL	C31-C32-C33-C34
32	l	701	PEE	C21-C22-C23-C24
32	l	702	PEE	C20-C21-C22-C23
33	p	201	8Q1	C11-C12-C13-C14
31	n	101	CDL	CB5-C51-C52-C53
32	l	702	PEE	C33-C34-C35-C36
31	i	401	CDL	OA9-CA7-OA8-CA6
30	U	101	PLX	C33-C34-C35-C36
31	V	201	CDL	C71-C72-C73-C74
31	l	704	CDL	C51-C52-C53-C54
31	l	703	CDL	CB7-C71-C72-C73
31	l	704	CDL	CA7-C31-C32-C33
31	l	704	CDL	CB7-C71-C72-C73
30	g	202	PLX	C14-C15-C16-C17
30	U	101	PLX	C19-C20-C21-C22
30	r	501	PLX	C13-C14-C15-C16
32	V	202	PEE	C12-C13-C14-C15
31	l	703	CDL	OB9-CB7-OB8-CB6
32	l	702	PEE	C21-C22-C23-C24
30	V	203	PLX	C25-C26-C27-C28
31	l	703	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
30	r	502	PLX	C11-C12-C13-C14
32	V	202	PEE	C40-C41-C42-C43
33	p	201	8Q1	C6-C7-C8-C9
30	U	101	PLX	C12-C13-C14-C15
30	U	101	PLX	C10-C11-C12-C13
30	V	203	PLX	C32-C33-C34-C35
30	b	201	PLX	C16-C17-C18-C19
30	r	502	PLX	C14-C15-C16-C17
30	r	502	PLX	C10-C11-C12-C13
30	U	101	PLX	C35-C36-C37-C38
30	b	201	PLX	C27-C28-C29-C30
30	g	203	PLX	C15-C16-C17-C18
31	l	703	CDL	C11-C12-C13-C14
30	r	502	PLX	C32-C33-C34-C35
30	V	203	PLX	C10-C11-C12-C13
30	s	401	PLX	C28-C29-C30-C31
30	g	203	PLX	C17-C18-C19-C20
31	V	201	CDL	C11-CA5-OA6-CA4
30	r	502	PLX	C25-C26-C27-C28
31	n	101	CDL	CB7-C71-C72-C73
31	i	401	CDL	C13-C14-C15-C16
31	l	704	CDL	C32-C33-C34-C35
32	V	202	PEE	C14-C15-C16-C17
32	l	702	PEE	C34-C35-C36-C37
32	l	702	PEE	C40-C41-C42-C43
31	V	201	CDL	OA7-CA5-OA6-CA4
30	b	201	PLX	C29-C30-C31-C32
31	n	101	CDL	C55-C56-C57-C58
30	U	101	PLX	C9-C10-C11-C12
30	b	201	PLX	C18-C19-C20-C21
30	g	201	PLX	C16-C17-C18-C19
30	g	203	PLX	C14-C15-C16-C17
30	g	203	PLX	C7-C8-C9-C10
30	r	501	PLX	C7-C8-C9-C10
30	r	502	PLX	C9-C10-C11-C12
30	s	401	PLX	C9-C10-C11-C12
31	i	401	CDL	C11-C12-C13-C14
30	U	101	PLX	C7-C8-C9-C10
30	b	201	PLX	C25-C26-C27-C28
30	g	201	PLX	C10-C11-C12-C13
31	l	703	CDL	C51-C52-C53-C54
31	i	401	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
31	i	401	CDL	C51-CB5-OB6-CB4
31	V	201	CDL	CB5-C51-C52-C53
30	V	203	PLX	C11-C12-C13-C14
32	W	201	PEE	C23-C24-C25-C26
31	i	401	CDL	CB5-C51-C52-C53
30	r	502	PLX	C20-C21-C22-C23
30	r	502	PLX	C36-C37-C38-C39
30	g	201	PLX	C32-C33-C34-C35
31	n	101	CDL	C51-C52-C53-C54
30	g	202	PLX	C9-C10-C11-C12
31	l	703	CDL	OA9-CA7-OA8-CA6
31	i	401	CDL	C73-C74-C75-C76
32	V	202	PEE	C31-C32-C33-C34
32	l	701	PEE	C20-C21-C22-C23
30	s	401	PLX	C12-C13-C14-C15
32	V	202	PEE	C34-C35-C36-C37
30	g	203	PLX	C10-C11-C12-C13
30	r	502	PLX	C26-C27-C28-C29
32	l	701	PEE	C15-C16-C17-C18
32	l	702	PEE	C19-C20-C21-C22
32	l	702	PEE	C31-C32-C33-C34
31	l	703	CDL	C33-C34-C35-C36
30	g	202	PLX	C11-C12-C13-C14
32	l	701	PEE	C16-C17-C18-C19
33	p	201	8Q1	C7-C8-C9-C10
31	i	401	CDL	C32-C33-C34-C35
31	i	401	CDL	C34-C35-C36-C37
30	r	501	PLX	C35-C36-C37-C38
31	l	704	CDL	CB2-C1-CA2-OA2
30	b	201	PLX	C30-C31-C32-C33
32	W	201	PEE	C43-C44-C45-C46
32	l	701	PEE	C13-C14-C15-C16
32	l	701	PEE	C41-C42-C43-C44
31	n	101	CDL	C71-C72-C73-C74
32	V	202	PEE	C43-C44-C45-C46
30	b	201	PLX	C32-C33-C34-C35
31	V	201	CDL	C14-C15-C16-C17
33	p	201	8Q1	C12-C13-C14-C15
30	g	203	PLX	C35-C36-C37-C38
30	r	501	PLX	C26-C27-C28-C29
32	V	202	PEE	C19-C20-C21-C22
32	W	201	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
31	l	704	CDL	OB5-CB3-CB4-CB6
32	l	701	PEE	O3P-C1-C2-C3
32	l	701	PEE	C23-C24-C25-C26
30	r	502	PLX	C7-C8-C9-C10
32	W	201	PEE	C41-C42-C43-C44
31	i	401	CDL	OB9-CB7-OB8-CB6
30	U	101	PLX	O8-C24-C25-C26
30	r	501	PLX	C3-C4-C5-O8
31	l	703	CDL	CA3-CA4-CA6-OA8
33	p	201	8Q1	C13-C14-C15-C16
30	g	202	PLX	C26-C27-C28-C29
31	n	101	CDL	C33-C34-C35-C36
30	r	502	PLX	C35-C36-C37-C38
32	l	701	PEE	C2-C1-O3P-P
31	i	401	CDL	OB7-CB5-OB6-CB4
30	s	401	PLX	C29-C30-C31-C32
30	s	401	PLX	C11-C10-C9-C8
30	r	501	PLX	C9-C10-C11-C12
30	b	201	PLX	C11-C12-C13-C14
30	g	202	PLX	C11-C10-C9-C8
30	s	401	PLX	C15-C16-C17-C18
31	l	704	CDL	C13-C14-C15-C16
31	n	101	CDL	C34-C35-C36-C37
32	l	701	PEE	C40-C41-C42-C43
30	r	502	PLX	C17-C18-C19-C20
31	V	201	CDL	OA5-CA3-CA4-OA6
30	r	502	PLX	C15-C16-C17-C18
30	r	501	PLX	C18-C19-C20-C21
32	l	702	PEE	C42-C43-C44-C45
31	V	201	CDL	C12-C13-C14-C15
32	W	201	PEE	C33-C34-C35-C36
32	W	201	PEE	O2-C2-C3-O3
31	i	401	CDL	C35-C36-C37-C38
32	V	202	PEE	C41-C42-C43-C44
32	l	701	PEE	C42-C43-C44-C45
30	g	201	PLX	C26-C27-C28-C29
32	l	702	PEE	C44-C45-C46-C47
33	p	201	8Q1	C30-C29-C32-O33
32	W	201	PEE	C44-C45-C46-C47
32	l	702	PEE	C12-C13-C14-C15
30	b	201	PLX	C20-C21-C22-C23
30	r	502	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	V	203	PLX	C7-C8-C9-C10
30	U	101	PLX	C11-C10-C9-C8
30	U	101	PLX	C26-C27-C28-C29
31	l	703	CDL	OB5-CB3-CB4-CB6
32	W	201	PEE	O3P-C1-C2-C3
32	l	702	PEE	C11-C10-O2-C2
31	l	703	CDL	C75-C76-C77-C78
30	g	201	PLX	C27-C28-C29-C30
30	V	203	PLX	C16-C17-C18-C19
31	V	201	CDL	C72-C73-C74-C75
31	i	401	CDL	C52-C51-CB5-OB6
32	W	201	PEE	C34-C35-C36-C37
30	b	201	PLX	C36-C37-C38-C39
30	V	203	PLX	C12-C13-C14-C15
31	V	201	CDL	CB3-CB4-CB6-OB8
31	i	401	CDL	CA3-CA4-CA6-OA8
32	W	201	PEE	C1-C2-C3-O3
30	g	201	PLX	C17-C18-C19-C20
30	r	501	PLX	C25-C26-C27-C28
31	V	201	CDL	C52-C53-C54-C55
30	V	203	PLX	C31-C32-C33-C34
30	s	401	PLX	C30-C31-C32-C33
30	b	201	PLX	C11-C10-C9-C8
30	U	101	PLX	C28-C29-C30-C31
30	U	101	PLX	C27-C28-C29-C30
31	l	704	CDL	OA5-CA3-CA4-OA6
30	b	201	PLX	C13-C14-C15-C16
31	l	703	CDL	OA6-CA4-CA6-OA8
30	r	502	PLX	C27-C28-C29-C30
33	p	201	8Q1	C10-C11-C12-C13
30	r	501	PLX	C28-C29-C30-C31
32	W	201	PEE	C13-C14-C15-C16
31	V	201	CDL	C53-C54-C55-C56
30	b	201	PLX	C35-C36-C37-C38
30	V	203	PLX	C26-C27-C28-C29
32	W	201	PEE	C11-C10-O2-C2
31	V	201	CDL	C12-C11-CA5-OA6
31	l	704	CDL	C73-C74-C75-C76
30	g	201	PLX	C20-C21-C22-C23
30	r	501	PLX	C19-C20-C21-C22
30	s	401	PLX	C11-C12-C13-C14
31	l	703	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	W	201	PEE	O4-C10-O2-C2
32	l	702	PEE	O4-C10-O2-C2
30	g	202	PLX	O4-C3-C4-O6
31	V	201	CDL	OB5-CB3-CB4-OB6
31	l	703	CDL	OA5-CA3-CA4-OA6
30	g	201	PLX	C3-C4-C5-O8
30	g	202	PLX	C30-C31-C32-C33
30	b	201	PLX	C1-C2-O1-P1
30	g	203	PLX	C1-C2-O1-P1
31	n	101	CDL	CA5-C11-C12-C13
30	s	401	PLX	C32-C33-C34-C35
30	b	201	PLX	O6-C4-C5-O8
30	r	501	PLX	O6-C4-C5-O8
31	V	201	CDL	OA6-CA4-CA6-OA8
31	V	201	CDL	OB6-CB4-CB6-OB8
32	l	701	PEE	C31-C32-C33-C34
30	r	501	PLX	C30-C31-C32-C33
30	r	502	PLX	C24-C25-C26-C27
32	V	202	PEE	C33-C34-C35-C36
32	V	202	PEE	C32-C33-C34-C35
31	V	201	CDL	C75-C76-C77-C78
31	l	704	CDL	C12-C13-C14-C15
30	g	202	PLX	O7-C6-C7-C8
30	r	502	PLX	C34-C35-C36-C37
30	U	101	PLX	C25-C24-O8-C5
30	r	501	PLX	C25-C24-O8-C5
30	g	201	PLX	C35-C36-C37-C38
32	l	702	PEE	C11-C12-C13-C14
30	g	202	PLX	O4-C3-C4-C5
31	V	201	CDL	OA5-CA3-CA4-CA6
31	V	201	CDL	OB5-CB3-CB4-CB6
31	l	703	CDL	OA5-CA3-CA4-CA6
31	l	704	CDL	OA5-CA3-CA4-CA6
33	p	201	8Q1	O27-C28-C29-C31
30	r	501	PLX	C31-C32-C33-C34
31	n	101	CDL	C11-C12-C13-C14
32	W	201	PEE	C31-C32-C33-C34
30	r	501	PLX	C15-C16-C17-C18
32	l	701	PEE	C24-C25-C26-C27
30	r	502	PLX	O8-C24-C25-C26
31	l	704	CDL	OB5-CB3-CB4-OB6
32	l	701	PEE	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
31	n	101	CDL	C35-C36-C37-C38
30	g	203	PLX	C19-C20-C21-C22
30	V	203	PLX	C19-C20-C21-C22
31	V	201	CDL	C74-C75-C76-C77
30	g	203	PLX	O6-C4-C5-O8
30	r	502	PLX	O6-C4-C5-O8
31	l	704	CDL	OA6-CA4-CA6-OA8
30	g	203	PLX	C3-C4-C5-O8
30	r	502	PLX	C3-C4-C5-O8
30	V	203	PLX	C14-C15-C16-C17
30	V	203	PLX	C3-O4-P1-O2
30	b	201	PLX	C3-O4-P1-O2
30	g	202	PLX	C3-C4-O6-C6
30	g	202	PLX	C5-C4-O6-C6
30	g	202	PLX	C3-O4-P1-O1
30	g	202	PLX	C3-O4-P1-O2
30	g	202	PLX	C3-O4-P1-O3
30	r	502	PLX	C2-O1-P1-O3
31	i	401	CDL	CB2-OB2-PB2-OB3
31	i	401	CDL	CB3-OB5-PB2-OB2
31	l	703	CDL	CA2-OA2-PA1-OA4
31	l	704	CDL	CA3-OA5-PA1-OA3
31	l	704	CDL	CB3-OB5-PB2-OB3
31	n	101	CDL	CA3-OA5-PA1-OA3
32	V	202	PEE	C1-O3P-P-O1P
32	l	701	PEE	C4-O4P-P-O3P
32	l	701	PEE	O4P-C4-C5-N
32	l	702	PEE	C4-O4P-P-O1P
30	g	203	PLX	C4-C3-O4-P1
30	r	501	PLX	C4-C3-O4-P1
30	r	502	PLX	C4-C3-O4-P1
31	l	704	CDL	CA4-CA3-OA5-PA1
30	U	101	PLX	C36-C37-C38-C39
32	W	201	PEE	C10-C11-C12-C13
31	V	201	CDL	CA3-CA4-OA6-CA5
31	l	703	CDL	CB6-CB4-OB6-CB5
31	l	704	CDL	CA6-CA4-OA6-CA5
32	l	701	PEE	C3-C2-O2-C10
32	l	702	PEE	C3-C2-O2-C10
30	s	401	PLX	C20-C21-C22-C23
31	l	704	CDL	C15-C16-C17-C18
30	r	502	PLX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	n	101	CDL	C73-C74-C75-C76
30	g	201	PLX	C14-C15-C16-C17
32	V	202	PEE	C11-C10-O2-C2
31	V	201	CDL	C55-C56-C57-C58
32	V	202	PEE	C35-C36-C37-C38
31	i	401	CDL	C32-C31-CA7-OA8
31	n	101	CDL	C53-C54-C55-C56
30	V	203	PLX	C6-C7-C8-C9
30	g	201	PLX	C24-C25-C26-C27
30	s	401	PLX	C6-C7-C8-C9
31	n	101	CDL	C15-C16-C17-C18
31	V	201	CDL	CB7-C71-C72-C73
30	r	501	PLX	O7-C6-C7-C8
30	V	203	PLX	O6-C6-C7-C8
30	g	201	PLX	O6-C6-C7-C8
30	r	501	PLX	C11-C10-C9-C8
30	b	201	PLX	C28-C29-C30-C31
32	V	202	PEE	C23-C24-C25-C26
30	V	203	PLX	C29-C30-C31-C32
31	l	703	CDL	CA7-C31-C32-C33
31	l	703	CDL	C34-C35-C36-C37
30	g	202	PLX	C15-C16-C17-C18
32	V	202	PEE	O4-C10-O2-C2
32	l	702	PEE	C23-C24-C25-C26
31	l	704	CDL	C1-CB2-OB2-PB2
30	V	203	PLX	C3-C4-C5-O8
30	g	201	PLX	C19-C20-C21-C22
30	g	201	PLX	C25-C26-C27-C28
31	V	201	CDL	C11-C12-C13-C14
32	W	201	PEE	C11-C12-C13-C14
31	i	401	CDL	C1-CB2-OB2-PB2
31	i	401	CDL	CB4-CB3-OB5-PB2
30	g	201	PLX	O6-C4-C5-O8
32	V	202	PEE	C21-C22-C23-C24
31	i	401	CDL	C72-C71-CB7-OB8
30	V	203	PLX	C24-C25-C26-C27
30	V	203	PLX	C33-C34-C35-C36
31	l	703	CDL	CB5-C51-C52-C53
30	b	201	PLX	C3-C4-C5-O8
31	l	704	CDL	CA3-CA4-CA6-OA8
30	s	401	PLX	O9-C24-C25-C26
31	i	401	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
30	s	401	PLX	C7-C8-C9-C10
30	g	201	PLX	O4-C3-C4-O6
30	r	502	PLX	C28-C29-C30-C31
31	l	703	CDL	CA4-CA3-OA5-PA1
31	V	201	CDL	C73-C74-C75-C76
30	g	202	PLX	C16-C17-C18-C19
32	W	201	PEE	C1-C2-O2-C10
32	W	201	PEE	C35-C36-C37-C38
30	g	202	PLX	C27-C28-C29-C30
31	V	201	CDL	CA3-CA4-CA6-OA8
32	l	701	PEE	C38-C39-C40-C41
30	V	203	PLX	C35-C36-C37-C38
30	s	401	PLX	C14-C15-C16-C17
31	l	704	CDL	C32-C31-CA7-OA8
31	l	703	CDL	C32-C31-CA7-OA8
30	r	502	PLX	C33-C34-C35-C36
31	l	704	CDL	C35-C36-C37-C38
32	V	202	PEE	C30-C31-C32-C33
30	b	201	PLX	C24-C25-C26-C27
32	l	702	PEE	C1-C2-C3-O3
30	b	201	PLX	C25-C24-O8-C5
30	g	202	PLX	C25-C24-O8-C5
32	l	702	PEE	C18-C19-C20-C21
32	l	702	PEE	C22-C23-C24-C25
30	V	203	PLX	C17-C18-C19-C20
33	p	201	8Q1	O27-C28-C29-C30
31	l	703	CDL	C32-C33-C34-C35
31	V	201	CDL	C12-C11-CA5-OA7
30	s	401	PLX	C4-C3-O4-P1
30	g	202	PLX	C6-C7-C8-C9
30	g	202	PLX	C24-C25-C26-C27
32	l	701	PEE	C33-C34-C35-C36
31	l	703	CDL	C32-C31-CA7-OA9
32	V	202	PEE	C39-C40-C41-C42
32	l	702	PEE	C41-C42-C43-C44
30	V	203	PLX	C15-C16-C17-C18
30	r	501	PLX	C14-C15-C16-C17
30	U	101	PLX	O9-C24-O8-C5
30	s	401	PLX	O9-C24-O8-C5
32	l	701	PEE	C11-C12-C13-C14
31	l	704	CDL	C32-C31-CA7-OA9
30	g	201	PLX	C4-C5-O8-C24

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Mol	Chain	Res	Type	Atoms
32	l	702	PEE	O2-C2-C3-O3
33	p	201	8Q1	O33-C32-C34-N36
30	g	203	PLX	C36-C37-C38-C39
32	l	702	PEE	C32-C33-C34-C35
30	V	203	PLX	C34-C35-C36-C37
31	l	704	CDL	C74-C75-C76-C77
31	l	704	CDL	C52-C51-CB5-OB6

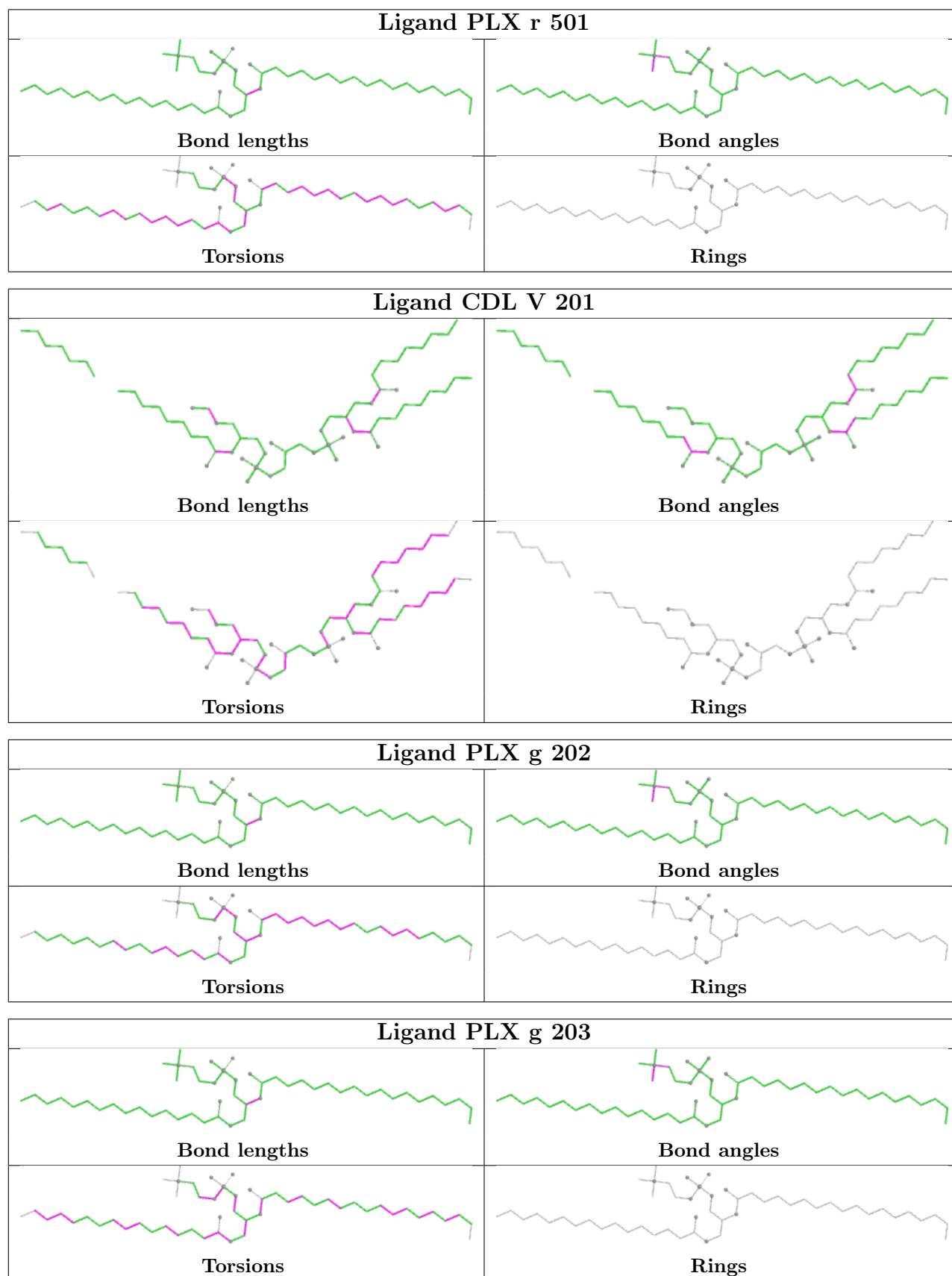
There are no ring outliers.

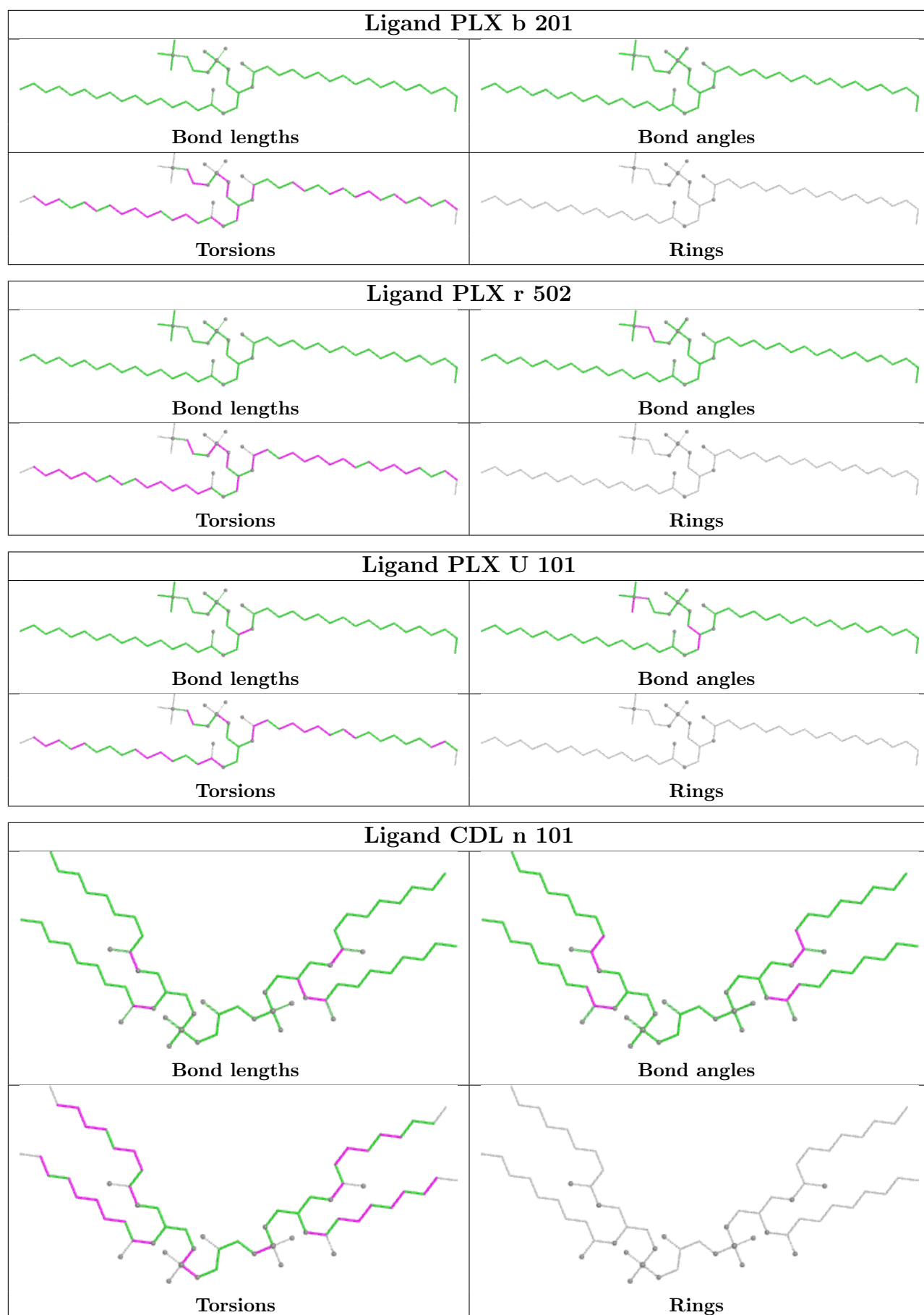
19 monomers are involved in 221 short contacts:

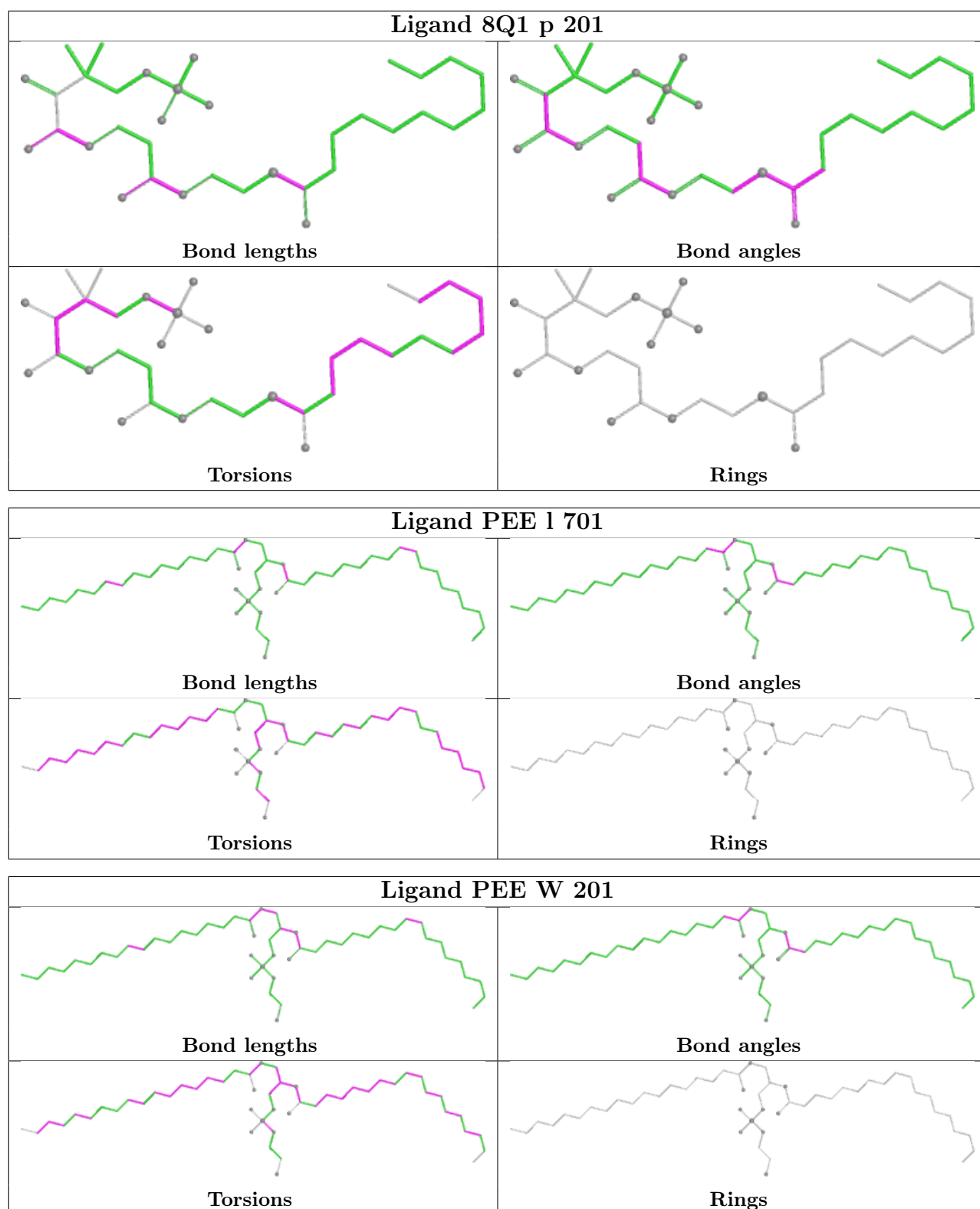
Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	r	501	PLX	6	0
31	V	201	CDL	8	0
30	g	202	PLX	3	0
30	g	203	PLX	8	0
30	b	201	PLX	38	0
30	r	502	PLX	16	0
30	U	101	PLX	3	0
31	n	101	CDL	10	0
33	p	201	8Q1	12	0
32	l	701	PEE	50	0
32	W	201	PEE	18	0
31	l	704	CDL	3	0
31	l	703	CDL	2	0
30	V	203	PLX	5	0
30	s	401	PLX	2	0
32	l	702	PEE	18	0
31	i	401	CDL	3	0
30	g	201	PLX	2	0
32	V	202	PEE	21	0

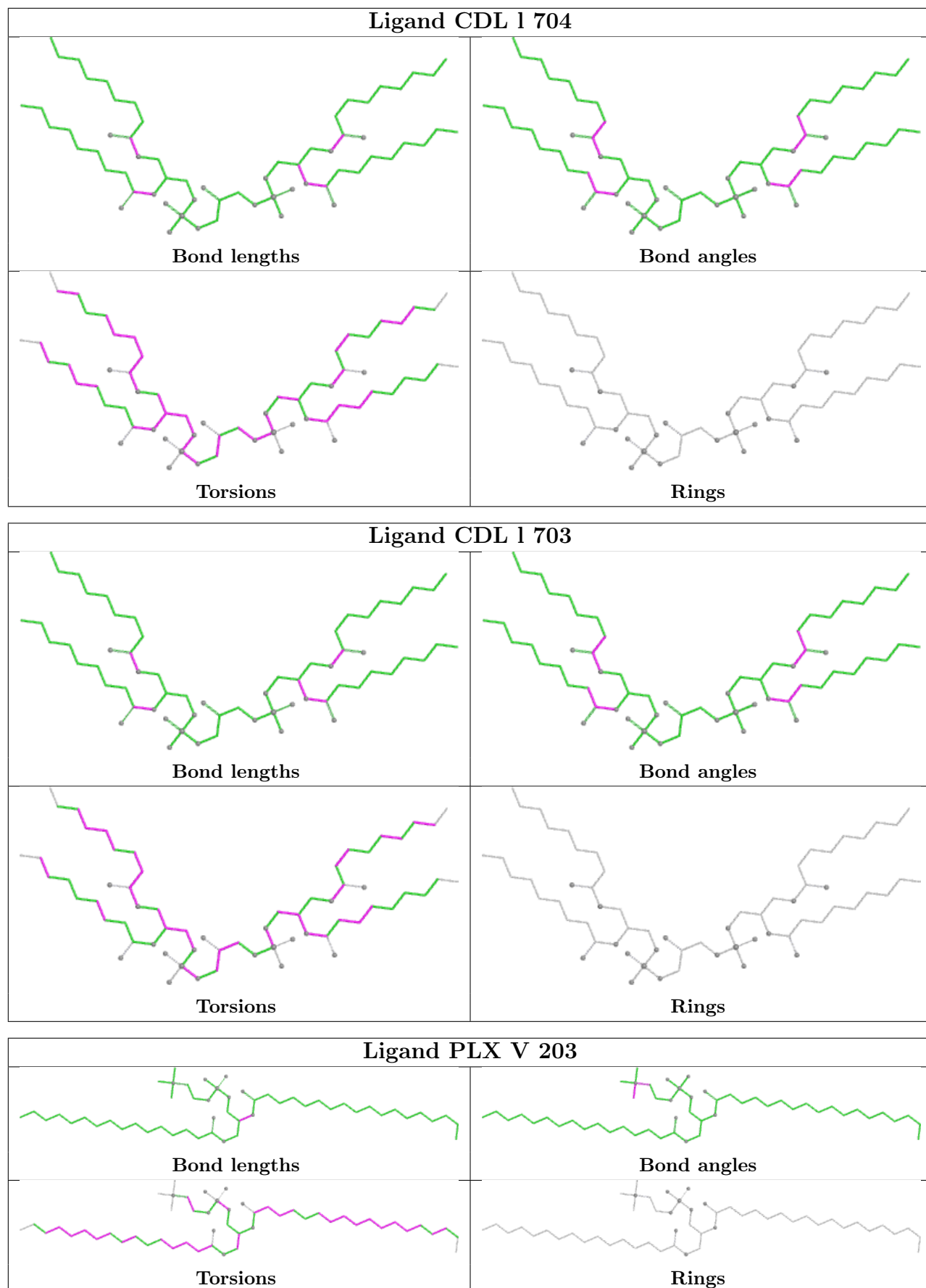
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

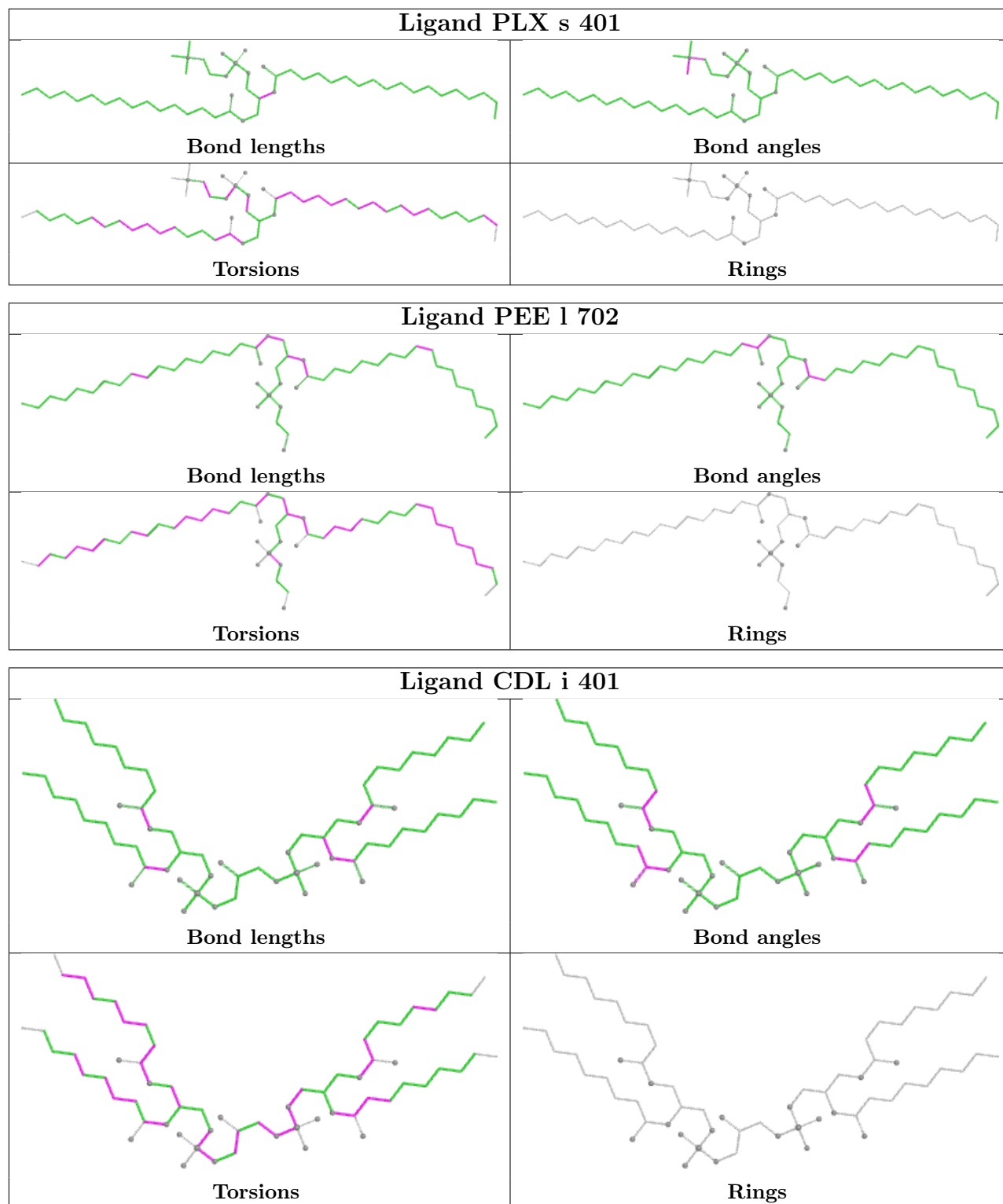
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

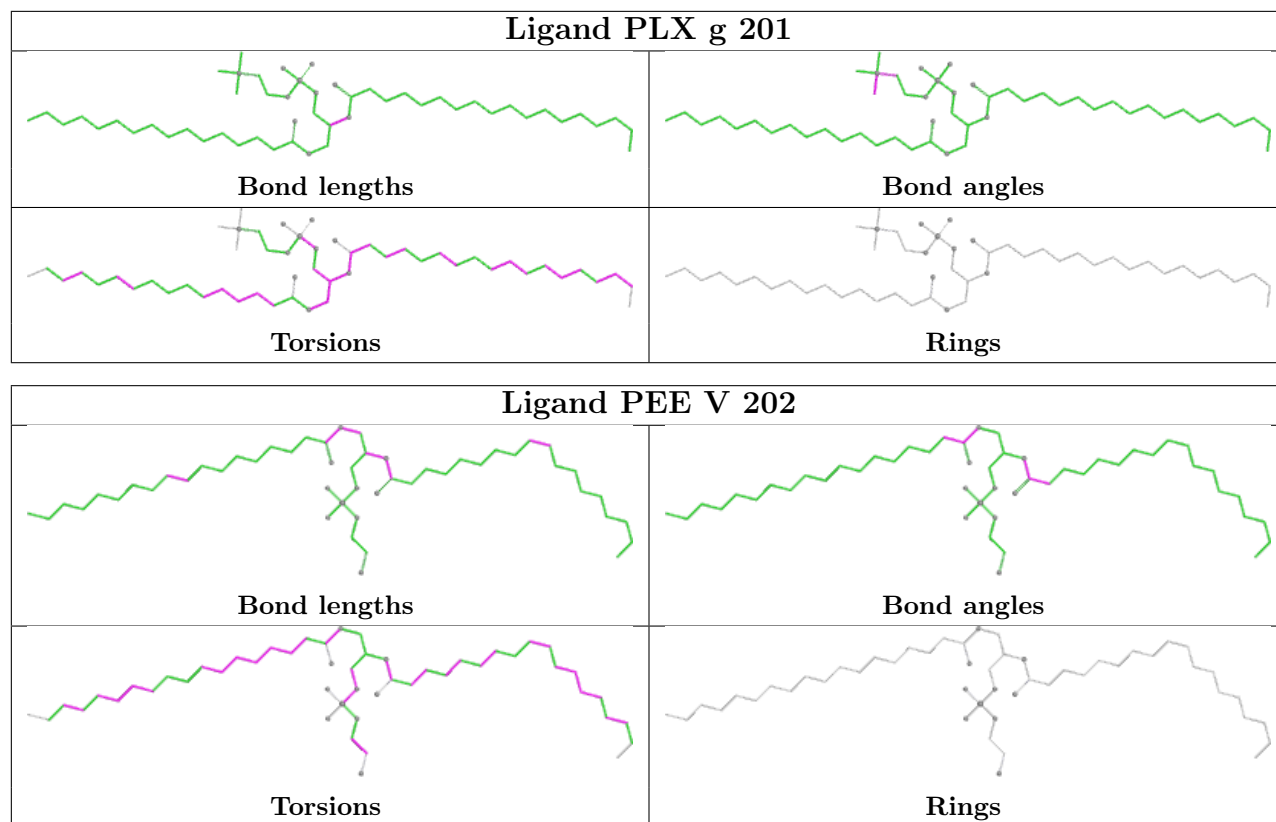












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

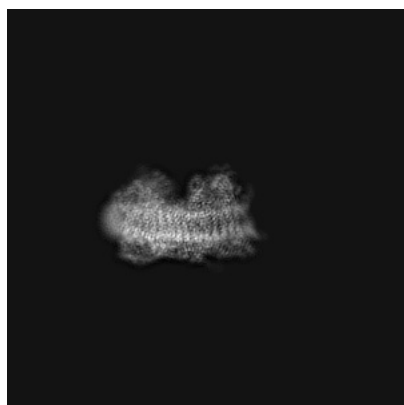
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6772. These allow visual inspection of the internal detail of the map and identification of artifacts.

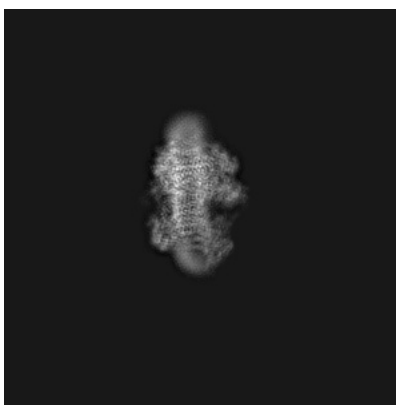
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

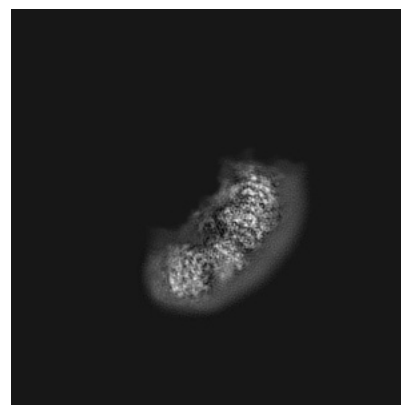
#### 6.1.1 Primary map



X



Y

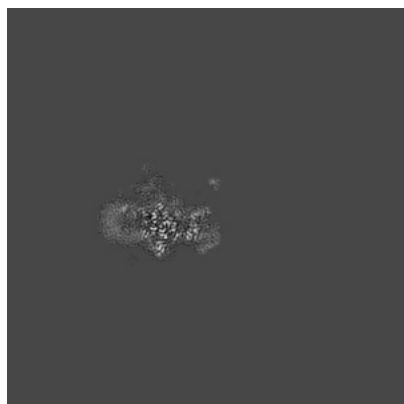


Z

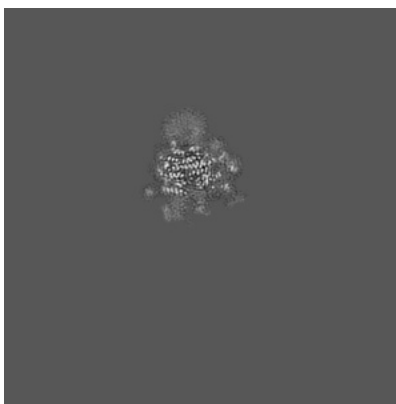
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

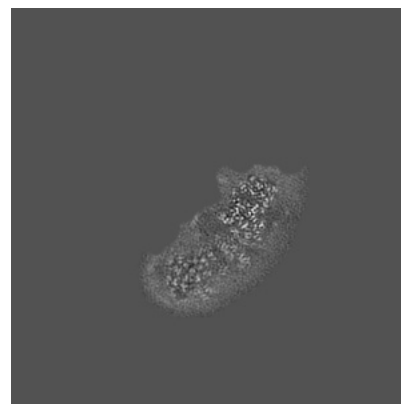
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

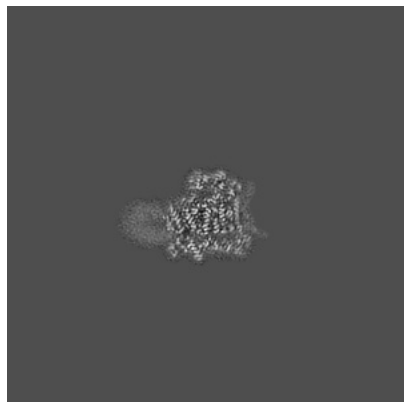


Z Index: 240

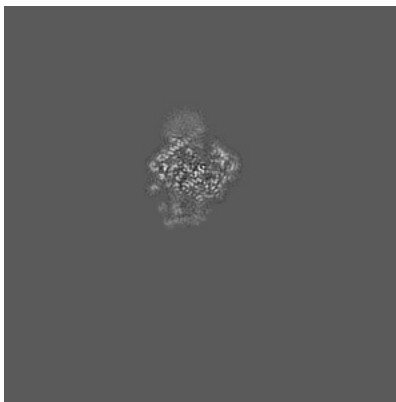
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

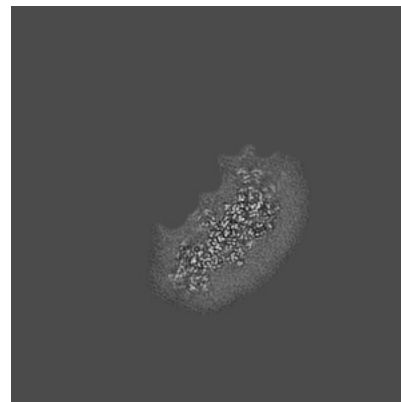
### 6.3.1 Primary map



X Index: 290



Y Index: 232

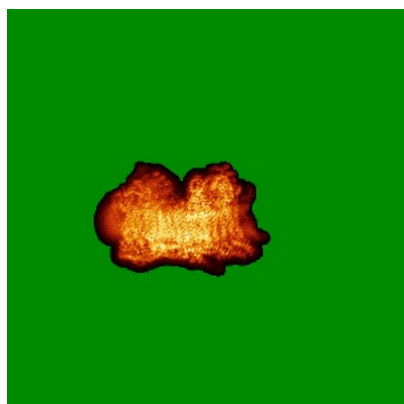


Z Index: 207

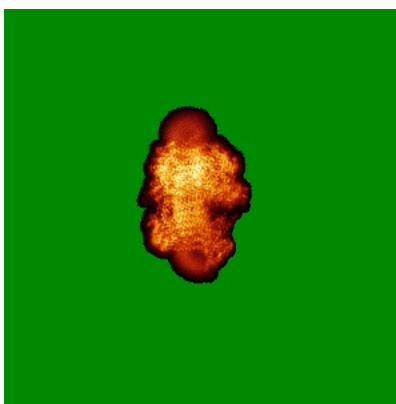
The images above show the largest variance slices of the map in three orthogonal directions.

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

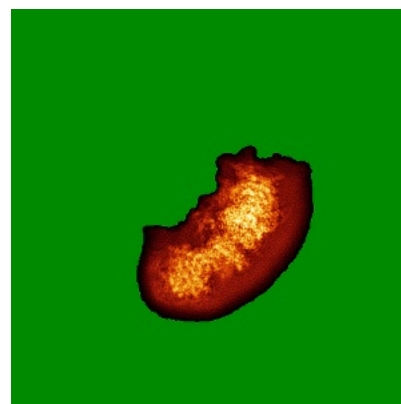
### 6.4.1 Primary map



X



Y

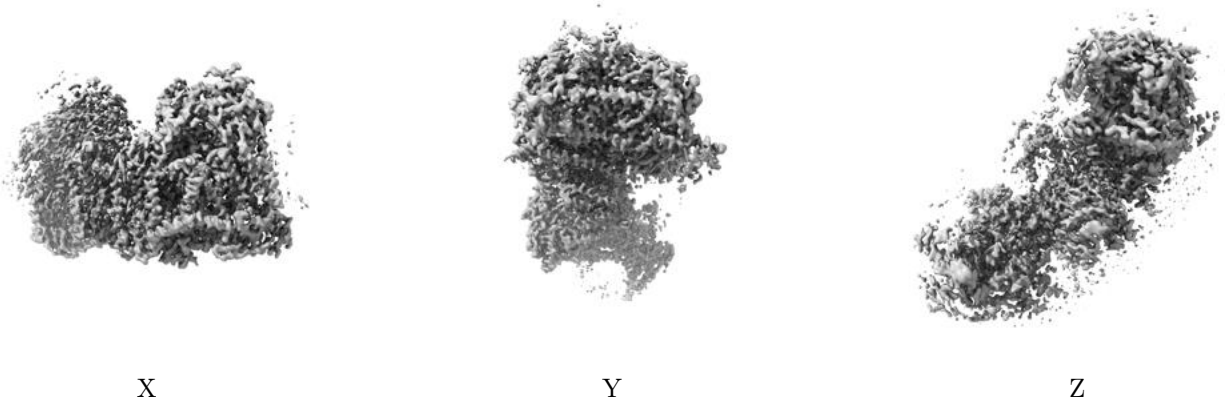


Z

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 0.0677. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

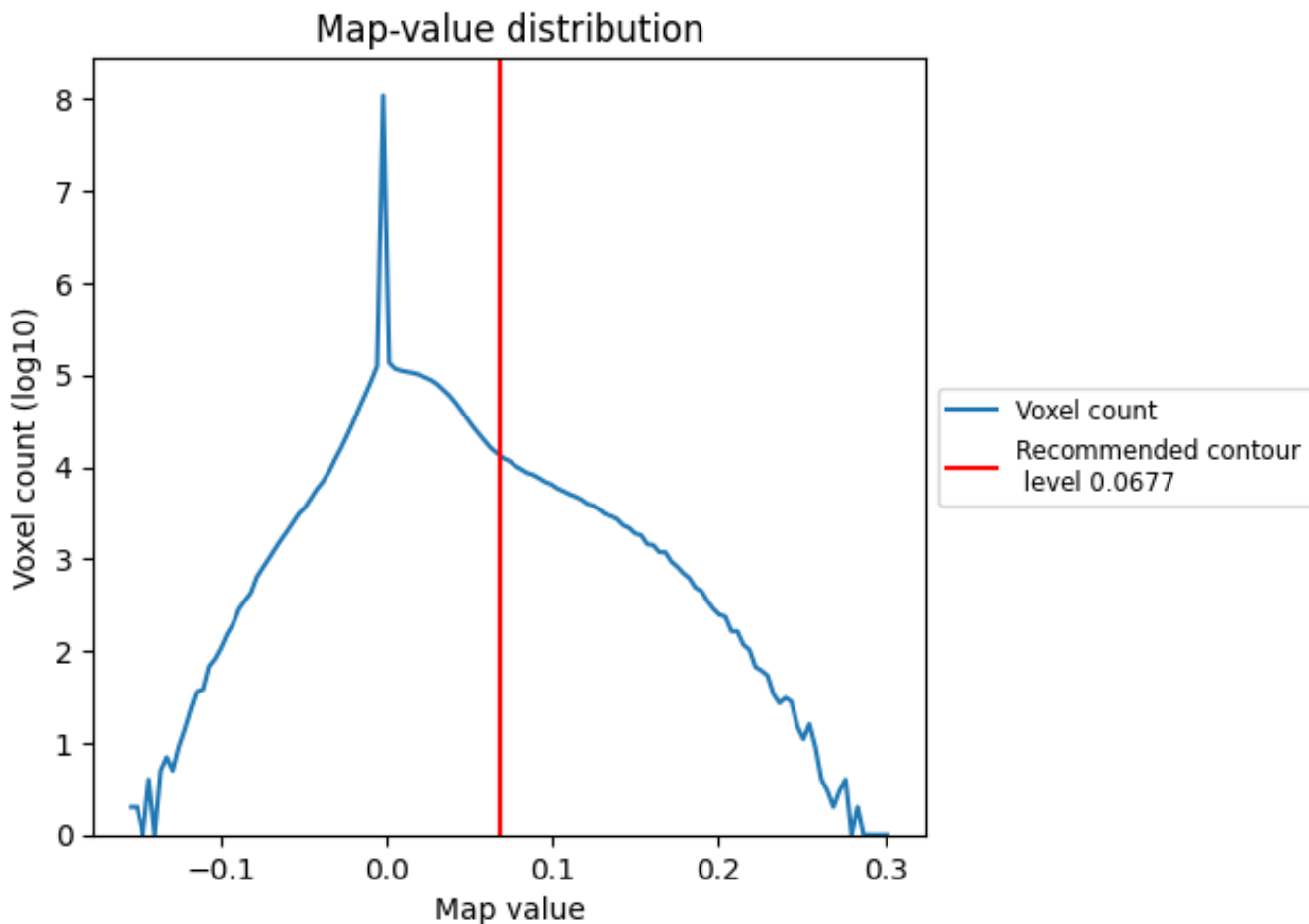
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

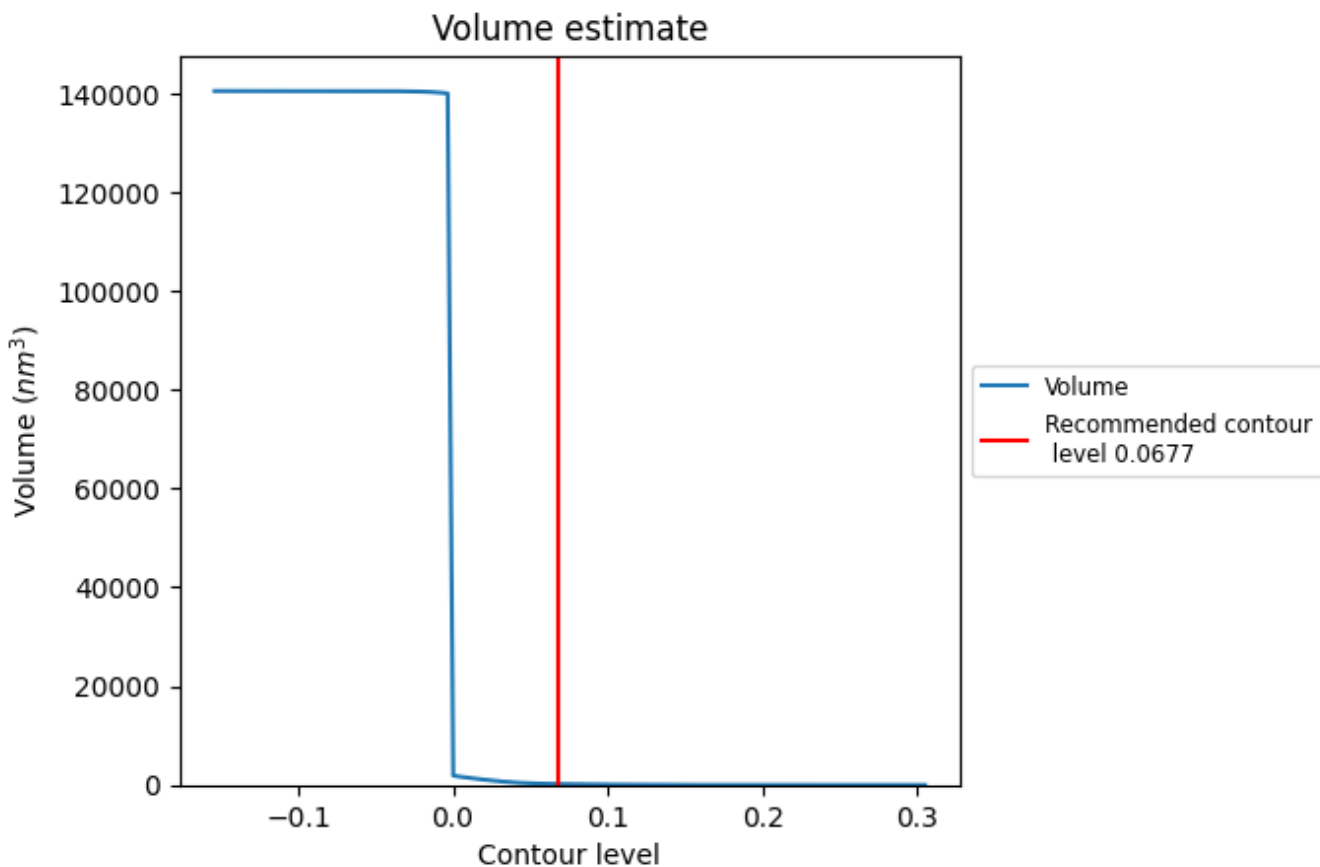
This section contains the results of statistical analysis of the map.

### 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.

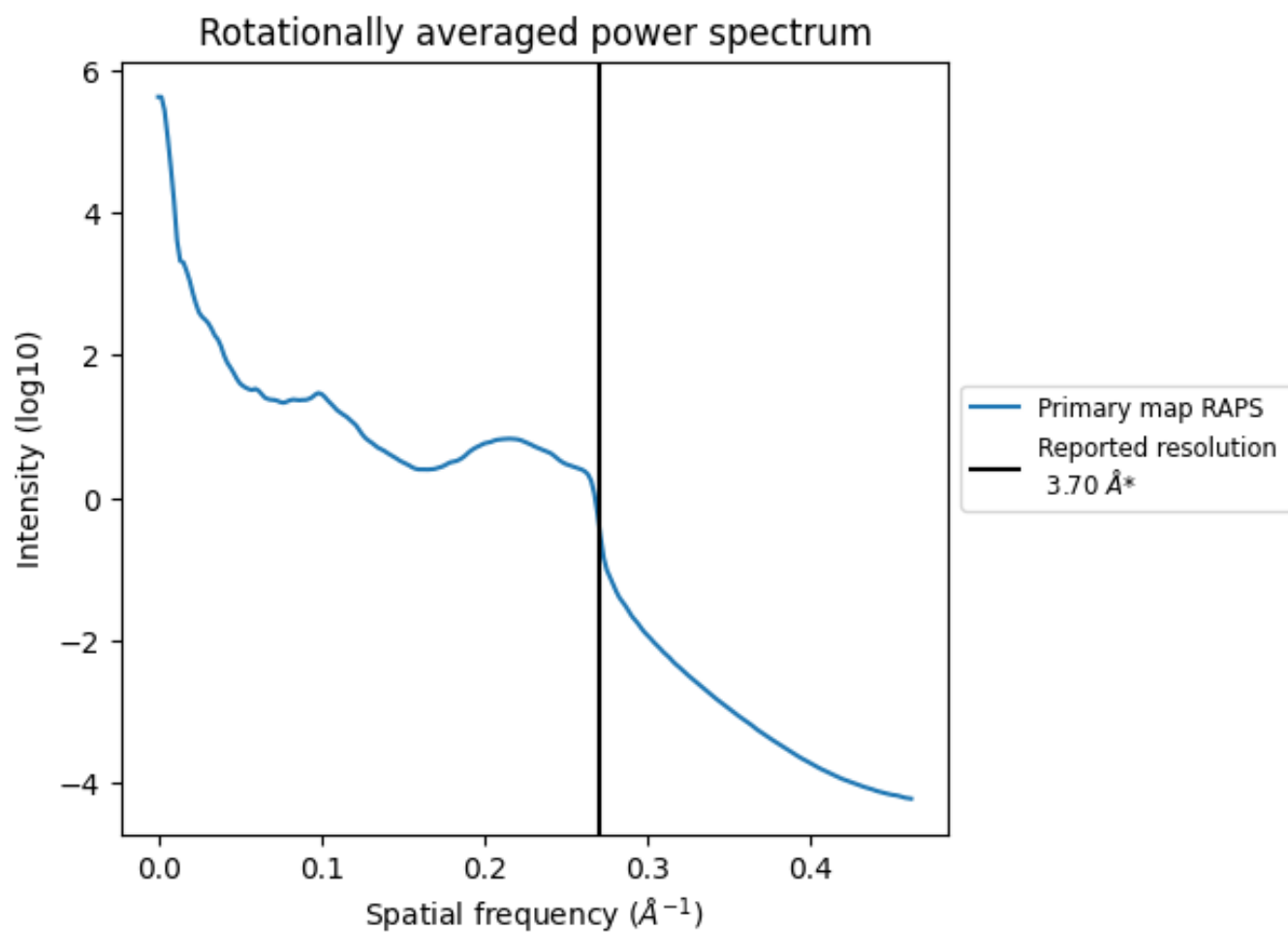
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 198 nm<sup>3</sup>; this corresponds to an approximate mass of 179 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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.270 \text{\AA}^{-1}$

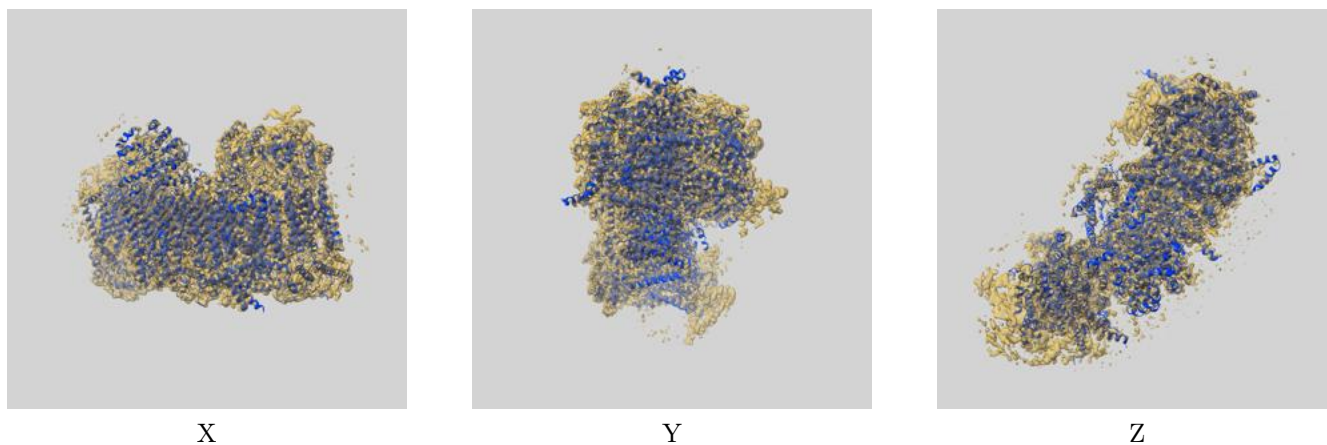
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

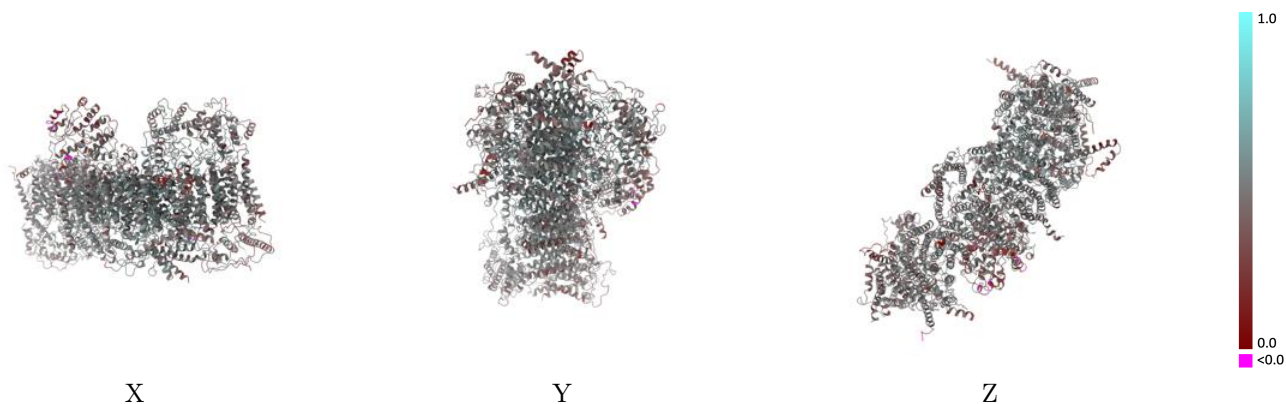
This section contains information regarding the fit between EMDB map EMD-6772 and PDB model 5XTC. Per-residue inclusion information can be found in section 3 on page 13.

### 9.1 Map-model overlay [i](#)



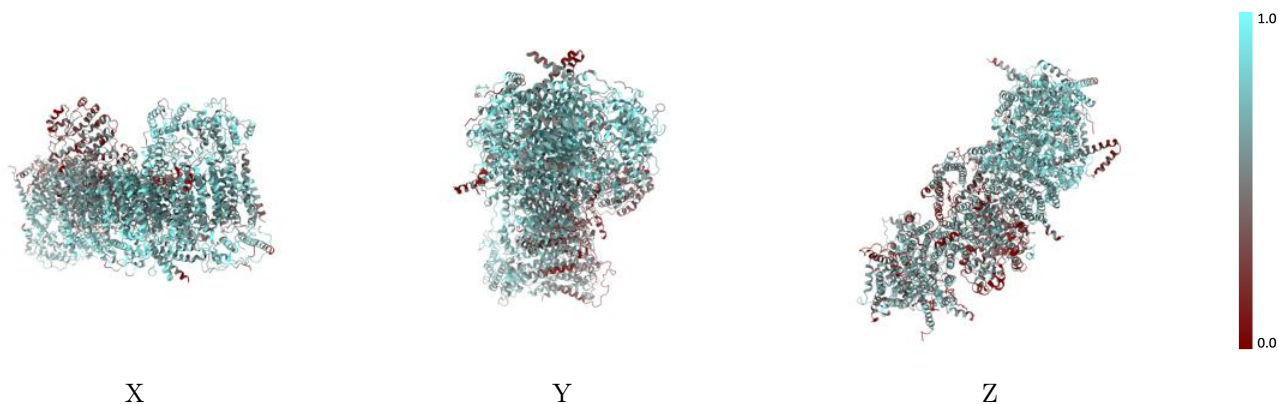
The images above show the 3D surface view of the map at the recommended contour level 0.0677 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



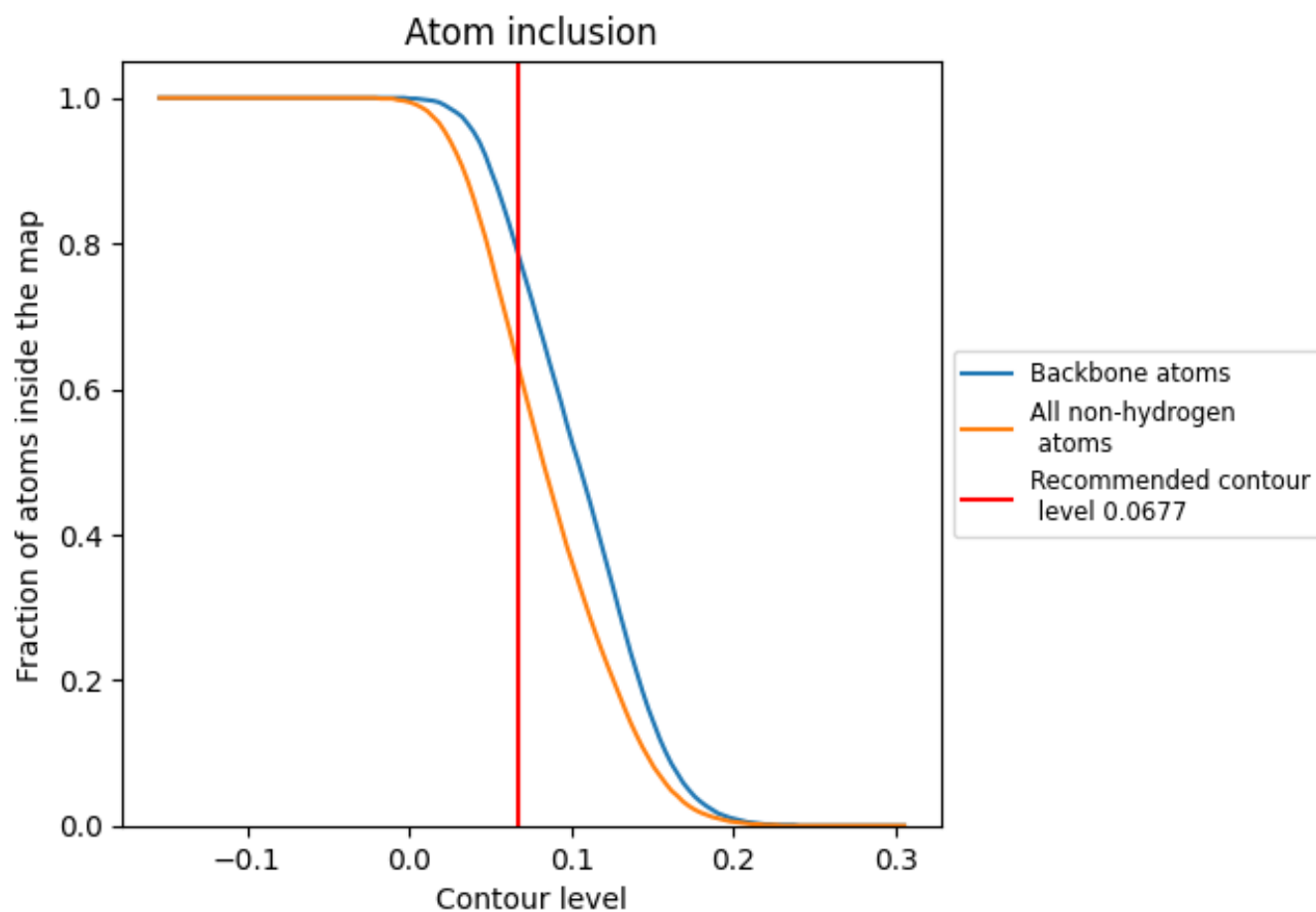
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0677).





























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 63% 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 (0.0677) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6260	 0.4550
Q	 0.1600	 0.3760
S	 0.6490	 0.4460
U	 0.5820	 0.4320
V	 0.4690	 0.4430
W	 0.6980	 0.4530
X	 0.6870	 0.4460
Y	 0.7120	 0.4390
Z	 0.6150	 0.4280
a	 0.7780	 0.4990
b	 0.5620	 0.4050
c	 0.7210	 0.4830
d	 0.7260	 0.4660
e	 0.6580	 0.4670
f	 0.5350	 0.3810
g	 0.6660	 0.4870
h	 0.7160	 0.4550
i	 0.6630	 0.4960
j	 0.4020	 0.3850
k	 0.5780	 0.4600
l	 0.6490	 0.4770
m	 0.5340	 0.4350
n	 0.6050	 0.4470
o	 0.6720	 0.4730
p	 0.7260	 0.4700
r	 0.7260	 0.5070
s	 0.5710	 0.4410
u	 0.6960	 0.4390
v	 0.6050	 0.3870
w	 0.3810	 0.3740

