



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:01 PM UTC

PDB ID : 7W31 / pdb_00007w31
EMDB ID : EMD-32269
Title : Deactive state CI from DQ-NADH dataset, Subclass 1
Authors : Gu, J.K.; Yang, M.J.
Deposited on : 2021-11-24
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

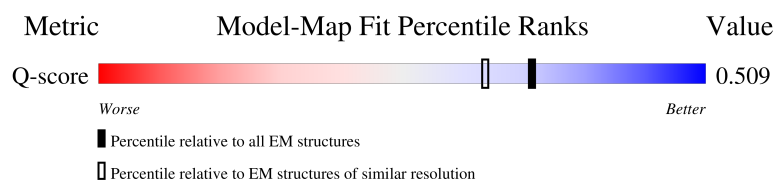
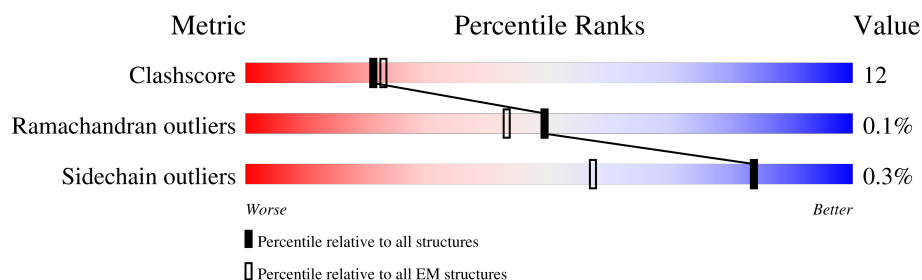
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	433	 72% 28%
2	B	176	 76% 23% .
3	C	156	 79% 21%
4	E	115	 75% 25%

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Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	

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Mol	Chain	Length	Quality of chain
29	f	49	
30	g	122	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	603	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	A	501	-	-	X	-

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 66476 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] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3314	2093	591	610	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1402	882	240	267	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1248	794	227	213	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	115	Total	C	N	O	S	0	0
			968	618	179	166	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			693	447	102	139	5		
6	X	88	Total	C	N	O	S	0	0
			692	447	103	137	5		

- Molecule 7 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			910	588	154	165	3		

- Molecule 8 is a protein called Complex I-B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	97	Total	C	N	O	S	0	0
			780	491	147	139	3		

- Molecule 9 is a protein called NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	331	Total	C	N	O	S	0	0
			2611	1693	459	451	8		

- Molecule 10 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	42	Total	C	N	O	S	0	0
			355	219	67	68	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	125	Total	C	N	O	S	0	0
			1016	642	181	190	3		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	690	Total	C	N	O	S	0	0
			5290	3317	923	1011	39		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	144	Total	C	N	O	S	0	0
			1204	770	218	212	4		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	217	Total	C	N	O	S	0	0
			1636	1042	272	312	10		

- Molecule 15 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	208	Total	C	N	O	S	0	0
			1735	1123	298	312	2		

- Molecule 16 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3377	2162	578	613	24		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 21 is a protein called Complex I-B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	142	Total	C	N	O	S	0	0
			1167	752	200	206	9		

- Molecule 22 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	70	Total	C	N	O	S	0	0
			571	379	88	103	1		

- Molecule 23 is a protein called Complex I-B12.

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

- Molecule 24 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	140	Total	C	N	O	S	0	0
			1159	759	199	198	3		

- Molecule 25 is a protein called Complex I-B17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			847	553	154	139	1		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1287	834	209	236	8		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	107	Total	C	N	O	S	0	0
			889	568	145	172	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	42	Total	C	N	O	0	0
			342	225	58	59		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	121	Total	C	N	O	S	0	0
			1000	650	173	171	6		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	99	Total	C	N	O	S	0	0
			800	545	118	132	5		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4704	3106	738	812	48		

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			915	611	137	159	8		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	128	Total	C	N	O	S	0	0
			1052	686	180	186			

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	178	Total	C	N	O	S	0	0
			1491	954	273	257	7		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	459	Total	C	N	O	S	0	0
			3629	2412	572	607	38		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	s	303	Total	C	N	O	S	0	0
			2394	1607	369	397	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	u	171	Total	C	N	O	S	0	0
			1396	886	250	250	10		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			987	619	178	181	9		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2582	1643	438	491	10		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



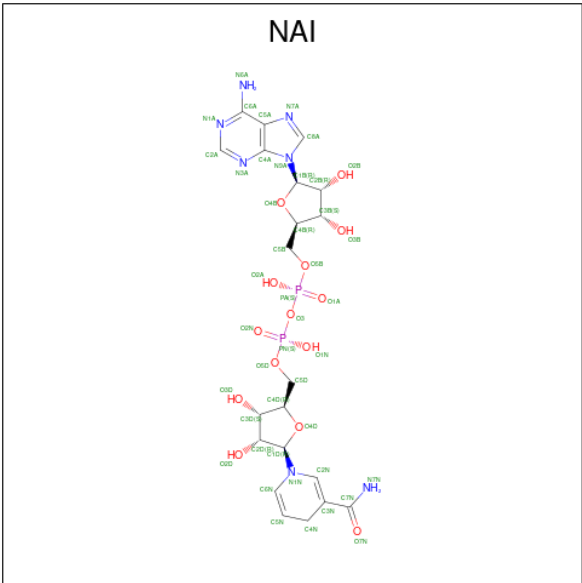
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



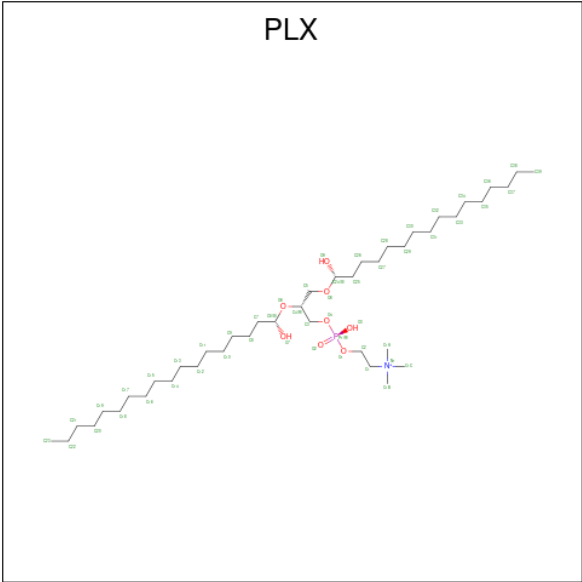
Mol	Chain	Residues	Atoms					AltConf
47	A	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 48 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



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

- Molecule 49 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: C₄₂H₈₉NO₈P).



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

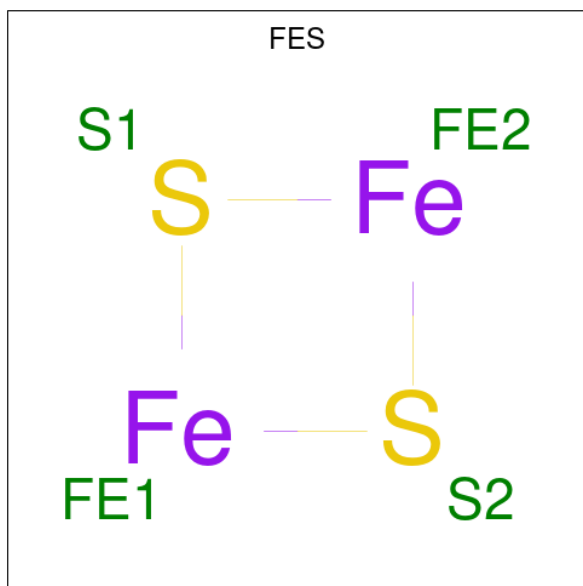
- Molecule 50 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: C₂₃H₄₅N₂O₈PS).



- Molecule 51 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



- Molecule 52 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

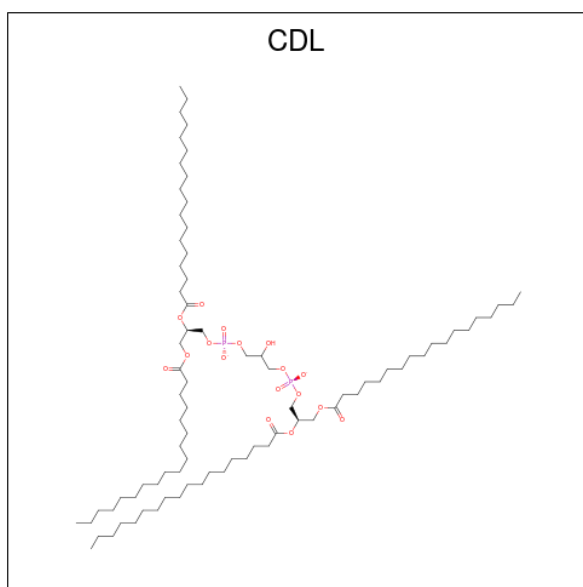


Mol	Chain	Residues	Atoms			AltConf
52	M	1	Total	Fe	S	0
			4	2	2	
52	O	1	Total	Fe	S	0
			4	2	2	

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	M	1	Total	Mg	0
			1	1	

- Molecule 54 is CARDIOLIPIN (CCD ID: CDL) (formula: $\text{C}_{81}\text{H}_{156}\text{O}_{17}\text{P}_2$).

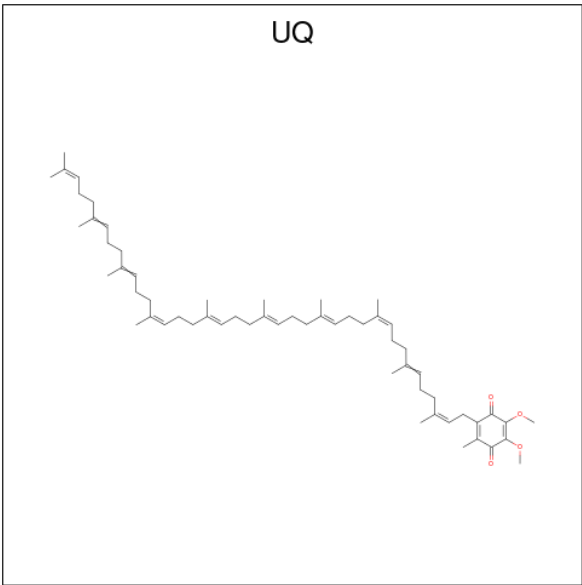


Mol	Chain	Residues	Atoms				AltConf
54	N	1	Total	C	O	P	0
			51	32	17	2	
54	a	1	Total	C	O	P	0
			91	72	17	2	
54	i	1	Total	C	O	P	0
			66	47	17	2	
54	r	1	Total	C	O	P	0
			99	80	17	2	
54	r	1	Total	C	O	P	0
			100	81	17	2	
54	u	1	Total	C	O	P	0
			78	59	17	2	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

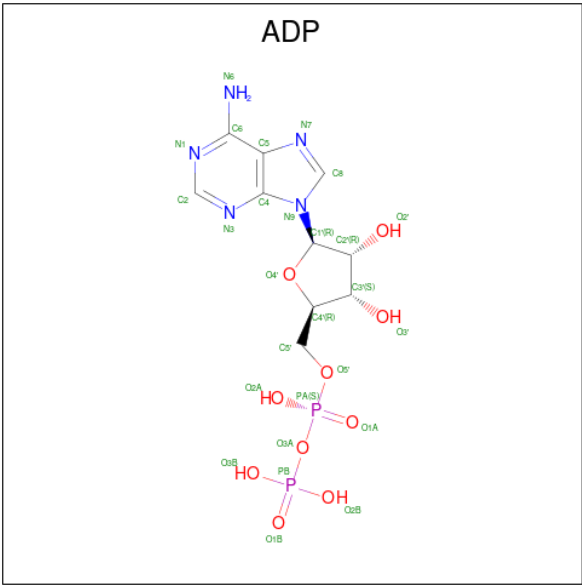
Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

- Molecule 56 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (CCD ID: UQ) (formula: C₅₉H₉₀O₄).



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

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

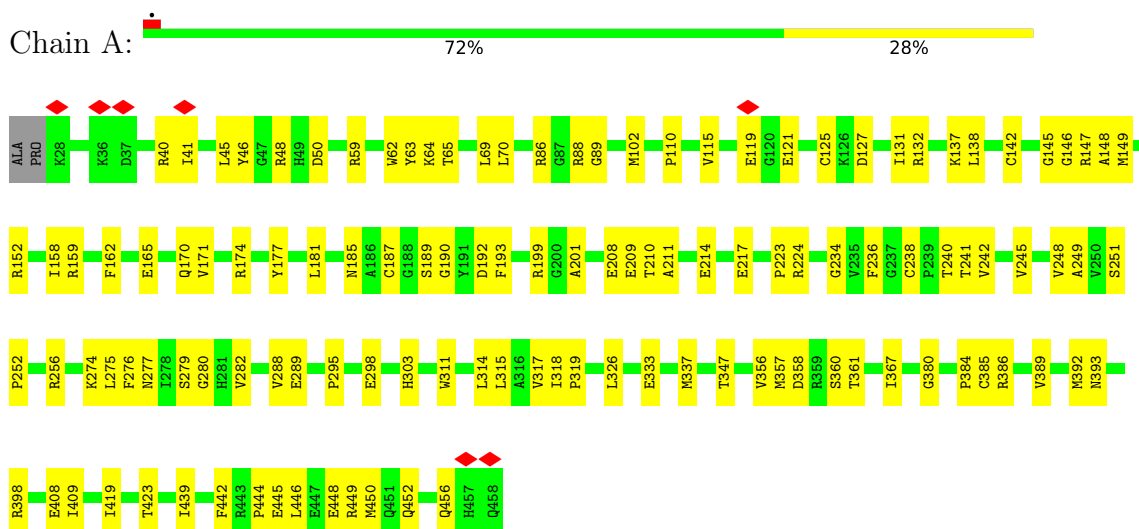


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

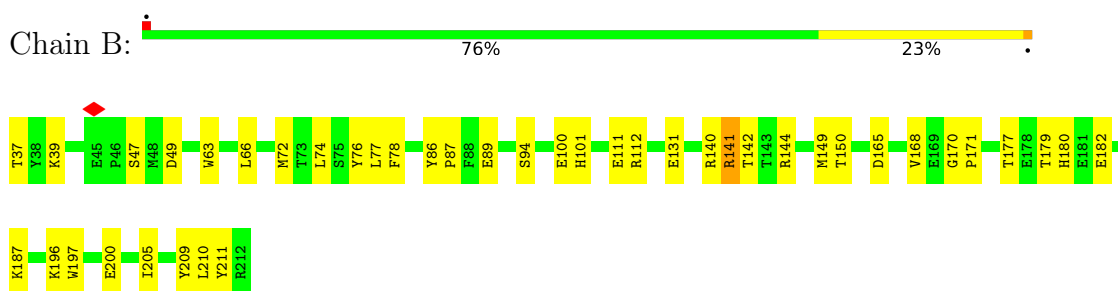
3 Residue-property plots

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

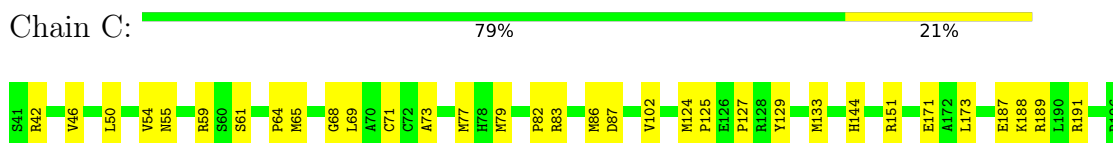
- Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

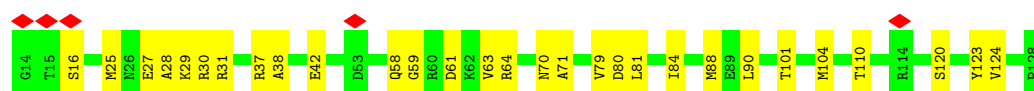


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:  75% 25%



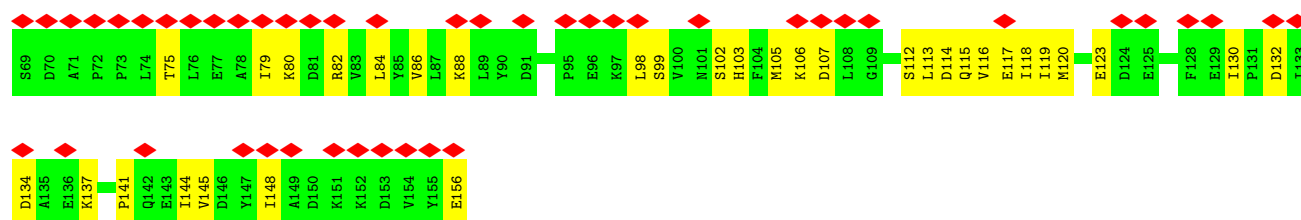
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F:  8% 72% 28%



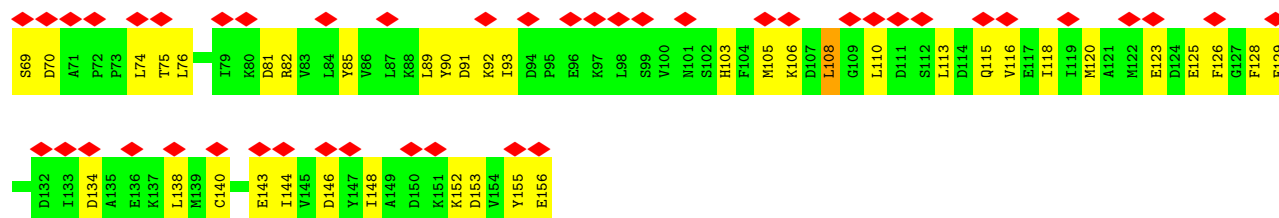
- Molecule 6: Acyl carrier protein

Chain G:  52% 63% 38%



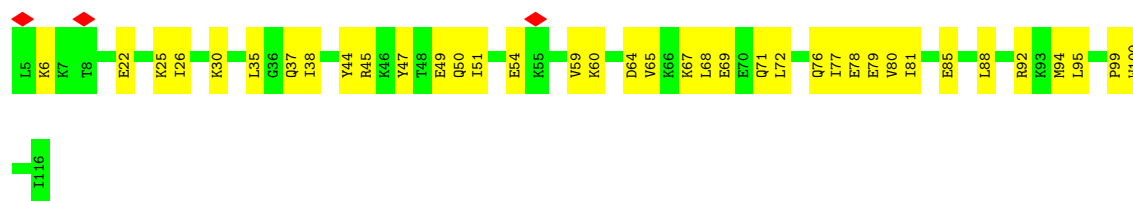
- Molecule 6: Acyl carrier protein

Chain X:  50% 56% 43%



- Molecule 7: Complex I subunit B13

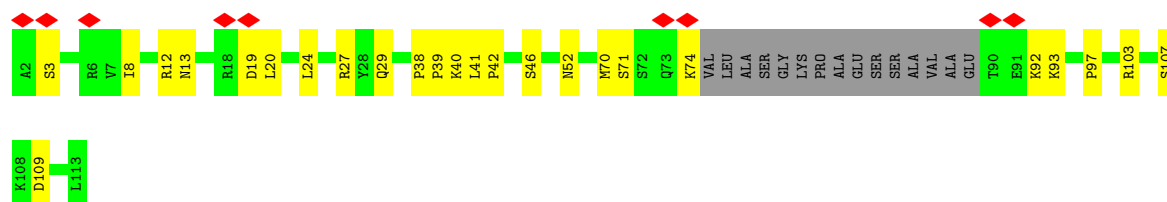
Chain H:  67% 33%



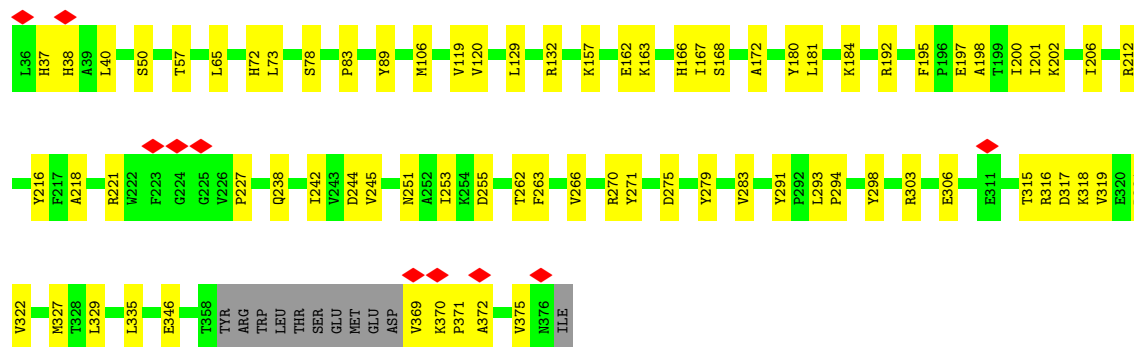
- Molecule 8: Complex I-B14.5a

Chain I:  8% 64% 22% 13%





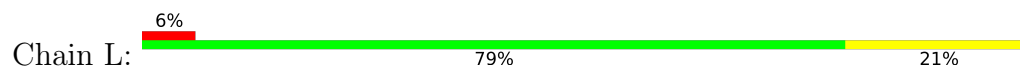
- Molecule 9: NADH dehydrogenase ubiquinone 1 alpha subcomplex subunit 9, mitochondrial



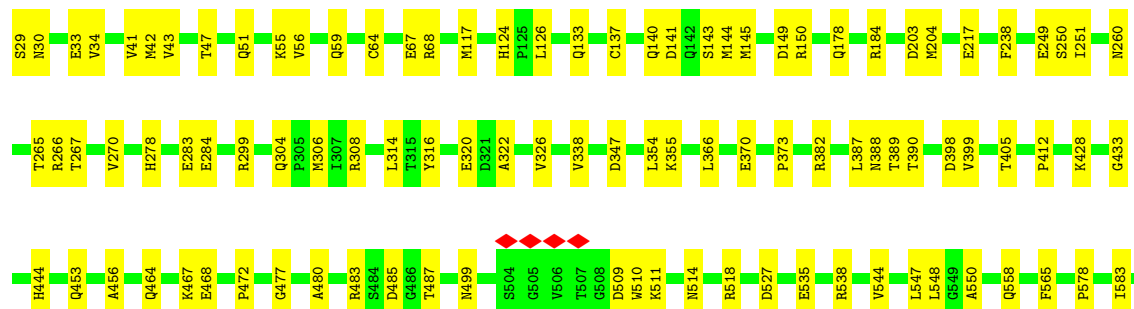
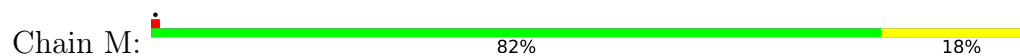
- Molecule 10: Complex I-9kD



- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

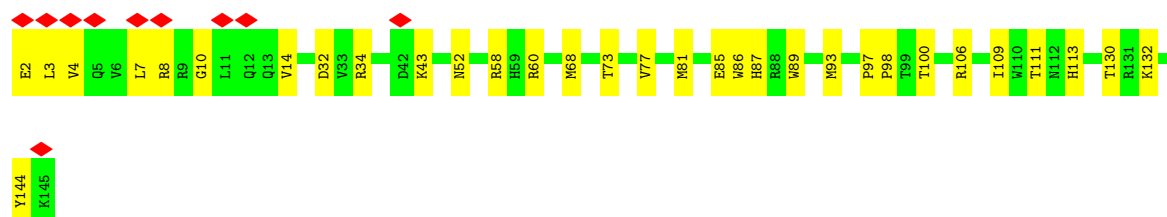
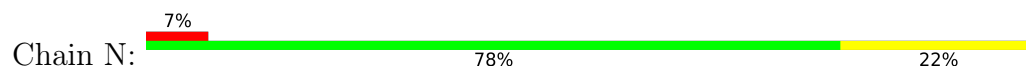


- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

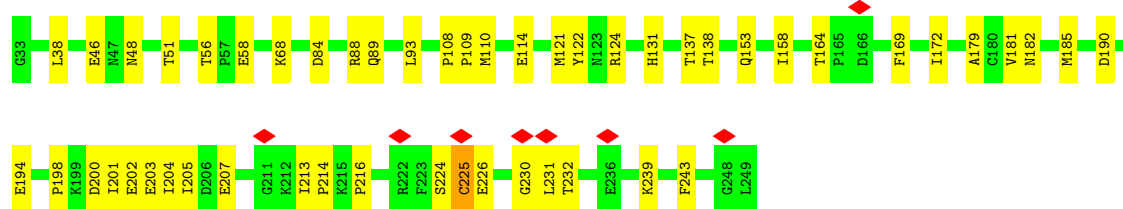
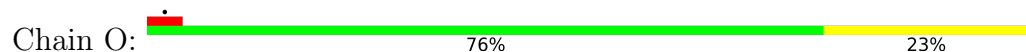




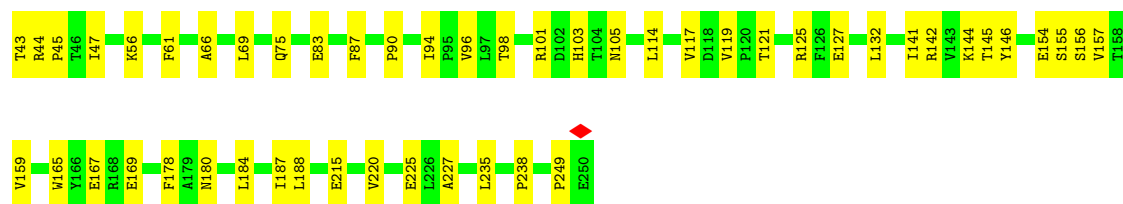
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



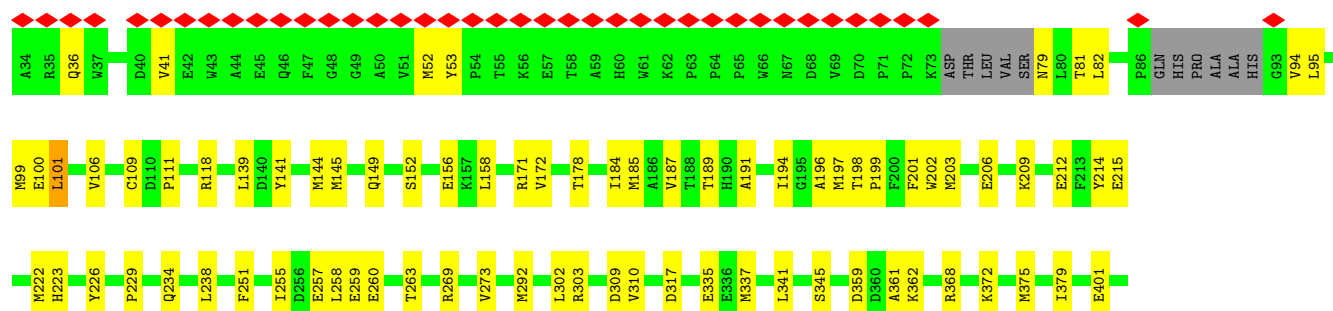
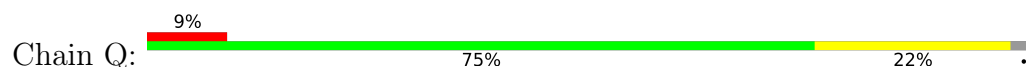
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 15: Complex I-30kD

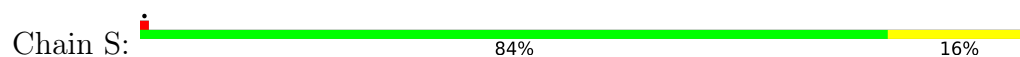


- Molecule 16: Complex I-49kD





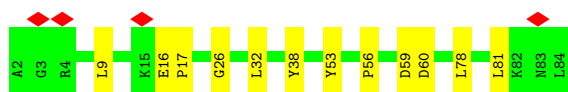
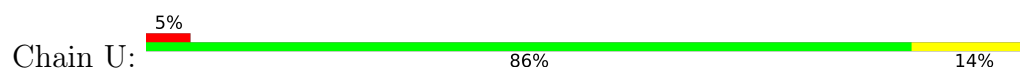
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



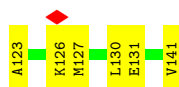
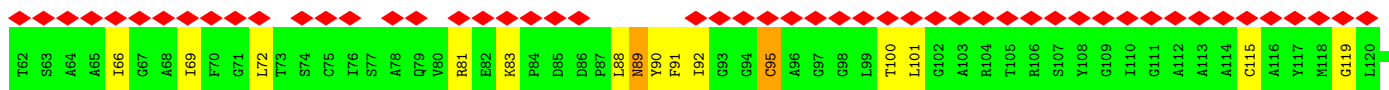
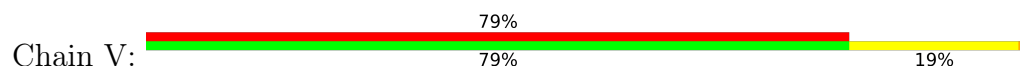
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



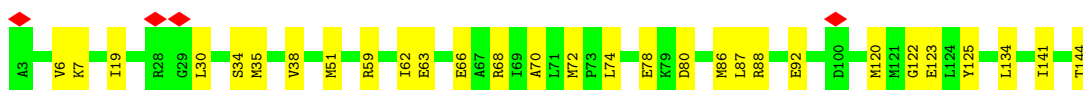
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



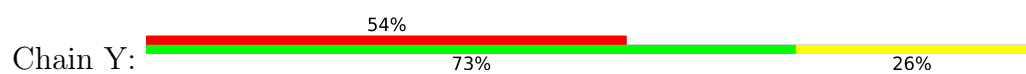
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



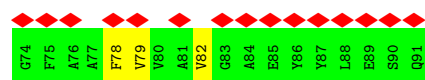
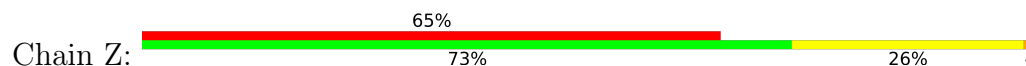
- Molecule 21: Complex I-B16.6



- Molecule 22: Complex I-AGGG



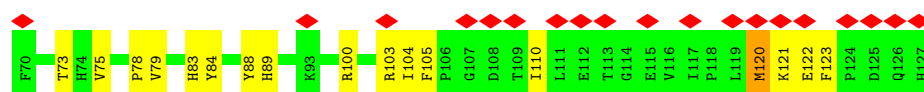
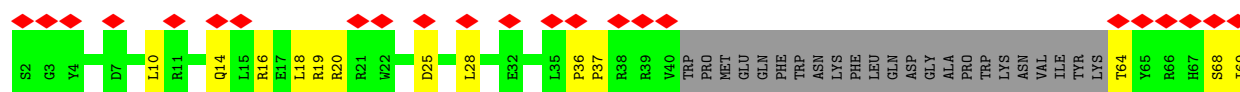
• Molecule 23: Complex I-B12



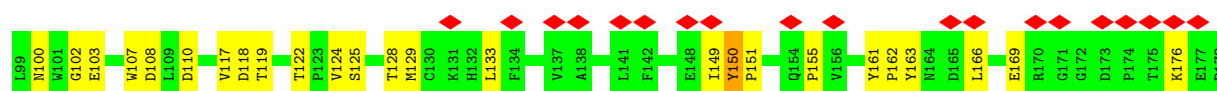
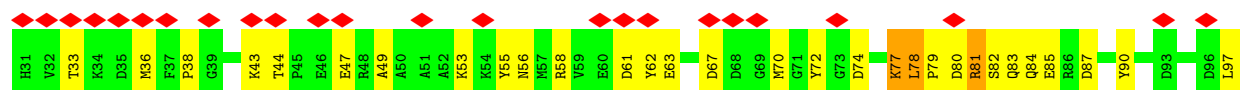
• Molecule 24: Complex I-SGDH

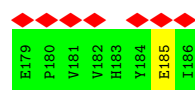


• Molecule 25: Complex I-B17

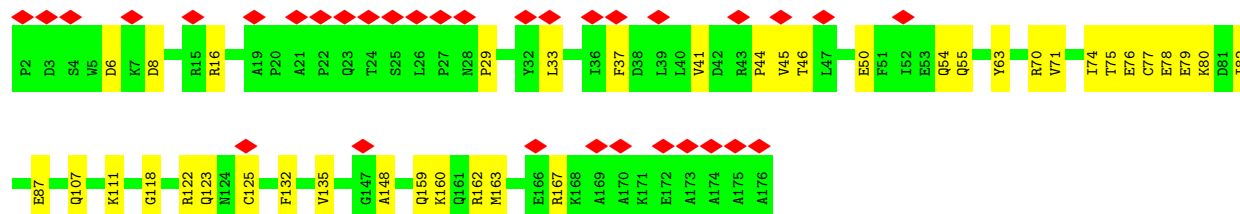
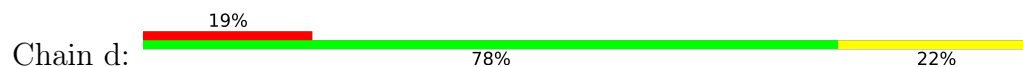


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

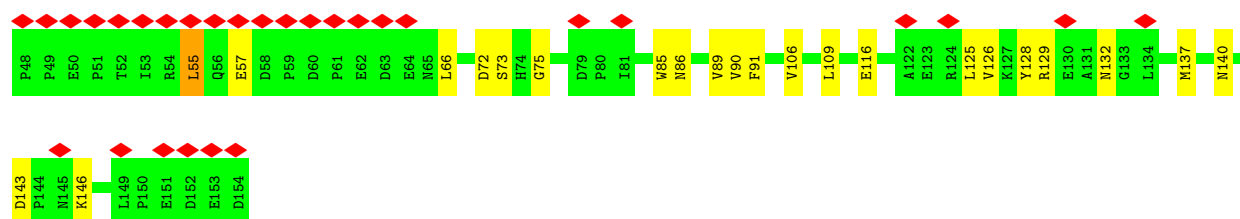
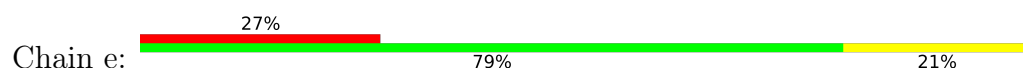




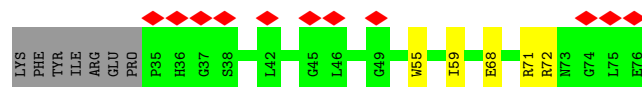
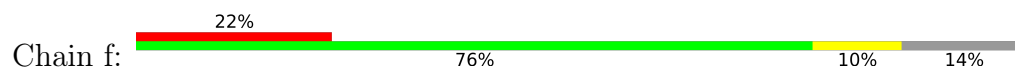
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



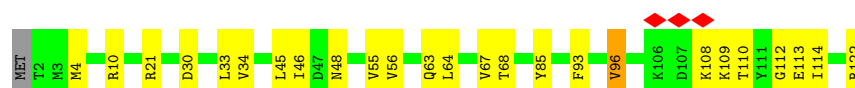
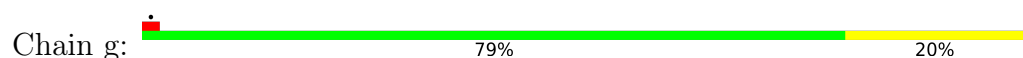
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



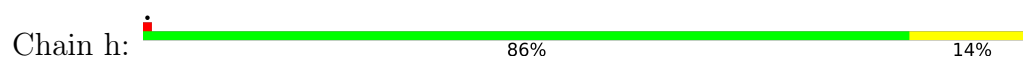
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



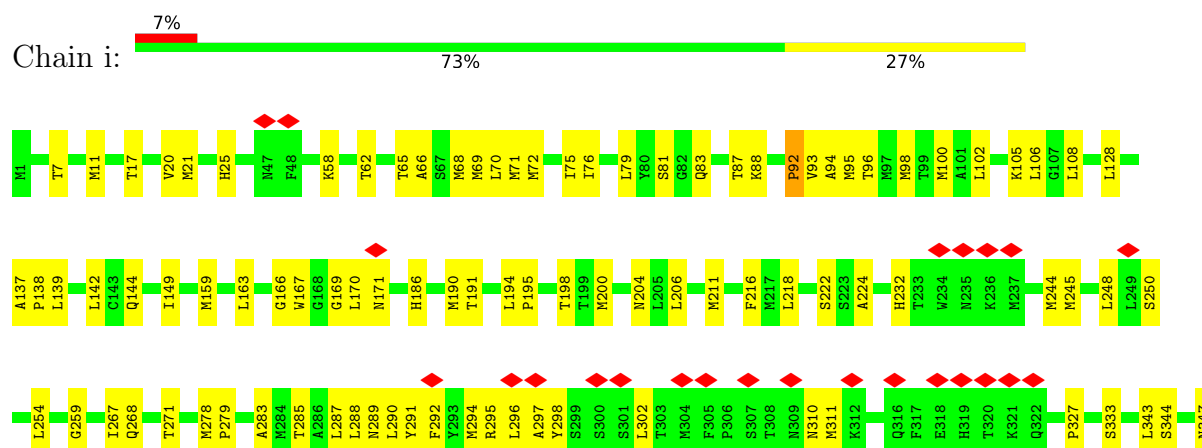
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2



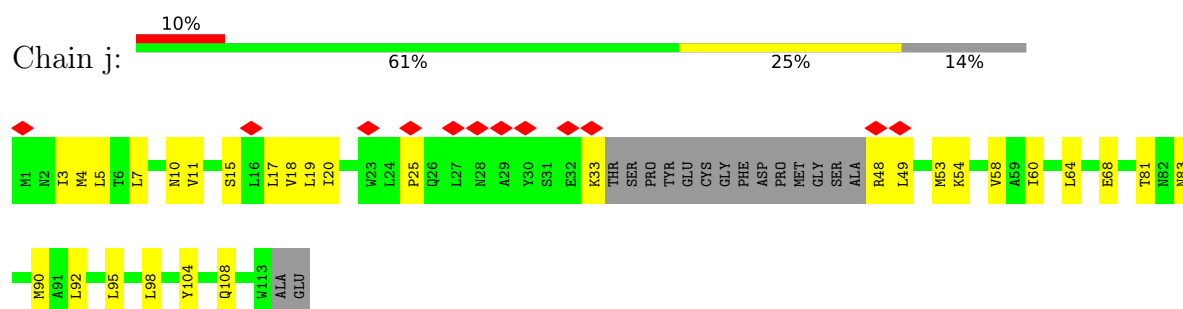
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



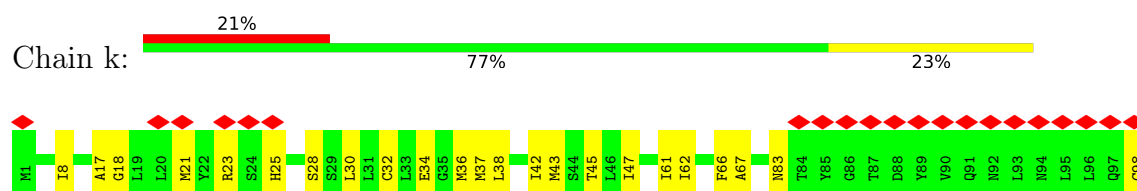
- Molecule 32: NADH-ubiquinone oxidoreductase chain 2



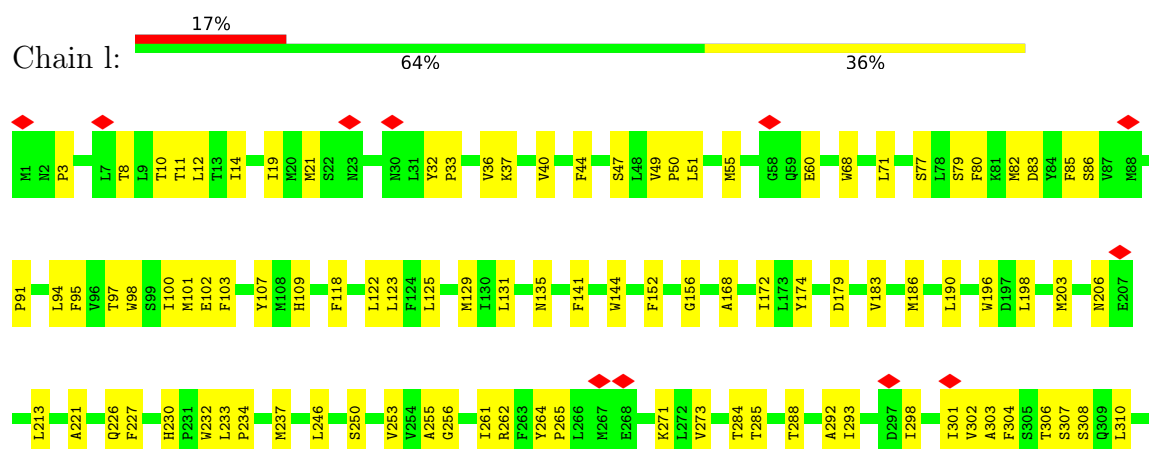
- Molecule 33: NADH-ubiquinone oxidoreductase chain 3

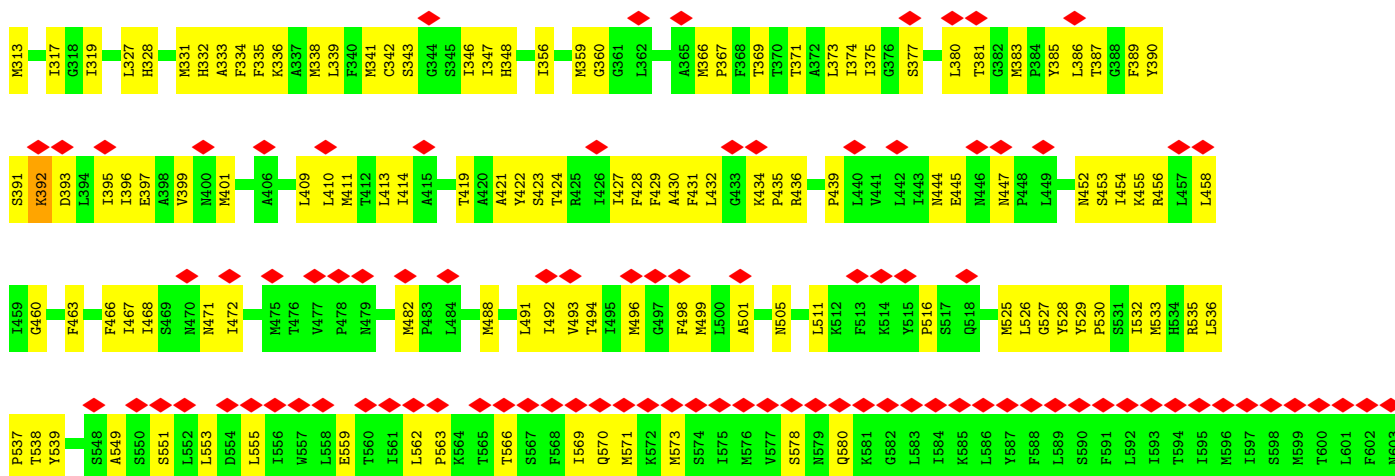


- Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

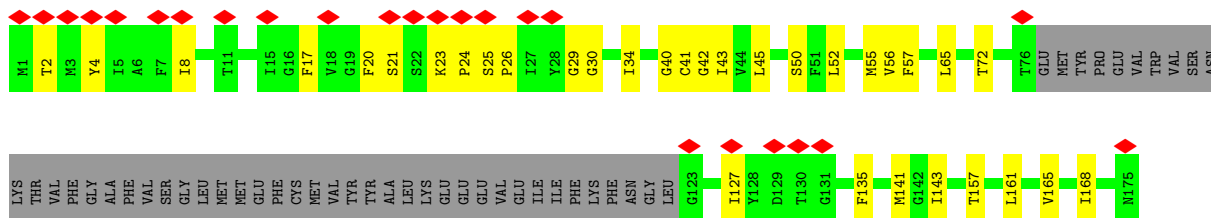


- Molecule 35: NADH-ubiquinone oxidoreductase chain 5

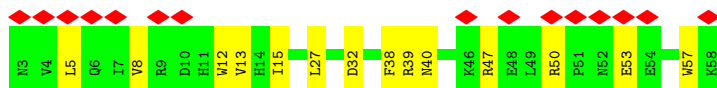
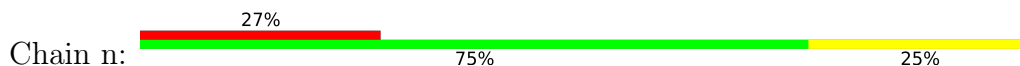




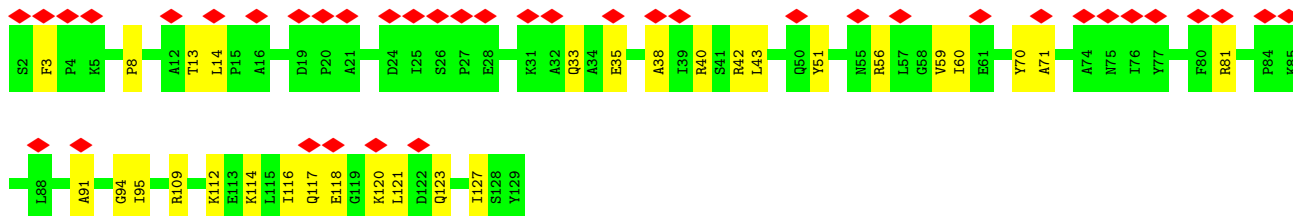
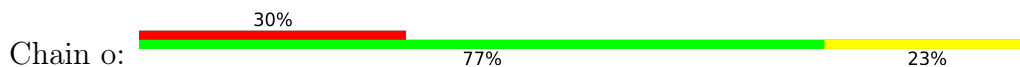
• Molecule 36: NADH-ubiquinone oxidoreductase chain 6



• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

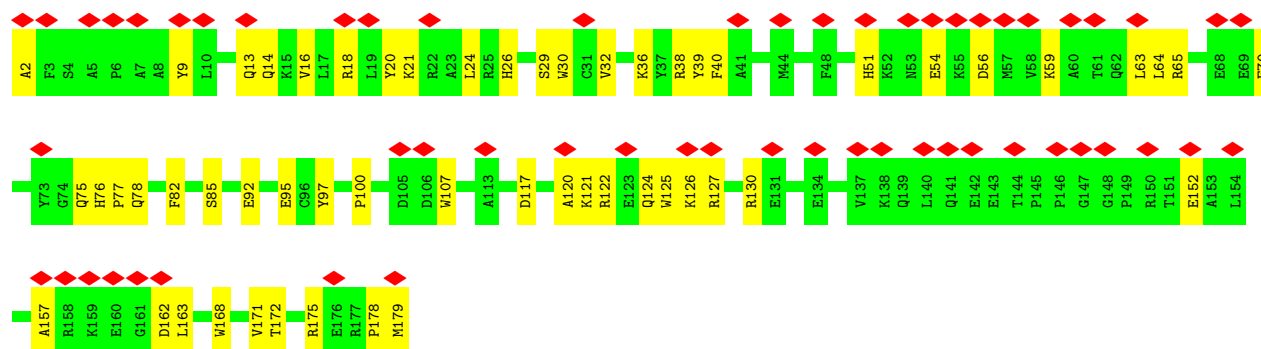


• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



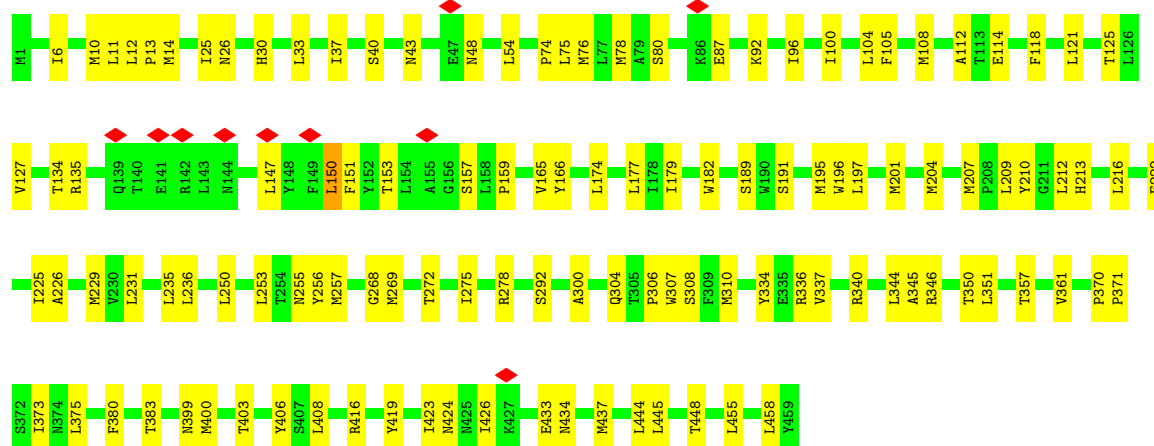
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9





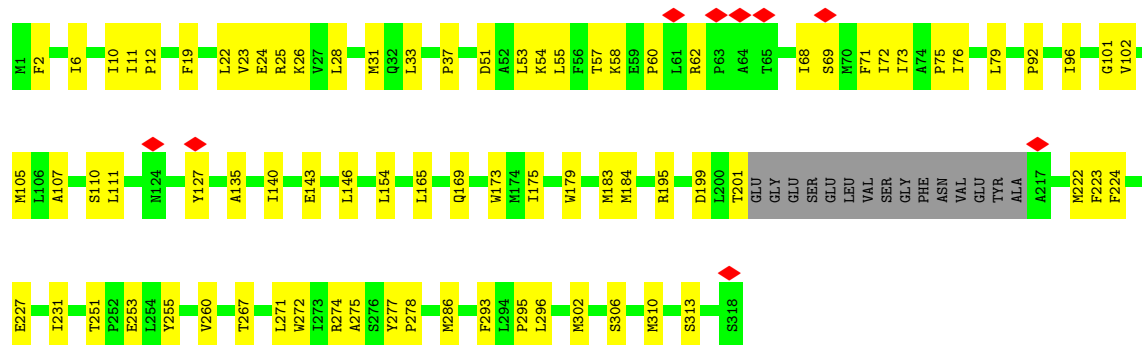
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r: 74% 26%



• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

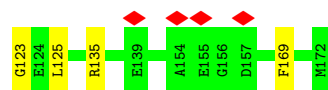
Chain s: 70% 25% 5%



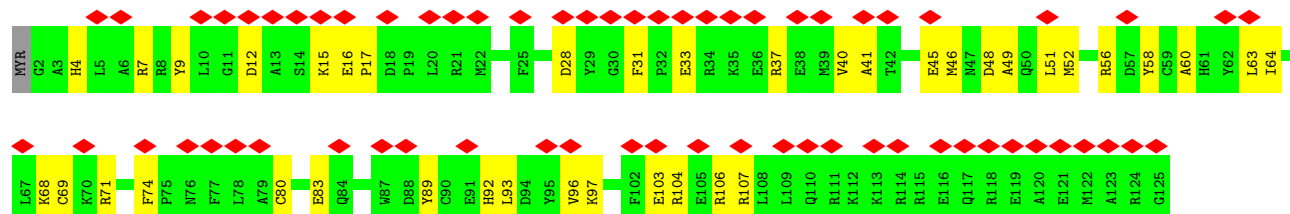
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 78% 21%

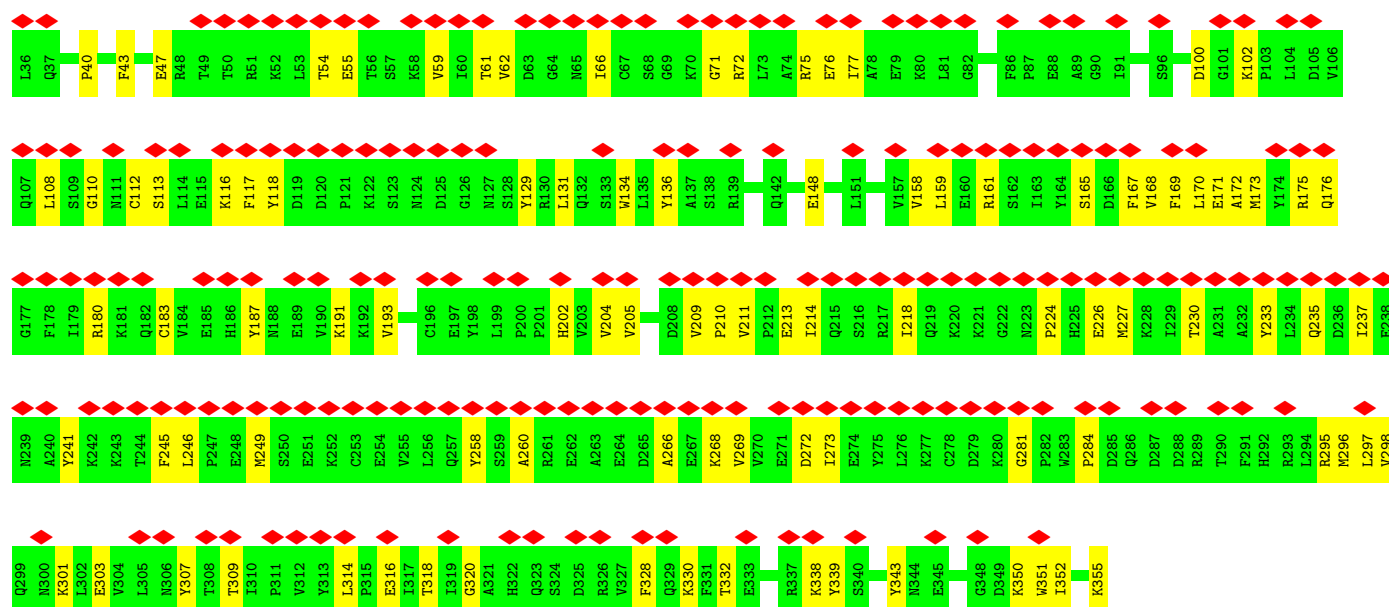




- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	89863	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0208	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, NDP, FMN, UQ, 2MR, 8Q1, PEE, SF4, PLX, CDL, NAI, MG, FES, ZN

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	A	0.14	0/3389	0.35	0/4579
2	B	0.16	0/1433	0.37	1/1940 (0.1%)
3	C	0.17	0/1279	0.43	2/1730 (0.1%)
4	E	0.17	0/992	0.38	0/1336
5	F	0.14	0/702	0.37	0/945
6	G	0.16	0/705	0.36	0/956
6	X	0.23	0/704	0.49	0/954
7	H	0.14	0/929	0.36	0/1258
8	I	0.12	0/798	0.34	0/1079
9	J	0.13	0/2680	0.31	0/3633
10	K	0.16	0/365	0.38	0/493
11	L	0.11	0/1039	0.29	0/1403
12	M	0.12	0/5378	0.33	1/7287 (0.0%)
13	N	0.14	0/1245	0.36	0/1694
14	O	0.16	0/1675	0.49	3/2287 (0.1%)
15	P	0.15	0/1786	0.39	1/2432 (0.0%)
16	Q	0.16	0/3451	0.36	0/4672
17	S	0.15	0/582	0.37	0/783
18	T	0.10	0/755	0.27	0/1018
19	U	0.11	0/664	0.32	0/912
20	V	0.17	0/1042	0.41	0/1411
21	W	0.13	0/1198	0.31	0/1617
22	Y	0.22	0/595	0.65	2/818 (0.2%)
23	Z	0.16	0/695	0.31	0/939
24	a	0.17	0/1193	0.51	4/1615 (0.2%)
25	b	0.19	0/873	0.45	0/1191
26	c	0.20	0/1341	0.49	3/1836 (0.2%)
27	d	0.13	0/1494	0.32	0/2015
28	e	0.15	0/915	0.39	0/1245
29	f	0.11	0/350	0.23	0/473
30	g	0.12	0/1031	0.28	0/1394
31	h	0.12	0/889	0.28	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.14	0/2773	0.35	0/3768
33	j	0.20	0/819	0.42	0/1117
34	k	0.15	0/759	0.34	0/1029
35	l	0.16	0/4828	0.40	1/6573 (0.0%)
36	m	0.18	0/934	0.52	2/1266 (0.2%)
37	n	0.17	0/491	0.44	0/663
38	o	0.20	0/1082	0.36	0/1469
39	p	0.15	0/1545	0.36	0/2099
40	r	0.15	0/3721	0.37	0/5076
41	s	0.19	0/2464	0.40	0/3369
42	u	0.13	0/1434	0.34	0/1935
43	v	0.21	0/1010	0.45	0/1362
44	w	0.13	0/2642	0.33	0/3580
All	All	0.15	0/66669	0.38	20/90441 (0.0%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	P	125	ARG	N-CA-C	7.21	119.14	111.28
24	a	128	GLY	CA-C-N	7.17	127.50	119.32
24	a	128	GLY	C-N-CA	7.17	127.50	119.32
24	a	124	THR	N-CA-C	7.00	118.99	111.36
14	O	232	THR	N-CA-C	6.92	118.83	111.28
14	O	230	GLY	N-CA-C	6.66	120.22	112.50
36	m	25	SER	CA-C-N	6.14	125.54	118.85
36	m	25	SER	C-N-CA	6.14	125.54	118.85
24	a	126	TYR	N-CA-C	6.05	119.34	109.24
26	c	150	TYR	CA-C-N	5.55	125.46	119.85
26	c	150	TYR	C-N-CA	5.55	125.46	119.85
2	B	112	ARG	N-CA-C	5.55	117.41	111.36
22	Y	84	PHE	CA-C-N	5.55	125.49	119.78
22	Y	84	PHE	C-N-CA	5.55	125.49	119.78
35	l	392	LYS	N-CA-C	5.42	116.99	111.14
3	C	124	MET	CA-C-N	5.31	125.72	119.99
3	C	124	MET	C-N-CA	5.31	125.72	119.99
12	M	695	TYR	N-CA-C	5.19	116.94	111.28
26	c	77	LYS	N-CA-C	-5.11	98.24	107.75
14	O	224	SER	N-CA-C	5.05	118.21	111.24

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3314	0	3276	90	0
2	B	1402	0	1348	39	0
3	C	1248	0	1254	28	0
4	E	968	0	973	29	0
5	F	691	0	704	20	0
6	G	693	0	671	29	0
6	X	692	0	667	51	0
7	H	910	0	950	25	0
8	I	780	0	808	25	0
9	J	2611	0	2630	63	0
10	K	355	0	329	15	0
11	L	1016	0	1016	18	0
12	M	5290	0	5317	86	0
13	N	1204	0	1162	24	0
14	O	1636	0	1604	31	0
15	P	1735	0	1691	37	0
16	Q	3377	0	3320	82	0
17	S	567	0	565	11	0
18	T	741	0	702	9	0
19	U	643	0	642	15	0
20	V	1021	0	1029	24	0
21	W	1167	0	1155	30	0
22	Y	571	0	500	36	0
23	Z	674	0	643	42	0
24	a	1159	0	1165	54	0
25	b	847	0	848	38	0
26	c	1287	0	1173	67	0
27	d	1461	0	1429	32	0
28	e	889	0	834	22	0
29	f	342	0	341	3	0
30	g	1000	0	994	20	0
31	h	867	0	871	10	0
32	i	2710	0	2874	82	0
33	j	800	0	855	29	0
34	k	748	0	799	31	0
35	l	4704	0	4770	177	0
36	m	915	0	908	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	n	479	0	486	18	0
38	o	1052	0	1055	30	0
39	p	1491	0	1405	42	0
40	r	3629	0	3833	101	0
41	s	2394	0	2508	75	0
42	u	1396	0	1373	28	0
43	v	987	0	903	47	0
44	w	2582	0	2531	62	0
45	A	8	0	0	2	0
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	2	0
47	A	44	0	27	3	0
48	B	51	0	82	1	0
48	C	47	0	71	3	0
48	b	46	0	69	4	0
48	i	47	0	71	4	0
48	j	51	0	82	6	0
48	l	46	0	69	0	0
48	m	41	0	59	6	0
48	r	51	0	82	5	0
49	C	52	0	88	5	0
49	g	52	0	88	2	0
49	j	52	0	88	3	0
49	l	52	0	88	3	0
49	r	52	0	88	3	0
50	G	35	0	0	8	0
50	X	35	0	0	2	0
51	J	48	0	25	2	0
52	M	4	0	0	0	0
52	O	4	0	0	0	0
53	M	1	0	0	0	0
54	N	51	0	46	1	0
54	a	91	0	132	9	0
54	i	66	0	76	4	0
54	r	199	0	307	17	0
54	u	78	0	103	13	0
55	T	1	0	0	0	0
56	s	28	0	31	5	0
57	w	27	0	11	1	0
All	All	66476	0	66713	1581	0

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

All (1581) 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)
6:G:112:SER:CB	50:G:201:8Q1:O1	1.66	1.43
26:c:78:LEU:CD2	26:c:79:PRO:HD2	1.60	1.31
41:s:24:GLU:OE1	41:s:271:LEU:HD22	1.42	1.18
35:l:383:MET:O	35:l:389:PHE:HB2	1.42	1.18
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.17
22:Y:56:ILE:HA	22:Y:59:GLU:OE1	1.44	1.17
35:l:391:SER:O	35:l:395:ILE:HG12	1.47	1.15
51:J:401:NDP:O4D	51:J:401:NDP:C4D	1.68	1.12
24:a:120:TRP:O	24:a:124:THR:HG22	1.52	1.10
25:b:104:ILE:HG13	43:v:48:ASP:HB3	1.34	1.08
26:c:78:LEU:HD23	26:c:79:PRO:CD	1.87	1.05
23:Z:9:HIS:CD2	24:a:52:LYS:HZ1	1.75	1.04
24:a:131:LYS:HE3	37:n:32:ASP:OD2	1.58	1.04
2:B:140:ARG:O	2:B:141:ARG:HD2	1.58	1.02
24:a:120:TRP:HE3	24:a:123:ARG:NH2	1.61	0.97
34:k:21:MET:HB2	36:m:23:LYS:NZ	1.79	0.97
26:c:78:LEU:HD23	26:c:79:PRO:HD2	0.99	0.96
22:Y:54:GLN:NE2	35:l:367:PRO:HD2	1.79	0.96
23:Z:9:HIS:CG	24:a:52:LYS:HZ1	1.83	0.95
6:X:90:TYR:HE1	23:Z:44:PRO:CB	1.82	0.93
20:V:95:CYS:HB2	20:V:115:CYS:SG	2.09	0.92
34:k:21:MET:HB2	36:m:23:LYS:HZ3	1.30	0.91
22:Y:74:TRP:CH2	23:Z:82:VAL:HG21	2.06	0.91
6:X:155:TYR:OH	24:a:54:LEU:HD11	1.72	0.90
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.34	0.90
12:M:544:VAL:HG23	12:M:565:PHE:HB3	1.52	0.88
6:G:112:SER:CB	50:G:201:8Q1:P24	2.60	0.88
6:X:146:ASP:HB3	25:b:16:ARG:HH21	1.40	0.87
6:X:90:TYR:CE1	23:Z:44:PRO:HB2	2.10	0.87
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.57	0.87
3:C:125:PRO:HG2	41:s:58:LYS:HE3	1.57	0.87
24:a:131:LYS:CE	37:n:32:ASP:OD2	2.24	0.86
6:X:90:TYR:CD1	23:Z:44:PRO:O	2.29	0.85
35:l:55:MET:HE1	35:l:472:ILE:HA	1.59	0.84
24:a:120:TRP:CE3	24:a:123:ARG:NH2	2.46	0.84
22:Y:54:GLN:HE22	35:l:367:PRO:HD2	1.39	0.83
6:X:90:TYR:CE1	23:Z:44:PRO:CB	2.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:56:ILE:O	22:Y:59:GLU:HG2	1.78	0.83
40:r:10:MET:O	40:r:13:PRO:HD2	1.78	0.82
35:l:103:PHE:HB2	35:l:341:MET:HE3	1.62	0.82
26:c:80:ASP:O	26:c:81:ARG:O	1.99	0.81
40:r:10:MET:C	40:r:13:PRO:HD2	2.05	0.81
1:A:170:GLN:HB3	10:K:89:LEU:HD23	1.63	0.81
2:B:140:ARG:C	2:B:141:ARG:HD2	2.05	0.80
9:J:293:LEU:HD22	9:J:298:TYR:HD1	1.46	0.80
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.65	0.79
20:V:88:LEU:O	20:V:92:ILE:HG13	1.83	0.79
22:Y:72:ARG:HB3	35:l:385:TYR:CG	2.18	0.79
43:v:16:GLU:HG3	43:v:17:PRO:HD2	1.65	0.78
26:c:78:LEU:CD2	26:c:79:PRO:CD	2.53	0.78
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.65	0.78
25:b:103:ARG:HH22	43:v:51:LEU:HD23	1.46	0.78
6:X:76:LEU:HD11	25:b:20:ARG:HH12	1.47	0.78
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.64	0.78
41:s:28:LEU:HD21	41:s:274:ARG:HD3	1.65	0.78
4:E:37:ARG:HA	6:G:120:MET:HE1	1.66	0.78
35:l:383:MET:O	35:l:389:PHE:CB	2.30	0.78
54:u:201:CDL:C58	54:u:201:CDL:H542	2.14	0.77
22:Y:54:GLN:NE2	35:l:367:PRO:CD	2.48	0.77
26:c:78:LEU:CG	26:c:79:PRO:HD2	2.14	0.77
24:a:110:TRP:CE3	24:a:123:ARG:HG3	2.19	0.77
32:i:87:THR:HG22	32:i:88:LYS:H	1.50	0.77
40:r:306:PRO:HA	40:r:458:LEU:HD23	1.65	0.77
1:A:152:ARG:HG2	1:A:152:ARG:HH11	1.50	0.77
8:I:71:SER:HB3	8:I:74:LYS:HE3	1.68	0.76
16:Q:82:LEU:HD12	16:Q:101:LEU:HD11	1.67	0.76
20:V:69:ILE:HG13	20:V:100:THR:HG21	1.66	0.76
6:G:103:HIS:ND1	6:G:106:LYS:HG2	2.01	0.76
21:W:120:MET:HG2	21:W:123:GLU:HG3	1.68	0.76
23:Z:9:HIS:CG	24:a:52:LYS:NZ	2.52	0.76
24:a:50:HIS:ND1	24:a:52:LYS:HD3	2.02	0.75
6:X:82:ARG:HD2	6:X:126:PHE:HE1	1.51	0.75
21:W:134:LEU:HD11	36:m:2:THR:HG23	1.68	0.75
27:d:54:GLN:HE22	27:d:55:GLN:HE21	1.34	0.74
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.21	0.74
32:i:218:LEU:HB3	32:i:244:MET:HE2	1.70	0.73
35:l:501:ALA:O	35:l:505:ASN:ND2	2.21	0.73
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.21	0.73
8:I:29:GLN:HE22	13:N:52:ASN:HB3	1.54	0.73
6:X:90:TYR:HD1	23:Z:44:PRO:O	1.72	0.73
32:i:295:ARG:NH1	48:i:402:PEE:O2P	2.22	0.73
32:i:72:MET:HE1	34:k:43:MET:HE1	1.71	0.72
34:k:23:ARG:HG2	36:m:23:LYS:HE3	1.69	0.72
39:p:56:ASP:HB3	39:p:59:LYS:HB2	1.70	0.72
54:u:201:CDL:H772	54:u:201:CDL:H271	1.71	0.72
6:X:90:TYR:CE1	23:Z:44:PRO:O	2.43	0.72
6:X:108:LEU:HB3	6:X:110:LEU:HD23	1.70	0.72
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.23	0.72
15:P:90:PRO:HA	15:P:145:THR:CG2	2.20	0.72
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.54	0.72
26:c:155:PRO:HG3	43:v:4:HIS:CD2	2.25	0.71
22:Y:72:ARG:HB3	35:l:385:TYR:CD1	2.24	0.71
1:A:138:LEU:HD13	1:A:245:VAL:HG13	1.72	0.71
26:c:150:TYR:HD1	43:v:9:TYR:CD1	2.07	0.71
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.72	0.71
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.73	0.71
35:l:97:THR:O	35:l:101:MET:HG3	1.90	0.71
9:J:212:ARG:O	9:J:216:TYR:HB2	1.90	0.71
24:a:110:TRP:CZ3	24:a:123:ARG:HG3	2.26	0.70
54:u:201:CDL:H542	54:u:201:CDL:H581	1.71	0.70
43:v:51:LEU:HD13	43:v:63:LEU:HD13	1.73	0.70
3:C:79:MET:HE3	3:C:86:MET:HE3	1.72	0.70
44:w:258:TYR:HE2	44:w:269:VAL:HG23	1.55	0.70
3:C:188:LYS:HE3	3:C:191:ARG:HH11	1.55	0.70
4:E:64:ARG:NH2	6:G:117:GLU:OE1	2.25	0.70
25:b:103:ARG:HH12	43:v:51:LEU:HA	1.56	0.70
40:r:96:ILE:O	40:r:100:ILE:HG12	1.92	0.70
26:c:67:ASP:OD1	38:o:81:ARG:NH2	2.25	0.70
41:s:24:GLU:OE1	41:s:271:LEU:CD2	2.32	0.70
26:c:80:ASP:O	26:c:81:ARG:C	2.33	0.70
5:F:40:ARG:HH12	5:F:84:ALA:HB1	1.57	0.69
40:r:166:TYR:CD1	40:r:195:MET:HE1	2.27	0.69
40:r:210:TYR:O	40:r:213:HIS:ND1	2.25	0.69
6:X:91:ASP:OD1	6:X:92:LYS:N	2.26	0.69
6:X:115:GLN:O	6:X:118:ILE:HG22	1.92	0.69
27:d:159:GLN:O	27:d:163:MET:HG3	1.93	0.69
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.73	0.69
32:i:159:MET:HG2	32:i:278:MET:HE3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:78:LEU:CG	26:c:79:PRO:CD	2.70	0.69
6:G:80:LYS:O	6:G:84:LEU:HG	1.91	0.69
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.74	0.69
26:c:102:GLY:HA3	38:o:43:LEU:HD22	1.75	0.69
54:r:503:CDL:H312	54:r:503:CDL:H742	1.74	0.69
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.75	0.69
40:r:14:MET:HE2	40:r:30:HIS:ND1	2.08	0.69
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.74	0.68
1:A:152:ARG:NH2	10:K:99:PRO:O	2.26	0.68
1:A:127:ASP:OD1	1:A:245:VAL:HB	1.93	0.68
20:V:69:ILE:HG21	20:V:100:THR:CG2	2.24	0.68
26:c:78:LEU:HG	26:c:79:PRO:CD	2.23	0.68
9:J:327:MET:HE2	9:J:329:LEU:HD11	1.75	0.68
48:r:501:PEE:H36	48:r:501:PEE:H79	1.76	0.67
9:J:192:ARG:NH1	9:J:198:ALA:O	2.27	0.67
26:c:161:TYR:HB3	26:c:166:LEU:HG	1.76	0.67
35:l:55:MET:HE2	35:l:55:MET:HA	1.76	0.67
17:S:1:MET:O	17:S:4:GLU:HG3	1.94	0.67
23:Z:36:LEU:HG	23:Z:41:LEU:HB2	1.76	0.67
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.75	0.67
29:f:55:TRP:O	29:f:59:ILE:HG12	1.95	0.67
6:G:141:PRO:O	6:G:145:VAL:HG23	1.94	0.67
24:a:84:ILE:O	24:a:88:LEU:HG	1.94	0.67
9:J:206:ILE:HG12	9:J:245:VAL:HG21	1.77	0.67
26:c:150:TYR:CD1	43:v:9:TYR:CD1	2.82	0.67
32:i:92:PRO:O	32:i:94:ALA:N	2.28	0.67
1:A:234:GLY:HA3	1:A:240:THR:HG22	1.77	0.66
20:V:69:ILE:HG21	20:V:100:THR:HG21	1.76	0.66
37:n:47:ARG:NH1	37:n:53:GLU:OE1	2.27	0.66
40:r:201:MET:HG2	48:r:501:PEE:H42	1.78	0.66
9:J:303:ARG:HD3	9:J:316:ARG:HD3	1.75	0.66
38:o:118:GLU:HG3	38:o:120:LYS:HG2	1.77	0.66
44:w:245:PHE:O	44:w:249:MET:HG2	1.95	0.66
24:a:135:LYS:HD2	37:n:32:ASP:OD1	1.96	0.66
2:B:76:TYR:HE1	41:s:33:LEU:HB2	1.60	0.66
32:i:142:LEU:HB3	32:i:194:LEU:HD21	1.78	0.66
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.28	0.66
33:j:7:LEU:HD21	48:m:201:PEE:H59	1.78	0.66
1:A:50:ASP:O	1:A:59:ARG:NH2	2.29	0.66
9:J:163:LYS:NZ	9:J:253:ILE:O	2.27	0.66
50:X:201:8Q1:N36	50:X:201:8Q1:O40	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.77	0.66
40:r:14:MET:SD	40:r:26:ASN:HB3	2.35	0.66
44:w:112:CYS:SG	44:w:113:SER:N	2.68	0.66
6:G:103:HIS:CE1	6:G:106:LYS:HE3	2.31	0.66
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.30	0.66
14:O:88:ARG:NH2	14:O:190:ASP:OD2	2.28	0.66
28:e:85:TRP:O	28:e:89:VAL:HG13	1.96	0.66
40:r:350:THR:HB	40:r:351:LEU:HD12	1.76	0.66
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.78	0.65
15:P:43:THR:HA	15:P:47:ILE:HD12	1.77	0.65
27:d:75:THR:HG23	30:g:112:GLY:HA3	1.78	0.65
12:M:464:GLN:NE2	12:M:468:GLU:OE2	2.29	0.65
40:r:75:LEU:HA	40:r:78:MET:HE2	1.78	0.65
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	1.76	0.65
40:r:201:MET:HE3	40:r:212:LEU:HD11	1.77	0.65
10:K:89:LEU:HD12	10:K:92:GLU:OE1	1.96	0.65
3:C:127:PRO:HB3	3:C:189:ARG:HH22	1.61	0.65
22:Y:74:TRP:CH2	23:Z:82:VAL:CG2	2.79	0.65
44:w:268:LYS:NZ	44:w:272:ASP:OD2	2.30	0.65
14:O:38:LEU:O	14:O:124:ARG:NH2	2.30	0.65
16:Q:81:THR:HG22	16:Q:100:GLU:HG3	1.79	0.64
28:e:116:GLU:N	28:e:116:GLU:OE1	2.27	0.64
54:u:201:CDL:H161	54:u:201:CDL:HB31	1.80	0.64
3:C:127:PRO:HA	9:J:89:TYR:OH	1.98	0.64
24:a:79:GLY:HA3	54:a:201:CDL:H222	1.78	0.64
30:g:63:GLN:O	30:g:67:VAL:HG23	1.97	0.64
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.30	0.64
7:H:59:VAL:HG23	7:H:68:LEU:HD21	1.79	0.64
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.80	0.64
21:W:144:THR:HB	41:s:96:ILE:HG23	1.78	0.64
26:c:125:SER:HB3	26:c:128:THR:HG23	1.79	0.64
12:M:306:MET:HB2	12:M:583:ILE:HB	1.79	0.64
14:O:182:ASN:HB3	14:O:194:GLU:HB3	1.79	0.64
24:a:160:MET:HE2	24:a:166:GLY:HA3	1.80	0.64
44:w:71:GLY:O	44:w:75:ARG:HG3	1.98	0.64
38:o:56:ARG:HH21	40:r:424:ASN:ND2	1.96	0.64
6:X:89:LEU:HD21	23:Z:22:TRP:HD1	1.63	0.63
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.32	0.63
34:k:66:PHE:HE1	36:m:157:THR:HG22	1.63	0.63
35:l:183:VAL:HG21	40:r:400:MET:HE1	1.81	0.63
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.81	0.63
1:A:409:ILE:HG23	1:A:439:ILE:HD12	1.79	0.63
9:J:238:GLN:NE2	9:J:266:VAL:HG12	2.13	0.63
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.32	0.63
44:w:338:LYS:HG3	44:w:339:TYR:CE1	2.34	0.63
2:B:72:MET:HE3	16:Q:257:GLU:HA	1.81	0.62
12:M:117:MET:HE2	12:M:143:SER:HB2	1.78	0.62
35:l:359:MET:O	35:l:436:ARG:NH2	2.32	0.62
21:W:51:MET:HA	41:s:313:SER:HB2	1.80	0.62
32:i:248:LEU:HD11	32:i:296:LEU:HD23	1.79	0.62
2:B:177:THR:HG22	2:B:179:THR:H	1.64	0.62
23:Z:9:HIS:CD2	24:a:52:LYS:NZ	2.59	0.62
20:V:126:LYS:HE3	20:V:130:LEU:HD21	1.80	0.62
6:X:89:LEU:O	23:Z:47:ARG:NH2	2.32	0.62
6:X:118:ILE:HD12	23:Z:45:TRP:HH2	1.64	0.62
6:G:79:ILE:HG22	6:G:145:VAL:HG13	1.81	0.62
32:i:291:TYR:CZ	48:i:402:PEE:H49	2.35	0.62
9:J:218:ALA:O	9:J:221:ARG:NH1	2.33	0.62
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.80	0.62
54:u:201:CDL:H581	54:u:201:CDL:C54	2.29	0.62
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.81	0.62
34:k:21:MET:CB	36:m:23:LYS:HZ3	2.06	0.62
26:c:43:LYS:NZ	26:c:67:ASP:OD2	2.33	0.62
44:w:72:ARG:O	44:w:76:GLU:HG2	1.99	0.62
23:Z:21:GLN:O	23:Z:23:LYS:NZ	2.33	0.62
26:c:78:LEU:HG	26:c:79:PRO:HD3	1.80	0.62
33:j:7:LEU:O	33:j:11:VAL:HG23	1.99	0.62
12:M:322:ALA:O	12:M:326:VAL:HG23	2.00	0.62
36:m:26:PRO:HB2	36:m:72:THR:HG21	1.82	0.61
43:v:7:ARG:HD2	43:v:16:GLU:OE1	2.00	0.61
43:v:93:LEU:O	43:v:97:LYS:HG3	1.99	0.61
1:A:319:PRO:HG2	1:A:347:THR:HG21	1.82	0.61
9:J:162:GLU:HG3	9:J:163:LYS:HG3	1.82	0.61
26:c:150:TYR:HD1	43:v:9:TYR:CE1	2.18	0.61
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.34	0.61
20:V:90:TYR:CE2	20:V:126:LYS:HD3	2.35	0.61
24:a:113:PHE:HB2	24:a:119:ARG:HG2	1.81	0.61
33:j:95:LEU:HD23	33:j:98:LEU:HD23	1.83	0.61
26:c:44:THR:N	26:c:47:GLU:OE1	2.25	0.61
16:Q:99:MET:HE1	16:Q:447:VAL:HG21	1.83	0.61
32:i:211:MET:HG2	32:i:333:SER:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:301:ILE:HD11	35:l:422:TYR:HB2	1.83	0.61
11:L:109:ASN:ND2	11:L:111:LEU:O	2.34	0.61
6:X:153:ASP:OD2	25:b:19:ARG:NH2	2.33	0.61
12:M:308:ARG:NH2	12:M:578:PRO:O	2.34	0.61
6:X:81:ASP:OD1	23:Z:16:LEU:HD22	2.00	0.61
44:w:246:LEU:HD13	44:w:249:MET:HE3	1.82	0.61
22:Y:68:TRP:CD2	35:l:463:PHE:HE1	2.19	0.60
32:i:96:THR:O	32:i:100:MET:HG2	2.00	0.60
20:V:66:ILE:HD11	20:V:101:LEU:HD13	1.81	0.60
5:F:40:ARG:O	5:F:43:GLU:HG2	2.01	0.60
12:M:388:ASN:HB3	12:M:511:LYS:HE2	1.82	0.60
16:Q:52:MET:O	32:i:171:ASN:ND2	2.32	0.60
33:j:17:LEU:HD22	41:s:222:MET:CE	2.31	0.60
37:n:40:ASN:ND2	37:n:40:ASN:O	2.35	0.60
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.83	0.60
22:Y:89:PRO:HB2	43:v:103:GLU:OE2	2.01	0.60
35:l:401:MET:HE2	35:l:482:MET:SD	2.41	0.60
1:A:41:ILE:O	1:A:137:LYS:NZ	2.30	0.60
22:Y:74:TRP:CZ2	23:Z:82:VAL:CG2	2.85	0.60
22:Y:67:PHE:CZ	22:Y:71:TRP:HE3	2.19	0.60
49:g:201:PLX:H301	32:i:347:ASN:HB3	1.84	0.60
35:l:237:MET:HE3	35:l:303:ALA:HB2	1.84	0.60
1:A:452:GLN:O	1:A:456:GLN:HG3	2.02	0.60
7:H:51:ILE:HA	7:H:54:GLU:OE1	2.01	0.60
3:C:59:ARG:NH1	49:C:303:PLX:O3	2.33	0.60
7:H:50:GLN:HE22	8:I:93:LYS:HD3	1.67	0.60
6:G:115:GLN:O	6:G:119:ILE:HG12	2.02	0.59
40:r:191:SER:HB3	48:r:501:PEE:H3	1.83	0.59
21:W:68:ARG:HD2	36:m:135:PHE:CD2	2.36	0.59
6:X:155:TYR:O	25:b:20:ARG:HD2	2.01	0.59
26:c:100:ASN:HB2	26:c:103:GLU:OE1	2.03	0.59
26:c:129:MET:HB3	35:l:532:ILE:HD11	1.84	0.59
35:l:331:MET:HB3	35:l:387:THR:HG22	1.84	0.59
35:l:335:PHE:O	35:l:339:LEU:HG	2.02	0.59
20:V:8:LYS:HZ2	20:V:24:ALA:HB2	1.67	0.59
23:Z:51:TRP:CZ3	23:Z:57:PHE:HE2	2.20	0.59
24:a:111:GLU:OE2	24:a:111:GLU:N	2.34	0.59
32:i:11:MET:HE1	54:i:401:CDL:H771	1.84	0.59
32:i:170:LEU:HD11	32:i:288:LEU:HD22	1.83	0.59
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.20	0.59
16:Q:53:TYR:CD1	35:l:571:MET:HE2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:86:ASN:O	28:e:90:VAL:HG13	2.01	0.59
42:u:169:PHE:HD1	54:u:201:CDL:H512	1.67	0.59
7:H:67:LYS:O	7:H:71:GLN:HG2	2.02	0.59
14:O:201:ILE:O	14:O:205:ILE:HG12	2.02	0.59
22:Y:84:PHE:CZ	43:v:89:TYR:HA	2.37	0.59
33:j:68:GLU:HG2	36:m:161:LEU:HD13	1.85	0.59
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.85	0.59
35:l:319:ILE:HG21	35:l:399:VAL:HG22	1.85	0.59
4:E:42:GLU:HG3	4:E:90:LEU:HD11	1.85	0.59
15:P:169:GLU:OE2	16:Q:463:ARG:NH2	2.35	0.59
54:a:201:CDL:HB21	48:b:201:PEE:H51	1.85	0.59
1:A:152:ARG:HH11	1:A:152:ARG:CG	2.13	0.59
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.84	0.59
32:i:149:ILE:HD11	32:i:195:PRO:HG3	1.85	0.59
3:C:50:LEU:HD13	48:C:302:PEE:H25	1.84	0.59
7:H:38:ILE:O	7:H:45:ARG:NH1	2.32	0.59
32:i:170:LEU:HD23	32:i:292:PHE:HB3	1.84	0.59
40:r:76:MET:HG2	40:r:229:MET:HE2	1.85	0.59
9:J:293:LEU:HD22	9:J:298:TYR:CD1	2.34	0.59
27:d:46:THR:O	27:d:50:GLU:HG2	2.02	0.59
31:h:38:LYS:O	31:h:42:GLU:HG3	2.02	0.59
44:w:113:SER:OG	44:w:116:LYS:HG2	2.02	0.59
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.37	0.59
44:w:204:VAL:HG11	44:w:249:MET:SD	2.43	0.59
16:Q:194:ILE:HG22	41:s:278:PRO:HB3	1.84	0.58
6:X:125:GLU:OE1	35:l:439:PRO:HG2	2.03	0.58
6:X:146:ASP:HB3	25:b:16:ARG:NH2	2.16	0.58
27:d:107:GLN:O	27:d:111:LYS:HG3	2.03	0.58
36:m:23:LYS:N	36:m:24:PRO:HD3	2.18	0.58
24:a:110:TRP:CZ2	24:a:123:ARG:HD3	2.38	0.58
27:d:82:ILE:HD13	40:r:182:TRP:HE1	1.67	0.58
11:L:89:SER:O	12:M:59:GLN:NE2	2.35	0.58
24:a:61:GLY:O	24:a:65:ARG:HG3	2.03	0.58
26:c:129:MET:HG2	35:l:528:TYR:CG	2.37	0.58
41:s:54:LYS:HE3	41:s:55:LEU:HD12	1.83	0.58
6:G:144:ILE:O	6:G:148:ILE:HG12	2.03	0.58
26:c:49:ALA:HB1	26:c:53:LYS:HZ1	1.69	0.58
35:l:11:THR:HG21	35:l:47:SER:HB3	1.85	0.58
40:r:403:THR:HA	40:r:406:TYR:CE2	2.39	0.58
3:C:188:LYS:HE3	3:C:191:ARG:NH1	2.19	0.58
45:C:301:SF4:S4	16:Q:223:HIS:HD2	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:279:TYR:O	9:J:283:VAL:HG23	2.04	0.58
36:m:42:GLY:CA	48:m:201:PEE:H22	2.33	0.58
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.85	0.58
12:M:373:PRO:HB3	12:M:487:THR:HG22	1.86	0.58
12:M:472:PRO:O	12:M:510:TRP:NE1	2.35	0.58
31:h:59:GLU:OE1	31:h:59:GLU:N	2.34	0.58
38:o:59:VAL:HG22	40:r:423:ILE:HD11	1.83	0.58
1:A:102:MET:HG3	1:A:241:THR:OG1	2.03	0.58
35:l:213:LEU:HB3	35:l:273:VAL:HG11	1.86	0.58
35:l:428:PHE:HD1	35:l:432:LEU:HD12	1.68	0.58
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.33	0.58
35:l:227:PHE:O	35:l:230:HIS:ND1	2.36	0.58
44:w:218:ILE:HG23	44:w:226:GLU:HG2	1.84	0.58
44:w:233:TYR:O	44:w:237:ILE:HG13	2.04	0.58
27:d:122:ARG:NH1	35:l:206:ASN:OD1	2.36	0.58
8:I:46:SER:O	8:I:52:ASN:ND2	2.36	0.58
12:M:464:GLN:HE22	12:M:467:LYS:HD2	1.69	0.57
6:X:120:MET:HE1	39:p:24:LEU:HB3	1.85	0.57
25:b:103:ARG:CZ	43:v:49:ALA:O	2.52	0.57
35:l:36:VAL:HG13	35:l:122:LEU:HD22	1.86	0.57
35:l:419:THR:HA	35:l:422:TYR:CE2	2.39	0.57
1:A:201:ALA:HA	14:O:121:MET:HE2	1.86	0.57
7:H:37:GLN:HB3	7:H:95:LEU:HD11	1.86	0.57
6:G:84:LEU:O	6:G:88:LYS:HG2	2.05	0.57
36:m:40:GLY:HA2	36:m:43:ILE:HD12	1.85	0.57
1:A:170:GLN:CB	10:K:89:LEU:HD23	2.32	0.57
7:H:72:LEU:HD13	7:H:80:VAL:HG11	1.86	0.57
43:v:4:HIS:HA	43:v:7:ARG:HG2	1.87	0.57
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.86	0.57
5:F:57:GLU:O	12:M:655:ARG:NH2	2.37	0.57
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.86	0.57
41:s:69:SER:O	41:s:73:ILE:HD12	2.03	0.57
6:G:116:VAL:O	6:G:120:MET:HG2	2.05	0.57
32:i:294:MET:SD	40:r:150:LEU:HD22	2.45	0.57
36:m:42:GLY:HA2	48:m:201:PEE:H22	1.86	0.57
39:p:92:GLU:HB3	39:p:95:GLU:HG3	1.85	0.57
41:s:25:ARG:HD2	56:s:401:UQ:HM21	1.85	0.57
3:C:69:LEU:HD23	16:Q:94:VAL:HG11	1.86	0.57
7:H:94:MET:SD	7:H:99:PRO:HG3	2.45	0.57
23:Z:30:GLU:O	23:Z:34:GLU:HG3	2.05	0.57
33:j:5:LEU:HD23	41:s:2:PHE:HD2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:169:GLU:HA	27:d:123:GLN:HB2	1.87	0.57
21:W:68:ARG:HD2	36:m:135:PHE:HD2	1.69	0.56
22:Y:67:PHE:CZ	22:Y:71:TRP:CE3	2.93	0.56
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.23	0.56
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.44	0.56
20:V:37:SER:HB3	20:V:56:THR:HG22	1.88	0.56
25:b:83:HIS:HD2	27:d:45:VAL:HG11	1.71	0.56
35:l:144:TRP:HH2	35:l:256:GLY:HA2	1.68	0.56
44:w:54:THR:O	44:w:55:GLU:HG3	2.05	0.56
1:A:46:TYR:CE1	14:O:226:GLU:CB	2.89	0.56
30:g:45:LEU:HD23	54:r:504:CDL:H752	1.87	0.56
35:l:397:GLU:HG2	35:l:482:MET:HE3	1.87	0.56
38:o:112:LYS:O	38:o:116:ILE:HG12	2.05	0.56
40:r:231:LEU:HA	40:r:235:LEU:HB2	1.85	0.56
43:v:33:GLU:H	43:v:33:GLU:CD	2.13	0.56
7:H:76:GLN:O	7:H:79:GLU:HG2	2.06	0.56
8:I:42:PRO:HB3	21:W:6:VAL:HG11	1.86	0.56
31:h:83:ARG:O	31:h:87:ILE:HG22	2.05	0.56
44:w:167:PHE:O	44:w:170:LEU:HB3	2.05	0.56
38:o:91:ALA:O	38:o:95:ILE:HB	2.05	0.56
41:s:135:ALA:HB2	41:s:201:THR:HG21	1.88	0.56
42:u:88:CYS:SG	42:u:89:ILE:N	2.78	0.56
6:G:112:SER:CA	50:G:201:8Q1:O1	2.47	0.56
25:b:19:ARG:HA	39:p:171:VAL:HG13	1.87	0.56
33:j:54:LYS:O	33:j:58:VAL:HG23	2.05	0.56
38:o:114:LYS:NZ	38:o:118:GLU:HB3	2.21	0.56
1:A:89:GLY:O	47:A:503:NAI:H2N	2.06	0.56
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.35	0.56
40:r:448:THR:HG21	54:r:503:CDL:H422	1.87	0.56
41:s:251:THR:HG23	41:s:253:GLU:OE1	2.06	0.56
1:A:208:GLU:OE1	1:A:210:THR:OG1	2.22	0.56
1:A:248:VAL:O	1:A:251:SER:OG	2.24	0.56
2:B:47:SER:OG	2:B:49:ASP:OD1	2.20	0.56
13:N:73:THR:HG22	13:N:73:THR:O	2.05	0.56
15:P:90:PRO:HA	15:P:145:THR:HG21	1.88	0.56
16:Q:79:ASN:HA	16:Q:101:LEU:O	2.05	0.56
25:b:100:ARG:HH11	35:l:60:GLU:HG3	1.70	0.56
32:i:87:THR:HG22	32:i:88:LYS:N	2.19	0.56
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.35	0.55
20:V:69:ILE:HD13	20:V:72:LEU:HD21	1.88	0.55
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:71:VAL:HG11	27:d:87:GLU:HB3	1.89	0.55
30:g:4:MET:O	30:g:10:ARG:NH1	2.39	0.55
35:l:343:SER:O	35:l:347:ILE:HG13	2.06	0.55
2:B:200:GLU:OE1	13:N:87:HIS:ND1	2.38	0.55
4:E:38:ALA:O	4:E:42:GLU:HG2	2.06	0.55
12:M:68:ARG:NH1	12:M:284:GLU:OE1	2.40	0.55
12:M:178:GLN:HG2	12:M:204:MET:HE3	1.88	0.55
35:l:342:CYS:SG	35:l:373:LEU:HB2	2.46	0.55
35:l:488:MET:O	35:l:492:ILE:HG23	2.06	0.55
20:V:81:ARG:O	20:V:81:ARG:HD3	2.07	0.55
54:r:503:CDL:H612	54:r:503:CDL:H451	1.89	0.55
20:V:131:GLU:OE1	40:r:189:SER:OG	2.24	0.55
25:b:110:ILE:HG12	27:d:16:ARG:HB3	1.87	0.55
30:g:109:LYS:HG3	30:g:113:GLU:HG3	1.87	0.55
40:r:33:LEU:O	40:r:37:ILE:HG12	2.06	0.55
1:A:318:ILE:HG13	1:A:357:MET:HE1	1.88	0.55
9:J:238:GLN:HE21	9:J:266:VAL:HG12	1.71	0.55
26:c:63:GLU:OE1	26:c:77:LYS:O	2.25	0.55
35:l:293:ILE:HD11	35:l:421:ALA:HB3	1.89	0.55
54:r:504:CDL:H662	54:r:504:CDL:H612	1.89	0.55
41:s:62:ARG:HH22	41:s:68:ILE:CA	2.20	0.55
1:A:445:GLU:OE2	1:A:449:ARG:NH2	2.35	0.55
14:O:131:HIS:NE2	14:O:172:ILE:HG13	2.21	0.55
12:M:456:ALA:O	12:M:499:ASN:ND2	2.39	0.55
21:W:63:GLU:OE1	42:u:119:ARG:NH2	2.39	0.55
27:d:41:VAL:O	27:d:45:VAL:HG12	2.06	0.55
4:E:104:MET:HE3	4:E:104:MET:HA	1.88	0.55
9:J:168:SER:O	9:J:202:LYS:HA	2.06	0.55
12:M:47:THR:HG23	12:M:51:GLN:HB2	1.87	0.55
24:a:156:VAL:O	24:a:160:MET:HG3	2.06	0.55
27:d:148:ALA:HB3	40:r:304:GLN:HG3	1.88	0.55
44:w:332:THR:HG22	44:w:338:LYS:HD3	1.89	0.55
1:A:127:ASP:O	1:A:131:ILE:HD12	2.07	0.55
9:J:212:ARG:O	9:J:216:TYR:CB	2.54	0.55
13:N:73:THR:HG21	13:N:81:MET:HE1	1.88	0.55
26:c:49:ALA:HB1	26:c:53:LYS:NZ	2.21	0.55
14:O:181:VAL:HG11	14:O:225:CYS:HB2	1.89	0.54
32:i:128:LEU:HD12	32:i:216:PHE:HB3	1.89	0.54
40:r:253:LEU:HD23	40:r:257:MET:HB2	1.89	0.54
4:E:25:MET:HE1	4:E:79:VAL:HG21	1.88	0.54
34:k:37:MET:HG3	34:k:67:ALA:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.73	0.54
43:v:31:PHE:HB2	43:v:33:GLU:OE2	2.07	0.54
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.89	0.54
20:V:126:LYS:O	20:V:130:LEU:HG	2.07	0.54
32:i:167:TRP:CZ3	35:l:573:MET:HB2	2.43	0.54
7:H:50:GLN:NE2	8:I:93:LYS:HD3	2.22	0.54
32:i:200:MET:HE1	32:i:343:LEU:HD13	1.89	0.54
35:l:19:ILE:HD12	35:l:123:LEU:HD22	1.90	0.54
41:s:195:ARG:HD3	41:s:231:ILE:HD11	1.88	0.54
6:X:69:SER:OG	6:X:70:ASP:N	2.40	0.54
32:i:290:LEU:O	32:i:294:MET:HG3	2.07	0.54
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.89	0.54
1:A:40:ARG:NH1	1:A:289:GLU:O	2.41	0.54
1:A:86:ARG:O	1:A:88:ARG:NH1	2.40	0.54
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.38	0.54
12:M:558:GLN:N	12:M:558:GLN:OE1	2.41	0.54
34:k:17:ALA:O	34:k:21:MET:HG3	2.07	0.54
35:l:551:SER:HA	35:l:555:LEU:HB2	1.88	0.54
44:w:209:VAL:HG12	44:w:260:ALA:HB2	1.89	0.54
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.90	0.54
22:Y:74:TRP:CZ3	23:Z:82:VAL:HG21	2.43	0.54
25:b:103:ARG:HH21	25:b:105:PHE:HE1	1.56	0.54
26:c:49:ALA:C	26:c:53:LYS:HZ2	2.14	0.54
1:A:380:GLY:O	1:A:386:ARG:NH1	2.40	0.54
31:h:3:PHE:HB2	32:i:144:GLN:CD	2.33	0.54
41:s:179:TRP:O	41:s:183:MET:HG3	2.08	0.54
43:v:12:ASP:HB3	43:v:15:LYS:HB2	1.90	0.54
9:J:50:SER:OG	15:P:225:GLU:OE2	2.26	0.54
9:J:303:ARG:CD	9:J:316:ARG:HD3	2.38	0.54
22:Y:74:TRP:CZ2	23:Z:82:VAL:HG23	2.43	0.54
23:Z:52:ARG:HG2	35:l:435:PRO:O	2.08	0.54
35:l:37:LYS:HD3	35:l:98:TRP:HE1	1.72	0.54
35:l:80:PHE:HB3	35:l:82:MET:HE2	1.90	0.54
35:l:429:PHE:HE1	39:p:32:VAL:HG11	1.72	0.54
35:l:468:ILE:O	35:l:472:ILE:HG23	2.08	0.54
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.43	0.54
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.89	0.54
33:j:15:SER:O	33:j:19:LEU:HG	2.08	0.54
35:l:516:PRO:HG3	39:p:30:TRP:CH2	2.43	0.54
44:w:136:TYR:OH	44:w:191:LYS:HG3	2.08	0.54
14:O:179:ALA:HB3	14:O:185:MET:HE3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:569:ILE:O	35:l:573:MET:HG2	2.08	0.53
1:A:192:ASP:HB3	10:K:98:MET:HE2	1.90	0.53
9:J:65:LEU:HG	9:J:129:LEU:HD21	1.90	0.53
26:c:62:TYR:OH	26:c:74:ASP:OD1	2.24	0.53
26:c:117:VAL:HG21	35:l:539:TYR:HB2	1.89	0.53
35:l:409:LEU:O	35:l:413:LEU:HG	2.08	0.53
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.90	0.53
24:a:134:GLU:OE2	37:n:57:TRP:NE1	2.27	0.53
1:A:384:PRO:HB2	1:A:423:THR:HG22	1.91	0.53
12:M:389:THR:O	12:M:390:THR:OG1	2.23	0.53
13:N:43:LYS:NZ	13:N:111:THR:O	2.32	0.53
25:b:69:ILE:O	25:b:73:THR:OG1	2.24	0.53
2:B:100:GLU:O	2:B:170:GLY:N	2.41	0.53
12:M:390:THR:HA	12:M:600:GLU:HG2	1.91	0.53
12:M:650:SER:OG	12:M:652:ASN:OD1	2.22	0.53
22:Y:74:TRP:CD1	22:Y:74:TRP:C	2.86	0.53
30:g:55:VAL:HG21	54:r:504:CDL:HB4	1.91	0.53
1:A:46:TYR:CD1	14:O:226:GLU:CB	2.92	0.53
6:X:82:ARG:HD3	6:X:125:GLU:OE2	2.09	0.53
35:l:467:ILE:O	35:l:471:ASN:HB2	2.09	0.53
1:A:145:GLY:O	1:A:148:ALA:N	2.42	0.53
3:C:133:MET:HE3	3:C:173:LEU:HD22	1.90	0.53
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.41	0.53
2:B:78:PHE:O	8:I:12:ARG:NH2	2.42	0.53
2:B:171:PRO:HB2	13:N:93:MET:HE1	1.90	0.53
9:J:157:LYS:NZ	9:J:197:GLU:OE2	2.36	0.53
16:Q:184:ILE:HG23	16:Q:203:MET:HB3	1.90	0.53
6:X:82:ARG:HD2	6:X:126:PHE:CE1	2.40	0.53
40:r:371:PRO:HD2	54:r:503:CDL:H391	1.89	0.53
2:B:171:PRO:HG2	2:B:200:GLU:OE2	2.08	0.53
12:M:605:GLN:OE1	12:M:643:ARG:NH1	2.42	0.53
35:l:288:THR:HG21	35:l:307:SER:HB3	1.91	0.53
40:r:336:ARG:HG2	40:r:426:ILE:HG22	1.90	0.53
6:X:76:LEU:CD1	25:b:20:ARG:HH12	2.20	0.53
6:X:90:TYR:HE1	23:Z:44:PRO:C	2.17	0.53
9:J:83:PRO:HG3	9:J:119:VAL:HG11	1.91	0.52
26:c:55:TYR:OH	26:c:74:ASP:O	2.20	0.52
35:l:338:MET:HE1	35:l:458:LEU:HD13	1.91	0.52
43:v:16:GLU:CG	43:v:17:PRO:HD2	2.38	0.52
1:A:185:ASN:OD1	1:A:190:GLY:N	2.25	0.52
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:509:ASP:OD1	12:M:509:ASP:N	2.38	0.52
20:V:8:LYS:NZ	20:V:24:ALA:HB2	2.24	0.52
24:a:114:LYS:HG2	27:d:63:TYR:CE2	2.44	0.52
40:r:310:MET:HB3	40:r:455:LEU:HD22	1.90	0.52
9:J:172:ALA:HA	9:J:181:LEU:HB3	1.91	0.52
26:c:124:VAL:HG12	26:c:128:THR:OG1	2.09	0.52
32:i:79:LEU:HB2	34:k:47:ILE:HD13	1.91	0.52
1:A:162:PHE:HB3	1:A:165:GLU:HB2	1.91	0.52
3:C:87:ASP:OD1	41:s:25:ARG:NH2	2.35	0.52
12:M:299:ARG:NH1	12:M:703:ALA:O	2.41	0.52
12:M:347:ASP:HB3	12:M:594:ALA:HB1	1.91	0.52
23:Z:51:TRP:HZ3	23:Z:57:PHE:HE2	1.57	0.52
30:g:122:ARG:O	38:o:109:ARG:NH2	2.39	0.52
35:l:411:MET:SD	35:l:411:MET:N	2.81	0.52
37:n:13:VAL:CG1	40:r:14:MET:HG2	2.38	0.52
9:J:37:HIS:CE1	18:T:49:ASP:HA	2.44	0.52
4:E:58:GLN:HA	4:E:61:ASP:OD2	2.10	0.52
9:J:206:ILE:CG1	9:J:245:VAL:HG21	2.40	0.52
41:s:69:SER:C	41:s:73:ILE:HD12	2.35	0.52
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.37	0.52
48:b:201:PEE:H29	54:r:503:CDL:H642	1.92	0.52
35:l:21:MET:SD	35:l:21:MET:N	2.83	0.52
26:c:107:TRP:HD1	26:c:108:ASP:OD1	1.93	0.52
6:X:138:LEU:HD13	6:X:144:ILE:HG12	1.92	0.52
31:h:65:GLU:OE2	31:h:71:LYS:HG3	2.10	0.52
35:l:261:ILE:HG12	35:l:317:ILE:HD11	1.91	0.52
41:s:306:SER:OG	41:s:310:MET:SD	2.68	0.52
16:Q:269:ARG:O	16:Q:273:VAL:HG23	2.10	0.52
24:a:120:TRP:HE3	24:a:123:ARG:HH22	1.52	0.52
34:k:38:LEU:O	34:k:42:ILE:HG12	2.09	0.52
35:l:356:ILE:HD11	35:l:430:ALA:HB2	1.91	0.52
40:r:74:PRO:O	40:r:78:MET:HG3	2.10	0.52
41:s:165:LEU:O	41:s:169:GLN:HG3	2.10	0.52
1:A:392:MET:HE3	1:A:419:ILE:HD12	1.91	0.51
12:M:697:THR:O	12:M:697:THR:HG22	2.09	0.51
17:S:20:GLY:O	17:S:23:THR:HG22	2.09	0.51
23:Z:78:PHE:O	23:Z:82:VAL:HG12	2.09	0.51
24:a:110:TRP:CE2	24:a:123:ARG:HD3	2.45	0.51
42:u:107:PHE:O	42:u:111:VAL:HG13	2.10	0.51
9:J:167:ILE:HD13	9:J:201:ILE:HB	1.92	0.51
20:V:91:PHE:HD1	20:V:119:GLY:C	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:LYS:HE3	16:Q:335:GLU:OE2	2.10	0.51
22:Y:54:GLN:HE21	35:l:367:PRO:CD	2.21	0.51
35:l:525:MET:SD	35:l:525:MET:N	2.83	0.51
42:u:83:THR:HA	42:u:86:TRP:CD1	2.45	0.51
43:v:51:LEU:HD22	43:v:63:LEU:HD22	1.92	0.51
18:T:69:ASP:O	18:T:73:GLU:HG3	2.10	0.51
30:g:21:ARG:HG2	30:g:21:ARG:HH11	1.74	0.51
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.92	0.51
44:w:100:ASP:HB2	44:w:102:LYS:HG2	1.93	0.51
12:M:34:VAL:HG23	12:M:41:VAL:HG13	1.93	0.51
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.46	0.51
19:U:26:GLY:HA3	48:j:201:PEE:H37	1.91	0.51
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.92	0.51
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.91	0.51
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.46	0.51
1:A:152:ARG:CG	1:A:152:ARG:NH1	2.73	0.51
1:A:185:ASN:O	1:A:187:CYS:N	2.44	0.51
12:M:464:GLN:NE2	12:M:467:LYS:HD2	2.26	0.51
21:W:70:ALA:HB2	42:u:125:LEU:HD13	1.92	0.51
54:a:201:CDL:H322	48:b:201:PEE:H62	1.92	0.51
28:e:125:LEU:O	28:e:129:ARG:HG3	2.11	0.51
43:v:52:MET:O	43:v:56:ARG:HG3	2.10	0.51
44:w:116:LYS:HD3	44:w:116:LYS:N	2.26	0.51
2:B:111:GLU:O	2:B:141:ARG:NH2	2.44	0.51
3:C:54:VAL:HG21	48:C:302:PEE:H52	1.92	0.51
21:W:30:LEU:HB3	21:W:35:MET:HE3	1.93	0.51
6:X:90:TYR:CE1	23:Z:44:PRO:HB3	2.46	0.51
26:c:84:GLN:O	26:c:84:GLN:NE2	2.37	0.51
33:j:10:ASN:OD1	41:s:10:ILE:HD11	2.10	0.51
44:w:129:TYR:OH	44:w:183:CYS:O	2.27	0.51
44:w:161:ARG:HD3	44:w:241:TYR:OH	2.10	0.51
5:F:33:VAL:O	5:F:36:PHE:HB3	2.11	0.51
8:I:40:LYS:HB3	21:W:7:LYS:H	1.75	0.51
16:Q:196:ALA:C	16:Q:197:MET:HG3	2.36	0.51
50:X:201:8Q1:O27	50:X:201:8Q1:O33	2.28	0.51
54:a:201:CDL:H432	27:d:44:PRO:HB3	1.91	0.51
35:l:392:LYS:O	35:l:396:ILE:HG12	2.11	0.51
40:r:370:PRO:HB3	40:r:375:LEU:HD22	1.92	0.51
44:w:112:CYS:SG	44:w:131:LEU:HB2	2.51	0.51
3:C:77:MET:HE1	16:Q:185:MET:HE1	1.92	0.51
12:M:124:HIS:HD2	16:Q:375:MET:HE2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:53:ARG:CZ	25:b:28:LEU:HD23	2.40	0.51
35:l:79:SER:HB3	35:l:135:ASN:HB3	1.93	0.51
35:l:174:TYR:CD2	35:l:232:TRP:HB3	2.46	0.51
1:A:314:LEU:HD12	1:A:315:LEU:N	2.26	0.50
7:H:35:LEU:HD13	7:H:49:GLU:HG3	1.92	0.50
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.93	0.50
12:M:265:THR:HG22	12:M:270:VAL:HA	1.91	0.50
34:k:23:ARG:NH1	36:m:24:PRO:HA	2.25	0.50
41:s:184:MET:HE1	41:s:296:LEU:HB3	1.93	0.50
3:C:144:HIS:O	3:C:151:ARG:NH1	2.42	0.50
32:i:65:THR:O	32:i:69:MET:HG3	2.11	0.50
35:l:492:ILE:O	35:l:496:MET:HG3	2.11	0.50
35:l:559:GLU:O	35:l:563:PRO:HD2	2.11	0.50
15:P:87:PHE:CE1	15:P:144:LYS:HD2	2.45	0.50
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.93	0.50
35:l:221:ALA:HA	35:l:226:GLN:HG2	1.93	0.50
13:N:3:LEU:O	13:N:7:LEU:HG	2.11	0.50
40:r:12:LEU:N	40:r:13:PRO:CD	2.74	0.50
43:v:92:HIS:O	43:v:96:VAL:HG13	2.12	0.50
44:w:350:LYS:HD2	44:w:351:TRP:H	1.77	0.50
1:A:444:PRO:O	1:A:448:GLU:HG3	2.12	0.50
9:J:72:HIS:NE2	15:P:215:GLU:OE1	2.45	0.50
28:e:125:LEU:HD12	28:e:129:ARG:NH2	2.26	0.50
9:J:318:LYS:O	9:J:322:VAL:HG12	2.10	0.50
34:k:21:MET:HB2	36:m:23:LYS:HZ2	1.69	0.50
38:o:51:TYR:HA	38:o:56:ARG:NH1	2.26	0.50
39:p:120:ALA:O	39:p:124:GLN:HG3	2.11	0.50
43:v:33:GLU:OE2	43:v:33:GLU:N	2.32	0.50
43:v:68:LYS:O	43:v:71:ARG:HG2	2.12	0.50
44:w:61:THR:HG22	44:w:159:LEU:HB3	1.92	0.50
15:P:155:SER:OG	15:P:157:VAL:HG23	2.12	0.50
17:S:49:GLU:OE1	17:S:52:ARG:NH1	2.44	0.50
6:X:103:HIS:CE1	6:X:105:MET:HG3	2.47	0.50
39:p:100:PRO:HG3	40:r:419:TYR:CZ	2.46	0.50
42:u:100:CYS:HB2	42:u:103:GLN:OE1	2.12	0.50
44:w:117:PHE:CE1	44:w:173:MET:HE3	2.47	0.50
8:I:27:ARG:NH1	16:Q:212:GLU:OE1	2.36	0.50
12:M:347:ASP:OD1	12:M:347:ASP:N	2.37	0.50
18:T:60:LYS:HG2	18:T:62:VAL:HG23	1.93	0.50
27:d:125:CYS:HB2	35:l:203:MET:HE1	1.94	0.50
42:u:38:LYS:HB3	42:u:39:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:103:GLU:OE1	43:v:106:ARG:HD3	2.12	0.50
1:A:217:GLU:OE2	1:A:236:PHE:N	2.44	0.50
15:P:156:SER:O	15:P:156:SER:OG	2.23	0.50
18:T:39:THR:HG22	18:T:62:VAL:HG22	1.94	0.50
40:r:445:LEU:HB3	54:r:503:CDL:H452	1.93	0.50
1:A:70:LEU:HD21	1:A:189:SER:HA	1.94	0.49
8:I:29:GLN:NE2	13:N:52:ASN:HB3	2.24	0.49
9:J:303:ARG:HD3	9:J:316:ARG:CD	2.42	0.49
15:P:114:LEU:HD21	15:P:167:GLU:HG3	1.94	0.49
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.32	0.49
26:c:162:PRO:HB3	43:v:58:TYR:HE1	1.77	0.49
2:B:168:VAL:HG11	2:B:205:ILE:HD11	1.94	0.49
16:Q:404:LYS:HE2	16:Q:457:VAL:HB	1.94	0.49
20:V:50:LEU:HD23	20:V:50:LEU:H	1.77	0.49
21:W:30:LEU:HD23	21:W:35:MET:HG3	1.94	0.49
6:X:129:GLU:OE1	39:p:82:PHE:HD1	1.95	0.49
24:a:71:MET:HE3	24:a:75:ILE:HD12	1.95	0.49
26:c:87:ASP:OD2	26:c:90:TYR:N	2.43	0.49
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.95	0.49
35:l:250:SER:HB2	35:l:333:ALA:HA	1.94	0.49
36:m:30:GLY:O	36:m:34:ILE:HG13	2.11	0.49
10:K:89:LEU:O	10:K:92:GLU:HG2	2.13	0.49
16:Q:185:MET:O	16:Q:189:THR:OG1	2.24	0.49
35:l:10:THR:O	35:l:14:ILE:HG23	2.11	0.49
43:v:41:ALA:HA	43:v:45:GLU:OE2	2.12	0.49
6:X:120:MET:HE1	39:p:24:LEU:CB	2.42	0.49
6:X:128:PHE:HZ	6:X:148:ILE:HG23	1.78	0.49
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.47	0.49
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.47	0.49
3:C:42:ARG:O	3:C:46:VAL:HG12	2.12	0.49
8:I:39:PRO:HB2	8:I:41:LEU:HD13	1.95	0.49
8:I:40:LYS:HB3	21:W:6:VAL:HA	1.94	0.49
6:X:134:ASP:OD1	39:p:2:ALA:N	2.46	0.49
26:c:129:MET:HG2	35:l:528:TYR:CD1	2.47	0.49
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.28	0.49
6:G:99:SER:N	6:G:102:SER:OG	2.45	0.49
35:l:293:ILE:HD12	35:l:422:TYR:HB3	1.95	0.49
35:l:390:TYR:CZ	35:l:466:PHE:HA	2.47	0.49
35:l:428:PHE:CD1	35:l:432:LEU:HD12	2.48	0.49
43:v:60:ALA:O	43:v:64:ILE:HG13	2.12	0.49
44:w:224:PRO:HA	44:w:227:MET:HE2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:112:SER:CB	50:G:201:8Q1:O2	2.61	0.49
12:M:355:LYS:HG3	12:M:366:LEU:HD13	1.94	0.49
12:M:483:ARG:HG3	12:M:485:ASP:OD1	2.13	0.49
12:M:547:LEU:HD22	12:M:550:ALA:HB3	1.93	0.49
19:U:56:PRO:HG2	42:u:45:LEU:HB2	1.95	0.49
20:V:81:ARG:HG3	20:V:83:LYS:HB2	1.93	0.49
33:j:3:ILE:HG12	48:m:201:PEE:H50	1.95	0.49
34:k:18:GLY:O	36:m:23:LYS:HD3	2.12	0.49
42:u:59:GLU:O	42:u:63:VAL:HG13	2.12	0.49
42:u:83:THR:HA	42:u:86:TRP:NE1	2.28	0.49
7:H:81:ILE:O	7:H:85:GLU:HG3	2.12	0.49
12:M:141:ASP:O	12:M:145:MET:HG2	2.12	0.49
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.94	0.49
15:P:90:PRO:HD3	15:P:146:TYR:CE1	2.48	0.49
6:X:74:LEU:HD21	6:X:152:LYS:HD3	1.95	0.49
27:d:160:LYS:NZ	30:g:114:ILE:O	2.42	0.49
30:g:64:LEU:O	30:g:68:THR:OG1	2.31	0.49
34:k:25:HIS:O	34:k:28:SER:N	2.38	0.49
35:l:445:GLU:O	35:l:447:ASN:N	2.46	0.49
41:s:224:PHE:O	41:s:227:GLU:HG2	2.13	0.49
10:K:76:LEU:HA	10:K:79:HIS:HD2	1.77	0.49
16:Q:431:HIS:O	16:Q:454:GLN:NE2	2.46	0.49
27:d:29:PRO:O	27:d:33:LEU:HB2	2.12	0.49
41:s:184:MET:HE2	41:s:293:PHE:HA	1.95	0.49
44:w:62:VAL:HG22	44:w:205:VAL:HB	1.94	0.49
1:A:249:ALA:O	1:A:252:PRO:HD2	2.13	0.48
11:L:78:ARG:NH2	12:M:249:GLU:OE1	2.41	0.48
19:U:53:TYR:HB2	21:W:72:MET:HE3	1.95	0.48
22:Y:65:MET:O	22:Y:69:ILE:HG13	2.13	0.48
26:c:149:ILE:O	26:c:151:PRO:HD3	2.13	0.48
32:i:17:THR:HG22	32:i:21:MET:HE2	1.93	0.48
35:l:341:MET:HB3	35:l:454:ILE:CD1	2.43	0.48
1:A:279:SER:OG	1:A:280:GLY:N	2.45	0.48
5:F:46:LYS:HD3	12:M:674:LEU:HD11	1.96	0.48
6:G:113:LEU:O	6:G:117:GLU:HG3	2.14	0.48
34:k:23:ARG:CG	36:m:23:LYS:HE3	2.42	0.48
35:l:373:LEU:HD23	35:l:431:PHE:HE2	1.77	0.48
38:o:59:VAL:HG11	40:r:344:LEU:HD21	1.95	0.48
44:w:211:VAL:HG21	44:w:235:GLN:OE1	2.13	0.48
16:Q:36:GLN:NE2	40:r:135:ARG:O	2.37	0.48
21:W:62:ILE:O	21:W:66:GLU:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Z:43:ASP:HB2	39:p:38:ARG:HH21	1.78	0.48
24:a:140:LEU:HD21	40:r:177:LEU:HB3	1.94	0.48
33:j:15:SER:HA	41:s:76:ILE:HD12	1.95	0.48
33:j:104:TYR:O	33:j:108:GLN:HG2	2.13	0.48
35:l:444:ASN:OD1	35:l:445:GLU:N	2.46	0.48
3:C:102:VAL:HA	3:C:129:TYR:O	2.13	0.48
5:F:41:TYR:CD1	5:F:41:TYR:C	2.91	0.48
14:O:58:GLU:H	14:O:58:GLU:CD	2.19	0.48
14:O:137:THR:HG22	14:O:138:THR:H	1.78	0.48
15:P:235:LEU:HD12	16:Q:418:ARG:HE	1.78	0.48
35:l:371:THR:O	35:l:375:ILE:HG13	2.13	0.48
39:p:122:ARG:O	39:p:126:LYS:HG2	2.13	0.48
41:s:286:MET:HE3	41:s:286:MET:HA	1.95	0.48
48:B:303:PEE:H14	41:s:293:PHE:HE1	1.78	0.48
17:S:17:PHE:HD1	41:s:260:VAL:HG21	1.79	0.48
20:V:89:ASN:N	20:V:89:ASN:ND2	2.60	0.48
22:Y:54:GLN:HE21	35:l:367:PRO:CG	2.26	0.48
35:l:327:LEU:O	35:l:331:MET:HG2	2.14	0.48
4:E:27:GLU:HA	4:E:30:ARG:HG2	1.96	0.48
5:F:23:LEU:O	5:F:57:GLU:HA	2.13	0.48
7:H:78:GLU:HA	7:H:81:ILE:HD12	1.94	0.48
10:K:76:LEU:HA	10:K:79:HIS:CD2	2.48	0.48
19:U:38:TYR:HB2	41:s:310:MET:O	2.13	0.48
22:Y:65:MET:CE	35:l:375:ILE:HG12	2.43	0.48
33:j:17:LEU:HD22	41:s:222:MET:HE2	1.95	0.48
34:k:62:ILE:HD12	36:m:157:THR:HG21	1.95	0.48
39:p:97:TYR:CD1	39:p:179:MET:HE3	2.48	0.48
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.95	0.48
16:Q:259:GLU:O	16:Q:263:THR:HG22	2.12	0.48
22:Y:65:MET:HE2	35:l:375:ILE:HG12	1.94	0.48
24:a:126:TYR:OH	40:r:40:SER:O	2.32	0.48
27:d:162:ARG:NH2	28:e:140:ASN:OD1	2.36	0.48
32:i:267:ILE:HG12	32:i:279:PRO:HB3	1.96	0.48
35:l:55:MET:HB3	43:v:74:PHE:HE1	1.79	0.48
35:l:298:ILE:O	35:l:302:VAL:HG23	2.13	0.48
3:C:82:PRO:HG3	16:Q:201:PHE:HB3	1.96	0.48
22:Y:99:ILE:HD11	43:v:107:ARG:HG3	1.95	0.48
26:c:185:GLU:OE2	43:v:37:ARG:HG2	2.13	0.48
32:i:190:MET:HG2	32:i:204:ASN:HB3	1.95	0.48
35:l:172:ILE:HG21	40:r:408:LEU:HD12	1.94	0.48
40:r:269:MET:HE3	40:r:399:ASN:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:v:28:ASP:N	43:v:28:ASP:OD1	2.47	0.48
43:v:103:GLU:O	43:v:107:ARG:HG2	2.13	0.48
44:w:66:ILE:HD11	44:w:169:PHE:HE2	1.78	0.48
7:H:38:ILE:HG21	7:H:45:ARG:HB2	1.96	0.48
12:M:140:GLN:HG2	16:Q:379:ILE:HG23	1.95	0.48
13:N:60:ARG:NH1	13:N:89:TRP:O	2.47	0.48
15:P:69:LEU:HD22	15:P:96:VAL:HG22	1.96	0.48
6:X:113:LEU:O	6:X:116:VAL:HG12	2.13	0.48
26:c:90:TYR:OH	39:p:152:GLU:OE2	2.26	0.48
35:l:306:THR:HG23	35:l:332:HIS:HE1	1.79	0.48
35:l:335:PHE:HA	35:l:338:MET:HG2	1.95	0.48
42:u:16:GLN:OE1	42:u:72:ARG:NH2	2.47	0.48
25:b:75:VAL:O	25:b:79:VAL:HG12	2.13	0.48
35:l:423:SER:O	35:l:427:ILE:HG22	2.14	0.48
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.49	0.47
17:S:66:LEU:HD13	42:u:82:PHE:HE2	1.78	0.47
30:g:48:ASN:HB3	30:g:55:VAL:HA	1.95	0.47
32:i:347:ASN:N	32:i:347:ASN:OD1	2.45	0.47
34:k:32:CYS:O	34:k:36:MET:HG3	2.14	0.47
35:l:377:SER:O	35:l:381:THR:HG23	2.13	0.47
39:p:14:GLN:O	39:p:18:ARG:HG2	2.14	0.47
40:r:11:LEU:HD13	40:r:100:ILE:HD12	1.95	0.47
40:r:121:LEU:O	40:r:125:THR:HG23	2.13	0.47
40:r:433:GLU:O	40:r:437:MET:HG2	2.14	0.47
2:B:37:THR:OG1	16:Q:317:ASP:OD1	2.24	0.47
12:M:354:LEU:HD22	12:M:548:LEU:HD22	1.96	0.47
13:N:85:GLU:HB2	13:N:98:PRO:HB3	1.95	0.47
21:W:120:MET:HG3	21:W:122:GLY:H	1.79	0.47
32:i:271:THR:HG21	40:r:165:VAL:HG23	1.96	0.47
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.95	0.47
39:p:175:ARG:HH11	39:p:178:PRO:HA	1.78	0.47
40:r:445:LEU:HD22	54:r:503:CDL:H401	1.96	0.47
1:A:214:GLU:OE2	1:A:224:ARG:NH2	2.41	0.47
7:H:44:TYR:CD2	7:H:94:MET:HG2	2.49	0.47
11:L:163:ASN:O	11:L:171:ARG:HA	2.14	0.47
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.40	0.47
24:a:110:TRP:CD2	24:a:123:ARG:HB2	2.49	0.47
54:a:201:CDL:H792	54:a:201:CDL:H762	1.61	0.47
26:c:100:ASN:HB2	26:c:103:GLU:CD	2.39	0.47
32:i:58:LYS:O	32:i:62:THR:HG23	2.14	0.47
32:i:167:TRP:HZ3	35:l:570:GLN:HA	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:o:38:ALA:O	38:o:42:ARG:HG2	2.15	0.47
54:u:201:CDL:H542	54:u:201:CDL:H582	1.91	0.47
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.97	0.47
2:B:86:TYR:CE1	3:C:171:GLU:HG2	2.49	0.47
9:J:166:HIS:HB3	9:J:200:ILE:HD13	1.94	0.47
12:M:405:THR:HG21	12:M:477:GLY:HA3	1.97	0.47
25:b:89:HIS:CE1	48:b:201:PEE:H50	2.49	0.47
32:i:186:HIS:O	32:i:190:MET:HG3	2.15	0.47
35:l:335:PHE:HE1	35:l:380:LEU:HD13	1.79	0.47
35:l:397:GLU:HG2	35:l:482:MET:CE	2.44	0.47
36:m:17:PHE:HA	36:m:20:PHE:CE1	2.49	0.47
36:m:41:CYS:SG	36:m:42:GLY:N	2.88	0.47
44:w:72:ARG:HH11	44:w:76:GLU:HG3	1.80	0.47
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.97	0.47
6:G:119:ILE:O	6:G:123:GLU:HG3	2.15	0.47
19:U:53:TYR:OH	42:u:41:LYS:NZ	2.42	0.47
40:r:272:THR:OG1	40:r:292:SER:OG	2.25	0.47
1:A:119:GLU:OE1	1:A:127:ASP:HB2	2.14	0.47
9:J:238:GLN:HE21	9:J:266:VAL:CG1	2.28	0.47
11:L:116:SER:OG	15:P:227:ALA:O	2.28	0.47
21:W:120:MET:HE3	36:m:127:ILE:HA	1.96	0.47
49:j:202:PLX:H151	49:j:202:PLX:H341	1.95	0.47
36:m:57:PHE:CE1	41:s:111:LEU:HD11	2.50	0.47
40:r:195:MET:HE3	40:r:195:MET:HB2	1.69	0.47
7:H:38:ILE:HD12	7:H:100:TRP:CH2	2.50	0.47
13:N:97:PRO:HG2	13:N:100:THR:HG23	1.95	0.47
15:P:94:ILE:O	15:P:98:THR:OG1	2.21	0.47
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.49	0.47
16:Q:206:GLU:OE2	16:Q:209:LYS:NZ	2.48	0.47
20:V:89:ASN:N	20:V:89:ASN:HD22	2.12	0.47
23:Z:18:ASP:OD1	23:Z:18:ASP:N	2.40	0.47
26:c:38:PRO:HG2	38:o:71:ALA:HB2	1.95	0.47
35:l:44:PHE:HB2	35:l:94:LEU:HB3	1.97	0.47
36:m:45:LEU:HD23	36:m:50:SER:HA	1.97	0.47
40:r:6:ILE:HD12	54:u:201:CDL:H261	1.95	0.47
3:C:71:CYS:HB3	16:Q:141:TYR:CG	2.50	0.47
4:E:71:ALA:HA	50:G:201:8Q1:O40	2.14	0.47
7:H:22:GLU:O	7:H:26:ILE:HG12	2.15	0.47
31:h:7:GLN:O	31:h:11:GLY:N	2.47	0.47
35:l:190:LEU:HD23	40:r:383:THR:HG21	1.96	0.47
35:l:342:CYS:SG	35:l:369:THR:HG22	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:36:LYS:HZ2	39:p:40:PHE:HE2	1.63	0.47
40:r:337:VAL:HG21	40:r:345:ALA:HB2	1.96	0.47
5:F:41:TYR:HE2	5:F:55:ILE:HD11	1.80	0.47
5:F:43:GLU:O	5:F:46:LYS:HB2	2.15	0.47
8:I:70:MET:HG3	15:P:66:ALA:HB1	1.97	0.47
16:Q:184:ILE:CG1	16:Q:337:MET:HE3	2.45	0.47
54:a:201:CDL:H341	54:a:201:CDL:H372	1.46	0.47
25:b:10:LEU:O	25:b:14:GLN:HG3	2.14	0.47
32:i:245:MET:HG3	32:i:297:ALA:HB1	1.96	0.47
33:j:64:LEU:O	33:j:68:GLU:HG3	2.15	0.47
38:o:3:PHE:CE2	39:p:70:GLU:HG2	2.50	0.47
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.50	0.47
9:J:316:ARG:HA	9:J:319:VAL:HG22	1.97	0.47
27:d:37:PHE:CE2	35:l:3:PRO:HB3	2.49	0.47
32:i:167:TRP:CZ3	35:l:570:GLN:HA	2.51	0.47
33:j:4:MET:HE1	48:m:201:PEE:H26	1.97	0.47
34:k:30:LEU:O	34:k:34:GLU:HG2	2.15	0.47
34:k:61:ILE:HG12	36:m:55:MET:SD	2.55	0.47
1:A:45:LEU:HD11	1:A:275:LEU:HD21	1.95	0.46
1:A:276:PHE:CE1	1:A:337:MET:HE3	2.50	0.46
9:J:201:ILE:HD13	9:J:263:PHE:HB2	1.97	0.46
13:N:2:GLU:HG3	13:N:4:VAL:HG22	1.97	0.46
13:N:4:VAL:O	13:N:8:ARG:HG2	2.15	0.46
14:O:56:THR:HG23	14:O:89:GLN:OE1	2.15	0.46
6:X:90:TYR:CE1	23:Z:44:PRO:C	2.92	0.46
24:a:66:ARG:HH12	28:e:72:ASP:HA	1.80	0.46
31:h:15:ASP:OD2	32:i:25:HIS:N	2.48	0.46
49:l:701:PLX:H301	49:l:701:PLX:H352	1.96	0.46
1:A:209:GLU:HB2	1:A:242:VAL:HG21	1.96	0.46
6:G:112:SER:N	50:G:201:8Q1:O1	2.49	0.46
16:Q:199:PRO:HA	16:Q:202:TRP:HB2	1.98	0.46
26:c:83:GLN:NE2	26:c:97:LEU:O	2.25	0.46
27:d:76:GLU:HG3	28:e:146:LYS:HD2	1.97	0.46
35:l:332:HIS:NE2	35:l:336:LYS:HG3	2.29	0.46
35:l:335:PHE:CE1	35:l:380:LEU:HD13	2.50	0.46
40:r:253:LEU:HD23	40:r:253:LEU:O	2.16	0.46
1:A:185:ASN:C	1:A:187:CYS:H	2.22	0.46
9:J:298:TYR:CD2	9:J:319:VAL:HB	2.51	0.46
15:P:132:LEU:HB2	15:P:141:ILE:HG22	1.95	0.46
16:Q:345:SER:HB2	21:W:19:ILE:HD12	1.96	0.46
26:c:44:THR:OG1	26:c:47:GLU:OE1	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:148:GLU:OE1	44:w:301:LYS:NZ	2.33	0.46
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.51	0.46
4:E:27:GLU:O	4:E:30:ARG:HG3	2.15	0.46
13:N:144:TYR:HD1	13:N:144:TYR:H	1.62	0.46
25:b:103:ARG:NH2	43:v:51:LEU:HD23	2.23	0.46
25:b:104:ILE:CG1	43:v:48:ASP:HB3	2.24	0.46
34:k:37:MET:HG3	34:k:67:ALA:HB1	1.97	0.46
35:l:100:ILE:HG21	35:l:246:LEU:HB2	1.97	0.46
40:r:268:GLY:O	40:r:272:THR:HG23	2.15	0.46
5:F:93:ASN:HD22	5:F:98:LYS:HE3	1.81	0.46
6:G:103:HIS:NE2	6:G:105:MET:HG2	2.31	0.46
11:L:78:ARG:NE	11:L:148:GLU:OE1	2.27	0.46
35:l:566:THR:O	35:l:570:GLN:HG2	2.15	0.46
39:p:117:ASP:O	39:p:121:LYS:HG3	2.16	0.46
12:M:55:LYS:HB3	12:M:55:LYS:HE3	1.61	0.46
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	1.97	0.46
6:X:126:PHE:CD2	6:X:148:ILE:HD13	2.51	0.46
54:a:201:CDL:H342	25:b:84:TYR:CD2	2.51	0.46
29:f:68:GLU:OE1	29:f:71:ARG:NH2	2.42	0.46
39:p:124:GLN:O	39:p:127:ARG:HG2	2.16	0.46
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.96	0.46
1:A:326:LEU:HD23	1:A:367:ILE:HD11	1.98	0.46
3:C:65:MET:O	3:C:65:MET:HG3	2.16	0.46
4:E:16:SER:HB3	11:L:52:LEU:HG	1.98	0.46
9:J:57:THR:HG21	9:J:120:VAL:HG12	1.97	0.46
9:J:162:GLU:CG	9:J:163:LYS:HG3	2.45	0.46
12:M:399:VAL:HG23	12:M:428:LYS:HB3	1.97	0.46
14:O:46:GLU:N	14:O:46:GLU:OE2	2.48	0.46
25:b:120:MET:SD	25:b:120:MET:N	2.89	0.46
32:i:232:HIS:HB3	32:i:311:MET:CE	2.46	0.46
35:l:424:THR:HA	35:l:427:ILE:HG22	1.97	0.46
9:J:132:ARG:HA	9:J:132:ARG:HD3	1.69	0.46
12:M:64:CYS:O	12:M:184:ARG:NH2	2.39	0.46
16:Q:292:MET:HE1	16:Q:438:MET:SD	2.55	0.46
39:p:26:HIS:ND1	39:p:75:GLN:O	2.48	0.46
14:O:110:MET:O	14:O:114:GLU:HG3	2.16	0.46
14:O:198:PRO:O	14:O:202:GLU:HG3	2.16	0.46
26:c:53:LYS:HD3	26:c:53:LYS:N	2.31	0.46
32:i:7:THR:HG23	54:i:401:CDL:H531	1.97	0.46
32:i:68:MET:HE2	32:i:68:MET:HA	1.97	0.46
34:k:66:PHE:CE1	36:m:157:THR:HG22	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:285:THR:HA	35:l:308:SER:HA	1.98	0.46
3:C:55:ASN:ND2	3:C:187:GLU:O	2.49	0.46
25:b:18:LEU:HD11	39:p:163:LEU:HD22	1.97	0.46
25:b:84:TYR:CD1	25:b:88:TYR:HD2	2.33	0.46
27:d:6:ASP:OD1	27:d:8:ASP:N	2.36	0.46
27:d:132:PHE:HA	27:d:135:VAL:HG12	1.98	0.46
32:i:171:ASN:OD1	35:l:578:SER:OG	2.29	0.46
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.97	0.46
36:m:21:SER:O	36:m:23:LYS:HG3	2.16	0.46
44:w:43:PHE:CD1	44:w:43:PHE:C	2.94	0.46
44:w:171:GLU:O	44:w:175:ARG:HG2	2.15	0.46
1:A:125:CYS:H	1:A:277:ASN:HD22	1.64	0.45
7:H:30:LYS:HE3	7:H:88:LEU:HD21	1.97	0.45
12:M:29:SER:OG	12:M:30:ASN:N	2.43	0.45
12:M:535:GLU:HA	12:M:538:ARG:HG3	1.98	0.45
14:O:231:LEU:N	14:O:231:LEU:HD12	2.31	0.45
16:Q:178:THR:OG1	16:Q:214:TYR:OH	2.30	0.45
19:U:78:LEU:HD12	42:u:123:GLY:HA3	1.96	0.45
22:Y:56:ILE:HA	22:Y:59:GLU:CD	2.34	0.45
25:b:100:ARG:HE	27:d:118:GLY:HA3	1.81	0.45
32:i:310:ASN:HB2	44:w:309:THR:HG22	1.97	0.45
41:s:140:ILE:HA	41:s:143:GLU:HG2	1.98	0.45
9:J:238:GLN:HG2	9:J:270:ARG:HG2	1.98	0.45
16:Q:82:LEU:HD21	41:s:127:TYR:CE1	2.51	0.45
20:V:123:ALA:O	20:V:127:MET:HG3	2.16	0.45
24:a:60:SER:HB3	39:p:107:TRP:HA	1.98	0.45
26:c:58:ARG:HD2	38:o:35:GLU:HG3	1.99	0.45
35:l:525:MET:CE	39:p:77:PRO:HB2	2.46	0.45
40:r:255:ASN:OD1	40:r:256:TYR:N	2.49	0.45
40:r:351:LEU:HD22	40:r:426:ILE:HD11	1.98	0.45
54:u:201:CDL:H752	54:u:201:CDL:H781	1.49	0.45
1:A:158:ILE:HD12	1:A:159:ARG:H	1.82	0.45
9:J:238:GLN:CG	9:J:270:ARG:HG2	2.47	0.45
10:K:79:HIS:ND1	14:O:216:PRO:HD2	2.32	0.45
6:X:103:HIS:ND1	6:X:106:LYS:HG2	2.31	0.45
26:c:33:THR:OG1	26:c:36:MET:HG2	2.15	0.45
26:c:163:TYR:OH	43:v:41:ALA:O	2.34	0.45
32:i:291:TYR:HA	40:r:151:PHE:HZ	1.80	0.45
40:r:87:GLU:O	40:r:92:LYS:NZ	2.50	0.45
40:r:225:ILE:O	40:r:229:MET:HG3	2.17	0.45
49:r:502:PLX:H51	49:r:502:PLX:H6	1.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:GLY:HA2	3:C:73:ALA:HB2	1.98	0.45
7:H:88:LEU:HG	7:H:92:ARG:NH1	2.31	0.45
10:K:75:ASN:O	10:K:78:HIS:ND1	2.43	0.45
6:X:120:MET:HE3	39:p:21:LYS:HD2	1.98	0.45
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.80	0.45
26:c:117:VAL:HB	35:l:538:THR:OG1	2.17	0.45
32:i:167:TRP:CH2	35:l:573:MET:HB2	2.51	0.45
54:i:401:CDL:H142	54:i:401:CDL:H171	1.48	0.45
35:l:334:PHE:CE1	35:l:460:GLY:HA3	2.51	0.45
40:r:174:LEU:HD23	40:r:179:ILE:HD11	1.99	0.45
4:E:70:ASN:HB2	50:G:201:8Q1:C43	2.47	0.45
16:Q:462:ASP:OD1	16:Q:462:ASP:N	2.49	0.45
17:S:5:ILE:HG12	41:s:26:LYS:HG2	1.99	0.45
20:V:141:VAL:HG22	24:a:157:ARG:HB3	1.98	0.45
21:W:80:ASP:HB3	42:u:53:PRO:HB3	1.98	0.45
6:X:115:GLN:NE2	6:X:138:LEU:O	2.50	0.45
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.75	0.45
24:a:59:PRO:HG2	40:r:351:LEU:HA	1.98	0.45
24:a:165:ASP:OD1	24:a:165:ASP:N	2.44	0.45
27:d:78:GLU:CD	30:g:108:LYS:HB3	2.41	0.45
28:e:73:SER:O	28:e:75:GLY:N	2.49	0.45
28:e:106:VAL:HA	28:e:109:LEU:HG	1.98	0.45
30:g:110:THR:OG1	30:g:113:GLU:OE2	2.34	0.45
31:h:3:PHE:HD1	32:i:144:GLN:HE22	1.64	0.45
38:o:121:LEU:O	38:o:121:LEU:HD23	2.17	0.45
44:w:230:THR:HG23	44:w:233:TYR:H	1.81	0.45
44:w:343:TYR:HA	44:w:352:ILE:HD12	1.98	0.45
3:C:61:SER:OG	41:s:54:LYS:HD3	2.17	0.45
26:c:70:MET:HE2	26:c:72:TYR:HE2	1.81	0.45
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.98	0.45
32:i:170:LEU:O	32:i:295:ARG:NH2	2.49	0.45
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.97	0.45
38:o:117:GLN:OE1	38:o:117:GLN:HA	2.17	0.45
40:r:114:GLU:OE1	40:r:174:LEU:HB2	2.17	0.45
40:r:204:MET:HG3	40:r:209:LEU:HB2	1.99	0.45
41:s:28:LEU:CD2	41:s:274:ARG:NH1	2.80	0.45
44:w:172:ALA:O	44:w:176:GLN:HG2	2.15	0.45
3:C:64:PRO:HB3	3:C:102:VAL:HG13	1.99	0.45
14:O:181:VAL:CG1	14:O:225:CYS:HB2	2.46	0.45
16:Q:52:MET:HG3	16:Q:53:TYR:CG	2.52	0.45
16:Q:185:MET:HE3	16:Q:189:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:34:LYS:HE3	17:S:34:LYS:HB2	1.84	0.45
49:l:701:PLX:H131	54:r:503:CDL:H462	1.99	0.45
1:A:357:MET:HB3	1:A:361:THR:HG21	1.99	0.45
48:C:302:PEE:H26	48:C:302:PEE:H20	1.66	0.45
11:L:76:LYS:HE2	11:L:146:ASP:OD2	2.17	0.45
6:X:155:TYR:HH	24:a:54:LEU:HD11	1.79	0.45
34:k:45:THR:HG23	36:m:52:LEU:HD13	1.99	0.45
37:n:5:LEU:HD12	37:n:5:LEU:O	2.16	0.45
42:u:26:LYS:NZ	42:u:95:GLN:O	2.33	0.45
5:F:69:TYR:HE2	5:F:75:LYS:HD3	1.81	0.45
15:P:167:GLU:HG2	15:P:178:PHE:CD2	2.52	0.45
32:i:102:LEU:HD13	32:i:142:LEU:HG	1.99	0.45
35:l:399:VAL:HG12	35:l:409:LEU:HD12	1.99	0.45
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.98	0.45
9:J:346:GLU:HG2	9:J:371:PRO:HB3	1.99	0.45
11:L:115:SER:HB2	12:M:267:THR:HB	1.99	0.45
12:M:398:ASP:OD1	12:M:398:ASP:N	2.51	0.45
14:O:93:LEU:HD12	14:O:122:TYR:HB3	1.99	0.45
16:Q:196:ALA:O	16:Q:197:MET:HG3	2.17	0.45
32:i:7:THR:HG22	32:i:11:MET:SD	2.57	0.45
32:i:139:LEU:HD11	32:i:190:MET:HE1	1.99	0.45
40:r:300:ALA:O	40:r:308:SER:HB3	2.17	0.45
41:s:51:ASP:HB3	56:s:401:UQ:H8	2.00	0.45
1:A:147:ARG:HA	1:A:147:ARG:HD2	1.84	0.44
6:G:114:ASP:O	6:G:118:ILE:HG13	2.17	0.44
21:W:74:LEU:O	21:W:78:GLU:HG3	2.17	0.44
30:g:46:ILE:HG22	32:i:327:PRO:HB3	1.99	0.44
38:o:56:ARG:NH1	38:o:60:ILE:HD11	2.31	0.44
40:r:196:TRP:CE3	40:r:257:MET:HG2	2.52	0.44
4:E:37:ARG:HH22	6:G:132:ASP:HB2	1.80	0.44
9:J:270:ARG:HB2	9:J:375:VAL:O	2.17	0.44
12:M:638:THR:O	12:M:642:VAL:HG23	2.17	0.44
16:Q:372:LYS:NZ	18:T:94:GLY:O	2.35	0.44
25:b:75:VAL:C	25:b:78:PRO:HD2	2.43	0.44
40:r:112:ALA:HB1	40:r:118:PHE:HB2	1.99	0.44
40:r:159:PRO:HG2	48:r:501:PEE:H38	1.99	0.44
2:B:77:LEU:HD13	41:s:31:MET:HE2	1.98	0.44
21:W:86:MET:HE1	21:W:125:TYR:CZ	2.51	0.44
26:c:162:PRO:HB3	43:v:58:TYR:CE1	2.51	0.44
28:e:57:GLU:OE1	44:w:320:GLY:HA3	2.17	0.44
35:l:144:TRP:CH2	35:l:256:GLY:HA2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:186:MET:HG2	35:l:196:TRP:NE1	2.33	0.44
35:l:371:THR:O	35:l:374:ILE:HG22	2.17	0.44
40:r:147:LEU:HD22	40:r:151:PHE:HE2	1.82	0.44
40:r:222:GLU:HA	40:r:222:GLU:OE1	2.17	0.44
41:s:107:ALA:O	41:s:110:SER:OG	2.27	0.44
54:u:201:CDL:H201	54:u:201:CDL:H171	1.81	0.44
44:w:165:SER:HB3	44:w:245:PHE:CZ	2.52	0.44
4:E:104:MET:HE3	4:E:104:MET:CA	2.47	0.44
7:H:69:GLU:HG3	7:H:77:ILE:HG13	1.99	0.44
12:M:133:GLN:O	12:M:137:CYS:HB2	2.18	0.44
12:M:690:THR:HG23	12:M:692:LYS:HG2	1.99	0.44
6:X:93:ILE:HG23	6:X:108:LEU:HD21	2.00	0.44
24:a:131:LYS:HE3	37:n:32:ASP:CG	2.37	0.44
25:b:25:ASP:OD2	39:p:125:TRP:NE1	2.31	0.44
26:c:133:LEU:HD13	35:l:527:GLY:O	2.17	0.44
32:i:87:THR:CG2	32:i:88:LYS:H	2.26	0.44
35:l:233:LEU:HB3	35:l:234:PRO:HD3	2.00	0.44
37:n:8:VAL:O	37:n:12:TRP:HB3	2.18	0.44
1:A:358:ASP:OD1	1:A:360:SER:OG	2.30	0.44
12:M:29:SER:HG	12:M:30:ASN:H	1.64	0.44
17:S:1:MET:HE3	17:S:1:MET:HB2	1.72	0.44
22:Y:72:ARG:CB	35:l:385:TYR:CG	2.95	0.44
26:c:176:LYS:HA	26:c:176:LYS:HD2	1.77	0.44
30:g:85:TYR:CZ	32:i:344:SER:HB3	2.53	0.44
34:k:23:ARG:HG2	36:m:23:LYS:CE	2.45	0.44
35:l:12:LEU:HD22	35:l:129:MET:HB3	1.99	0.44
35:l:51:LEU:HD22	35:l:91:PRO:HG2	1.98	0.44
35:l:390:TYR:OH	35:l:466:PHE:HB2	2.18	0.44
35:l:498:PHE:HB3	35:l:499:MET:HE2	1.98	0.44
39:p:157:ALA:HB1	39:p:162:ASP:HB2	1.99	0.44
42:u:47:ARG:NH2	42:u:53:PRO:HG3	2.33	0.44
1:A:210:THR:HB	1:A:224:ARG:HG2	1.99	0.44
2:B:72:MET:HE2	16:Q:260:GLU:HG2	1.99	0.44
4:E:120:SER:O	4:E:124:VAL:HG22	2.18	0.44
12:M:382:ARG:HE	12:M:527:ASP:CG	2.26	0.44
16:Q:41:VAL:HG23	28:e:55:LEU:HD23	1.98	0.44
17:S:16:LEU:HB3	41:s:260:VAL:HG22	1.99	0.44
26:c:56:ASN:ND2	38:o:43:LEU:HD21	2.32	0.44
32:i:232:HIS:HB3	32:i:311:MET:HE3	1.99	0.44
40:r:104:LEU:O	40:r:108:MET:HG3	2.17	0.44
9:J:227:PRO:HB2	9:J:298:TYR:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:131:LYS:HD2	11:L:147:VAL:HG11	2.00	0.44
12:M:370:GLU:OE2	12:M:518:ARG:HD3	2.17	0.44
15:P:101:ARG:HE	15:P:159:VAL:HG13	1.82	0.44
16:Q:251:PHE:O	16:Q:255:ILE:HG13	2.17	0.44
20:V:22:ALA:O	20:V:26:THR:OG1	2.35	0.44
31:h:72:THR:O	31:h:76:LEU:HD13	2.17	0.44
32:i:72:MET:HE1	34:k:43:MET:CE	2.43	0.44
35:l:131:LEU:HD21	35:l:255:ALA:HB1	2.00	0.44
54:r:503:CDL:H202	54:r:503:CDL:H231	1.71	0.44
56:s:401:UQ:H101	56:s:401:UQ:H121	1.73	0.44
42:u:18:VAL:HG12	42:u:20:VAL:HG22	1.99	0.44
43:v:69:CYS:HB3	43:v:80:CYS:HB2	1.74	0.44
1:A:152:ARG:CZ	10:K:101:PRO:HD3	2.48	0.44
14:O:48:ASN:OD1	14:O:51:THR:OG1	2.32	0.44
23:Z:78:PHE:C	23:Z:78:PHE:CD1	2.95	0.44
28:e:137:MET:HE3	28:e:137:MET:HB2	1.88	0.44
54:u:201:CDL:H712	54:u:201:CDL:H741	1.54	0.44
4:E:27:GLU:O	4:E:31:ARG:HG2	2.17	0.44
4:E:37:ARG:HA	6:G:120:MET:CE	2.45	0.44
9:J:271:TYR:OH	9:J:346:GLU:OE2	2.30	0.44
12:M:690:THR:OG1	12:M:691:ILE:N	2.51	0.44
14:O:213:ILE:HD12	14:O:214:PRO:HD2	1.98	0.44
28:e:143:ASP:OD1	28:e:143:ASP:N	2.49	0.44
32:i:72:MET:HE3	32:i:76:ILE:HG13	1.99	0.44
35:l:107:TYR:HE1	35:l:348:HIS:HB2	1.82	0.44
41:s:143:GLU:HA	41:s:146:LEU:HB2	2.00	0.44
1:A:146:GLY:HA3	1:A:193:PHE:CE1	2.53	0.43
1:A:210:THR:HB	1:A:224:ARG:H	1.83	0.43
9:J:244:ASP:HB3	9:J:335:LEU:HD21	1.99	0.43
15:P:117:VAL:HB	15:P:127:GLU:HG2	1.99	0.43
16:Q:52:MET:HG3	16:Q:53:TYR:N	2.32	0.43
16:Q:172:VAL:HG21	16:Q:310:VAL:HG22	1.99	0.43
25:b:103:ARG:NH1	43:v:49:ALA:O	2.50	0.43
26:c:90:TYR:OH	38:o:40:ARG:HD3	2.18	0.43
28:e:126:VAL:HA	28:e:129:ARG:HD2	2.01	0.43
31:h:36:PHE:CD1	31:h:62:ASP:HB3	2.53	0.43
35:l:529:TYR:HB3	35:l:530:PRO:HD3	1.98	0.43
40:r:80:SER:OG	40:r:226:ALA:HB2	2.17	0.43
41:s:72:ILE:O	41:s:76:ILE:HG12	2.17	0.43
41:s:173:TRP:HB2	41:s:175:ILE:HG22	2.00	0.43
41:s:267:THR:O	41:s:271:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:47:GLU:CD	44:w:295:ARG:HH12	2.27	0.43
4:E:104:MET:HA	4:E:104:MET:CE	2.47	0.43
9:J:73:LEU:O	9:J:78:SER:OG	2.31	0.43
9:J:83:PRO:HA	9:J:106:MET:O	2.17	0.43
12:M:29:SER:OG	12:M:30:ASN:OD1	2.36	0.43
12:M:33:GLU:HG3	12:M:42:MET:HE1	1.99	0.43
48:i:402:PEE:H27	35:l:563:PRO:HA	1.99	0.43
1:A:288:VAL:HG21	1:A:303:HIS:ND1	2.33	0.43
1:A:446:LEU:O	1:A:450:MET:HG3	2.18	0.43
6:X:75:THR:OG1	6:X:156:GLU:O	2.30	0.43
22:Y:105:ASP:N	22:Y:105:ASP:OD1	2.51	0.43
24:a:110:TRP:CG	24:a:123:ARG:HB2	2.54	0.43
32:i:163:LEU:HA	32:i:285:THR:HG21	2.00	0.43
33:j:17:LEU:HA	33:j:20:ILE:HG12	2.00	0.43
48:j:201:PEE:H35	48:j:201:PEE:H30	1.82	0.43
40:r:153:THR:O	40:r:157:SER:N	2.51	0.43
41:s:53:LEU:O	41:s:57:THR:HG23	2.18	0.43
1:A:65:THR:O	1:A:69:LEU:HD23	2.18	0.43
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.53	0.43
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.53	0.43
4:E:80:ASP:C	4:E:80:ASP:OD1	2.62	0.43
4:E:84:ILE:O	4:E:88:MET:HG3	2.18	0.43
16:Q:184:ILE:HG12	16:Q:337:MET:HE3	2.00	0.43
19:U:59:ASP:OD1	19:U:60:ASP:N	2.51	0.43
22:Y:71:TRP:CD1	22:Y:71:TRP:C	2.96	0.43
24:a:94:GLY:HA2	24:a:116:PRO:HG3	2.00	0.43
24:a:95:GLU:OE2	54:a:201:CDL:O1	2.27	0.43
32:i:95:MET:HE2	32:i:149:ILE:HG22	2.00	0.43
34:k:61:ILE:HD11	36:m:143:ILE:HG12	1.99	0.43
35:l:33:PRO:HB3	35:l:118:PHE:CZ	2.54	0.43
35:l:536:LEU:HB3	35:l:537:PRO:HD3	2.00	0.43
35:l:553:LEU:HD11	38:o:94:GLY:HA3	2.00	0.43
41:s:75:PRO:HD3	41:s:223:PHE:CZ	2.54	0.43
4:E:88:MET:HE2	15:P:184:LEU:O	2.19	0.43
7:H:50:GLN:O	7:H:54:GLU:HG3	2.18	0.43
9:J:180:TYR:HB2	9:J:317:ASP:OD2	2.18	0.43
10:K:80:GLU:N	10:K:80:GLU:OE1	2.51	0.43
12:M:144:MET:O	16:Q:362:LYS:NZ	2.47	0.43
14:O:164:THR:CG2	14:O:169:PHE:H	2.31	0.43
16:Q:145:MET:HG3	16:Q:214:TYR:CZ	2.53	0.43
6:X:89:LEU:HD13	23:Z:48:ASN:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:66:LEU:HB3	28:e:73:SER:OG	2.18	0.43
38:o:8:PRO:HG3	38:o:14:LEU:HD13	2.00	0.43
56:s:401:UQ:H72	56:s:401:UQ:H111	1.85	0.43
44:w:211:VAL:HA	44:w:214:ILE:HG12	1.99	0.43
12:M:251:ILE:HB	12:M:606:THR:HG22	2.00	0.43
13:N:10:GLY:O	13:N:14:VAL:HG23	2.19	0.43
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	2.00	0.43
22:Y:60:PHE:CD1	22:Y:60:PHE:C	2.97	0.43
25:b:123:PHE:HB3	43:v:40:VAL:HG21	1.99	0.43
32:i:206:LEU:HD12	32:i:347:ASN:HD22	1.84	0.43
1:A:295:PRO:HD2	1:A:298:GLU:OE1	2.19	0.43
1:A:385:CYS:O	1:A:389:VAL:HB	2.19	0.43
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.54	0.43
2:B:150:THR:HG21	2:B:180:HIS:CD2	2.54	0.43
9:J:38:HIS:NE2	13:N:132:LYS:HD2	2.34	0.43
9:J:195:PHE:HB3	9:J:198:ALA:HB2	2.01	0.43
12:M:126:LEU:O	18:T:113:TYR:OH	2.28	0.43
12:M:433:GLY:O	12:M:444:HIS:NE2	2.35	0.43
22:Y:59:GLU:HG3	23:Z:73:TRP:HZ3	1.83	0.43
24:a:131:LYS:NZ	37:n:32:ASP:OD2	2.51	0.43
26:c:38:PRO:HD2	38:o:70:TYR:HD2	1.82	0.43
26:c:110:ASP:CG	40:r:278:ARG:HE	2.26	0.43
27:d:54:GLN:NE2	27:d:55:GLN:HG2	2.33	0.43
30:g:30:ASP:O	30:g:34:VAL:HG23	2.19	0.43
32:i:302:LEU:HD13	40:r:134:THR:HG21	2.00	0.43
35:l:95:PHE:CZ	35:l:456:ARG:HG2	2.54	0.43
35:l:313:MET:HG2	35:l:328:HIS:HD2	1.83	0.43
37:n:12:TRP:O	37:n:15:ILE:HG22	2.18	0.43
39:p:63:LEU:C	39:p:65:ARG:H	2.27	0.43
40:r:48:ASN:OD1	40:r:48:ASN:N	2.50	0.43
40:r:196:TRP:NE1	40:r:250:LEU:HB3	2.34	0.43
40:r:351:LEU:CD2	40:r:426:ILE:HD11	2.49	0.43
54:r:503:CDL:H591	54:r:503:CDL:H332	2.00	0.43
4:E:25:MET:O	4:E:29:LYS:HG3	2.19	0.43
8:I:92:LYS:HD2	8:I:92:LYS:HA	1.63	0.43
9:J:303:ARG:HD2	9:J:303:ARG:HA	1.58	0.43
12:M:591:GLU:HG2	12:M:610:VAL:HG23	2.01	0.43
16:Q:144:MET:HE3	16:Q:222:MET:O	2.19	0.43
16:Q:184:ILE:CG2	16:Q:203:MET:HB3	2.49	0.43
16:Q:187:VAL:HG11	16:Q:258:LEU:HD21	1.99	0.43
21:W:34:SER:O	21:W:38:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:Y:74:TRP:CZ2	23:Z:82:VAL:HG21	2.47	0.43
24:a:131:LYS:HD3	37:n:57:TRP:CE3	2.54	0.43
27:d:70:ARG:HD2	27:d:70:ARG:HA	1.89	0.43
30:g:110:THR:O	30:g:114:ILE:HG13	2.18	0.43
33:j:33:LYS:HD2	33:j:33:LYS:HA	1.71	0.43
35:l:32:TYR:O	35:l:36:VAL:HG23	2.18	0.43
39:p:20:TYR:CZ	39:p:24:LEU:HD11	2.54	0.43
40:r:216:LEU:HD11	40:r:236:LEU:HD11	2.01	0.43
40:r:357:THR:O	40:r:361:VAL:HG23	2.19	0.43
1:A:274:LYS:HB3	1:A:276:PHE:CZ	2.54	0.43
46:A:502:FMN:N1	46:A:502:FMN:O3'	2.49	0.43
8:I:13:ASN:ND2	8:I:19:ASP:HA	2.33	0.43
12:M:306:MET:HB3	12:M:314:LEU:HD22	2.00	0.43
13:N:73:THR:HG22	13:N:77:VAL:HG12	2.01	0.43
19:U:53:TYR:CD1	21:W:72:MET:HE3	2.54	0.43
21:W:88:ARG:HD3	42:u:9:THR:HA	2.00	0.43
24:a:50:HIS:CE1	24:a:52:LYS:HD3	2.53	0.43
26:c:119:THR:HB	38:o:13:THR:HG23	2.01	0.43
49:g:201:PLX:H22	49:g:201:PLX:H1C3	1.77	0.43
54:i:401:CDL:H372	54:i:401:CDL:H402	1.87	0.43
41:s:101:GLY:O	41:s:105:MET:HG3	2.19	0.43
44:w:165:SER:O	44:w:168:VAL:HG22	2.19	0.43
2:B:94:SER:HB3	16:Q:215:GLU:OE2	2.18	0.43
2:B:142:THR:O	2:B:187:LYS:NZ	2.51	0.43
4:E:59:GLY:O	4:E:63:VAL:HG23	2.19	0.43
9:J:206:ILE:HG21	9:J:242:ILE:HD13	2.01	0.43
12:M:718:ILE:HD12	12:M:718:ILE:HA	1.93	0.43
16:Q:414:ASP:OD1	16:Q:414:ASP:N	2.46	0.43
19:U:81:LEU:O	21:W:59:ARG:NH1	2.51	0.43
6:X:123:GLU:HG2	6:X:129:GLU:HA	2.01	0.43
24:a:141:GLN:OE1	37:n:38:PHE:HE1	2.00	0.43
48:j:201:PEE:H59	48:j:201:PEE:H64	1.57	0.43
49:j:202:PLX:H372	49:j:202:PLX:H342	1.84	0.43
49:l:701:PLX:H152	49:l:701:PLX:H121	1.48	0.43
36:m:23:LYS:HB2	36:m:23:LYS:HE3	1.92	0.43
40:r:346:ARG:O	40:r:419:TYR:HA	2.19	0.43
42:u:60:GLY:O	42:u:63:VAL:HG22	2.18	0.43
44:w:129:TYR:OH	44:w:187:TYR:HB2	2.19	0.43
1:A:115:VAL:HG21	1:A:142:CYS:SG	2.58	0.42
1:A:192:ASP:CB	10:K:98:MET:HE2	2.49	0.42
2:B:66:LEU:O	41:s:277:TYR:OH	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:G:201:8Q1:O40	50:G:201:8Q1:N36	2.52	0.42
12:M:260:ASN:HD21	12:M:278:HIS:HD2	1.66	0.42
22:Y:97:LEU:HD12	43:v:104:ARG:HB2	2.00	0.42
25:b:105:PHE:CE2	43:v:71:ARG:HD2	2.54	0.42
28:e:73:SER:C	28:e:75:GLY:H	2.27	0.42
35:l:386:LEU:O	35:l:389:PHE:HB3	2.19	0.42
35:l:511:LEU:HD12	39:p:39:TYR:CD2	2.54	0.42
40:r:307:TRP:HA	40:r:310:MET:HE2	2.00	0.42
54:u:201:CDL:H781	54:u:201:CDL:H812	1.82	0.42
5:F:16:LEU:HD12	5:F:16:LEU:HA	1.90	0.42
12:M:203:ASP:OD1	12:M:203:ASP:N	2.49	0.42
16:Q:158:LEU:HD12	16:Q:411:LEU:HD23	2.01	0.42
16:Q:226:TYR:OH	16:Q:234:GLN:O	2.21	0.42
6:X:140:CYS:HB2	6:X:143:GLU:HG2	2.01	0.42
54:a:201:CDL:H511	54:a:201:CDL:H131	2.01	0.42
32:i:291:TYR:HE1	32:i:295:ARG:HD3	1.83	0.42
48:j:201:PEE:H39	41:s:302:MET:HE1	2.00	0.42
35:l:152:PHE:CD1	35:l:168:ALA:HB1	2.54	0.42
37:n:13:VAL:HG13	40:r:14:MET:HG2	2.01	0.42
37:n:39:ARG:HG3	37:n:57:TRP:CE2	2.54	0.42
39:p:82:PHE:HB2	39:p:85:SER:OG	2.18	0.42
1:A:314:LEU:HD11	1:A:317:VAL:HG23	2.00	0.42
7:H:25:LYS:HE2	7:H:60:LYS:HG2	2.01	0.42
8:I:8:ILE:HD13	8:I:8:ILE:HA	1.92	0.42
9:J:227:PRO:HB3	9:J:291:TYR:CZ	2.54	0.42
11:L:156:LYS:HD2	12:M:67:GLU:HB3	2.02	0.42
26:c:151:PRO:O	43:v:9:TYR:OH	2.27	0.42
27:d:54:GLN:NE2	27:d:55:GLN:HE21	2.09	0.42
33:j:53:MET:HE2	33:j:53:MET:HB2	1.94	0.42
33:j:53:MET:HE1	34:k:83:ASN:ND2	2.35	0.42
39:p:63:LEU:O	39:p:64:LEU:HB3	2.19	0.42
40:r:166:TYR:CE1	40:r:195:MET:HE1	2.54	0.42
44:w:129:TYR:CZ	44:w:183:CYS:HB3	2.54	0.42
44:w:210:PRO:HD2	44:w:213:GLU:HB3	2.02	0.42
3:C:59:ARG:HH12	49:C:303:PLX:P1	2.43	0.42
7:H:6:LYS:NZ	7:H:78:GLU:OE1	2.52	0.42
8:I:12:ARG:HD3	8:I:20:LEU:HD22	2.01	0.42
35:l:190:LEU:HB2	35:l:196:TRP:NE1	2.34	0.42
35:l:293:ILE:HD11	35:l:421:ALA:CB	2.49	0.42
35:l:419:THR:HA	35:l:422:TYR:CZ	2.54	0.42
36:m:41:CYS:SG	36:m:57:PHE:HD2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:76:HIS:O	39:p:78:GLN:N	2.53	0.42
49:r:502:PLX:H121	49:r:502:PLX:H92	1.71	0.42
1:A:125:CYS:SG	1:A:277:ASN:ND2	2.92	0.42
9:J:37:HIS:O	9:J:40:LEU:N	2.40	0.42
11:L:101:PHE:CE1	11:L:124:LEU:HD23	2.55	0.42
12:M:698:ASP:OD1	12:M:698:ASP:N	2.52	0.42
17:S:66:LEU:HD13	42:u:82:PHE:CE2	2.53	0.42
30:g:93:PHE:O	30:g:96:VAL:HG12	2.20	0.42
32:i:222:SER:O	32:i:224:ALA:N	2.52	0.42
33:j:48:ARG:HB2	33:j:49:LEU:H	1.61	0.42
35:l:533:MET:HA	35:l:533:MET:HE2	2.02	0.42
4:E:28:ALA:HB1	4:E:79:VAL:HG11	2.02	0.42
4:E:81:LEU:HD12	4:E:81:LEU:HA	1.90	0.42
9:J:279:TYR:HB2	9:J:372:ALA:HB2	2.01	0.42
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.49	0.42
12:M:453:GLN:HE21	12:M:453:GLN:HB2	1.67	0.42
12:M:480:ALA:O	12:M:483:ARG:HG2	2.19	0.42
16:Q:152:SER:HB3	16:Q:229:PRO:HA	2.00	0.42
32:i:72:MET:CE	34:k:43:MET:HE1	2.44	0.42
35:l:109:HIS:C	35:l:109:HIS:HD1	2.27	0.42
35:l:179:ASP:O	35:l:183:VAL:HG23	2.19	0.42
54:r:504:CDL:H231	54:r:504:CDL:H262	1.87	0.42
54:r:504:CDL:H832	54:r:504:CDL:H862	1.86	0.42
1:A:48:ARG:HD3	10:K:70:ASN:O	2.20	0.42
4:E:110:THR:HG21	15:P:220:VAL:HG11	2.01	0.42
5:F:26:ARG:CZ	5:F:26:ARG:HB2	2.49	0.42
14:O:153:GLN:HG2	14:O:158:ILE:O	2.20	0.42
14:O:203:GLU:O	14:O:207:GLU:HG3	2.20	0.42
14:O:239:LYS:HG3	14:O:243:PHE:CD2	2.54	0.42
16:Q:269:ARG:HG2	16:Q:273:VAL:HG21	2.00	0.42
26:c:82:SER:HB3	26:c:119:THR:H	1.84	0.42
30:g:55:VAL:HG23	30:g:56:VAL:HG23	2.01	0.42
48:i:402:PEE:H28	48:i:402:PEE:H33	1.44	0.42
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.54	0.42
35:l:366:MET:HE2	35:l:369:THR:OG1	2.20	0.42
35:l:410:LEU:O	35:l:414:ILE:HG13	2.20	0.42
36:m:20:PHE:HB2	36:m:29:GLY:HA2	2.02	0.42
36:m:57:PHE:HE1	41:s:111:LEU:HD11	1.85	0.42
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.27	0.42
2:B:197:TRP:CE3	2:B:200:GLU:OE2	2.73	0.42
11:L:77:VAL:HG23	11:L:145:PHE:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:68:MET:SD	13:N:81:MET:HB3	2.60	0.42
15:P:56:LYS:HA	15:P:56:LYS:HD3	1.94	0.42
15:P:165:TRP:CZ2	16:Q:111:PRO:HG2	2.54	0.42
26:c:85:GLU:OE2	26:c:119:THR:OG1	2.36	0.42
32:i:169:GLY:HA3	32:i:292:PHE:CE2	2.55	0.42
35:l:86:SER:OG	35:l:262:ARG:NH2	2.53	0.42
38:o:33:GLN:OE1	39:p:9:TYR:HB3	2.19	0.42
44:w:266:ALA:O	44:w:269:VAL:HG12	2.19	0.42
49:C:303:PLX:H21	49:C:303:PLX:H1C3	1.78	0.42
6:G:123:GLU:HG2	6:G:130:ILE:HG13	2.01	0.42
14:O:200:ASP:O	14:O:204:ILE:HG13	2.19	0.42
16:Q:106:VAL:HG22	16:Q:442:HIS:O	2.19	0.42
22:Y:68:TRP:CE3	35:l:463:PHE:HE1	2.38	0.42
23:Z:79:VAL:HA	23:Z:82:VAL:HG12	2.02	0.42
32:i:250:SER:O	32:i:259:GLY:HA3	2.20	0.42
33:j:68:GLU:OE1	33:j:98:LEU:HD13	2.19	0.42
35:l:198:LEU:HD23	35:l:198:LEU:HA	1.88	0.42
36:m:17:PHE:O	36:m:21:SER:OG	2.33	0.42
39:p:51:HIS:HB3	39:p:54:GLU:HG3	2.01	0.42
42:u:100:CYS:O	42:u:100:CYS:SG	2.78	0.42
44:w:108:LEU:HD21	44:w:330:LYS:HB3	2.02	0.42
1:A:63:TYR:CE2	1:A:64:LYS:HG3	2.55	0.42
1:A:171:VAL:HG23	1:A:174:ARG:HH21	1.85	0.42
5:F:30:SER:OG	5:F:63:PRO:HG3	2.20	0.42
14:O:68:LYS:HB2	14:O:68:LYS:HE3	1.88	0.42
15:P:119:VAL:HG12	15:P:121:THR:HG22	2.02	0.42
16:Q:198:THR:OG1	41:s:275:ALA:O	2.35	0.42
48:j:201:PEE:H29	41:s:295:PRO:HB3	2.02	0.42
48:j:201:PEE:H73	48:j:201:PEE:H67	1.86	0.42
35:l:60:GLU:OE2	35:l:83:ASP:HA	2.20	0.42
36:m:141:MET:HE2	36:m:141:MET:HA	2.01	0.42
38:o:94:GLY:C	38:o:95:ILE:HD13	2.45	0.42
1:A:110:PRO:O	1:A:238:CYS:HB3	2.20	0.41
1:A:145:GLY:C	1:A:149:MET:HE2	2.45	0.41
13:N:85:GLU:HG2	13:N:86:TRP:H	1.85	0.41
19:U:53:TYR:HB2	21:W:72:MET:CE	2.49	0.41
19:U:78:LEU:HD23	19:U:78:LEU:HA	1.91	0.41
20:V:141:VAL:CG2	24:a:157:ARG:HB3	2.51	0.41
25:b:36:PRO:HA	25:b:37:PRO:HD3	1.92	0.41
26:c:118:ASP:O	35:l:535:ARG:HD3	2.20	0.41
32:i:70:LEU:HD12	32:i:98:MET:HE1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:253:VAL:HG23	35:l:310:LEU:HD21	2.00	0.41
35:l:360:GLY:HA3	35:l:435:PRO:HA	2.02	0.41
40:r:334:TYR:CD2	40:r:340:ARG:HB2	2.55	0.41
1:A:199:ARG:NH1	14:O:84:ASP:OD2	2.43	0.41
9:J:251:ASN:O	9:J:255:ASP:N	2.49	0.41
9:J:317:ASP:O	9:J:321:ARG:HG3	2.19	0.41
19:U:16:GLU:N	19:U:17:PRO:HD3	2.35	0.41
35:l:156:GLY:O	40:r:416:ARG:NH1	2.53	0.41
40:r:105:PHE:HB3	40:r:125:THR:HG22	2.02	0.41
40:r:197:LEU:HD13	48:r:501:PEE:H73	2.00	0.41
41:s:199:ASP:OD1	41:s:199:ASP:N	2.47	0.41
44:w:297:LEU:HD12	44:w:303:GLU:OE2	2.20	0.41
1:A:63:TYR:HD2	1:A:256:ARG:HD3	1.84	0.41
1:A:69:LEU:HD13	1:A:147:ARG:HG2	2.01	0.41
2:B:205:ILE:O	2:B:209:TYR:HB3	2.20	0.41
4:E:16:SER:HA	11:L:54:ALA:HA	2.02	0.41
5:F:64:LYS:HZ3	5:F:64:LYS:HB2	1.85	0.41
11:L:84:ARG:NH1	11:L:88:GLN:O	2.52	0.41
14:O:108:PRO:HA	14:O:109:PRO:HD3	1.98	0.41
21:W:88:ARG:O	21:W:92:GLU:HG2	2.19	0.41
6:X:118:ILE:HD12	23:Z:45:TRP:CH2	2.51	0.41
32:i:222:SER:O	32:i:222:SER:OG	2.35	0.41
32:i:268:GLN:O	32:i:271:THR:OG1	2.34	0.41
32:i:283:ALA:O	32:i:287:LEU:HD13	2.20	0.41
32:i:311:MET:HG2	44:w:309:THR:HG21	2.01	0.41
35:l:141:PHE:HE2	40:r:375:LEU:HD11	1.84	0.41
35:l:271:LYS:HD2	35:l:271:LYS:N	2.35	0.41
35:l:511:LEU:HD12	39:p:39:TYR:HD2	1.85	0.41
36:m:23:LYS:N	36:m:24:PRO:CD	2.82	0.41
44:w:281:GLY:O	44:w:284:PRO:HD2	2.19	0.41
1:A:234:GLY:HA3	1:A:240:THR:CG2	2.46	0.41
5:F:40:ARG:NH1	5:F:84:ALA:HB1	2.31	0.41
8:I:24:LEU:HD23	8:I:24:LEU:HA	1.90	0.41
12:M:43:VAL:HG12	12:M:55:LYS:HD3	2.01	0.41
19:U:53:TYR:HD1	21:W:72:MET:HE3	1.86	0.41
24:a:67:PHE:CE2	40:r:434:ASN:HB3	2.54	0.41
25:b:103:ARG:HE	25:b:105:PHE:HZ	1.68	0.41
26:c:70:MET:HE2	26:c:72:TYR:CE2	2.56	0.41
32:i:248:LEU:HD23	32:i:248:LEU:HA	1.90	0.41
32:i:298:TYR:HE1	40:r:134:THR:HG21	1.85	0.41
33:j:81:THR:C	33:j:83:ASN:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:304:PHE:CZ	35:l:526:LEU:HD22	2.55	0.41
35:l:492:ILE:HG13	35:l:493:VAL:N	2.34	0.41
38:o:116:ILE:HA	38:o:116:ILE:HD13	1.85	0.41
38:o:127:ILE:HD13	38:o:127:ILE:HA	1.86	0.41
39:p:126:LYS:O	39:p:130:ARG:HG3	2.20	0.41
1:A:315:LEU:HD11	1:A:442:PHE:HE2	1.86	0.41
2:B:171:PRO:HG2	2:B:200:GLU:CD	2.45	0.41
49:C:303:PLX:H82	49:C:303:PLX:H252	2.03	0.41
6:G:134:ASP:O	6:G:137:LYS:HG2	2.21	0.41
8:I:107:SER:C	8:I:109:ASP:H	2.29	0.41
9:J:293:LEU:HD23	9:J:294:PRO:O	2.20	0.41
14:O:225:CYS:O	14:O:225:CYS:SG	2.78	0.41
15:P:75:GLN:HB3	15:P:87:PHE:CD2	2.55	0.41
19:U:9:LEU:HD23	19:U:9:LEU:HA	1.93	0.41
34:k:23:ARG:HD3	36:m:23:LYS:O	2.20	0.41
35:l:389:PHE:CD1	35:l:393:ASP:HB2	2.56	0.41
41:s:22:LEU:CD1	41:s:37:PRO:HG2	2.51	0.41
41:s:184:MET:HE1	41:s:296:LEU:CB	2.51	0.41
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.54	0.41
44:w:328:PHE:O	44:w:332:THR:OG1	2.28	0.41
44:w:351:TRP:O	44:w:355:LYS:HG3	2.20	0.41
1:A:177:TYR:CD2	10:K:93:LEU:HD21	2.55	0.41
1:A:282:VAL:HG13	1:A:356:VAL:CG2	2.49	0.41
2:B:101:HIS:ND1	2:B:149:MET:HE1	2.36	0.41
3:C:188:LYS:HE3	3:C:188:LYS:HB3	1.84	0.41
4:E:80:ASP:OD1	4:E:81:LEU:N	2.54	0.41
11:L:105:GLU:HA	12:M:611:THR:HG21	2.03	0.41
12:M:304:GLN:HB2	12:M:316:TYR:CD1	2.55	0.41
16:Q:53:TYR:OH	32:i:295:ARG:NH1	2.52	0.41
22:Y:59:GLU:HG3	23:Z:73:TRP:CZ3	2.55	0.41
24:a:124:THR:HG23	24:a:125:PHE:CD2	2.56	0.41
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.01	0.41
35:l:47:SER:O	35:l:50:PRO:HD2	2.21	0.41
48:m:201:PEE:H56	48:m:201:PEE:H25	2.02	0.41
49:r:502:PLX:H301	49:r:502:PLX:H331	1.64	0.41
41:s:22:LEU:HD12	41:s:37:PRO:HG2	2.02	0.41
41:s:62:ARG:NH2	41:s:68:ILE:HB	2.35	0.41
43:v:46:MET:HE2	43:v:56:ARG:HG2	2.01	0.41
2:B:196:LYS:HE3	13:N:113:HIS:CE1	2.56	0.41
2:B:210:LEU:HD12	8:I:38:PRO:HB3	2.03	0.41
6:G:82:ARG:O	6:G:86:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:64:ASP:OD1	7:H:65:VAL:N	2.54	0.41
12:M:56:VAL:O	15:P:249:PRO:HG3	2.21	0.41
16:Q:450:ILE:O	16:Q:453:THR:HG22	2.20	0.41
18:T:104:LYS:HD2	18:T:107:LYS:HE3	2.02	0.41
21:W:141:ILE:HD12	21:W:141:ILE:H	1.86	0.41
24:a:74:TYR:CD2	28:e:91:PHE:HB3	2.55	0.41
24:a:184:LYS:C	24:a:186:THR:H	2.28	0.41
36:m:34:ILE:HG12	36:m:65:LEU:HD13	2.01	0.41
39:p:168:TRP:O	39:p:172:THR:OG1	2.29	0.41
44:w:40:PRO:HD3	44:w:296:MET:HE1	2.02	0.41
1:A:125:CYS:N	1:A:277:ASN:HD22	2.18	0.41
7:H:47:TYR:OH	8:I:92:LYS:HG3	2.20	0.41
8:I:103:ARG:HG2	8:I:103:ARG:HH11	1.85	0.41
12:M:338:VAL:HG12	12:M:544:VAL:HG12	2.02	0.41
16:Q:238:LEU:HD23	16:Q:238:LEU:HA	1.87	0.41
25:b:121:LYS:C	25:b:122:GLU:HG3	2.46	0.41
26:c:80:ASP:C	26:c:81:ARG:O	2.61	0.41
35:l:71:LEU:HD21	40:r:380:PHE:CZ	2.56	0.41
35:l:83:ASP:OD1	35:l:85:PHE:N	2.53	0.41
35:l:102:GLU:HG2	35:l:453:SER:HB3	2.02	0.41
41:s:71:PHE:CD1	41:s:71:PHE:C	2.98	0.41
41:s:222:MET:N	41:s:222:MET:SD	2.91	0.41
42:u:80:GLU:HB2	42:u:81:PRO:HD3	2.03	0.41
43:v:83:GLU:OE1	43:v:83:GLU:N	2.49	0.41
44:w:269:VAL:O	44:w:273:ILE:HG12	2.20	0.41
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.60	0.41
2:B:76:TYR:CE1	41:s:33:LEU:HD13	2.56	0.41
49:C:303:PLX:H311	49:C:303:PLX:H281	1.76	0.41
9:J:293:LEU:HA	9:J:294:PRO:HD3	1.95	0.41
12:M:670:GLU:HA	12:M:673:LYS:HG3	2.03	0.41
15:P:165:TRP:HZ2	16:Q:111:PRO:HG2	1.85	0.41
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	2.02	0.41
16:Q:303:ARG:HG3	16:Q:401:GLU:HB3	2.03	0.41
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	2.03	0.41
19:U:32:LEU:HD23	19:U:32:LEU:HA	1.82	0.41
6:X:75:THR:OG1	6:X:76:LEU:N	2.54	0.41
24:a:50:HIS:CD2	24:a:52:LYS:HB3	2.56	0.41
26:c:58:ARG:HB2	26:c:61:ASP:HB2	2.01	0.41
26:c:97:LEU:HD11	40:r:346:ARG:NH1	2.36	0.41
27:d:163:MET:O	27:d:167:ARG:HG2	2.21	0.41
32:i:194:LEU:HD12	32:i:198:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:j:92:LEU:HD22	41:s:302:MET:HG2	2.03	0.41
35:l:8:THR:HG23	35:l:82:MET:HE3	2.01	0.41
35:l:40:VAL:HG11	35:l:101:MET:SD	2.61	0.41
35:l:360:GLY:HA3	35:l:434:LYS:O	2.21	0.41
35:l:549:ALA:HB1	40:r:275:ILE:HG13	2.03	0.41
41:s:11:ILE:HB	41:s:12:PRO:HD3	2.03	0.41
41:s:92:PRO:HB3	41:s:255:TYR:CD1	2.55	0.41
56:s:401:UQ:H72	56:s:401:UQ:HM53	1.71	0.41
42:u:85:TYR:CE1	42:u:104:GLN:HB2	2.56	0.41
2:B:131:GLU:OE1	13:N:130:THR:HG21	2.21	0.41
5:F:19:ILE:HD12	5:F:51:LEU:HD21	2.02	0.41
9:J:132:ARG:NH2	51:J:401:NDP:O2X	2.54	0.41
12:M:250:SER:OG	12:M:251:ILE:N	2.49	0.41
16:Q:184:ILE:HD11	16:Q:251:PHE:HZ	1.81	0.41
17:S:17:PHE:CD1	41:s:260:VAL:HG21	2.56	0.41
27:d:74:ILE:O	27:d:77:CYS:HB2	2.21	0.41
27:d:79:GLU:OE1	27:d:80:LYS:HG2	2.21	0.41
32:i:71:MET:O	32:i:75:ILE:HG12	2.21	0.41
32:i:137:ALA:HB3	32:i:138:PRO:HD3	2.03	0.41
35:l:491:LEU:O	35:l:494:THR:HG22	2.21	0.41
54:r:504:CDL:H182	54:r:504:CDL:H331	2.03	0.41
44:w:193:VAL:HG11	44:w:307:TYR:CD2	2.56	0.41
5:F:37:ILE:HA	5:F:41:TYR:HB2	2.03	0.40
9:J:181:LEU:HA	9:J:184:LYS:HB2	2.03	0.40
28:e:128:TYR:CD1	28:e:128:TYR:C	2.99	0.40
32:i:81:SER:O	32:i:83:GLN:N	2.48	0.40
39:p:13:GLN:O	39:p:16:VAL:HG12	2.20	0.40
40:r:166:TYR:CD1	40:r:166:TYR:C	2.98	0.40
41:s:79:LEU:HD22	41:s:222:MET:HE3	2.02	0.40
42:u:28:ALA:HB1	42:u:70:PHE:HE2	1.85	0.40
1:A:251:SER:OG	1:A:252:PRO:HD3	2.21	0.40
1:A:393:ASN:OD1	1:A:393:ASN:C	2.64	0.40
8:I:3:SER:O	54:N:201:CDL:H1	2.21	0.40
16:Q:99:MET:HE3	16:Q:109:CYS:SG	2.60	0.40
29:f:68:GLU:OE2	29:f:72:ARG:NE	2.42	0.40
32:i:166:GLY:HA2	32:i:289:ASN:OD1	2.21	0.40
35:l:68:TRP:H	35:l:77:SER:HA	1.86	0.40
42:u:100:CYS:HB2	42:u:103:GLN:CD	2.46	0.40
44:w:314:LEU:O	44:w:318:THR:HG22	2.22	0.40
5:F:26:ARG:HB2	5:F:26:ARG:NH1	2.36	0.40
6:G:103:HIS:O	6:G:107:ASP:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:275:ASP:OD1	9:J:275:ASP:N	2.54	0.40
21:W:87:LEU:HD23	21:W:87:LEU:HA	1.92	0.40
26:c:83:GLN:NE2	26:c:98:ARG:O	2.54	0.40
28:e:109:LEU:HD22	40:r:43:ASN:HB2	2.03	0.40
33:j:95:LEU:HD13	41:s:302:MET:HG3	2.03	0.40
35:l:292:ALA:HB2	35:l:304:PHE:CB	2.51	0.40
36:m:4:TYR:O	36:m:8:ILE:HD12	2.22	0.40
38:o:116:ILE:CD1	38:o:123:GLN:OE1	2.70	0.40
41:s:2:PHE:CE2	41:s:6:ILE:HD11	2.56	0.40
41:s:19:PHE:O	41:s:23:VAL:HG23	2.20	0.40
44:w:295:ARG:HA	44:w:298:VAL:HG22	2.02	0.40
6:G:75:THR:OG1	6:G:156:GLU:OE1	2.37	0.40
23:Z:9:HIS:CB	24:a:52:LYS:NZ	2.84	0.40
25:b:64:THR:O	25:b:68:SER:N	2.46	0.40
27:d:75:THR:HG21	28:e:146:LYS:HG2	2.03	0.40
32:i:66:ALA:HB1	32:i:105:LYS:HG3	2.03	0.40
35:l:227:PHE:N	35:l:284:THR:OG1	2.53	0.40
38:o:114:LYS:NZ	38:o:118:GLU:OE2	2.35	0.40
44:w:59:VAL:HG13	44:w:202:HIS:H	1.87	0.40
44:w:77:ILE:HG22	44:w:158:VAL:HG21	2.03	0.40
18:T:49:ASP:O	18:T:52:ARG:HG3	2.22	0.40
18:T:122:HIS:O	18:T:122:HIS:ND1	2.55	0.40
30:g:33:LEU:HD12	30:g:33:LEU:HA	1.88	0.40
33:j:90:MET:HE1	49:j:202:PLX:H281	2.03	0.40
37:n:27:LEU:HD11	54:u:201:CDL:H112	2.04	0.40
40:r:127:VAL:HG11	54:r:504:CDL:H451	2.02	0.40
43:v:31:PHE:CD1	43:v:33:GLU:OE2	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/433 (99%)	413 (96%)	16 (4%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
4	E	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
5	F	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
6	G	86/88 (98%)	85 (99%)	1 (1%)	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	102 (93%)	8 (7%)	0	100	100
8	I	93/112 (83%)	82 (88%)	11 (12%)	0	100	100
9	J	327/342 (96%)	314 (96%)	13 (4%)	0	100	100
10	K	40/43 (93%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	120 (98%)	3 (2%)	0	100	100
12	M	688/690 (100%)	666 (97%)	21 (3%)	1 (0%)	48	78
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	207 (96%)	8 (4%)	0	100	100
15	P	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
16	Q	412/430 (96%)	400 (97%)	12 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	91 (97%)	3 (3%)	0	100	100
19	U	81/83 (98%)	77 (95%)	4 (5%)	0	100	100
20	V	138/140 (99%)	131 (95%)	6 (4%)	1 (1%)	18	49
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
23	Z	82/84 (98%)	79 (96%)	3 (4%)	0	100	100
24	a	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
25	b	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	144 (94%)	9 (6%)	1 (1%)	21	52
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
30	g	119/122 (98%)	114 (96%)	5 (4%)	0	100	100
31	h	103/105 (98%)	98 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	i	345/347 (99%)	332 (96%)	11 (3%)	2 (1%)	21	52
33	j	95/115 (83%)	89 (94%)	6 (6%)	0	100	100
34	k	96/98 (98%)	86 (90%)	10 (10%)	0	100	100
35	l	601/603 (100%)	572 (95%)	29 (5%)	0	100	100
36	m	125/175 (71%)	116 (93%)	9 (7%)	0	100	100
37	n	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
38	o	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
39	p	176/178 (99%)	166 (94%)	10 (6%)	0	100	100
40	r	457/459 (100%)	443 (97%)	14 (3%)	0	100	100
41	s	299/318 (94%)	285 (95%)	14 (5%)	0	100	100
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/125 (98%)	114 (93%)	8 (7%)	0	100	100
44	w	318/320 (99%)	306 (96%)	12 (4%)	0	100	100
All	All	8067/8323 (97%)	7746 (96%)	316 (4%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	c	81	ARG
32	i	93	VAL
32	i	92	PRO
12	M	283	GLU
20	V	46	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/346 (99%)	344 (100%)	0	100	100
2	B	149/151 (99%)	148 (99%)	1 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	132/132 (100%)	132 (100%)	0	100	100
4	E	106/107 (99%)	105 (99%)	1 (1%)	70	80
5	F	76/76 (100%)	75 (99%)	1 (1%)	61	77
6	G	76/81 (94%)	76 (100%)	0	100	100
6	X	74/81 (91%)	73 (99%)	1 (1%)	59	76
7	H	99/99 (100%)	99 (100%)	0	100	100
8	I	87/97 (90%)	87 (100%)	0	100	100
9	J	276/296 (93%)	276 (100%)	0	100	100
10	K	41/42 (98%)	41 (100%)	0	100	100
11	L	113/113 (100%)	112 (99%)	1 (1%)	70	80
12	M	578/580 (100%)	578 (100%)	0	100	100
13	N	130/130 (100%)	130 (100%)	0	100	100
14	O	175/183 (96%)	174 (99%)	1 (1%)	78	83
15	P	189/190 (100%)	189 (100%)	0	100	100
16	Q	361/370 (98%)	360 (100%)	1 (0%)	86	87
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	79 (100%)	0	100	100
19	U	69/69 (100%)	69 (100%)	0	100	100
20	V	101/101 (100%)	99 (98%)	2 (2%)	48	72
21	W	122/123 (99%)	122 (100%)	0	100	100
22	Y	56/63 (89%)	56 (100%)	0	100	100
23	Z	65/65 (100%)	64 (98%)	1 (2%)	57	75
24	a	120/122 (98%)	118 (98%)	2 (2%)	53	74
25	b	90/119 (76%)	89 (99%)	1 (1%)	65	78
26	c	136/141 (96%)	134 (98%)	2 (2%)	57	75
27	d	155/155 (100%)	155 (100%)	0	100	100
28	e	98/99 (99%)	96 (98%)	2 (2%)	48	72
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/109 (99%)	107 (99%)	1 (1%)	70	80
31	h	93/93 (100%)	93 (100%)	0	100	100
32	i	311/311 (100%)	310 (100%)	1 (0%)	86	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	j	88/100 (88%)	88 (100%)	0	100	100
34	k	85/85 (100%)	85 (100%)	0	100	100
35	l	514/537 (96%)	513 (100%)	1 (0%)	87	89
36	m	89/141 (63%)	88 (99%)	1 (1%)	65	78
37	n	53/53 (100%)	53 (100%)	0	100	100
38	o	110/113 (97%)	110 (100%)	0	100	100
39	p	149/159 (94%)	149 (100%)	0	100	100
40	r	408/410 (100%)	406 (100%)	2 (0%)	81	85
41	s	263/275 (96%)	263 (100%)	0	100	100
42	u	152/153 (99%)	151 (99%)	1 (1%)	76	82
43	v	96/111 (86%)	96 (100%)	0	100	100
44	w	281/283 (99%)	281 (100%)	0	100	100
All	All	6990/7246 (96%)	6966 (100%)	24 (0%)	84	87

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	141	ARG
4	E	101	THR
5	F	85	ASP
11	L	70	GLU
14	O	225	CYS
16	Q	101	LEU
20	V	89	ASN
20	V	95	CYS
6	X	108	LEU
23	Z	73	TRP
24	a	54	LEU
24	a	151	LEU
25	b	120	MET
26	c	78	LEU
26	c	122	THR
28	e	55	LEU
28	e	132	ASN
30	g	96	VAL
32	i	254	LEU
35	l	346	ILE
36	m	56	VAL

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Mol	Chain	Res	Type
40	r	150	LEU
40	r	207	MET
42	u	88	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	244	ASN
1	A	270	ASN
1	A	281	HIS
1	A	436	GLN
1	A	456	GLN
3	C	123	GLN
5	F	62	GLN
5	F	80	ASN
5	F	93	ASN
6	G	101	ASN
7	H	50	GLN
8	I	13	ASN
8	I	29	GLN
8	I	110	GLN
9	J	72	HIS
9	J	122	HIS
9	J	238	GLN
9	J	356	HIS
9	J	376	ASN
10	K	79	HIS
12	M	123	ASN
12	M	278	HIS
12	M	453	GLN
12	M	604	GLN
12	M	678	GLN
13	N	52	ASN
13	N	113	HIS
13	N	116	ASN
14	O	69	ASN
15	P	196	HIS
16	Q	83	ASN
16	Q	147	ASN
16	Q	160	ASN
16	Q	190	HIS

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Mol	Chain	Res	Type
16	Q	233	HIS
16	Q	234	GLN
16	Q	339	GLN
18	T	120	GLN
19	U	40	ASN
20	V	89	ASN
22	Y	54	GLN
22	Y	57	GLN
23	Z	9	HIS
25	b	14	GLN
27	d	54	GLN
27	d	56	HIS
28	e	132	ASN
29	f	62	HIS
30	g	119	HIS
31	h	7	GLN
32	i	91	ASN
32	i	144	GLN
33	j	108	GLN
35	l	192	HIS
35	l	447	ASN
35	l	505	ASN
37	n	3	ASN
39	p	75	GLN
39	p	78	GLN
40	r	20	HIS
40	r	144	ASN
40	r	175	ASN
40	r	399	ASN
40	r	415	GLN
40	r	440	HIS
41	s	47	GLN
41	s	317	GLN
42	u	30	HIS
42	u	35	GLN
42	u	143	HIS
43	v	82	HIS
43	v	84	GLN
44	w	127	ASN
44	w	155	GLN
44	w	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
16	2MR	Q	118	16	10,12,13	1.99	1 (10%)	5,13,15	6.11	3 (60%)

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
16	2MR	Q	118	16	-	2/10/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.69	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	118	2MR	NE-CZ-NH2	12.41	130.85	119.48
16	Q	118	2MR	CD-NE-CZ	4.72	132.22	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.14	130.40	123.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	Q	118	2MR	NE-CD-CG-CB
16	Q	118	2MR	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 2 are monoatomic - leaving 34 for Mogul analysis.

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	$\# Z > 2$
48	PEE	m	201	-	40,40,50	1.18	5 (12%)	43,45,55	1.01	3 (6%)
50	8Q1	X	201	-	32,34,34	1.62	6 (18%)	39,43,43	1.56	7 (17%)
46	FMN	A	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.23	8 (16%)
56	UQ	s	401	-	28,28,63	3.29	8 (28%)	36,37,79	2.87	11 (30%)
52	FES	M	803	12	0,4,4	-	-	-	-	-
54	CDL	r	504	-	99,99,99	1.12	9 (9%)	105,111,111	0.86	4 (3%)
45	SF4	M	801	12	0,12,12	-	-	-	-	-
49	PLX	l	701	-	51,51,51	1.21	4 (7%)	53,59,59	0.62	1 (1%)
45	SF4	B	301	2	0,12,12	-	-	-	-	-
48	PEE	l	702	-	45,45,50	1.24	6 (13%)	48,50,55	0.98	2 (4%)
48	PEE	j	201	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
51	NDP	J	401	-	51,52,52	4.28	25 (49%)	71,80,80	2.21	15 (21%)
54	CDL	N	201	-	50,50,99	1.42	9 (18%)	56,62,111	1.16	4 (7%)
45	SF4	M	802	12	0,12,12	-	-	-	-	-
45	SF4	A	501	1	0,12,12	-	-	-	-	-
49	PLX	r	502	-	51,51,51	1.20	4 (7%)	53,59,59	0.62	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	SF4	C	301	16,3	0,12,12	-	-	-		
52	FES	O	301	14	0,4,4	-	-	-		
54	CDL	a	201	-	90,90,99	1.16	8 (8%)	96,102,111	0.89	4 (4%)
49	PLX	g	201	-	51,51,51	1.21	3 (5%)	53,59,59	0.62	1 (1%)
54	CDL	i	401	-	65,65,99	1.31	8 (12%)	71,77,111	1.03	4 (5%)
57	ADP	w	401	-	28,29,29	3.18	9 (32%)	43,45,45	1.93	9 (20%)
47	NAI	A	503	-	47,48,48	4.02	22 (46%)	64,73,73	1.68	12 (18%)
49	PLX	C	303	-	51,51,51	1.21	4 (7%)	53,59,59	0.63	1 (1%)
45	SF4	B	302	2	0,12,12	-	-	-		
48	PEE	i	402	-	46,46,50	1.23	6 (13%)	49,51,55	0.97	2 (4%)
48	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	1.00	2 (3%)
48	PEE	C	302	-	46,46,50	1.23	6 (13%)	49,51,55	1.00	2 (4%)
50	8Q1	G	201	-	32,34,34	1.63	6 (18%)	39,43,43	1.65	6 (15%)
54	CDL	r	503	-	98,98,99	1.11	8 (8%)	104,110,111	0.89	4 (3%)
49	PLX	j	202	-	51,51,51	1.22	4 (7%)	53,59,59	0.59	1 (1%)
48	PEE	b	201	-	45,45,50	1.24	6 (13%)	48,50,55	0.99	2 (4%)
48	PEE	B	303	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
54	CDL	u	201	-	77,77,99	1.04	4 (5%)	83,89,111	1.10	4 (4%)

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
48	PEE	m	201	-	-	23/44/44/54	-
50	8Q1	X	201	-	-	18/41/41/41	-
46	FMN	A	502	-	-	9/18/18/18	0/3/3/3
56	UQ	s	401	-	-	10/21/45/87	0/1/1/1
52	FES	M	803	12	-	-	0/1/1/1
54	CDL	r	504	-	-	58/110/110/110	-
45	SF4	M	801	12	-	-	0/6/5/5
49	PLX	l	701	-	-	32/55/55/55	-
45	SF4	B	301	2	-	-	0/6/5/5
48	PEE	l	702	-	-	21/49/49/54	-
54	CDL	N	201	-	-	35/61/61/110	-
48	PEE	j	201	-	-	28/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	NDP	J	401	-	-	5/34/77/77	0/5/5/5
45	SF4	M	802	12	-	-	0/6/5/5
45	SF4	A	501	1	-	-	0/6/5/5
49	PLX	r	502	-	-	28/55/55/55	-
45	SF4	C	301	16,3	-	-	0/6/5/5
52	FES	O	301	14	-	-	0/1/1/1
54	CDL	a	201	-	-	37/101/101/110	-
49	PLX	g	201	-	-	21/55/55/55	-
54	CDL	i	401	-	-	43/76/76/110	-
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
47	NAI	A	503	-	-	6/29/72/72	0/5/5/5
49	PLX	C	303	-	-	25/55/55/55	-
45	SF4	B	302	2	-	-	0/6/5/5
48	PEE	i	402	-	-	22/50/50/54	-
48	PEE	r	501	-	-	27/54/54/54	-
48	PEE	C	302	-	-	29/50/50/54	-
50	8Q1	G	201	-	-	14/41/41/41	-
54	CDL	r	503	-	-	53/109/109/110	-
49	PLX	j	202	-	-	31/55/55/55	-
48	PEE	b	201	-	-	28/49/49/54	-
48	PEE	B	303	-	-	26/54/54/54	-
54	CDL	u	201	-	-	28/88/88/110	-

All (190) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	J	401	NDP	C3B-C2B	-13.12	1.24	1.53
51	J	401	NDP	O4D-C4D	10.75	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.15	1.27	1.53
51	J	401	NDP	C3D-C4D	-9.89	1.27	1.53
56	s	401	UQ	C13-C14	9.58	1.55	1.33
47	A	503	NAI	O4B-C1B	9.39	1.63	1.42
56	s	401	UQ	C8-C9	9.16	1.54	1.33
57	w	401	ADP	C3'-C4'	-9.06	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.29	1.26	1.45
56	s	401	UQ	C18-C19	7.88	1.56	1.32
51	J	401	NDP	O4B-C4B	-7.81	1.27	1.45
47	A	503	NAI	C2D-C1D	-7.80	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	w	401	ADP	O4'-C4'	7.65	1.62	1.45
51	J	401	NDP	C2N-C3N	7.51	1.55	1.35
47	A	503	NAI	C2B-C1B	-7.31	1.30	1.53
51	J	401	NDP	C6N-C5N	7.28	1.55	1.33
47	A	503	NAI	O4D-C4D	7.08	1.60	1.45
51	J	401	NDP	PN-O3	6.54	1.66	1.59
57	w	401	ADP	PA-O3A	6.49	1.66	1.59
47	A	503	NAI	PA-O3	6.46	1.66	1.59
51	J	401	NDP	P2B-O2B	6.00	1.70	1.59
47	A	503	NAI	C2D-C3D	5.95	1.69	1.53
51	J	401	NDP	C6A-N6A	5.84	1.49	1.34
47	A	503	NAI	PN-O3	5.62	1.65	1.59
51	J	401	NDP	PA-O3	5.60	1.65	1.59
47	A	503	NAI	O4D-C1D	5.59	1.54	1.42
51	J	401	NDP	C3B-C4B	5.48	1.66	1.53
57	w	401	ADP	C6-N6	5.45	1.48	1.34
47	A	503	NAI	C7N-N7N	5.33	1.48	1.33
47	A	503	NAI	C4N-C3N	-5.23	1.40	1.50
50	X	201	8Q1	C39-N41	5.20	1.45	1.33
51	J	401	NDP	C6N-N1N	5.16	1.49	1.37
50	G	201	8Q1	C34-N36	5.13	1.45	1.33
47	A	503	NAI	C6A-N6A	5.10	1.47	1.34
50	G	201	8Q1	C39-N41	5.05	1.45	1.33
50	X	201	8Q1	C34-N36	5.03	1.45	1.33
51	J	401	NDP	O4D-C1D	-5.01	1.30	1.42
51	J	401	NDP	O4B-C1B	4.77	1.53	1.42
51	J	401	NDP	C1B-N9A	-4.56	1.33	1.46
57	w	401	ADP	O4'-C1'	-4.55	1.31	1.42
47	A	503	NAI	O2B-C2B	4.36	1.53	1.43
54	u	201	CDL	OA8-CA7	4.23	1.45	1.33
54	u	201	CDL	OB8-CB7	4.21	1.45	1.33
54	u	201	CDL	OA6-CA5	4.19	1.46	1.34
54	u	201	CDL	OB6-CB5	3.97	1.45	1.34
51	J	401	NDP	O2D-C2D	-3.90	1.33	1.43
51	J	401	NDP	C7N-N7N	3.89	1.44	1.33
48	m	201	PEE	C18-C19	3.86	1.53	1.31
48	i	402	PEE	C18-C19	3.83	1.53	1.31
48	j	201	PEE	C18-C19	3.83	1.53	1.31
48	C	302	PEE	C18-C19	3.82	1.53	1.31
48	r	501	PEE	C18-C19	3.82	1.53	1.31
48	B	303	PEE	C18-C19	3.81	1.53	1.31
48	b	201	PEE	C18-C19	3.81	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	l	702	PEE	C18-C19	3.81	1.53	1.31
48	C	302	PEE	C39-C38	3.75	1.53	1.31
48	r	501	PEE	C39-C38	3.74	1.53	1.31
48	i	402	PEE	C39-C38	3.74	1.52	1.31
48	l	702	PEE	C39-C38	3.73	1.52	1.31
48	j	201	PEE	C39-C38	3.73	1.52	1.31
48	B	303	PEE	C39-C38	3.73	1.52	1.31
48	b	201	PEE	C39-C38	3.72	1.52	1.31
47	A	503	NAI	C7N-C3N	3.62	1.56	1.48
54	i	401	CDL	OA8-CA7	3.51	1.43	1.33
54	r	504	CDL	OA8-CA7	3.46	1.43	1.33
54	N	201	CDL	OA8-CA7	3.45	1.43	1.33
46	A	502	FMN	C4A-N5	3.45	1.38	1.30
54	a	201	CDL	OA8-CA7	3.44	1.43	1.33
57	w	401	ADP	C8-N9	-3.40	1.31	1.37
54	r	503	CDL	OA8-CA7	3.38	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.38	1.40	1.49
51	J	401	NDP	C8A-N9A	-3.18	1.32	1.37
57	w	401	ADP	O2'-C2'	-3.14	1.35	1.43
54	a	201	CDL	OB6-CB5	3.13	1.43	1.34
54	r	504	CDL	OB6-CB5	3.13	1.43	1.34
54	N	201	CDL	OA6-CA5	3.12	1.43	1.34
54	i	401	CDL	OB6-CB5	3.05	1.42	1.34
51	J	401	NDP	C7N-C3N	3.04	1.55	1.48
54	r	504	CDL	OB8-CB7	3.04	1.42	1.33
54	a	201	CDL	OA6-CA5	3.04	1.42	1.34
54	i	401	CDL	OB8-CB7	3.03	1.42	1.33
51	J	401	NDP	C5A-N7A	-3.02	1.33	1.39
54	N	201	CDL	OB8-CB7	3.02	1.42	1.33
54	a	201	CDL	OB8-CB7	3.00	1.42	1.33
57	w	401	ADP	O3'-C3'	3.00	1.50	1.43
54	r	503	CDL	OB6-CB5	3.00	1.42	1.34
54	r	503	CDL	OB8-CB7	2.99	1.42	1.33
51	J	401	NDP	O3D-C3D	2.98	1.50	1.43
54	r	504	CDL	OA6-CA5	2.98	1.42	1.34
54	i	401	CDL	OA6-CA5	2.98	1.42	1.34
54	N	201	CDL	OB6-CB5	2.97	1.42	1.34
49	l	701	PLX	O6-C4	-2.92	1.40	1.44
54	r	503	CDL	OA6-CA5	2.89	1.42	1.34
49	C	303	PLX	O6-C4	-2.86	1.41	1.44
49	g	201	PLX	O6-C4	-2.83	1.41	1.44
47	A	503	NAI	C8A-N9A	-2.73	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	j	202	PLX	O6-C4	-2.65	1.41	1.44
48	r	501	PEE	O2-C2	-2.63	1.40	1.46
56	s	401	UQ	C6-C1	2.62	1.53	1.46
51	J	401	NDP	O2B-C2B	2.61	1.53	1.44
54	r	503	CDL	OA6-CA4	-2.58	1.40	1.46
48	B	303	PEE	O2-C2	-2.55	1.40	1.46
48	b	201	PEE	O2-C2	-2.54	1.40	1.46
48	C	302	PEE	O2-C2	-2.54	1.40	1.46
46	A	502	FMN	C10-N1	2.54	1.38	1.33
54	r	504	CDL	OA6-CA4	-2.54	1.40	1.46
47	A	503	NAI	PN-O5D	2.53	1.69	1.59
48	b	201	PEE	O3-C30	2.52	1.40	1.33
48	l	702	PEE	O2-C2	-2.52	1.40	1.46
48	i	402	PEE	O2-C2	-2.52	1.40	1.46
48	i	402	PEE	O3-C30	2.52	1.40	1.33
54	i	401	CDL	OA6-CA4	-2.51	1.40	1.46
48	j	201	PEE	O2-C2	-2.50	1.40	1.46
54	a	201	CDL	OA6-CA4	-2.49	1.40	1.46
57	w	401	ADP	C5-N7	-2.48	1.34	1.39
48	l	702	PEE	O3-C30	2.48	1.40	1.33
47	A	503	NAI	C6N-C5N	2.47	1.40	1.33
48	C	302	PEE	O3-C30	2.44	1.40	1.33
49	g	201	PLX	C7-C6	2.42	1.55	1.50
50	X	201	8Q1	C1-S44	2.42	1.82	1.76
49	r	502	PLX	C7-C6	2.42	1.55	1.50
51	J	401	NDP	C2D-C3D	2.41	1.59	1.53
48	r	501	PEE	O3-C30	2.41	1.40	1.33
49	j	202	PLX	C7-C6	2.41	1.55	1.50
48	B	303	PEE	O3-C30	2.40	1.40	1.33
48	m	201	PEE	O2-C10	2.40	1.41	1.34
48	j	201	PEE	O3-C30	2.40	1.40	1.33
48	m	201	PEE	O2-C2	-2.39	1.41	1.46
50	G	201	8Q1	O35-C34	-2.39	1.18	1.23
50	G	201	8Q1	C1-S44	2.37	1.81	1.76
48	m	201	PEE	O3-C30	2.37	1.40	1.33
54	r	503	CDL	OB6-CB4	-2.37	1.41	1.46
50	X	201	8Q1	O35-C34	-2.36	1.18	1.23
49	l	701	PLX	C7-C6	2.35	1.55	1.50
49	r	502	PLX	O6-C4	-2.35	1.41	1.44
49	C	303	PLX	C7-C6	2.34	1.55	1.50
47	A	503	NAI	C5B-C4B	2.34	1.58	1.51
54	N	201	CDL	OB6-CB4	-2.33	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	G	201	8Q1	O40-C39	-2.30	1.18	1.23
47	A	503	NAI	O3B-C3B	-2.30	1.37	1.43
48	i	402	PEE	O2-C10	2.29	1.40	1.34
48	C	302	PEE	O2-C10	2.28	1.40	1.34
48	l	702	PEE	O2-C10	2.28	1.40	1.34
48	j	201	PEE	O2-C10	2.27	1.40	1.34
54	i	401	CDL	PB2-OB2	2.27	1.68	1.59
54	r	503	CDL	PB2-OB2	2.27	1.68	1.59
48	b	201	PEE	O2-C10	2.26	1.40	1.34
54	r	504	CDL	PB2-OB2	2.26	1.68	1.59
54	i	401	CDL	OB6-CB4	-2.26	1.41	1.46
54	i	401	CDL	PB2-OB5	2.25	1.68	1.59
50	X	201	8Q1	C6-C1	2.25	1.53	1.50
48	B	303	PEE	O2-C10	2.24	1.40	1.34
54	N	201	CDL	OA6-CA4	-2.24	1.41	1.46
54	r	504	CDL	PB2-OB5	2.24	1.68	1.59
50	G	201	8Q1	C6-C1	2.24	1.53	1.50
54	a	201	CDL	PB2-OB2	2.23	1.68	1.59
54	a	201	CDL	OB6-CB4	-2.23	1.41	1.46
54	N	201	CDL	PB2-OB5	2.23	1.68	1.59
49	r	502	PLX	P1-O4	2.23	1.68	1.59
54	r	503	CDL	PB2-OB5	2.22	1.68	1.59
49	j	202	PLX	P1-O4	2.22	1.68	1.59
54	a	201	CDL	PB2-OB5	2.21	1.68	1.59
54	N	201	CDL	PB2-OB2	2.21	1.68	1.59
48	r	501	PEE	O2-C10	2.19	1.40	1.34
50	X	201	8Q1	O40-C39	-2.19	1.18	1.23
48	m	201	PEE	O3-C3	-2.19	1.40	1.45
51	J	401	NDP	PA-O5B	2.18	1.67	1.59
48	r	501	PEE	O3-C3	-2.18	1.40	1.45
49	C	303	PLX	P1-O4	2.17	1.67	1.59
49	g	201	PLX	P1-O4	2.17	1.67	1.59
51	J	401	NDP	O7N-C7N	-2.14	1.19	1.24
54	r	504	CDL	OB6-CB4	-2.14	1.41	1.46
49	l	701	PLX	P1-O4	2.14	1.67	1.59
48	j	201	PEE	O3-C3	-2.12	1.40	1.45
49	r	502	PLX	P1-O1	2.12	1.67	1.59
48	l	702	PEE	O3-C3	-2.11	1.40	1.45
48	B	303	PEE	O3-C3	-2.10	1.40	1.45
48	C	302	PEE	O3-C3	-2.10	1.40	1.45
49	j	202	PLX	P1-O1	2.10	1.67	1.59
56	s	401	UQ	O3-CM3	-2.08	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	i	402	PEE	O3-C3	-2.08	1.40	1.45
49	C	303	PLX	P1-O1	2.07	1.67	1.59
56	s	401	UQ	O4-C4	-2.07	1.18	1.23
48	b	201	PEE	O3-C3	-2.07	1.40	1.45
47	A	503	NAI	C5A-N7A	-2.05	1.35	1.39
49	l	701	PLX	P1-O1	2.04	1.67	1.59
56	s	401	UQ	C7-C8	2.04	1.53	1.50
54	r	504	CDL	C11-CA5	2.03	1.56	1.50
54	N	201	CDL	C11-CA5	2.03	1.56	1.50
56	s	401	UQ	O2-CM2	-2.01	1.40	1.45

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C7-C8-C9	-9.85	109.85	126.83
51	J	401	NDP	C3N-C2N-N1N	-7.48	112.22	123.20
51	J	401	NDP	C1D-N1N-C2N	-7.37	108.99	121.14
56	s	401	UQ	C12-C13-C14	-6.49	112.77	127.62
51	J	401	NDP	C6N-N1N-C2N	-6.02	112.87	119.32
50	X	201	8Q1	C6-C1-S44	5.76	120.27	113.40
50	G	201	8Q1	C6-C1-S44	5.63	120.11	113.40
51	J	401	NDP	C5A-C4A-N3A	-5.59	119.03	126.72
57	w	401	ADP	C5-C4-N3	-5.46	119.20	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.42	119.26	126.72
51	J	401	NDP	C1D-N1N-C6N	-5.34	109.47	120.77
56	s	401	UQ	C11-C9-C8	-4.93	110.11	121.17
56	s	401	UQ	C10-C9-C8	-4.80	111.29	123.63
47	A	503	NAI	N3A-C2A-N1A	-4.49	121.78	128.58
57	w	401	ADP	N3-C2-N1	-4.39	121.94	128.58
57	w	401	ADP	N3-C4-N9	4.24	134.38	127.17
54	u	201	CDL	OA6-CA5-C11	4.22	120.62	111.48
56	s	401	UQ	C15-C14-C13	-4.21	112.81	123.63
51	J	401	NDP	N3A-C2A-N1A	-4.16	122.28	128.58
56	s	401	UQ	C17-C18-C19	-4.14	113.83	127.64
54	N	201	CDL	OA6-CA5-C11	4.11	120.37	111.48
54	N	201	CDL	OB6-CB5-C51	4.11	120.36	111.48
51	J	401	NDP	N3A-C4A-N9A	4.03	134.02	127.17
54	r	504	CDL	OB6-CB5-C51	4.02	120.17	111.48
54	a	201	CDL	OA6-CA5-C11	4.01	120.16	111.48
54	i	401	CDL	OA6-CA5-C11	4.01	120.15	111.48
48	r	501	PEE	O2-C10-C11	4.00	120.14	111.48
48	C	302	PEE	O2-C10-C11	3.94	120.01	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	s	401	UQ	C16-C14-C13	-3.94	112.33	121.17
48	j	201	PEE	O2-C10-C11	3.93	119.99	111.48
54	i	401	CDL	OB6-CB5-C51	3.92	119.96	111.48
47	A	503	NAI	N3A-C4A-N9A	3.91	133.81	127.17
54	r	503	CDL	OA6-CA5-C11	3.91	119.93	111.48
54	r	504	CDL	OA6-CA5-C11	3.90	119.91	111.48
48	B	303	PEE	O2-C10-C11	3.88	119.88	111.48
48	m	201	PEE	O2-C10-C11	3.88	119.87	111.48
48	i	402	PEE	O2-C10-C11	3.88	119.86	111.48
54	r	503	CDL	OB6-CB5-C51	3.86	119.84	111.48
54	a	201	CDL	OB6-CB5-C51	3.80	119.71	111.48
48	b	201	PEE	O2-C10-C11	3.78	119.66	111.48
57	w	401	ADP	N9-C8-N7	-3.72	108.66	113.94
47	A	503	NAI	C2A-N3A-C4A	3.68	120.81	111.83
48	l	702	PEE	O2-C10-C11	3.65	119.38	111.48
51	J	401	NDP	C2A-N3A-C4A	3.57	120.55	111.83
50	G	201	8Q1	O4-C1-C6	-3.56	119.87	123.98
50	G	201	8Q1	C37-C38-C39	3.55	118.31	112.39
54	u	201	CDL	OB6-CB5-C51	3.55	119.16	111.48
57	w	401	ADP	C2-N3-C4	3.48	120.32	111.83
50	X	201	8Q1	O4-C1-C6	-3.46	119.99	123.98
47	A	503	NAI	C5A-N7A-C8A	3.42	108.82	103.45
57	w	401	ADP	C5-N7-C8	3.42	108.82	103.45
47	A	503	NAI	C4A-C5A-N7A	-3.41	106.68	110.58
50	G	201	8Q1	C31-C29-C32	3.36	114.50	108.77
47	A	503	NAI	N9A-C8A-N7A	-3.35	109.19	113.94
51	J	401	NDP	C4A-C5A-N7A	-3.26	106.85	110.58
57	w	401	ADP	C4-N9-C8	3.26	109.16	105.74
56	s	401	UQ	C21-C19-C18	-3.25	112.90	122.66
57	w	401	ADP	C4-C5-N7	-3.19	106.93	110.58
51	J	401	NDP	N9A-C8A-N7A	-3.16	109.45	113.94
51	J	401	NDP	C5A-N7A-C8A	3.14	108.39	103.45
46	A	502	FMN	C4-N3-C2	-3.10	120.14	125.64
56	s	401	UQ	CM5-C5-C6	-3.06	119.42	124.45
56	s	401	UQ	C7-C6-C5	-3.04	119.67	124.89
56	s	401	UQ	C20-C19-C18	-3.01	113.61	122.66
48	r	501	PEE	O3-C30-C31	2.81	120.40	111.83
47	A	503	NAI	C2D-C3D-C4D	2.81	108.03	102.61
48	l	702	PEE	O3-C30-C31	2.80	120.38	111.83
54	i	401	CDL	OA8-CA7-C31	2.78	120.31	111.83
48	B	303	PEE	O3-C30-C31	2.77	120.28	111.83
54	u	201	CDL	OB8-CB7-C71	2.76	120.24	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	i	401	CDL	OB8-CB7-C71	2.73	120.17	111.83
48	b	201	PEE	O3-C30-C31	2.73	120.17	111.83
54	N	201	CDL	OB8-CB7-C71	2.73	120.16	111.83
48	j	201	PEE	O3-C30-C31	2.68	119.99	111.83
54	r	503	CDL	OB8-CB7-C71	2.67	119.99	111.83
54	a	201	CDL	OB8-CB7-C71	2.67	119.98	111.83
54	u	201	CDL	OA8-CA7-C31	2.65	119.93	111.83
54	r	503	CDL	OA8-CA7-C31	2.63	119.85	111.83
54	r	504	CDL	OB8-CB7-C71	2.62	119.84	111.83
46	A	502	FMN	C4A-C4-N3	2.61	119.89	113.25
54	N	201	CDL	OA8-CA7-C31	2.61	119.78	111.83
48	C	302	PEE	O3-C30-C31	2.60	119.76	111.83
49	g	201	PLX	C1A-N1-C1	2.57	120.11	109.91
48	m	201	PEE	O3-C30-C31	2.57	119.66	111.83
47	A	503	NAI	C4D-O4D-C1D	-2.56	103.80	109.47
47	A	503	NAI	C4A-N9A-C8A	2.52	108.39	105.74
46	A	502	FMN	C4A-C10-N10	2.52	120.09	116.48
51	J	401	NDP	C4A-N9A-C8A	2.49	108.36	105.74
54	r	504	CDL	OA8-CA7-C31	2.49	119.42	111.83
54	a	201	CDL	OA8-CA7-C31	2.49	119.42	111.83
49	r	502	PLX	C1A-N1-C1	2.49	119.80	109.91
46	A	502	FMN	O4-C4-C4A	-2.48	119.97	126.53
50	G	201	8Q1	C43-S44-C1	2.48	109.16	101.84
49	l	701	PLX	C1A-N1-C1	2.47	119.74	109.91
48	i	402	PEE	O3-C30-C31	2.46	119.35	111.83
49	j	202	PLX	C1A-N1-C1	2.38	119.38	109.91
47	A	503	NAI	C3D-C2D-C1D	2.36	105.94	101.46
46	A	502	FMN	C10-C4A-N5	-2.34	120.03	124.81
57	w	401	ADP	C4'-O4'-C1'	-2.32	104.34	109.47
50	X	201	8Q1	O4-C1-S44	-2.31	119.75	122.68
46	A	502	FMN	C9A-C5A-N5	-2.29	120.02	122.45
46	A	502	FMN	C5A-C9A-N10	2.29	120.03	117.97
49	C	303	PLX	C1A-N1-C1	2.28	118.98	109.91
51	J	401	NDP	C2B-C3B-C4B	2.26	106.86	101.99
50	X	201	8Q1	C38-C39-N41	2.26	120.46	116.34
50	X	201	8Q1	C37-C38-C39	2.21	116.08	112.39
50	X	201	8Q1	C43-S44-C1	2.16	108.22	101.84
51	J	401	NDP	C2D-C3D-C4D	2.12	106.71	102.61
50	G	201	8Q1	O4-C1-S44	-2.09	120.02	122.68
47	A	503	NAI	C3B-C2B-C1B	2.06	105.35	101.46
50	X	201	8Q1	C32-C34-N36	2.04	120.36	116.48
46	A	502	FMN	C4A-C10-N1	-2.04	119.59	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	m	201	PEE	O2-C10-O4	-2.03	118.95	123.70
51	J	401	NDP	P2B-O2B-C2B	-2.03	118.02	123.43

There are no chirality outliers.

All (661) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	C5'-O5'-P-O1P
47	A	503	NAI	C5B-O5B-PA-O1A
48	B	303	PEE	C37-C38-C39-C40
48	C	302	PEE	C1-O3P-P-O1P
48	C	302	PEE	C1-O3P-P-O4P
48	b	201	PEE	O4P-C4-C5-N
48	i	402	PEE	C11-C10-O2-C2
48	i	402	PEE	C4-O4P-P-O3P
48	i	402	PEE	C4-O4P-P-O1P
48	j	201	PEE	C11-C10-O2-C2
48	j	201	PEE	C1-O3P-P-O2P
48	j	201	PEE	C1-O3P-P-O1P
48	j	201	PEE	C1-O3P-P-O4P
48	j	201	PEE	C4-O4P-P-O3P
48	j	201	PEE	C4-O4P-P-O2P
48	j	201	PEE	C4-O4P-P-O1P
48	l	702	PEE	C11-C10-O2-C2
48	l	702	PEE	O3P-C1-C2-O2
48	l	702	PEE	C4-O4P-P-O3P
48	l	702	PEE	C4-O4P-P-O2P
48	l	702	PEE	C4-O4P-P-O1P
48	m	201	PEE	C11-C10-O2-C2
48	m	201	PEE	O4P-C4-C5-N
48	r	501	PEE	C1-O3P-P-O1P
48	r	501	PEE	C1-O3P-P-O4P
48	r	501	PEE	C4-O4P-P-O3P
48	r	501	PEE	C4-O4P-P-O1P
49	C	303	PLX	O4-C3-C4-O6
49	C	303	PLX	C3-O4-P1-O1
49	C	303	PLX	C3-O4-P1-O2
49	C	303	PLX	C3-O4-P1-O3
49	g	201	PLX	O7-C6-O6-C4
49	j	202	PLX	O7-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	O7-C6-O6-C4
49	j	202	PLX	O9-C24-C25-C26
49	l	701	PLX	O7-C6-O6-C4
49	l	701	PLX	C25-C24-O8-C5
49	l	701	PLX	O9-C24-C25-C26
49	r	502	PLX	O7-C6-O6-C4
49	r	502	PLX	C5-C4-O6-C6
49	r	502	PLX	C3-O4-P1-O2
49	r	502	PLX	O9-C24-O8-C5
49	r	502	PLX	O9-C24-C25-C26
50	G	201	8Q1	O4-C1-S44-C43
50	G	201	8Q1	C6-C1-S44-C43
50	G	201	8Q1	C28-C29-C32-C34
50	G	201	8Q1	C28-C29-C32-O33
50	G	201	8Q1	C30-C29-C32-C34
50	G	201	8Q1	C30-C29-C32-O33
50	G	201	8Q1	C31-C29-C32-C34
50	G	201	8Q1	C31-C29-C32-O33
50	G	201	8Q1	N36-C37-C38-C39
50	G	201	8Q1	C42-C43-S44-C1
50	X	201	8Q1	C28-C29-C32-C34
50	X	201	8Q1	C28-C29-C32-O33
50	X	201	8Q1	C30-C29-C32-C34
50	X	201	8Q1	C30-C29-C32-O33
50	X	201	8Q1	C31-C29-C32-C34
50	X	201	8Q1	C31-C29-C32-O33
50	X	201	8Q1	C29-C32-C34-O35
50	X	201	8Q1	N36-C37-C38-C39
50	X	201	8Q1	C28-O27-P24-O2
54	N	201	CDL	CA2-C1-CB2-OB2
54	N	201	CDL	CA2-OA2-PA1-OA3
54	N	201	CDL	CA2-OA2-PA1-OA4
54	N	201	CDL	CA2-OA2-PA1-OA5
54	N	201	CDL	CA3-OA5-PA1-OA2
54	N	201	CDL	CA3-OA5-PA1-OA4
54	N	201	CDL	C11-CA5-OA6-CA4
54	N	201	CDL	CB2-OB2-PB2-OB3
54	N	201	CDL	CB2-OB2-PB2-OB4
54	N	201	CDL	CB2-OB2-PB2-OB5
54	N	201	CDL	CB3-OB5-PB2-OB2
54	N	201	CDL	CB3-OB5-PB2-OB3
54	N	201	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
54	a	201	CDL	CA2-OA2-PA1-OA3
54	a	201	CDL	CA2-OA2-PA1-OA4
54	a	201	CDL	CA2-OA2-PA1-OA5
54	a	201	CDL	CA3-OA5-PA1-OA2
54	a	201	CDL	CA3-OA5-PA1-OA4
54	a	201	CDL	CB3-OB5-PB2-OB2
54	a	201	CDL	CB3-OB5-PB2-OB3
54	i	401	CDL	CA2-OA2-PA1-OA3
54	i	401	CDL	CA2-OA2-PA1-OA4
54	i	401	CDL	CA2-OA2-PA1-OA5
54	i	401	CDL	CA3-OA5-PA1-OA2
54	i	401	CDL	CA3-OA5-PA1-OA3
54	i	401	CDL	CA3-OA5-PA1-OA4
54	i	401	CDL	CB2-OB2-PB2-OB4
54	i	401	CDL	CB2-OB2-PB2-OB5
54	i	401	CDL	CB3-OB5-PB2-OB3
54	i	401	CDL	OB6-CB4-CB6-OB8
54	r	503	CDL	O1-C1-CA2-OA2
54	r	503	CDL	OA5-CA3-CA4-OA6
54	r	504	CDL	CA3-OA5-PA1-OA2
54	r	504	CDL	CA3-OA5-PA1-OA3
54	r	504	CDL	OA6-CA4-CA6-OA8
54	r	504	CDL	C51-CB5-OB6-CB4
54	u	201	CDL	CA2-OA2-PA1-OA3
54	u	201	CDL	CA2-OA2-PA1-OA5
54	u	201	CDL	CA3-OA5-PA1-OA2
54	u	201	CDL	CB3-OB5-PB2-OB2
54	u	201	CDL	CB3-OB5-PB2-OB3
56	s	401	UQ	C7-C8-C9-C10
56	s	401	UQ	C7-C8-C9-C11
56	s	401	UQ	C12-C13-C14-C16
57	w	401	ADP	C5'-O5'-PA-O2A
56	s	401	UQ	C17-C18-C19-C21
54	r	503	CDL	C31-CA7-OA8-CA6
48	b	201	PEE	O5-C30-O3-C3
48	l	702	PEE	O5-C30-O3-C3
54	r	503	CDL	OA9-CA7-OA8-CA6
48	i	402	PEE	O4-C10-O2-C2
48	j	201	PEE	O4-C10-O2-C2
48	l	702	PEE	O4-C10-O2-C2
48	m	201	PEE	O4-C10-O2-C2
54	N	201	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
54	r	504	CDL	OB7-CB5-OB6-CB4
56	s	401	UQ	C12-C11-C9-C8
54	i	401	CDL	OA9-CA7-OA8-CA6
48	b	201	PEE	C31-C30-O3-C3
48	l	702	PEE	C31-C30-O3-C3
48	i	402	PEE	C17-C18-C19-C20
48	j	201	PEE	C17-C18-C19-C20
48	r	501	PEE	C17-C18-C19-C20
49	g	201	PLX	C7-C8-C9-C10
54	N	201	CDL	O1-C1-CB2-OB2
54	i	401	CDL	O1-C1-CA2-OA2
54	r	504	CDL	C71-CB7-OB8-CB6
48	r	501	PEE	C11-C10-O2-C2
54	i	401	CDL	C31-CA7-OA8-CA6
49	l	701	PLX	C12-C13-C14-C15
54	r	504	CDL	OB9-CB7-OB8-CB6
54	r	503	CDL	C62-C63-C64-C65
48	m	201	PEE	C31-C30-O3-C3
56	s	401	UQ	C12-C13-C14-C15
48	b	201	PEE	C37-C38-C39-C40
48	m	201	PEE	C13-C14-C15-C16
49	j	202	PLX	C28-C29-C30-C31
48	m	201	PEE	O5-C30-O3-C3
54	r	503	CDL	CB2-C1-CA2-OA2
54	N	201	CDL	C31-CA7-OA8-CA6
54	i	401	CDL	C14-C15-C16-C17
54	i	401	CDL	C31-C32-C33-C34
48	C	302	PEE	C14-C15-C16-C17
54	r	503	CDL	C32-C33-C34-C35
48	r	501	PEE	C41-C42-C43-C44
49	r	502	PLX	C9-C10-C11-C12
54	i	401	CDL	C37-C38-C39-C40
48	r	501	PEE	O4-C10-O2-C2
51	J	401	NDP	C2D-C1D-N1N-C6N
54	a	201	CDL	CB5-C51-C52-C53
54	a	201	CDL	C34-C35-C36-C37
49	r	502	PLX	C11-C12-C13-C14
54	i	401	CDL	CA7-C31-C32-C33
49	l	701	PLX	C2-C1-N1-C1A
48	r	501	PEE	C10-C11-C12-C13
54	N	201	CDL	CB5-C51-C52-C53
54	r	503	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
48	B	303	PEE	C30-C31-C32-C33
48	C	302	PEE	C30-C31-C32-C33
54	N	201	CDL	CA7-C31-C32-C33
54	r	504	CDL	CA7-C31-C32-C33
49	j	202	PLX	C15-C16-C17-C18
48	b	201	PEE	C34-C35-C36-C37
49	C	303	PLX	C28-C29-C30-C31
49	r	502	PLX	C30-C31-C32-C33
48	i	402	PEE	C31-C30-O3-C3
54	a	201	CDL	C71-CB7-OB8-CB6
54	N	201	CDL	OA9-CA7-OA8-CA6
49	g	201	PLX	C12-C13-C14-C15
56	s	401	UQ	C13-C14-C16-C17
54	u	201	CDL	C75-C76-C77-C78
48	b	201	PEE	C10-C11-C12-C13
48	l	702	PEE	C30-C31-C32-C33
48	r	501	PEE	C30-C31-C32-C33
54	i	401	CDL	CB2-C1-CA2-OA2
54	r	503	CDL	C71-CB7-OB8-CB6
49	l	701	PLX	C2-C1-N1-C1C
48	B	303	PEE	C10-C11-C12-C13
56	s	401	UQ	C12-C11-C9-C10
48	b	201	PEE	C11-C10-O2-C2
54	N	201	CDL	C51-CB5-OB6-CB4
48	b	201	PEE	O4-C10-O2-C2
54	N	201	CDL	OB7-CB5-OB6-CB4
54	r	503	CDL	O1-C1-CB2-OB2
54	r	504	CDL	O1-C1-CA2-OA2
54	a	201	CDL	OB9-CB7-OB8-CB6
48	r	501	PEE	C33-C34-C35-C36
54	r	504	CDL	C78-C79-C80-C81
54	r	503	CDL	OB9-CB7-OB8-CB6
48	j	201	PEE	C23-C24-C25-C26
49	C	303	PLX	C7-C8-C9-C10
54	r	504	CDL	C12-C13-C14-C15
49	g	201	PLX	C11-C10-C9-C8
49	j	202	PLX	C25-C26-C27-C28
49	r	502	PLX	C27-C28-C29-C30
48	i	402	PEE	O5-C30-O3-C3
49	C	303	PLX	O7-C6-C7-C8
48	C	302	PEE	C42-C43-C44-C45
49	j	202	PLX	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
49	j	202	PLX	C27-C28-C29-C30
49	l	701	PLX	C33-C34-C35-C36
54	a	201	CDL	C75-C76-C77-C78
54	i	401	CDL	C35-C36-C37-C38
48	b	201	PEE	C32-C33-C34-C35
49	C	303	PLX	C17-C18-C19-C20
49	g	201	PLX	C27-C28-C29-C30
54	r	503	CDL	C73-C74-C75-C76
48	b	201	PEE	C14-C15-C16-C17
54	u	201	CDL	C11-CA5-OA6-CA4
49	r	502	PLX	C31-C32-C33-C34
54	N	201	CDL	C11-C12-C13-C14
49	j	202	PLX	C7-C8-C9-C10
54	a	201	CDL	C76-C77-C78-C79
54	r	503	CDL	C56-C57-C58-C59
50	X	201	8Q1	C7-C8-C9-C10
54	i	401	CDL	C12-C13-C14-C15
54	r	504	CDL	C55-C56-C57-C58
54	r	504	CDL	C75-C76-C77-C78
49	l	701	PLX	C29-C30-C31-C32
48	B	303	PEE	C33-C34-C35-C36
48	C	302	PEE	C43-C44-C45-C46
54	r	504	CDL	C73-C74-C75-C76
54	r	503	CDL	C71-C72-C73-C74
54	r	504	CDL	C43-C44-C45-C46
54	r	503	CDL	CB3-CB4-CB6-OB8
49	g	201	PLX	C28-C29-C30-C31
54	r	503	CDL	C20-C21-C22-C23
54	r	503	CDL	C75-C76-C77-C78
54	r	503	CDL	CB5-C51-C52-C53
48	m	201	PEE	C12-C13-C14-C15
49	g	201	PLX	C10-C11-C12-C13
54	a	201	CDL	C37-C38-C39-C40
54	i	401	CDL	C13-C14-C15-C16
54	r	504	CDL	C76-C77-C78-C79
49	g	201	PLX	C35-C36-C37-C38
48	b	201	PEE	C13-C14-C15-C16
48	i	402	PEE	C22-C23-C24-C25
49	j	202	PLX	C10-C11-C12-C13
49	l	701	PLX	C2-C1-N1-C1B
48	j	201	PEE	C32-C33-C34-C35
49	l	701	PLX	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
54	a	201	CDL	C33-C34-C35-C36
48	B	303	PEE	C11-C10-O2-C2
46	A	502	FMN	O2'-C2'-C3'-C4'
48	B	303	PEE	C39-C40-C41-C42
48	C	302	PEE	C15-C16-C17-C18
48	i	402	PEE	C37-C38-C39-C40
48	l	702	PEE	C37-C38-C39-C40
48	m	201	PEE	C11-C12-C13-C14
49	r	502	PLX	C28-C29-C30-C31
54	r	504	CDL	C52-C53-C54-C55
49	C	303	PLX	C13-C14-C15-C16
54	a	201	CDL	C54-C55-C56-C57
48	B	303	PEE	C23-C24-C25-C26
54	r	503	CDL	C37-C38-C39-C40
48	l	702	PEE	C21-C22-C23-C24
54	r	504	CDL	C13-C14-C15-C16
48	b	201	PEE	C31-C32-C33-C34
49	l	701	PLX	C14-C15-C16-C17
54	r	503	CDL	C42-C43-C44-C45
48	C	302	PEE	C11-C10-O2-C2
54	r	503	CDL	C11-CA5-OA6-CA4
54	r	503	CDL	OA7-CA5-OA6-CA4
54	u	201	CDL	OA7-CA5-OA6-CA4
54	r	504	CDL	C41-C42-C43-C44
54	r	504	CDL	C80-C81-C82-C83
48	B	303	PEE	C15-C16-C17-C18
48	C	302	PEE	C39-C40-C41-C42
48	r	501	PEE	C19-C20-C21-C22
49	l	701	PLX	C16-C17-C18-C19
54	N	201	CDL	CB7-C71-C72-C73
48	j	201	PEE	C37-C38-C39-C40
54	r	503	CDL	C81-C82-C83-C84
54	r	504	CDL	C72-C73-C74-C75
54	i	401	CDL	C52-C53-C54-C55
54	r	504	CDL	C14-C15-C16-C17
54	a	201	CDL	OA5-CA3-CA4-OA6
49	l	701	PLX	C9-C10-C11-C12
54	r	504	CDL	C71-C72-C73-C74
54	r	504	CDL	CB7-C71-C72-C73
49	C	303	PLX	C33-C34-C35-C36
54	i	401	CDL	C11-C12-C13-C14
48	i	402	PEE	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
48	i	402	PEE	C35-C36-C37-C38
54	r	503	CDL	OB6-CB4-CB6-OB8
54	i	401	CDL	C71-C72-C73-C74
48	b	201	PEE	C33-C34-C35-C36
49	j	202	PLX	C9-C10-C11-C12
49	l	701	PLX	C31-C32-C33-C34
49	l	701	PLX	C11-C12-C13-C14
48	j	201	PEE	C36-C37-C38-C39
48	r	501	PEE	C36-C37-C38-C39
48	b	201	PEE	C22-C23-C24-C25
46	A	502	FMN	C3'-C4'-C5'-O5'
49	r	502	PLX	C12-C13-C14-C15
49	r	502	PLX	C33-C34-C35-C36
48	m	201	PEE	C22-C23-C24-C25
49	g	201	PLX	C9-C10-C11-C12
54	r	503	CDL	C51-C52-C53-C54
49	r	502	PLX	C14-C15-C16-C17
54	a	201	CDL	C71-C72-C73-C74
54	r	504	CDL	C56-C57-C58-C59
49	C	303	PLX	C11-C12-C13-C14
48	l	702	PEE	C31-C32-C33-C34
48	l	702	PEE	C15-C16-C17-C18
54	r	503	CDL	C82-C83-C84-C85
48	l	702	PEE	O3P-C1-C2-C3
54	a	201	CDL	OA5-CA3-CA4-CA6
48	C	302	PEE	O4-C10-O2-C2
48	j	201	PEE	C43-C44-C45-C46
48	B	303	PEE	C13-C14-C15-C16
49	r	502	PLX	C15-C16-C17-C18
54	i	401	CDL	C11-CA5-OA6-CA4
49	j	202	PLX	C14-C15-C16-C17
54	r	504	CDL	C60-C61-C62-C63
48	j	201	PEE	C31-C30-O3-C3
48	i	402	PEE	C14-C15-C16-C17
48	B	303	PEE	O4-C10-O2-C2
48	b	201	PEE	C1-C2-C3-O3
48	r	501	PEE	C1-C2-C3-O3
54	i	401	CDL	CB3-CB4-CB6-OB8
54	r	504	CDL	CA3-CA4-CA6-OA8
56	s	401	UQ	C14-C16-C17-C18
49	C	303	PLX	C27-C28-C29-C30
48	r	501	PEE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
49	g	201	PLX	C30-C31-C32-C33
54	r	503	CDL	C54-C55-C56-C57
54	r	504	CDL	C62-C63-C64-C65
49	j	202	PLX	C26-C27-C28-C29
49	l	701	PLX	C26-C27-C28-C29
54	r	503	CDL	C58-C59-C60-C61
54	r	504	CDL	C82-C83-C84-C85
54	r	504	CDL	CB5-C51-C52-C53
48	B	303	PEE	C22-C23-C24-C25
54	N	201	CDL	CA6-CA4-OA6-CA5
54	u	201	CDL	CA6-CA4-OA6-CA5
48	B	303	PEE	C35-C36-C37-C38
50	G	201	8Q1	C12-C13-C14-C15
48	b	201	PEE	C17-C18-C19-C20
54	i	401	CDL	C33-C34-C35-C36
54	u	201	CDL	C57-C58-C59-C60
48	j	201	PEE	C44-C45-C46-C47
54	a	201	CDL	C14-C15-C16-C17
49	r	502	PLX	C13-C14-C15-C16
54	a	201	CDL	C72-C73-C74-C75
49	C	303	PLX	C36-C37-C38-C39
48	B	303	PEE	C34-C35-C36-C37
54	a	201	CDL	C24-C25-C26-C27
49	C	303	PLX	C31-C32-C33-C34
54	i	401	CDL	C73-C74-C75-C76
54	i	401	CDL	C39-C40-C41-C42
49	g	201	PLX	C32-C33-C34-C35
48	j	201	PEE	O5-C30-O3-C3
54	r	503	CDL	C76-C77-C78-C79
54	i	401	CDL	CB5-C51-C52-C53
48	B	303	PEE	C17-C18-C19-C20
49	l	701	PLX	C28-C29-C30-C31
50	X	201	8Q1	C9-C10-C11-C12
49	j	202	PLX	C34-C35-C36-C37
49	C	303	PLX	O4-C3-C4-C5
54	i	401	CDL	OA5-CA3-CA4-CA6
54	r	503	CDL	OA5-CA3-CA4-CA6
50	X	201	8Q1	C29-C32-C34-N36
48	C	302	PEE	C13-C14-C15-C16
54	a	201	CDL	C21-C22-C23-C24
48	C	302	PEE	C31-C30-O3-C3
54	r	503	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
54	r	504	CDL	C35-C36-C37-C38
49	r	502	PLX	C10-C11-C12-C13
54	i	401	CDL	C32-C33-C34-C35
49	j	202	PLX	C3-C4-C5-O8
50	X	201	8Q1	O33-C32-C34-N36
54	u	201	CDL	CA3-CA4-CA6-OA8
54	i	401	CDL	C15-C16-C17-C18
49	j	202	PLX	C13-C14-C15-C16
49	l	701	PLX	C25-C26-C27-C28
48	j	201	PEE	C30-C31-C32-C33
49	l	701	PLX	C30-C31-C32-C33
48	B	303	PEE	O3P-C1-C2-O2
54	r	503	CDL	C11-C12-C13-C14
50	X	201	8Q1	O4-C1-S44-C43
48	l	702	PEE	C13-C14-C15-C16
48	i	402	PEE	C20-C21-C22-C23
48	B	303	PEE	C20-C21-C22-C23
49	C	303	PLX	C30-C31-C32-C33
48	b	201	PEE	O2-C2-C3-O3
48	i	402	PEE	O2-C2-C3-O3
49	j	202	PLX	C30-C31-C32-C33
54	u	201	CDL	C53-C54-C55-C56
54	r	503	CDL	C35-C36-C37-C38
48	r	501	PEE	C24-C25-C26-C27
54	a	201	CDL	C58-C59-C60-C61
48	m	201	PEE	C31-C32-C33-C34
54	r	503	CDL	C21-C22-C23-C24
50	X	201	8Q1	C6-C1-S44-C43
54	a	201	CDL	C22-C23-C24-C25
49	g	201	PLX	C14-C15-C16-C17
49	l	701	PLX	C7-C8-C9-C10
49	r	502	PLX	C25-C26-C27-C28
54	r	503	CDL	C33-C34-C35-C36
48	b	201	PEE	C23-C24-C25-C26
46	A	502	FMN	C1'-C2'-C3'-O3'
54	N	201	CDL	OA5-CA3-CA4-CA6
54	N	201	CDL	OB5-CB3-CB4-CB6
48	j	201	PEE	C38-C39-C40-C41
49	C	303	PLX	C25-C26-C27-C28
54	r	503	CDL	CA7-C31-C32-C33
48	B	303	PEE	C31-C32-C33-C34
49	C	303	PLX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
54	r	504	CDL	C59-C60-C61-C62
54	i	401	CDL	CB7-C71-C72-C73
54	r	503	CDL	C23-C24-C25-C26
54	i	401	CDL	OA7-CA5-OA6-CA4
54	N	201	CDL	C71-CB7-OB8-CB6
48	m	201	PEE	C3-C2-O2-C10
48	C	302	PEE	O5-C30-O3-C3
49	r	502	PLX	C20-C21-C22-C23
49	g	201	PLX	O4-C3-C4-O6
54	i	401	CDL	OA5-CA3-CA4-OA6
49	g	201	PLX	C25-C26-C27-C28
48	i	402	PEE	C1-C2-C3-O3
49	l	701	PLX	C3-C4-C5-O8
54	r	504	CDL	C31-C32-C33-C34
54	r	504	CDL	C64-C65-C66-C67
54	r	503	CDL	C84-C85-C86-C87
48	C	302	PEE	C37-C38-C39-C40
48	j	201	PEE	C15-C16-C17-C18
49	j	202	PLX	O6-C4-C5-O8
49	l	701	PLX	O6-C4-C5-O8
54	u	201	CDL	CB7-C71-C72-C73
49	j	202	PLX	C31-C32-C33-C34
54	u	201	CDL	C77-C78-C79-C80
48	m	201	PEE	C14-C15-C16-C17
54	r	504	CDL	C33-C34-C35-C36
49	j	202	PLX	C7-C6-O6-C4
49	l	701	PLX	C24-C25-C26-C27
48	j	201	PEE	C34-C35-C36-C37
54	r	503	CDL	C60-C61-C62-C63
54	r	504	CDL	C32-C33-C34-C35
54	u	201	CDL	C22-C23-C24-C25
49	C	303	PLX	N1-C1-C2-O1
54	a	201	CDL	C55-C56-C57-C58
54	N	201	CDL	OB9-CB7-OB8-CB6
54	i	401	CDL	C75-C76-C77-C78
49	g	201	PLX	C25-C24-O8-C5
49	j	202	PLX	C25-C24-O8-C5
48	m	201	PEE	C23-C24-C25-C26
48	r	501	PEE	C16-C17-C18-C19
47	A	503	NAI	C2D-C1D-N1N-C2N
49	g	201	PLX	O4-C3-C4-C5
49	j	202	PLX	O4-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
49	C	303	PLX	C9-C10-C11-C12
54	r	503	CDL	C55-C56-C57-C58
50	X	201	8Q1	C42-C43-S44-C1
49	l	701	PLX	O8-C24-C25-C26
48	b	201	PEE	O3P-C1-C2-O2
48	r	501	PEE	O3P-C1-C2-O2
49	j	202	PLX	O4-C3-C4-O6
54	N	201	CDL	OB5-CB3-CB4-OB6
54	u	201	CDL	C71-C72-C73-C74
48	l	702	PEE	C32-C33-C34-C35
54	r	504	CDL	C37-C38-C39-C40
48	C	302	PEE	C20-C21-C22-C23
49	C	303	PLX	C15-C16-C17-C18
48	C	302	PEE	O2-C2-C3-O3
49	r	502	PLX	O6-C4-C5-O8
54	u	201	CDL	OA6-CA4-CA6-OA8
54	r	504	CDL	CB2-C1-CA2-OA2
54	a	201	CDL	C11-C12-C13-C14
54	r	504	CDL	C40-C41-C42-C43
48	C	302	PEE	C1-C2-C3-O3
48	m	201	PEE	C21-C22-C23-C24
54	a	201	CDL	C20-C21-C22-C23
48	b	201	PEE	C18-C19-C20-C21
48	m	201	PEE	C18-C19-C20-C21
54	i	401	CDL	CA5-C11-C12-C13
54	r	503	CDL	C17-C18-C19-C20
48	C	302	PEE	C1-O3P-P-O2P
48	C	302	PEE	C4-O4P-P-O3P
48	C	302	PEE	C4-O4P-P-O2P
48	b	201	PEE	C1-O3P-P-O1P
48	m	201	PEE	C4-O4P-P-O3P
48	m	201	PEE	C4-O4P-P-O2P
48	m	201	PEE	C4-O4P-P-O1P
49	C	303	PLX	C2-O1-P1-O3
49	g	201	PLX	C3-O4-P1-O2
49	g	201	PLX	C2-O1-P1-O2
49	l	701	PLX	C2-O1-P1-O4
49	l	701	PLX	C2-O1-P1-O2
49	l	701	PLX	C2-O1-P1-O3
49	r	502	PLX	C2-O1-P1-O4
49	r	502	PLX	C2-O1-P1-O3
51	J	401	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
54	i	401	CDL	CB2-OB2-PB2-OB3
54	r	503	CDL	CA2-OA2-PA1-OA3
54	r	503	CDL	CA3-OA5-PA1-OA2
54	r	503	CDL	CA3-OA5-PA1-OA4
54	r	503	CDL	CB3-OB5-PB2-OB3
54	r	504	CDL	CA2-OA2-PA1-OA3
54	r	504	CDL	CB2-OB2-PB2-OB3
54	r	504	CDL	CB2-OB2-PB2-OB4
54	r	504	CDL	CB2-OB2-PB2-OB5
54	r	504	CDL	CB3-OB5-PB2-OB3
54	u	201	CDL	CA2-OA2-PA1-OA4
54	u	201	CDL	CA3-OA5-PA1-OA3
54	u	201	CDL	CB2-OB2-PB2-OB4
54	u	201	CDL	CB3-OB5-PB2-OB4
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O3A
50	X	201	8Q1	C28-O27-P24-O3
54	r	504	CDL	C39-C40-C41-C42
48	b	201	PEE	C11-C12-C13-C14
49	r	502	PLX	C7-C8-C9-C10
48	B	303	PEE	O3P-C1-C2-C3
48	b	201	PEE	O3P-C1-C2-C3
48	r	501	PEE	O3P-C1-C2-C3
54	a	201	CDL	C60-C61-C62-C63
48	b	201	PEE	C38-C39-C40-C41
48	b	201	PEE	C30-C31-C32-C33
48	i	402	PEE	C34-C35-C36-C37
48	r	501	PEE	C12-C13-C14-C15
48	j	201	PEE	C41-C42-C43-C44
54	r	503	CDL	C61-C62-C63-C64
54	r	504	CDL	C15-C16-C17-C18
48	r	501	PEE	O2-C2-C3-O3
54	a	201	CDL	C35-C36-C37-C38
47	A	503	NAI	C2D-C1D-N1N-C6N
50	G	201	8Q1	C11-C10-C9-C8
48	j	201	PEE	C12-C13-C14-C15
48	C	302	PEE	C18-C19-C20-C21
48	C	302	PEE	C38-C39-C40-C41
54	r	504	CDL	CA5-C11-C12-C13
54	N	201	CDL	C52-C53-C54-C55
48	m	201	PEE	O3-C30-C31-C32
49	r	502	PLX	O8-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
50	G	201	8Q1	C11-C12-C13-C14
51	J	401	NDP	C2B-O2B-P2B-O3X
49	r	502	PLX	C16-C17-C18-C19
48	m	201	PEE	C24-C25-C26-C27
54	r	504	CDL	C74-C75-C76-C77
54	N	201	CDL	C31-C32-C33-C34
48	r	501	PEE	C31-C30-O3-C3
54	u	201	CDL	OA5-CA3-CA4-OA6
48	m	201	PEE	C16-C17-C18-C19
49	g	201	PLX	C18-C19-C20-C21
54	r	504	CDL	C84-C85-C86-C87
46	A	502	FMN	O2'-C2'-C3'-O3'
48	C	302	PEE	C16-C17-C18-C19
48	b	201	PEE	C16-C17-C18-C19
49	C	303	PLX	C19-C20-C21-C22
48	r	501	PEE	O5-C30-O3-C3
54	a	201	CDL	C36-C37-C38-C39
48	B	303	PEE	C42-C43-C44-C45
47	A	503	NAI	O4D-C1D-N1N-C2N
49	j	202	PLX	C32-C33-C34-C35
54	r	503	CDL	C36-C37-C38-C39
54	r	504	CDL	C57-C58-C59-C60
54	a	201	CDL	C74-C75-C76-C77
49	C	303	PLX	C18-C19-C20-C21
49	l	701	PLX	C36-C37-C38-C39
48	j	201	PEE	C19-C20-C21-C22
54	r	504	CDL	C23-C24-C25-C26
48	i	402	PEE	C21-C22-C23-C24
54	a	201	CDL	OB5-CB3-CB4-CB6
49	j	202	PLX	C19-C20-C21-C22
48	j	201	PEE	C21-C22-C23-C24
48	r	501	PEE	C11-C12-C13-C14
47	A	503	NAI	C2N-C3N-C7N-N7N
51	J	401	NDP	O4D-C1D-N1N-C6N
48	i	402	PEE	C31-C32-C33-C34
49	j	202	PLX	O6-C6-C7-C8
49	j	202	PLX	O8-C24-C25-C26
54	N	201	CDL	C72-C73-C74-C75
48	B	303	PEE	C14-C15-C16-C17
54	r	504	CDL	C1-CB2-OB2-PB2
54	r	504	CDL	C44-C45-C46-C47
54	i	401	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
49	r	502	PLX	C3-C4-C5-O8
56	s	401	UQ	C9-C11-C12-C13
48	b	201	PEE	C15-C16-C17-C18
54	a	201	CDL	OB7-CB5-OB6-CB4
48	C	302	PEE	C33-C34-C35-C36
54	r	503	CDL	CA2-C1-CB2-OB2
50	G	201	8Q1	C7-C8-C9-C10
48	r	501	PEE	C22-C23-C24-C25
48	i	402	PEE	C38-C39-C40-C41
48	i	402	PEE	C2-C1-O3P-P
48	B	303	PEE	C40-C41-C42-C43
49	j	202	PLX	C33-C34-C35-C36
46	A	502	FMN	C5'-O5'-P-O2P
49	l	701	PLX	C4-C5-O8-C24
50	X	201	8Q1	C28-O27-P24-O1
48	l	702	PEE	C16-C17-C18-C19
48	C	302	PEE	C36-C37-C38-C39
48	i	402	PEE	C16-C17-C18-C19
49	l	701	PLX	C10-C11-C12-C13
48	m	201	PEE	C33-C34-C35-C36
54	r	504	CDL	C20-C21-C22-C23
48	B	303	PEE	O5-C30-O3-C3
48	l	702	PEE	C1-C2-C3-O3
48	j	201	PEE	C16-C17-C18-C19
54	r	503	CDL	C12-C11-CA5-OA6
54	u	201	CDL	C17-C18-C19-C20
49	C	303	PLX	C12-C13-C14-C15
54	u	201	CDL	C55-C56-C57-C58
54	i	401	CDL	OA6-CA4-CA6-OA8
49	r	502	PLX	C35-C36-C37-C38
48	B	303	PEE	C18-C19-C20-C21
48	i	402	PEE	C36-C37-C38-C39
48	B	303	PEE	C31-C30-O3-C3
47	A	503	NAI	O4D-C1D-N1N-C6N
48	l	702	PEE	C36-C37-C38-C39
54	r	503	CDL	C79-C80-C81-C82
54	N	201	CDL	C12-C13-C14-C15
54	a	201	CDL	C51-CB5-OB6-CB4
48	B	303	PEE	C41-C42-C43-C44
48	l	702	PEE	C34-C35-C36-C37
54	r	504	CDL	C42-C43-C44-C45
54	r	504	CDL	C52-C51-CB5-OB6

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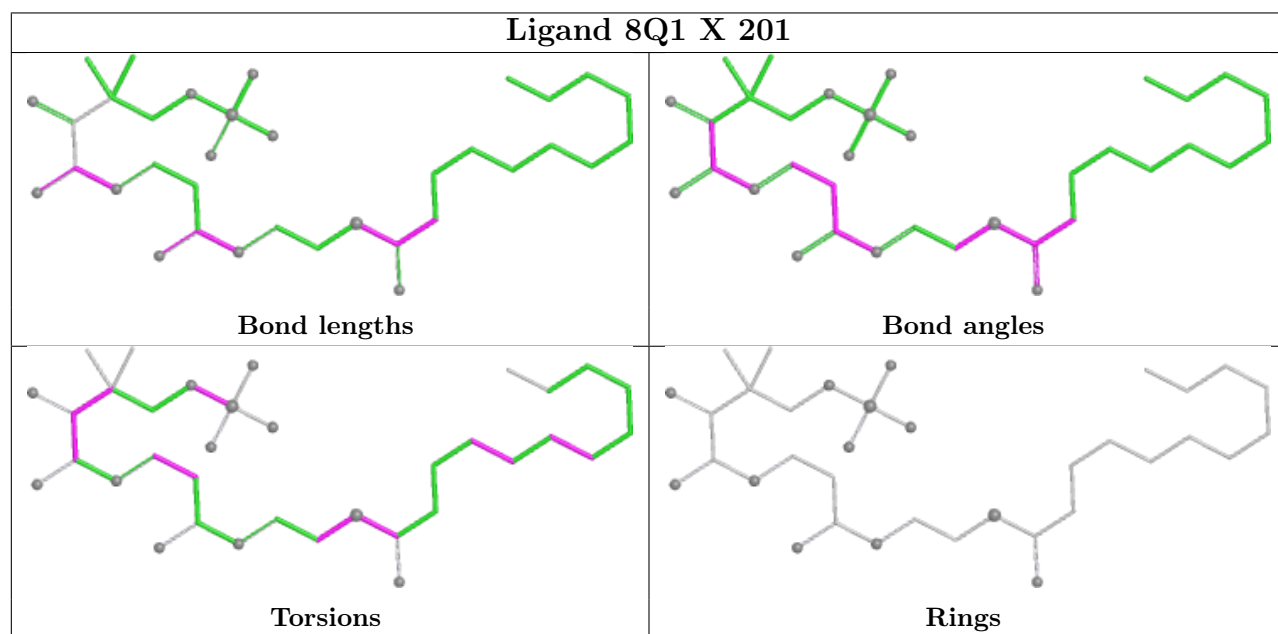
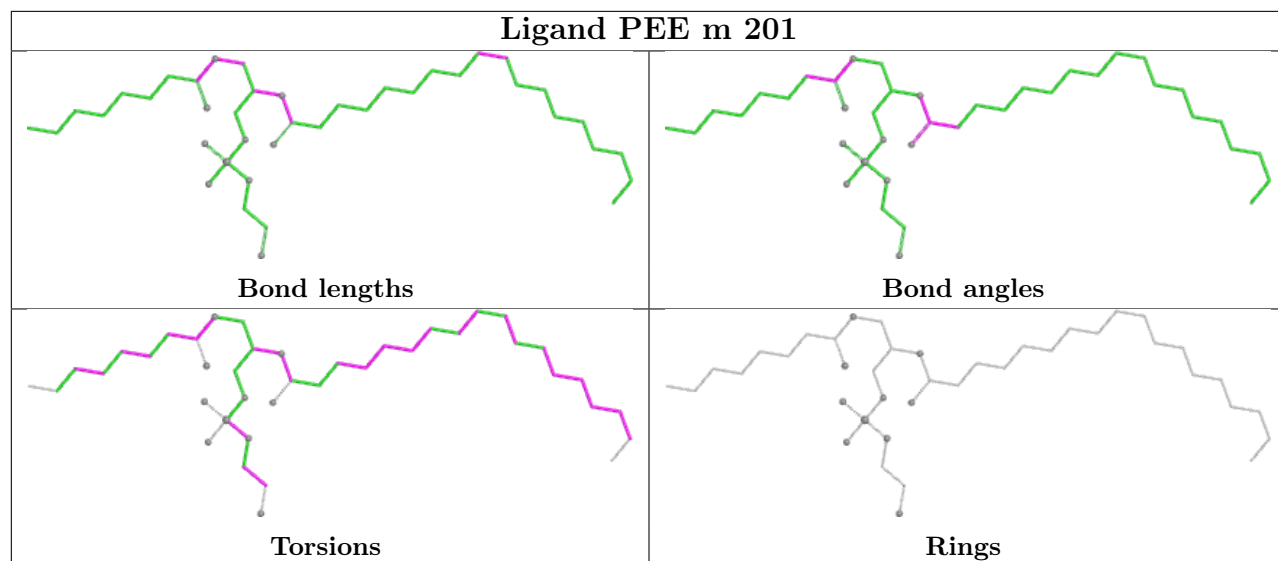
Mol	Chain	Res	Type	Atoms
54	r	503	CDL	C74-C75-C76-C77
48	C	302	PEE	O3-C30-C31-C32
48	j	201	PEE	O2-C10-C11-C12
48	C	302	PEE	C32-C33-C34-C35
54	u	201	CDL	C12-C11-CA5-OA6
54	i	401	CDL	CA3-CA4-CA6-OA8
54	N	201	CDL	C72-C71-CB7-OB8
46	A	502	FMN	O4'-C4'-C5'-O5'
48	r	501	PEE	C23-C24-C25-C26
49	j	202	PLX	C18-C19-C20-C21
54	u	201	CDL	C54-C55-C56-C57
48	b	201	PEE	C2-C3-O3-C30
54	a	201	CDL	C13-C14-C15-C16
48	C	302	PEE	C44-C45-C46-C47
54	u	201	CDL	C52-C51-CB5-OB6
54	r	504	CDL	C52-C51-CB5-OB7
49	g	201	PLX	O9-C24-O8-C5
49	j	202	PLX	O9-C24-O8-C5
49	l	701	PLX	O9-C24-O8-C5
54	r	503	CDL	C52-C53-C54-C55
49	r	502	PLX	C18-C19-C20-C21
49	l	701	PLX	C35-C36-C37-C38
49	j	202	PLX	C4-C5-O8-C24
48	l	702	PEE	O2-C2-C3-O3
54	r	504	CDL	C17-C18-C19-C20
48	C	302	PEE	O5-C30-C31-C32
54	r	503	CDL	C12-C11-CA5-OA7
54	N	201	CDL	C72-C71-CB7-OB9
54	a	201	CDL	CA4-CA3-OA5-PA1
48	j	201	PEE	O4-C10-C11-C12
54	i	401	CDL	C53-C54-C55-C56
49	g	201	PLX	C29-C30-C31-C32
48	m	201	PEE	C20-C21-C22-C23
48	r	501	PEE	C42-C43-C44-C45
57	w	401	ADP	PB-O3A-PA-O2A
54	u	201	CDL	C12-C11-CA5-OA7
51	J	401	NDP	O4B-C4B-C5B-O5B
48	B	303	PEE	C24-C25-C26-C27

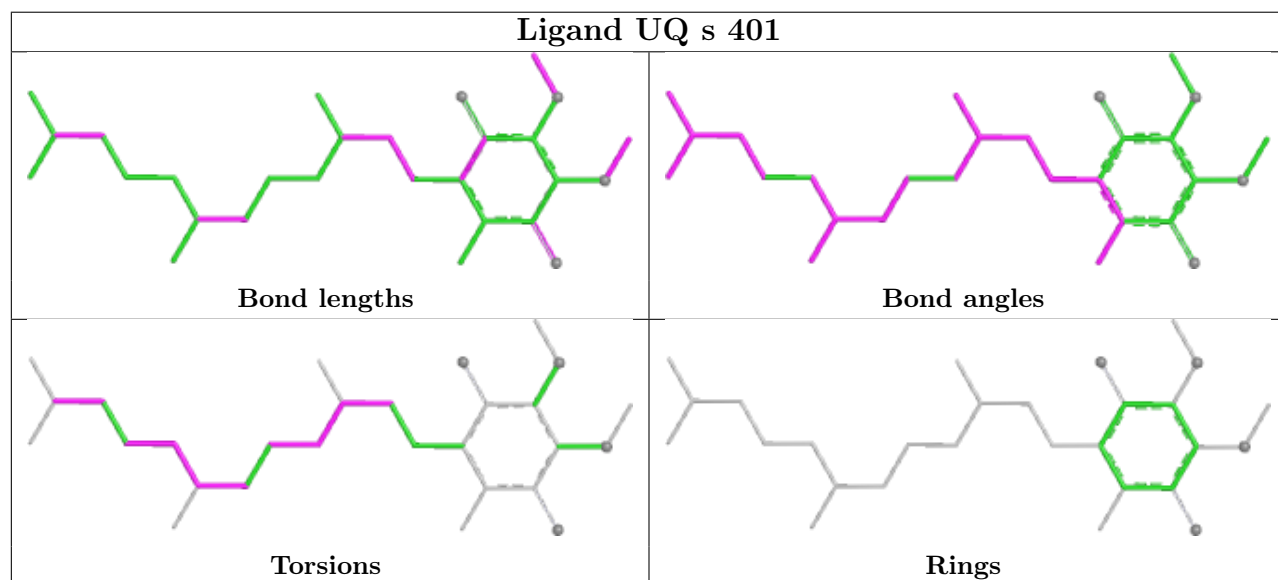
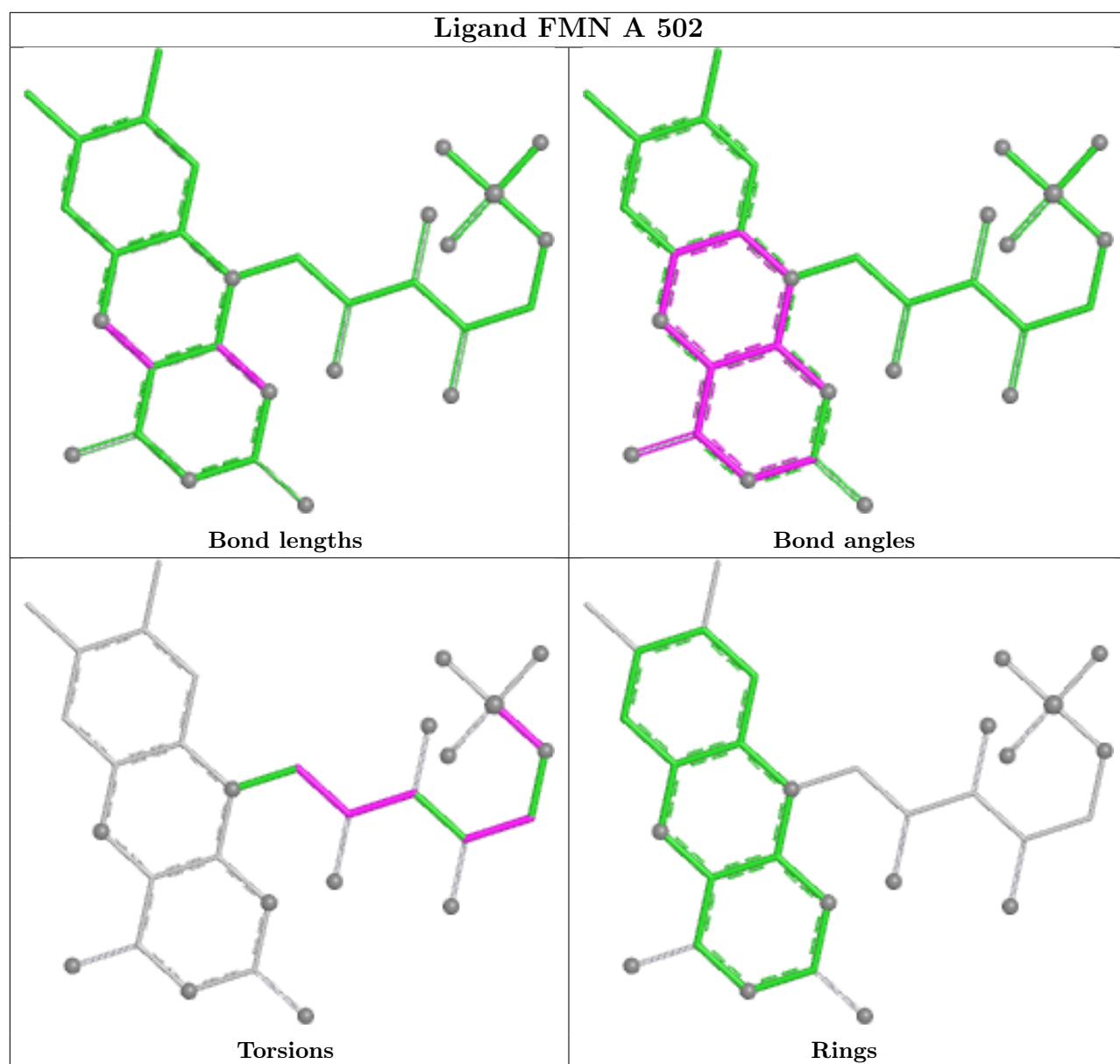
There are no ring outliers.

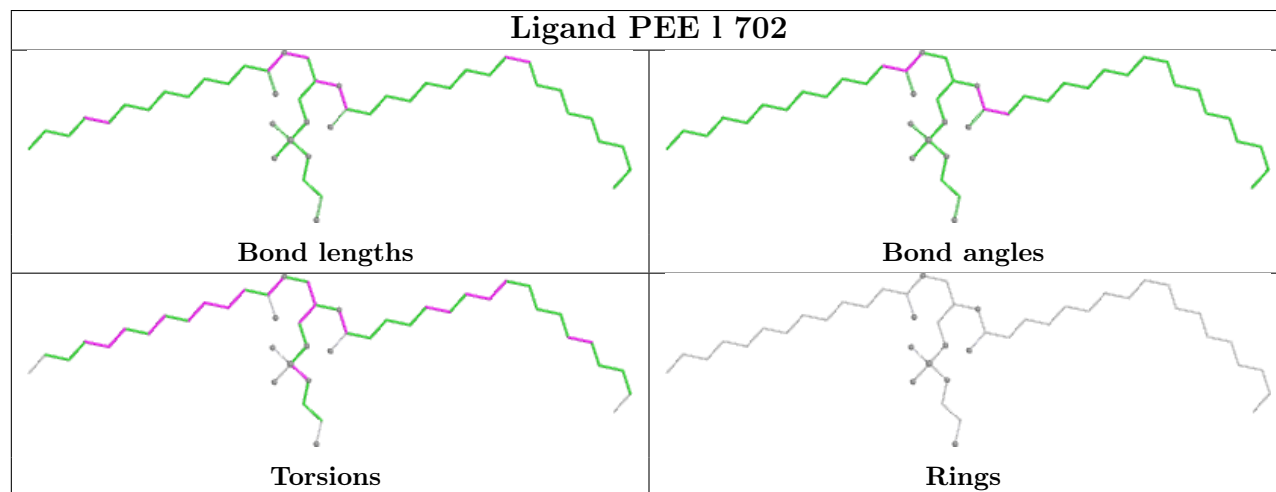
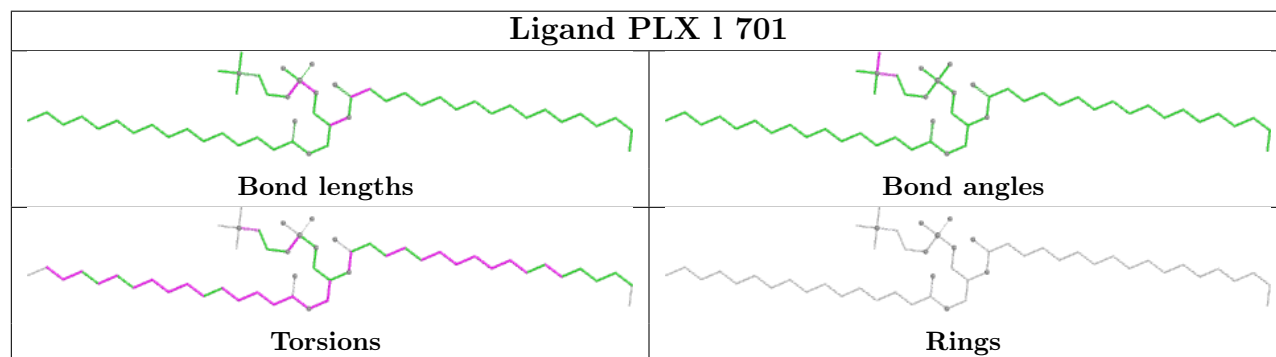
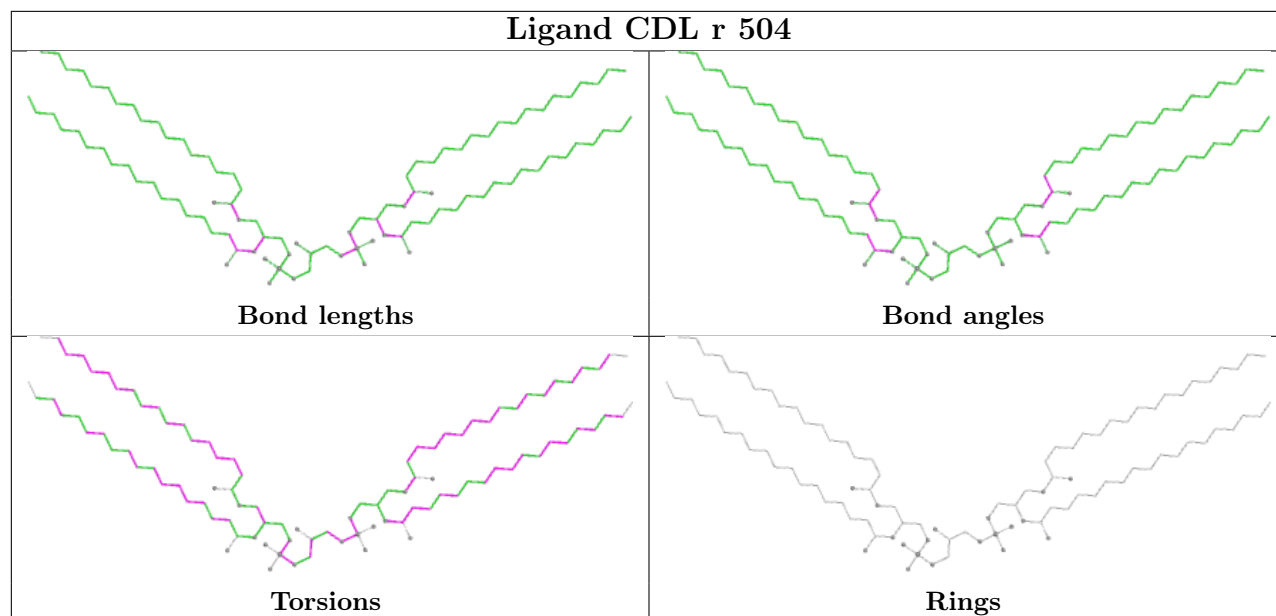
27 monomers are involved in 111 short contacts:

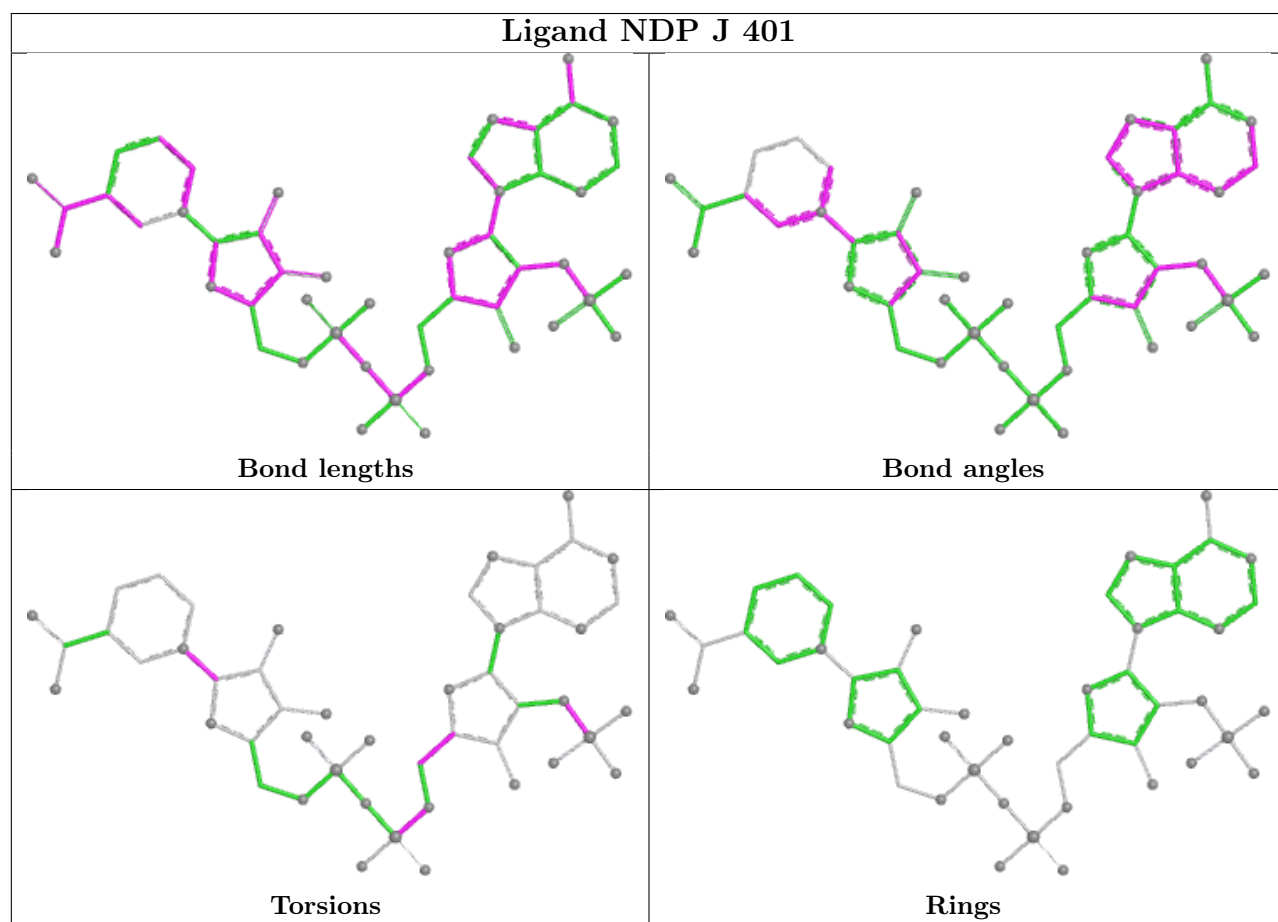
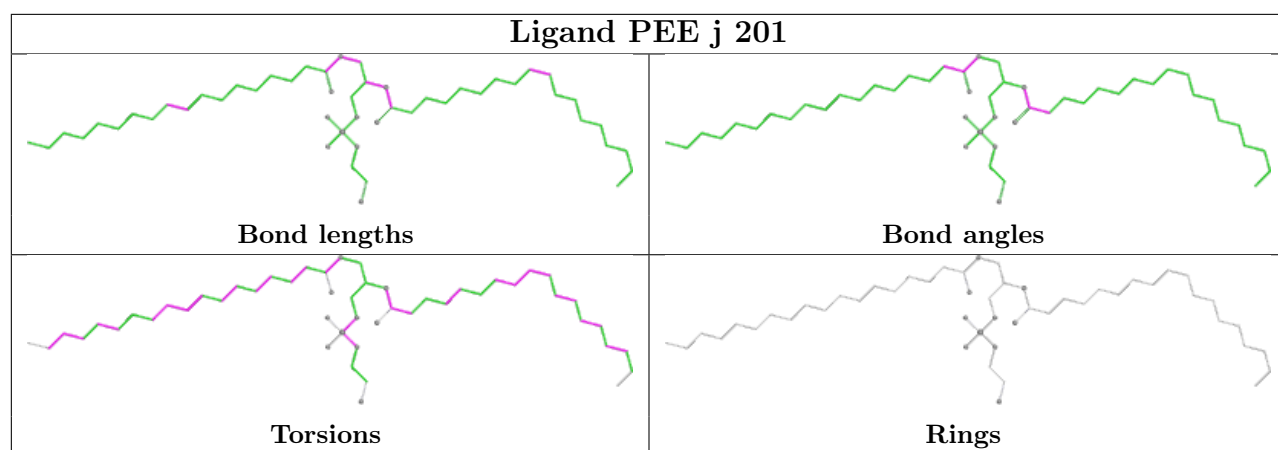
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	m	201	PEE	6	0
50	X	201	8Q1	2	0
46	A	502	FMN	2	0
56	s	401	UQ	5	0
54	r	504	CDL	7	0
49	l	701	PLX	3	0
48	j	201	PEE	6	0
51	J	401	NDP	2	0
54	N	201	CDL	1	0
45	A	501	SF4	2	0
49	r	502	PLX	3	0
45	C	301	SF4	1	0
54	a	201	CDL	9	0
49	g	201	PLX	2	0
54	i	401	CDL	4	0
57	w	401	ADP	1	0
47	A	503	NAI	3	0
49	C	303	PLX	5	0
48	i	402	PEE	4	0
48	r	501	PEE	5	0
48	C	302	PEE	3	0
50	G	201	8Q1	8	0
54	r	503	CDL	10	0
49	j	202	PLX	3	0
48	b	201	PEE	4	0
48	B	303	PEE	1	0
54	u	201	CDL	13	0

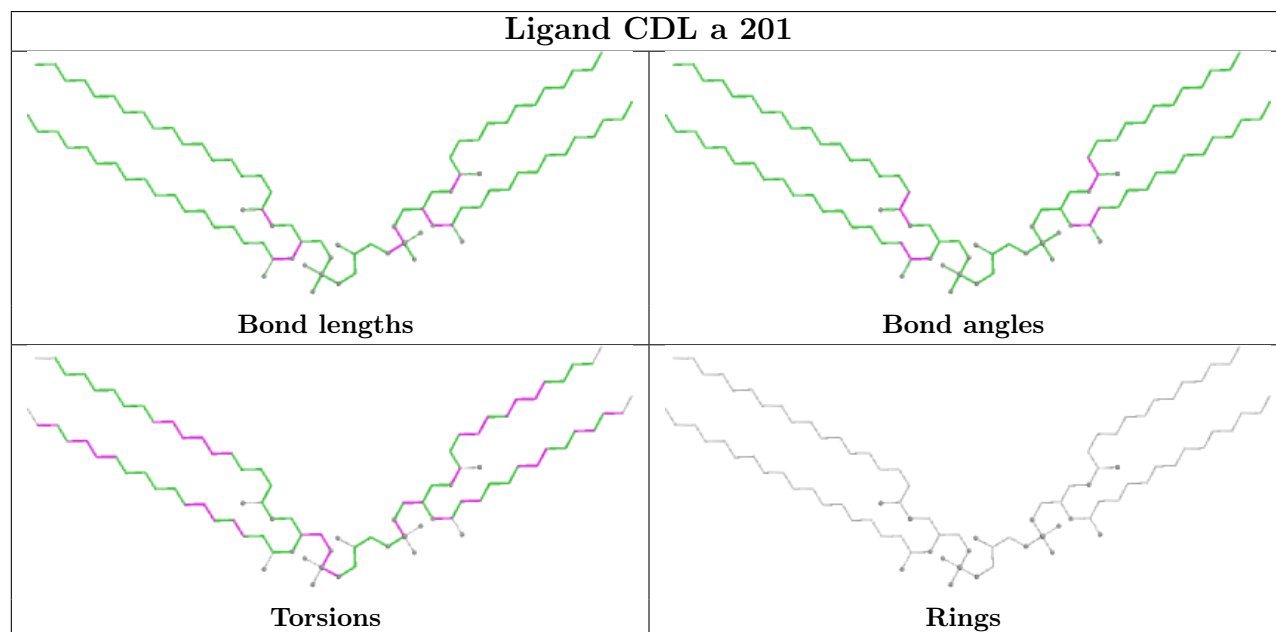
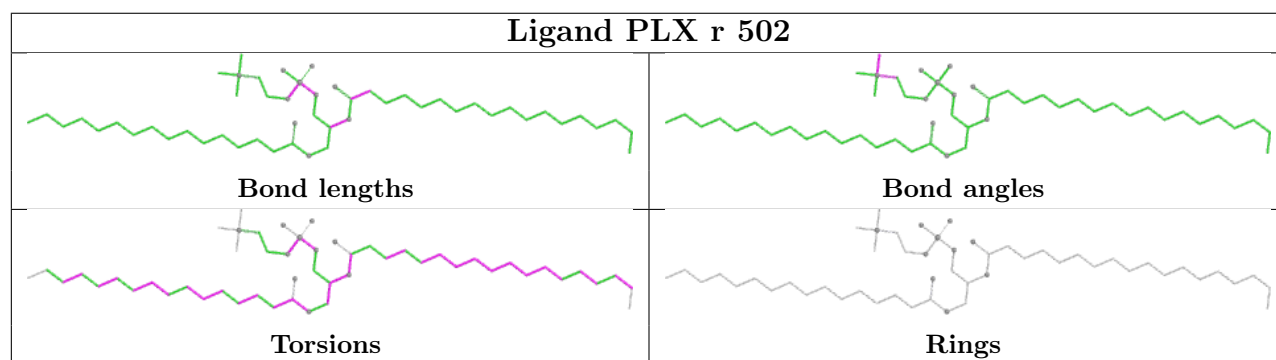
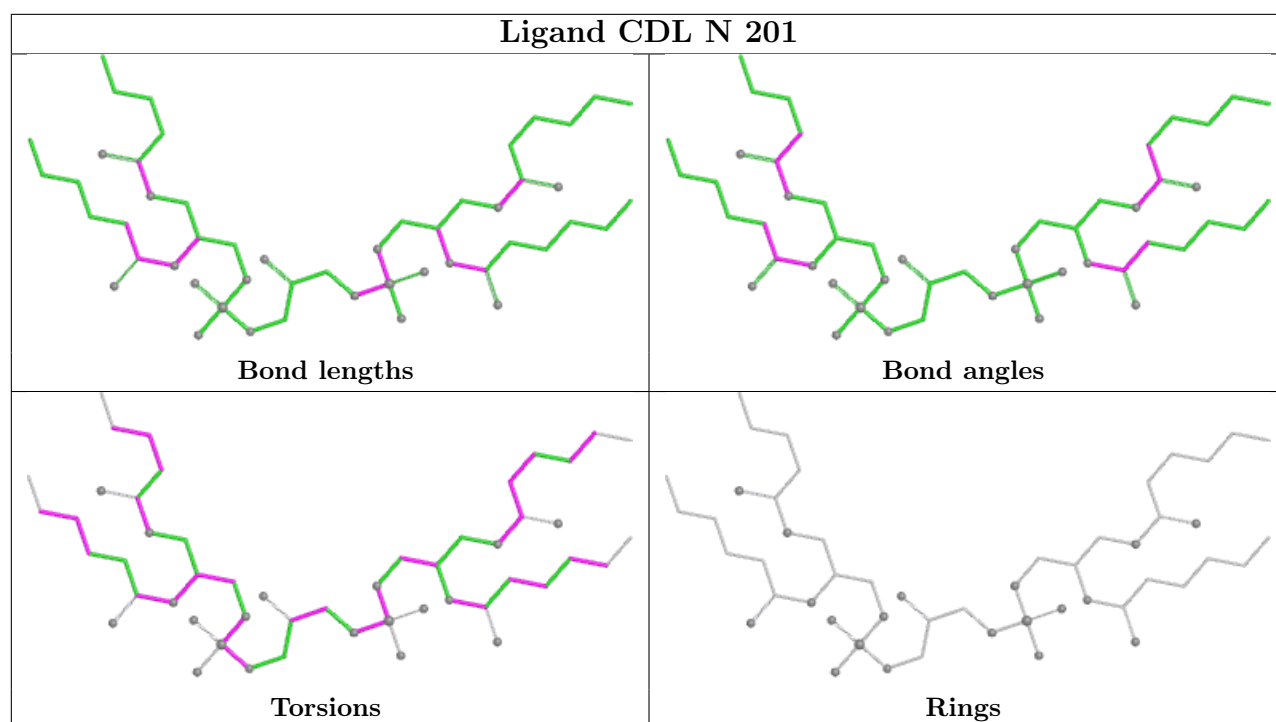
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

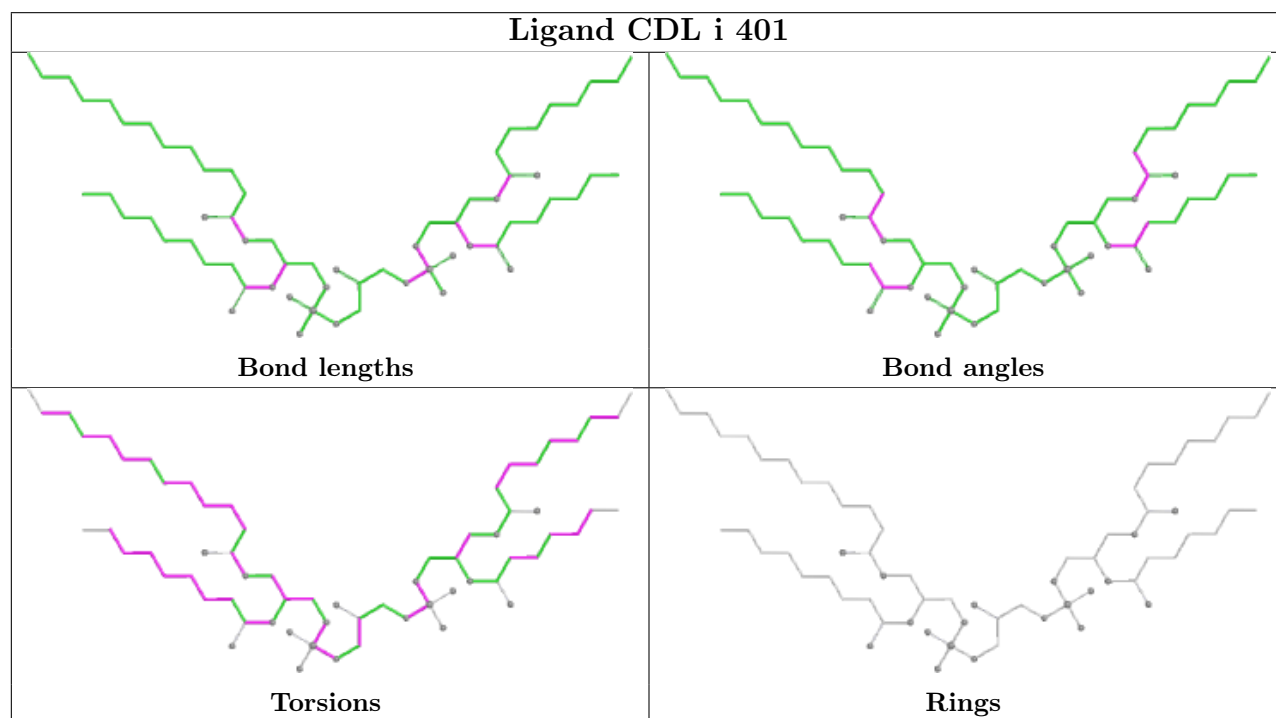


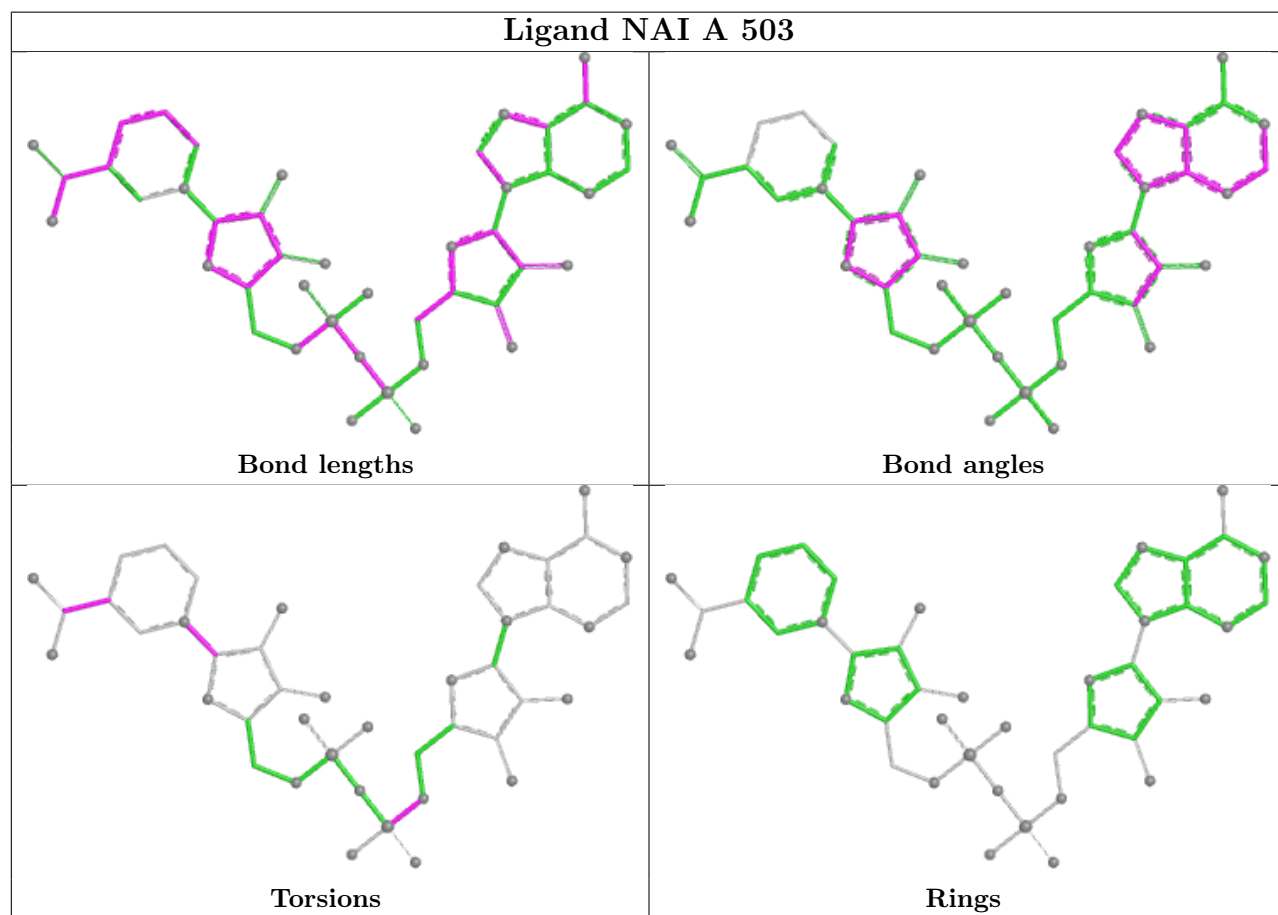
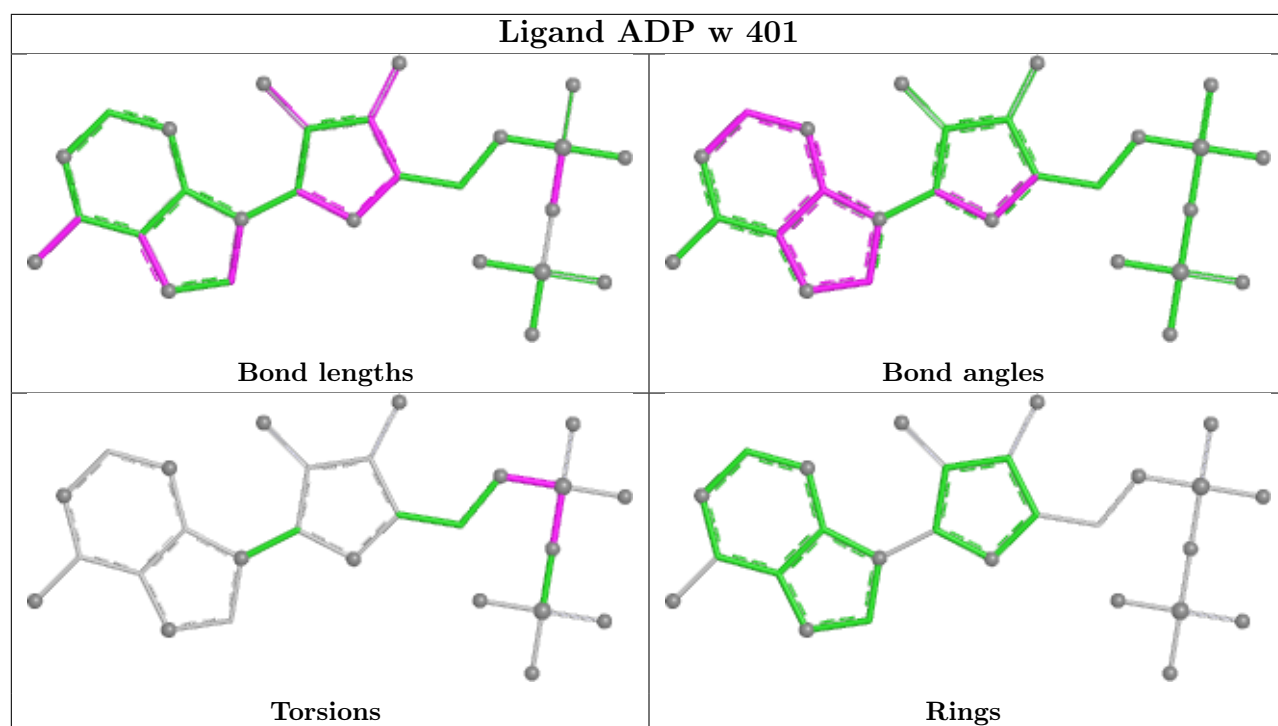


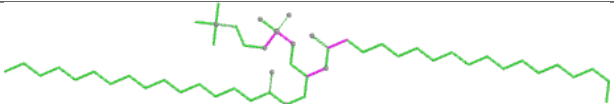
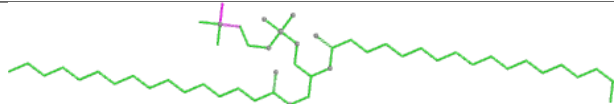
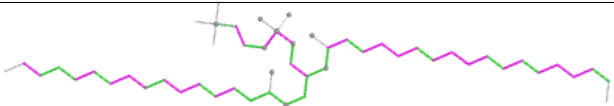
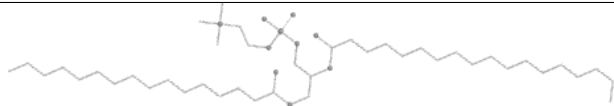


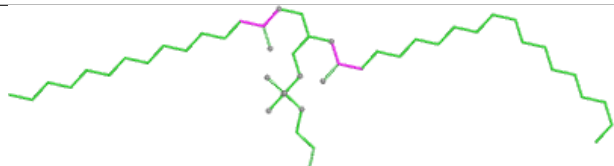
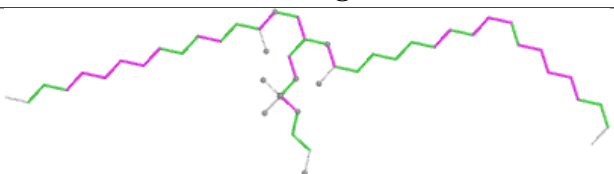
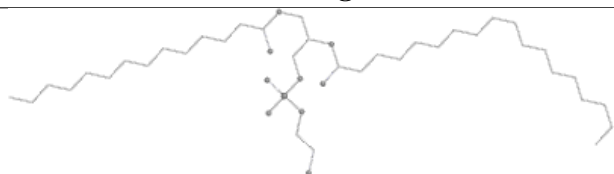


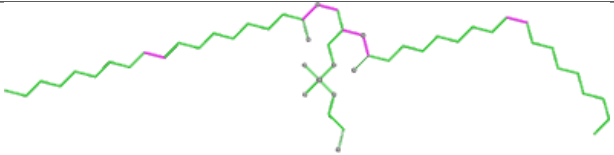
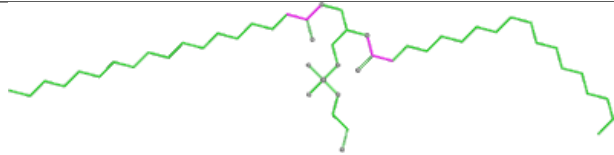
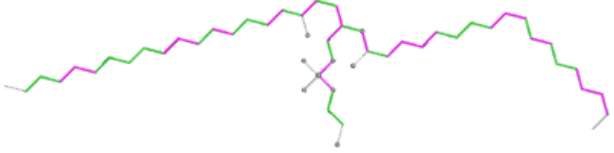
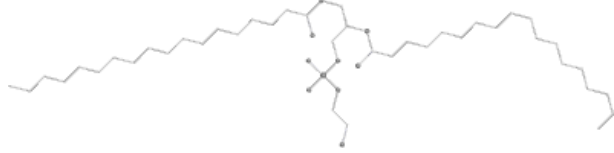


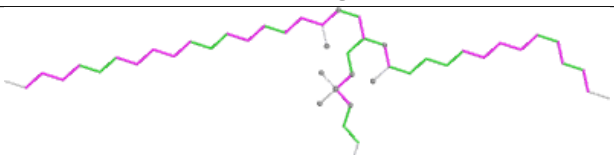
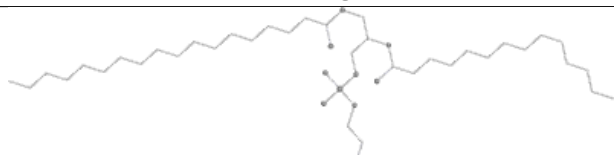


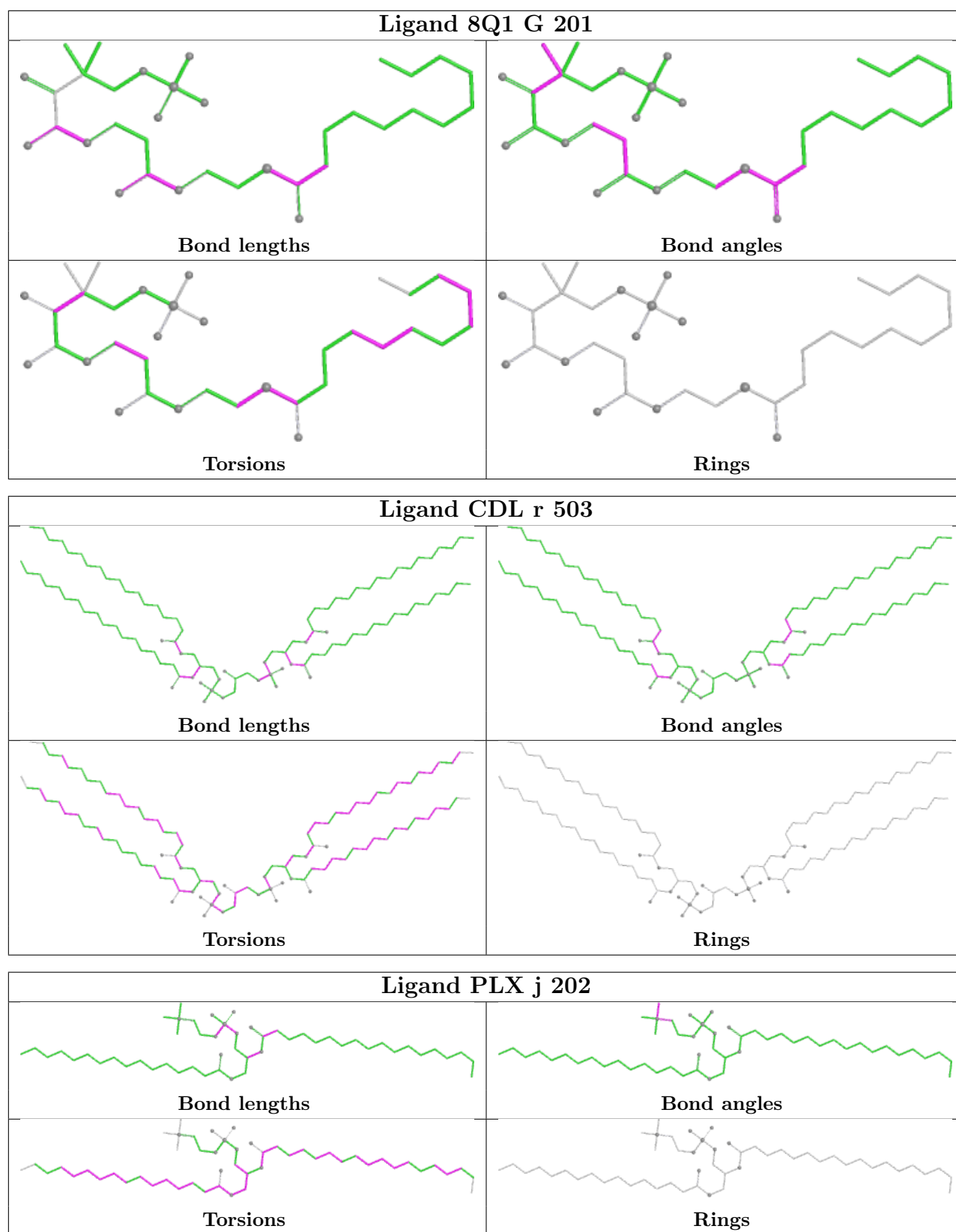


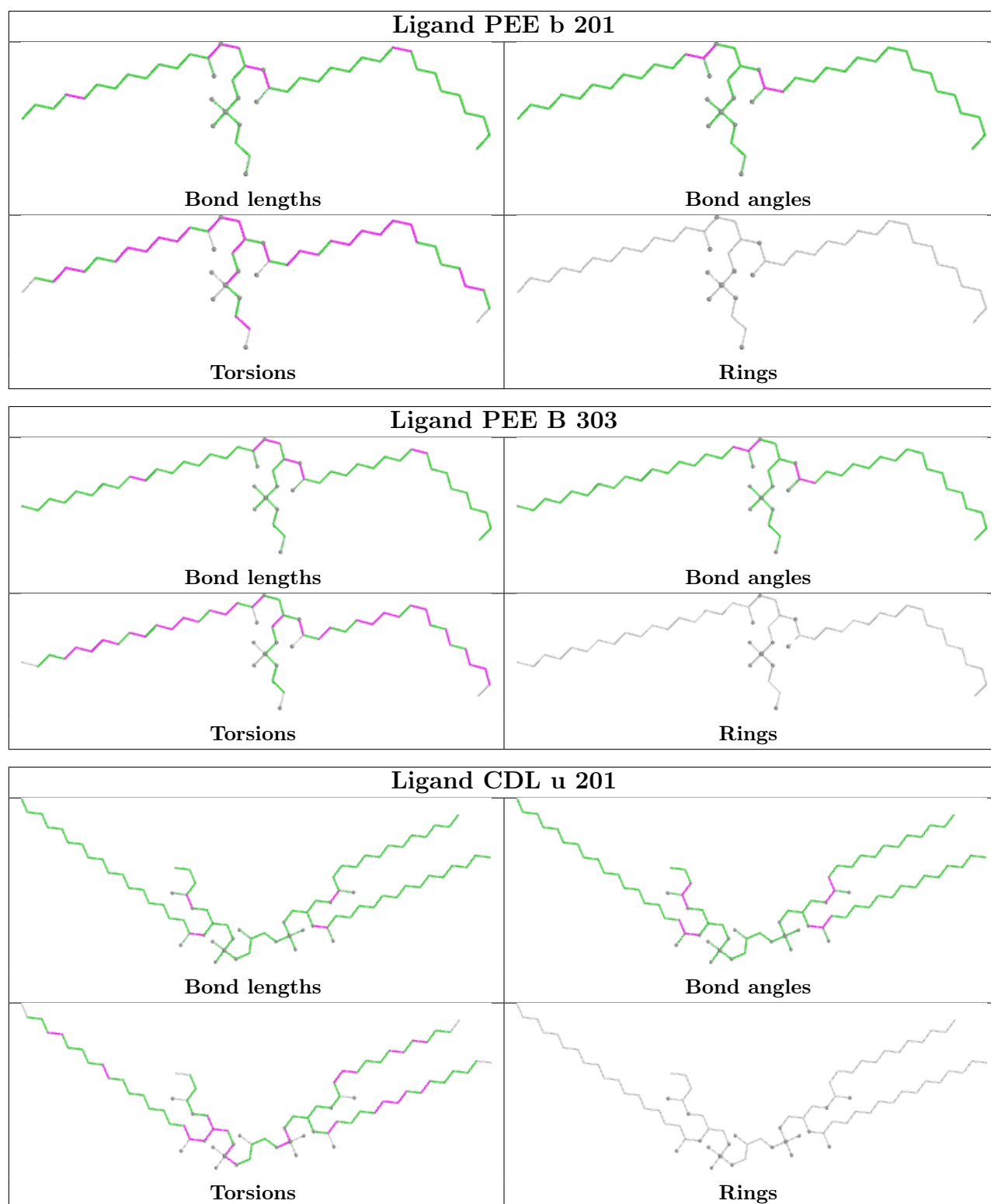
Ligand PLX C 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE i 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE r 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PEE C 302	
	
Bond lengths	Bond angles
	
Torsions	Rings





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

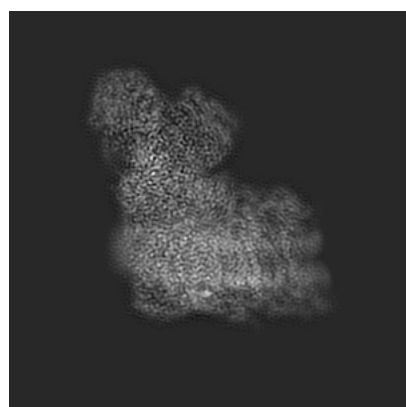
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32269. These allow visual inspection of the internal detail of the map and identification of artifacts.

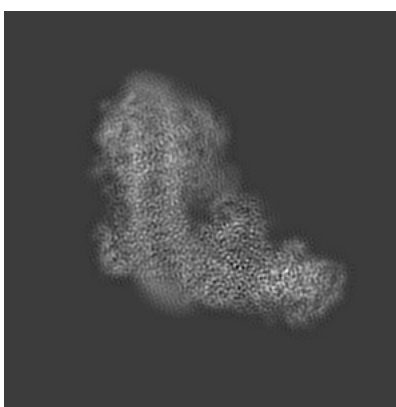
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

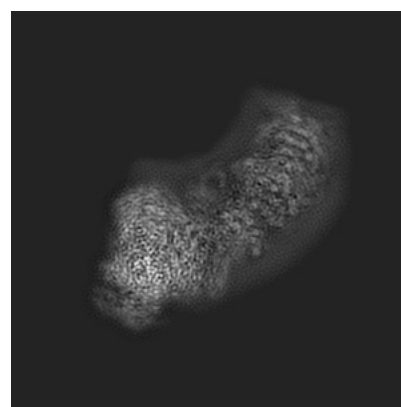
6.1.1 Primary map



X



Y

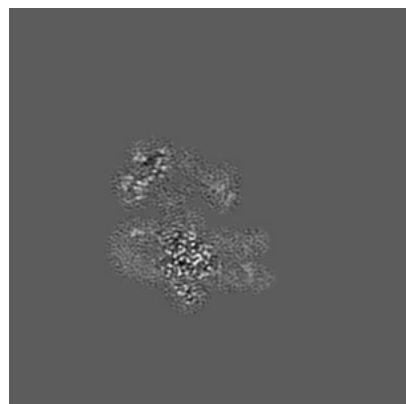


Z

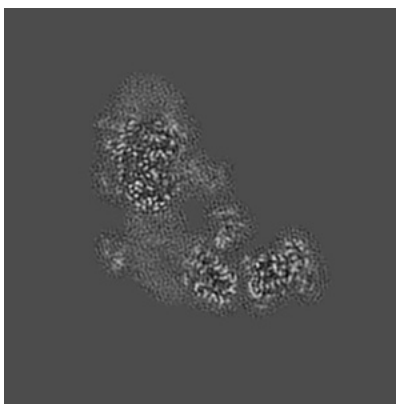
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

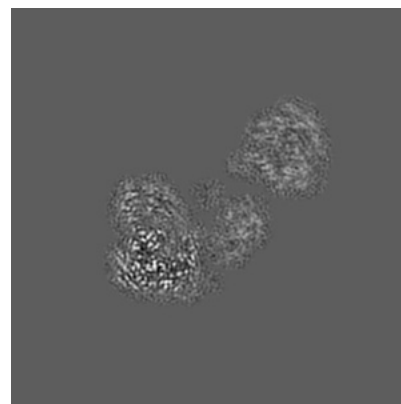
6.2.1 Primary map



X Index: 155



Y Index: 155

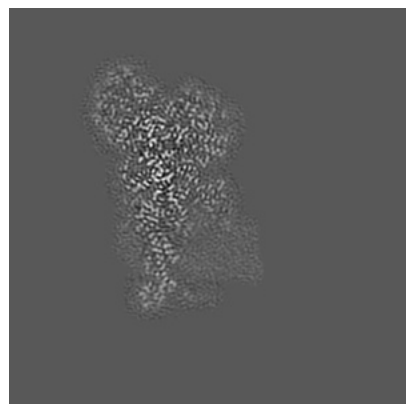


Z Index: 155

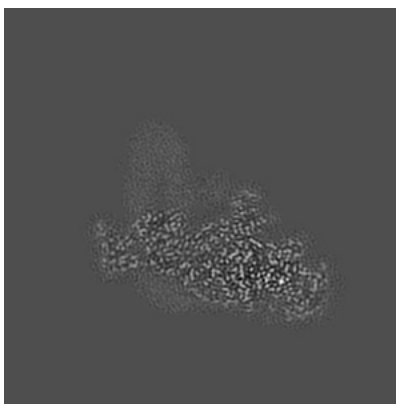
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

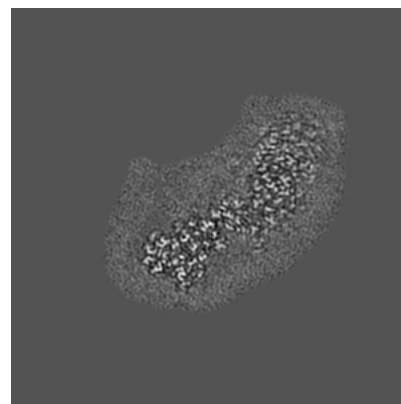
6.3.1 Primary map



X Index: 106



Y Index: 112

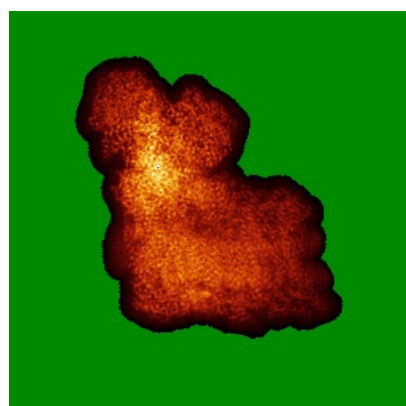


Z Index: 126

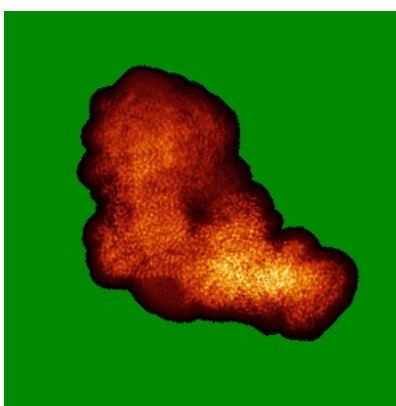
The images above show the largest variance slices of the map in three orthogonal directions.

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

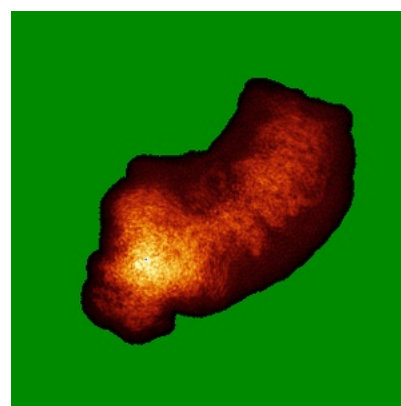
6.4.1 Primary map



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

This section was not generated.

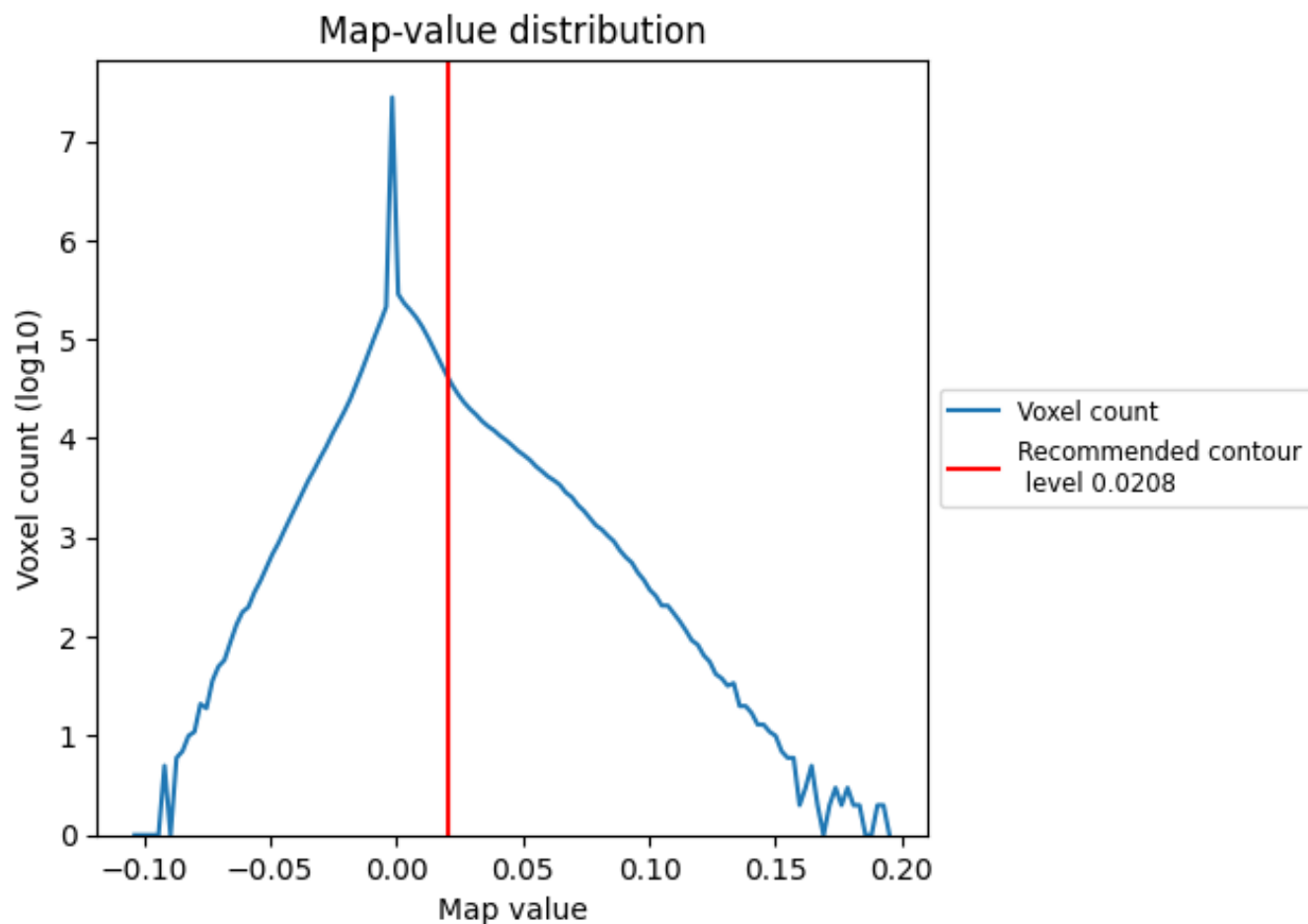
6.6 Mask visualisation

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

7 Map analysis [i](#)

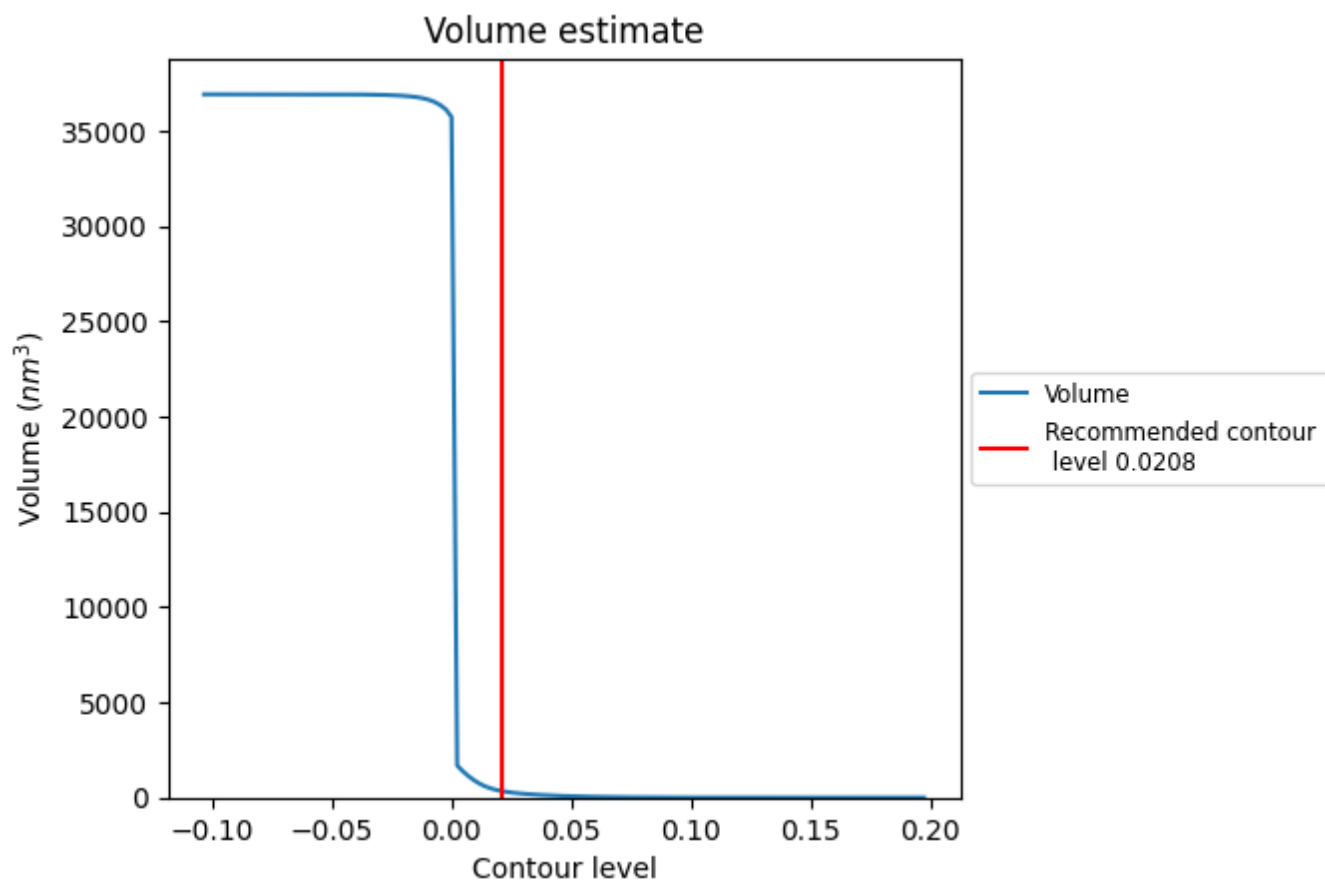
This section contains the results of statistical analysis of the map.

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.

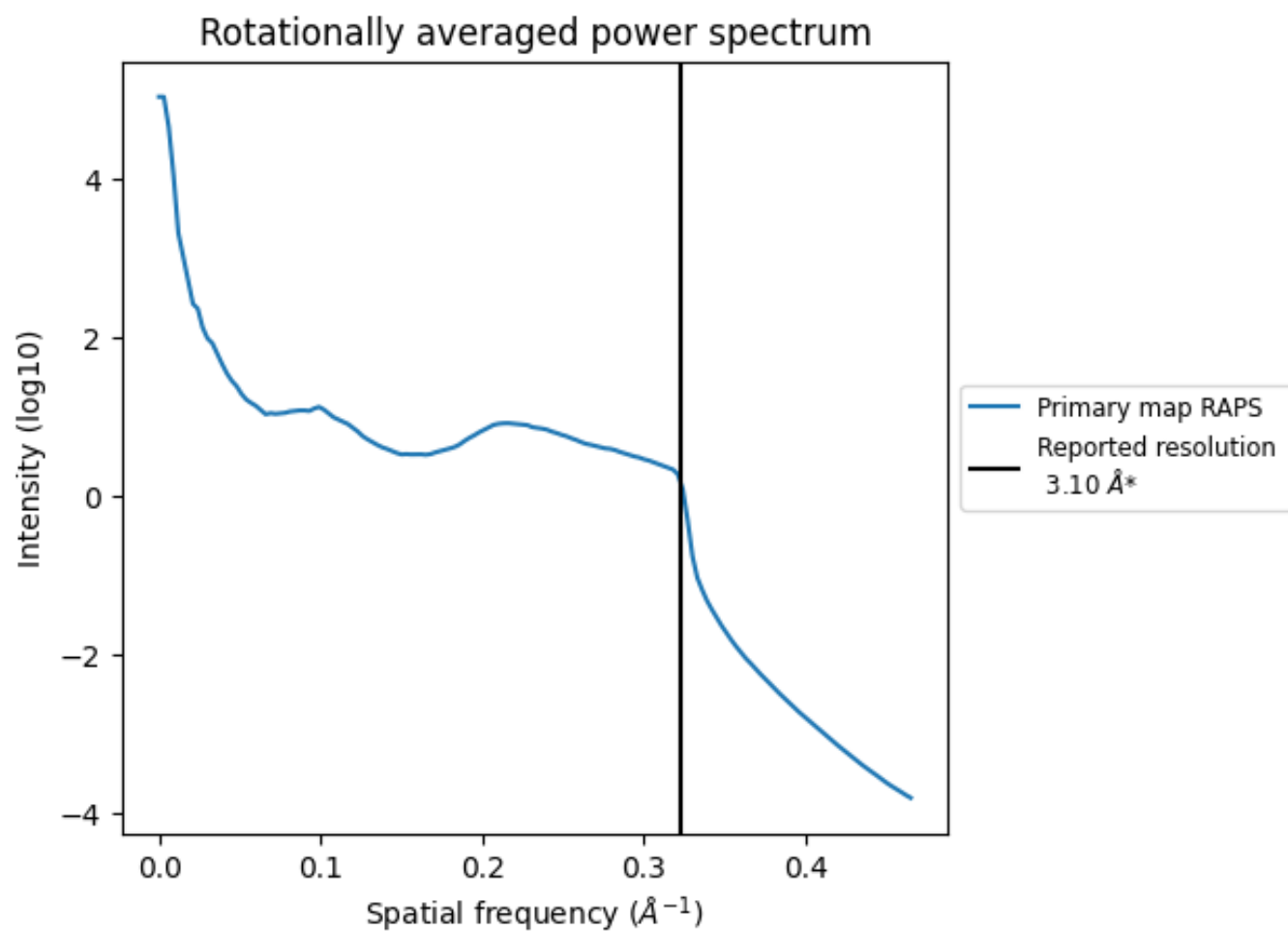
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 342 nm³; this corresponds to an approximate mass of 309 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation

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

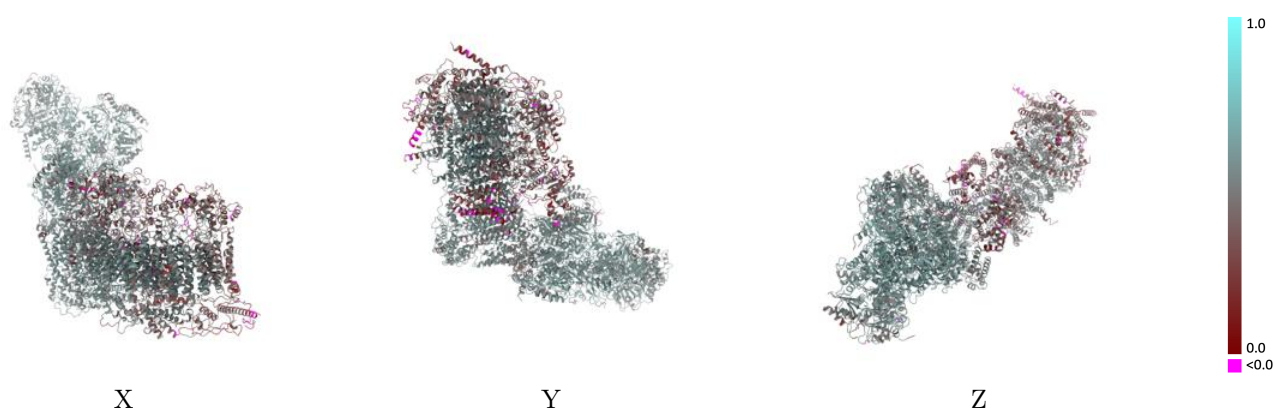
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32269 and PDB model 7W31. Per-residue inclusion information can be found in section 3 on page 20.

9.1 Map-model overlay [i](#)

This section was not generated.

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

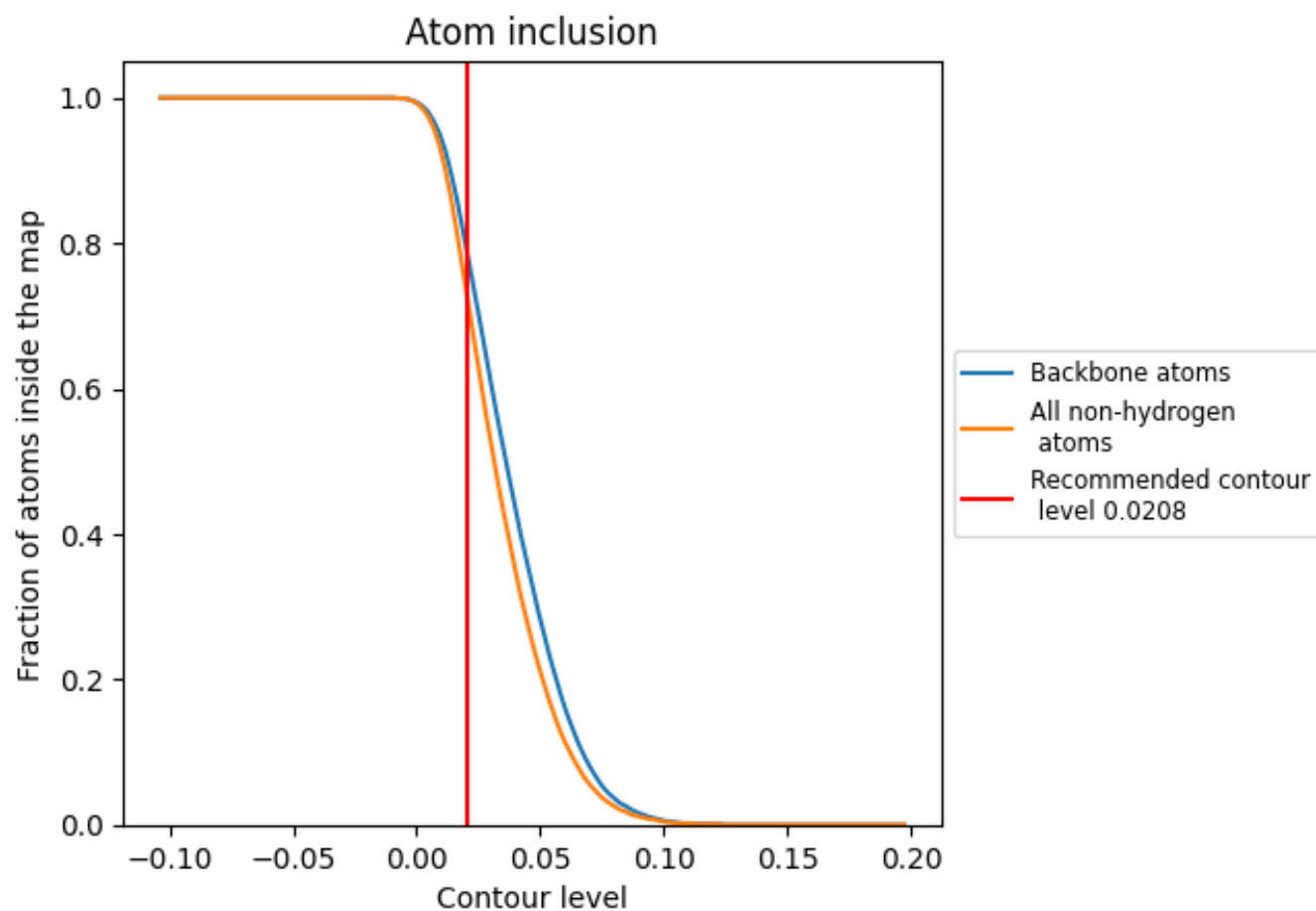


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.0208) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.5090
A	 0.8240	 0.5510
B	 0.9340	 0.6080
C	 0.8750	 0.5920
E	 0.7930	 0.5490
F	 0.7630	 0.5070
G	 0.4600	 0.3520
H	 0.7520	 0.5110
I	 0.7840	 0.5550
J	 0.7860	 0.5440
K	 0.7820	 0.5320
L	 0.8640	 0.5860
M	 0.8790	 0.5830
N	 0.7880	 0.5620
O	 0.7800	 0.5250
P	 0.9170	 0.6000
Q	 0.8290	 0.5750
S	 0.8660	 0.5730
T	 0.8020	 0.5770
U	 0.8160	 0.5400
V	 0.2410	 0.2310
W	 0.8290	 0.5550
X	 0.4400	 0.3530
Y	 0.3960	 0.3240
Z	 0.3270	 0.2910
a	 0.7170	 0.5120
b	 0.4470	 0.3450
c	 0.5670	 0.4260
d	 0.6390	 0.4550
e	 0.5710	 0.4470
f	 0.6080	 0.4500
g	 0.7840	 0.5360
h	 0.8230	 0.5640
i	 0.7760	 0.5470
j	 0.6830	 0.5020



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Chain	Atom inclusion	Q-score
k	 0.6500	 0.4750
l	 0.6300	 0.4850
m	 0.6820	 0.5010
n	 0.5840	 0.4480
o	 0.5600	 0.4180
p	 0.5370	 0.3970
r	 0.7660	 0.5470
s	 0.8370	 0.5600
u	 0.7960	 0.5460
v	 0.4120	 0.3250
w	 0.3310	 0.3590