



Full wwPDB EM Validation Report ⓘ

Mar 21, 2026 – 06:35 PM UTC

PDB ID : 7ARB / pdb_00007arb
EMDB ID : EMD-11878
Title : Cryo-EM structure of Arabidopsis thaliana Complex-I (complete composition)
Authors : Klusch, N.; Kuelbrandt, W.; Yildiz, O.
Deposited on : 2020-10-23
Resolution : 3.41 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

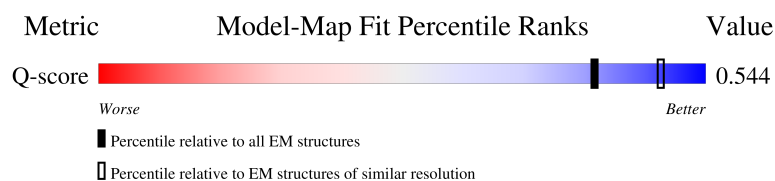
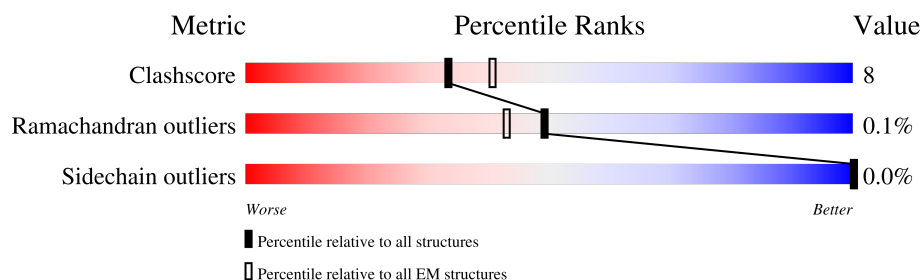
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.41 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	13997 (2.91 - 3.91)

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	119	10% 57% 20% 23%
2	B	218	55% 17% 28%
3	C	190	74% 23% .
4	D	394	76% 21% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	255	
6	F	486	
7	G	748	
8	H	325	
9	I	222	
10	J	205	
11	K	100	
12	L	669	
13	M	495	
14	N	499	
15	O	159	
16	P	402	
17	Q	154	
18	R	110	
19	S	97	
20	T	122	
21	U	126	
22	V	169	
23	W	133	
24	X	106	
25	Z	143	
26	a	65	
27	b	65	
28	c	88	
29	d	81	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	e	83	
31	f	106	
32	g	114	
33	i	98	
34	j	69	
35	k	72	
36	l	125	
37	m	71	
38	n	117	
39	o	103	
40	p	106	
41	q	159	
42	r	131	
43	u	30	
44	v	113	
45	x	256	
46	y	278	
47	z	275	

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
48	SF4	F	501	-	-	X	-
50	FES	E	500	-	-	X	-

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 61765 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-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	92	Total	C	N	O	S	0	0
			779	553	105	117	4		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1244	797	218	215	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	185	Total	C	N	O	S	0	0
			1581	1021	271	283	6		

- Molecule 4 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	385	Total	C	N	O	S	0	0
			3077	1954	542	557	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	363	SER	LEU	variant	UNP A0A2P2CLH2

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	192	Total	C	N	O	S	0	0
			1500	954	248	287	11		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	434	Total	C	N	O	S	0	0
			3368	2125	600	618	25		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5252	3291	921	1001	39		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	311	Total	C	N	O	S	0	0
			2439	1659	372	393	15		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	165	Total	C	N	O	S	0	0
			1349	849	229	261	10		

- Molecule 10 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	147	Total	C	N	O	S	0	0
			1162	784	179	191	8		

- Molecule 11 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	90	Total	C	N	O	S	0	0
			707	476	109	115	7		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	615	Total	C	N	O	S	0	0
			4807	3191	748	832	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP B5TM94

- Molecule 13 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	487	Total	C	N	O	S	0	0
			3887	2627	601	636	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	326	LEU	PRO	conflict	UNP B5TM93

- Molecule 14 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	488	Total	C	N	O	S	0	0
			3820	2573	577	642	28		

- Molecule 15 is a protein called AT3G07480.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	122	Total	C	N	O	S	0	0
			956	598	169	185	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	332	Total	C	N	O	S	0	0
			2560	1643	439	463	15		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	119	Total	C	N	O	S	0	0
			939	600	163	175	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	62	Total	C	N	O	S	0	0
			482	304	84	89	5		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	93	Total	C	N	O	S	0	0
			727	459	129	133	6		

- Molecule 20 is a protein called Acyl carrier protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	84	Total	C	N	O	S	0	0
			667	421	105	138	3		

- Molecule 21 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	83	Total	C	N	O	S	0	0
			650	411	103	135	1		

- Molecule 22 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	140	Total	C	N	O	S	0	0
			1123	712	187	219	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	112	Total	C	N	O	S	0	0
			904	578	161	162	3		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	97	Total	C	N	O	S	0	0
			767	480	132	143	12		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	125	Total	C	N	O	S	0	0
			997	640	175	177	5		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	58	Total	C	N	O	S	0	0
			469	302	84	78	5		

- Molecule 27 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	40	Total	C	N	O	S	0	0
			295	195	48	49	3		

- Molecule 28 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	76	Total	C	N	O	S	0	0
			617	396	115	100	6		

- Molecule 29 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	65	Total	C	N	O	S	0	0
			557	344	106	100	7		

- Molecule 31 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	101	Total	C	N	O	S	0	0
			763	490	126	142	5		

- Molecule 32 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	75	Total	C	N	O	S	0	0
			615	396	107	109	3		

- Molecule 33 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	85	Total	C	N	O	S	0	0
			737	466	135	131	5		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	51	Total	C	N	O	S	0	0
			415	275	73	64	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	47	Total	C	N	O	S	0	0
			374	238	71	62	3		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	66	Total	C	N	O	S	0	0
			502	328	80	93	1		

- Molecule 37 is a protein called B15 – 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	70	Total	C	N	O	S	0	0
			577	370	107	98	2		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	109	Total	C	N	O	S	0	0
			911	580	170	160	1		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	80	Total	C	N	O	S	0	0
			657	413	115	119	10		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	93	Total	C	N	O	S	0	0
			778	493	144	137	4		

- Molecule 41 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	q	65	Total	C	N	O	0	0
			536	342	95	99		

- Molecule 42 is a protein called Furry.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	r	10	Total	C	N	O	0	0
			89	56	18	15		

- Molecule 43 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	u	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 44 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	v	30	Total	C	N	O	0	0
			226	147	39	40		

- Molecule 45 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	214	Total	C	N	O	S	0	0
			1659	1063	285	306	5		

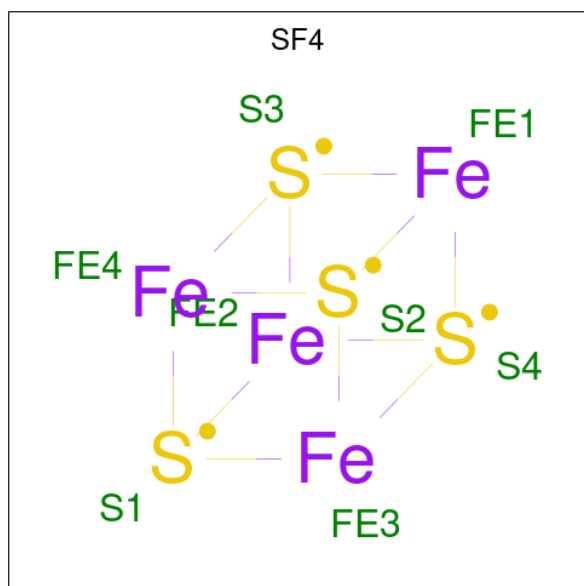
- Molecule 46 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	268	Total	C	N	O	S	0	0
			2032	1271	363	391	7		

- Molecule 47 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	233	Total	C	N	O	S	0	0
			1772	1111	325	330	6		

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



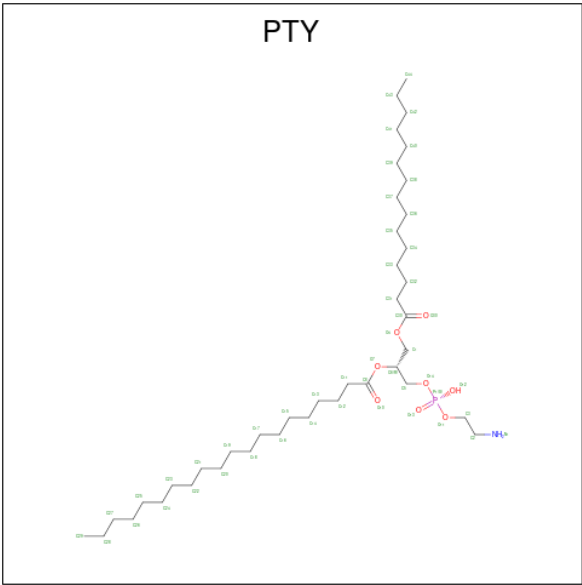
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	F	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

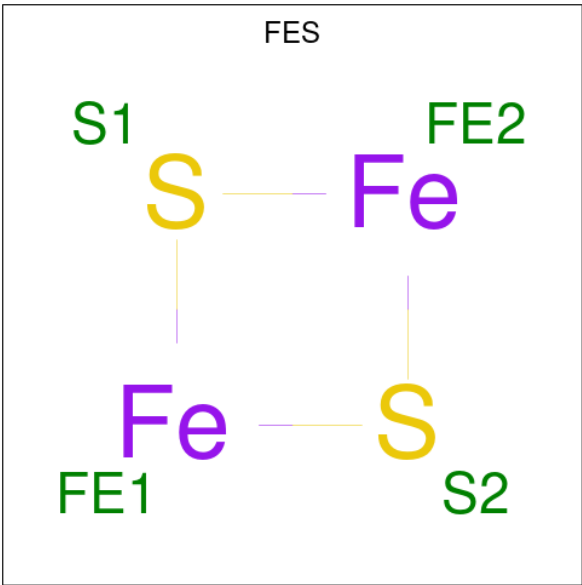
Mol	Chain	Residues	Atoms			AltConf
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



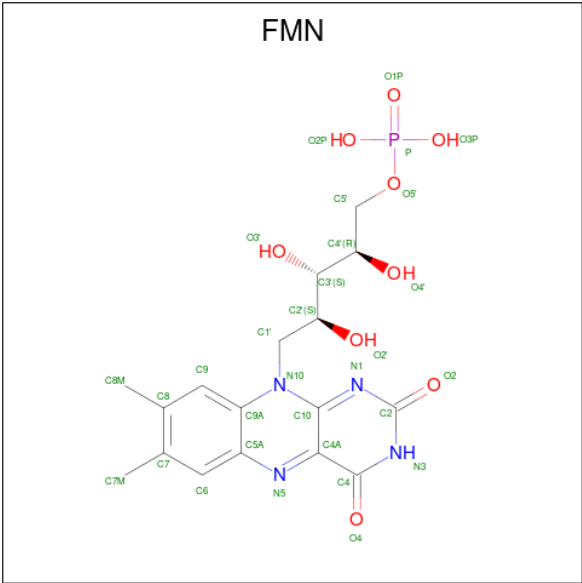
Mol	Chain	Residues	Atoms					AltConf
49	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
49	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
49	N	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



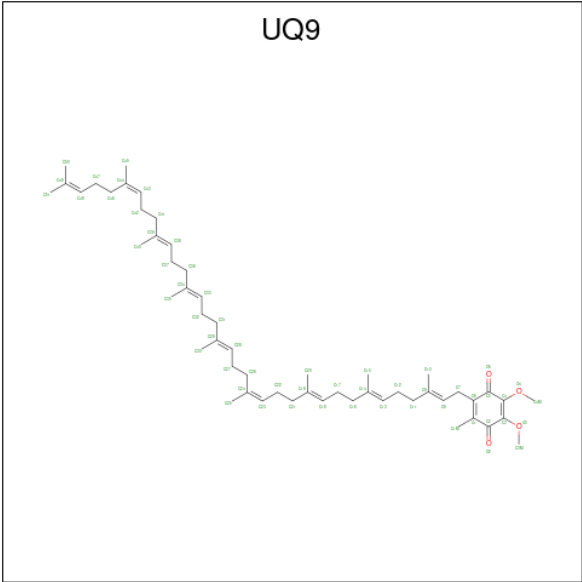
Mol	Chain	Residues	Atoms			AltConf
50	E	1	Total	Fe	S	0
			4	2	2	
50	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 51 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



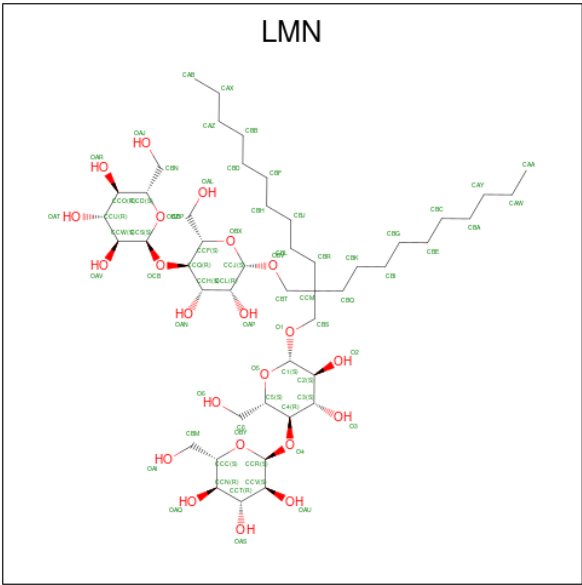
Mol	Chain	Residues	Atoms					AltConf
51	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 52 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$).



Mol	Chain	Residues	Atoms			AltConf
52	H	1	Total	C	O	0
			35	31	4	

- Molecule 53 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).

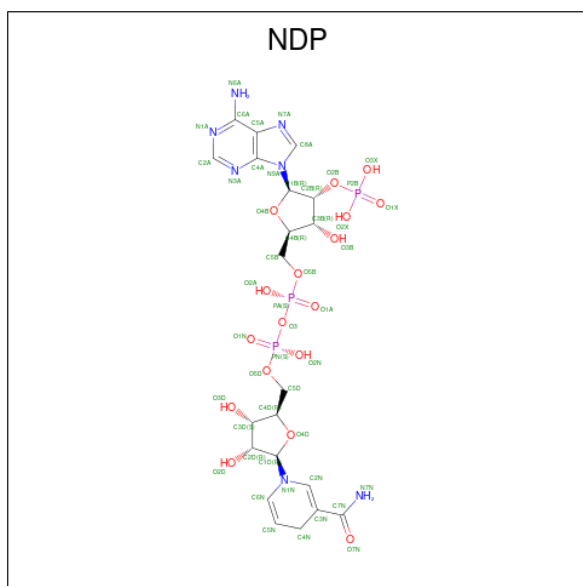


Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	C	O	0
			69	47	22	

- Molecule 54 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
54	O	1	Total	Fe	0
			1	1	

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					AltConf
55	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	R	1	Total	Zn	0
			1	1	
56	y	1	Total	Zn	0
			1	1	

- Molecule 57 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



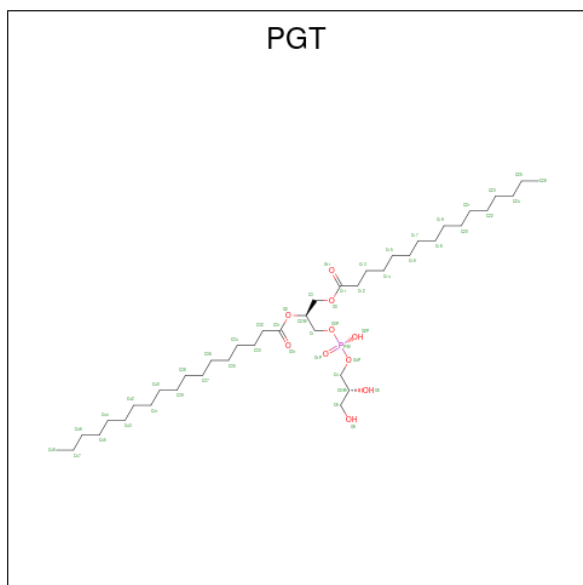
- Molecule 58 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: C₄₂H₈₅NO₈P).

Continued on next page...

Continued from previous page...

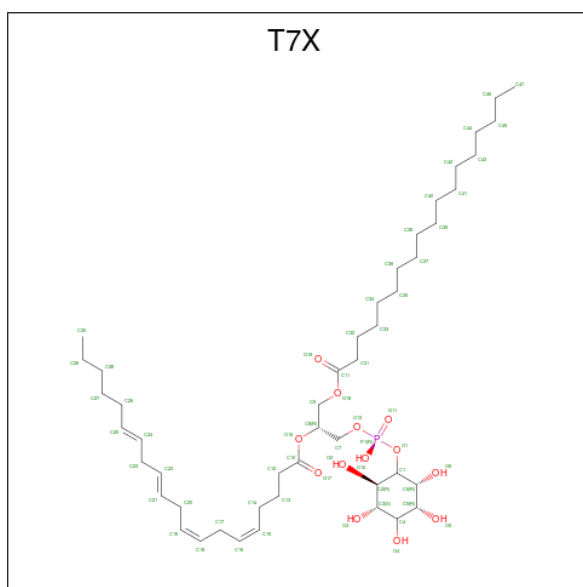
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	v	1	52	42	1	8	1	0

- Molecule 59 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



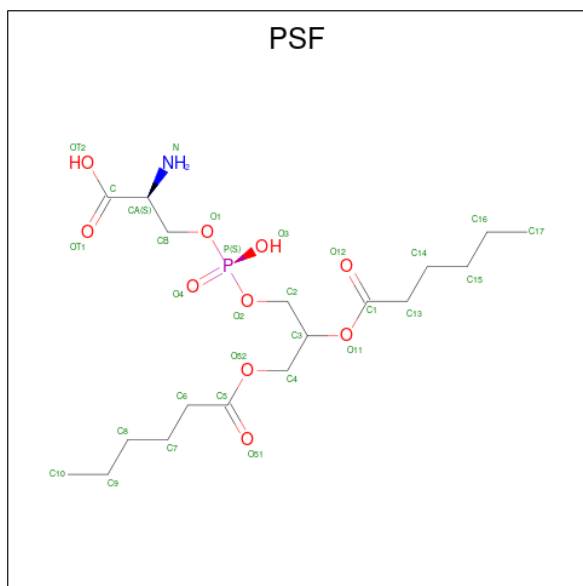
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
59	f	1	41	30	10	1	0

- Molecule 60 is Phosphatidylinositol (CCD ID: T7X) (formula: C₄₇H₈₃O₁₃P).

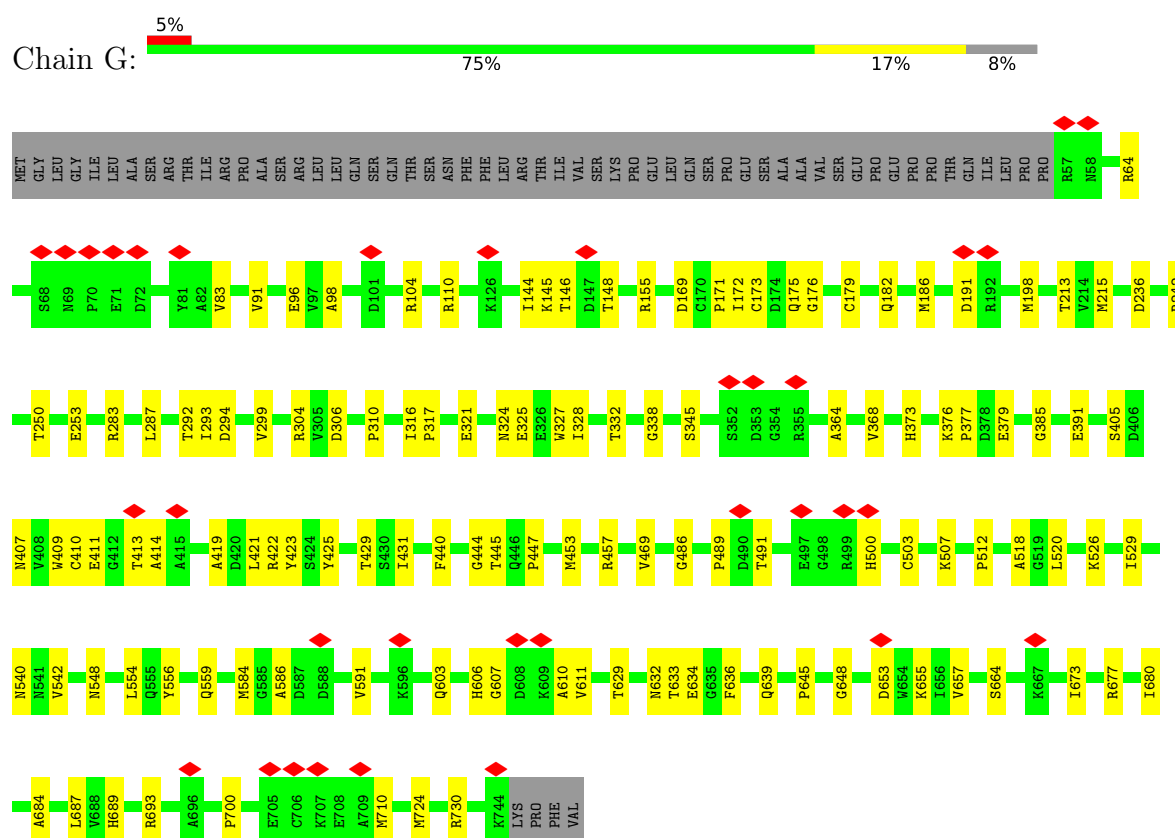


Mol	Chain	Residues	Atoms				AltConf
60	f	1	Total	C	O	P	0
			61	47	13	1	

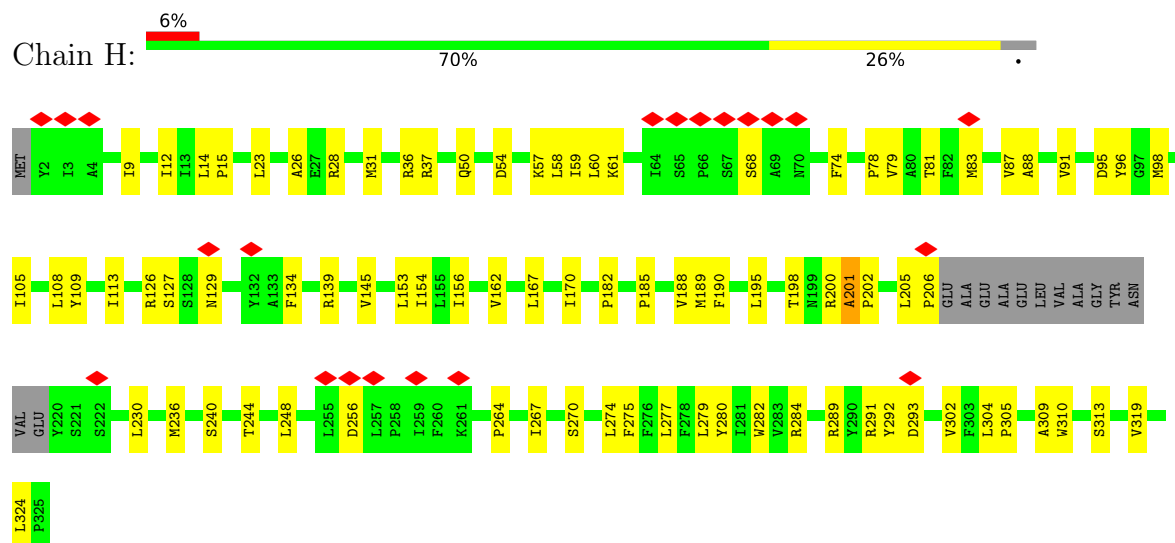
- Molecule 61 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (CCD ID: PSF) (formula: $C_{18}H_{34}NO_{10}P$).



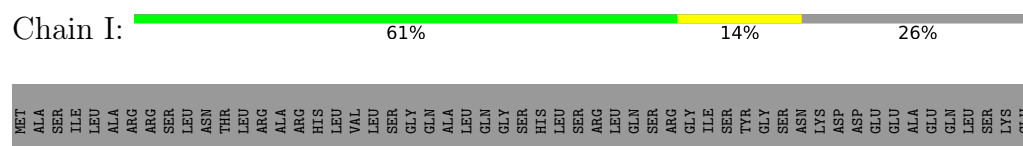
Mol	Chain	Residues	Atoms					AltConf
61	z	1	Total	C	N	O	P	0
			30	18	1	10	1	

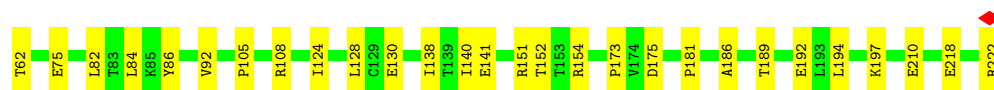


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

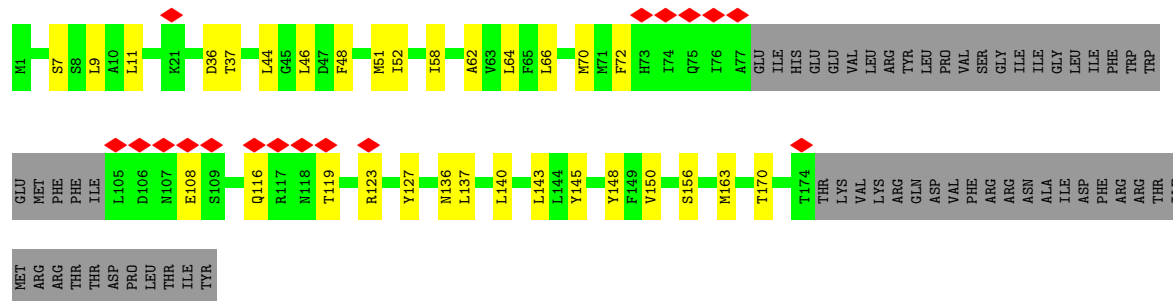


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial

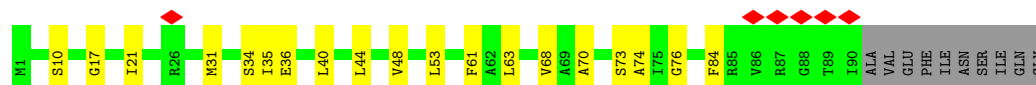
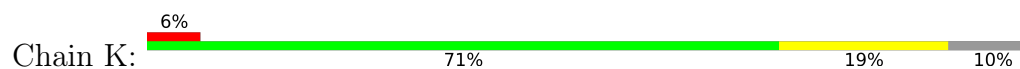




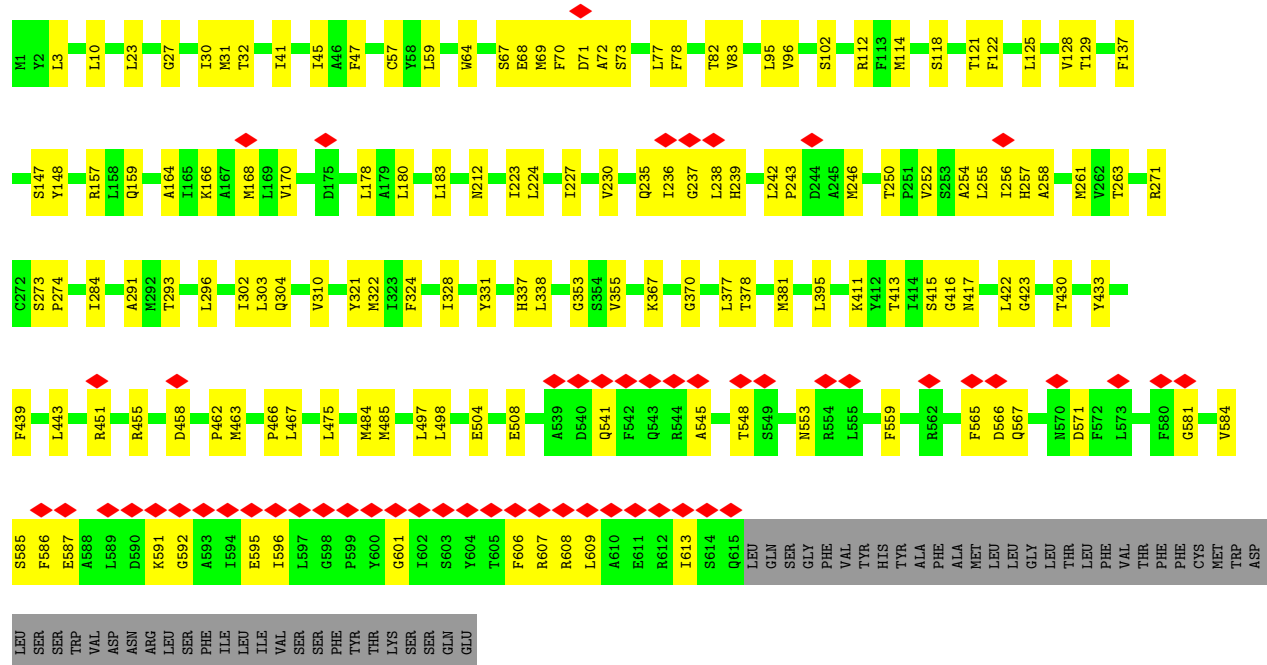
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



• Molecule 11: NADH dehydrogenase subunit 4L

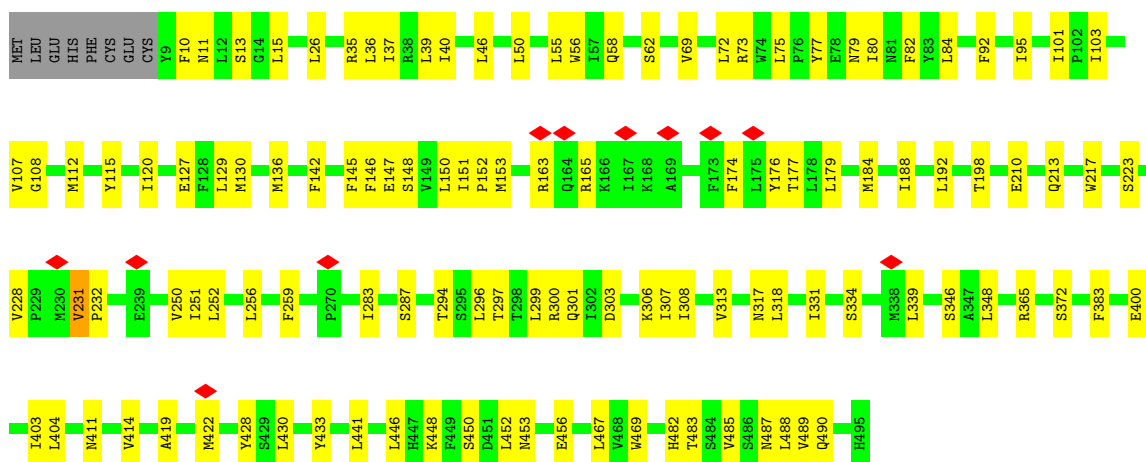


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



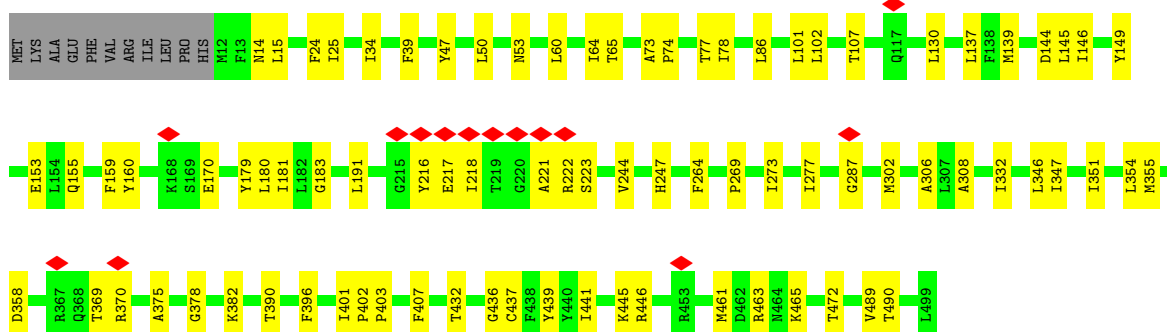
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 



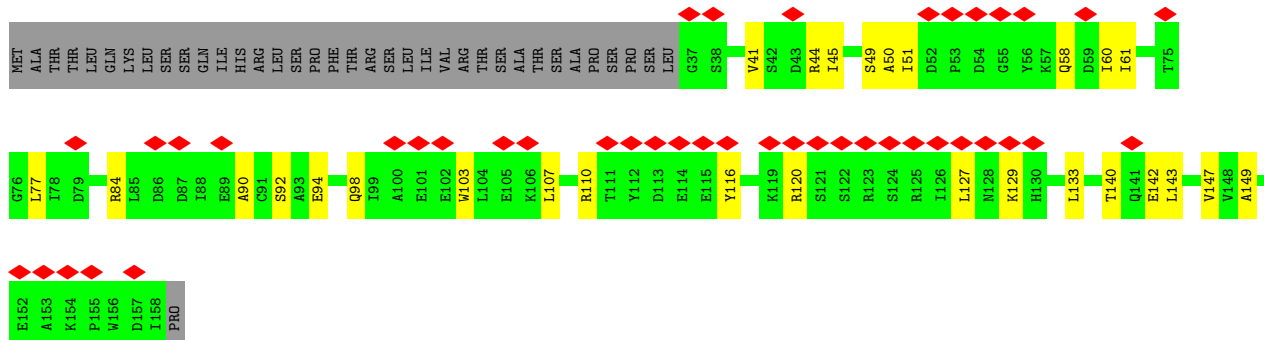
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 



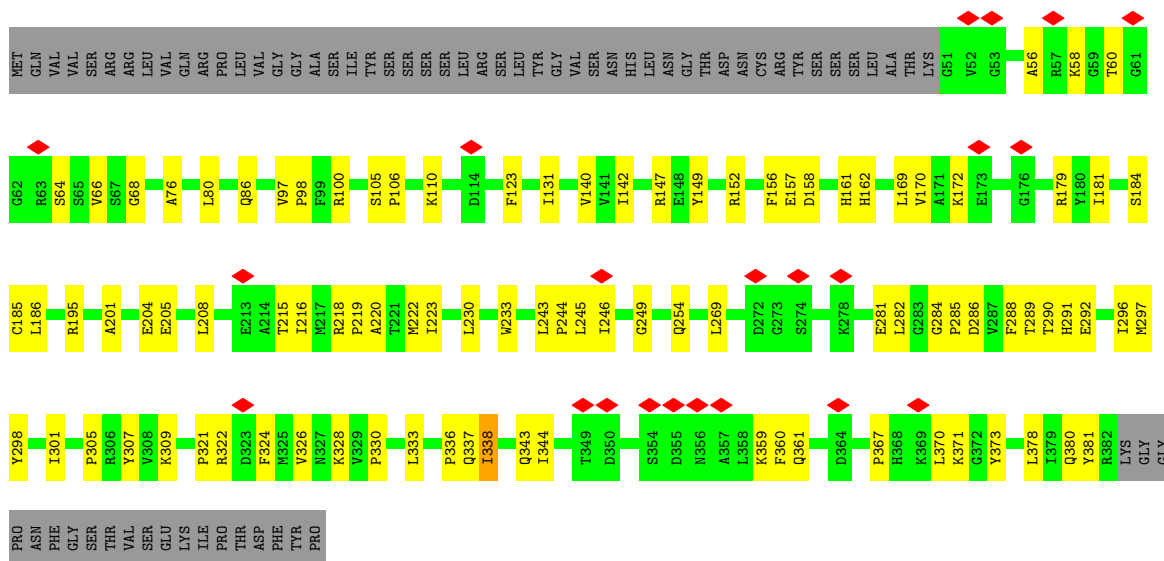
• Molecule 15: AT3G07480.1

Chain O: 

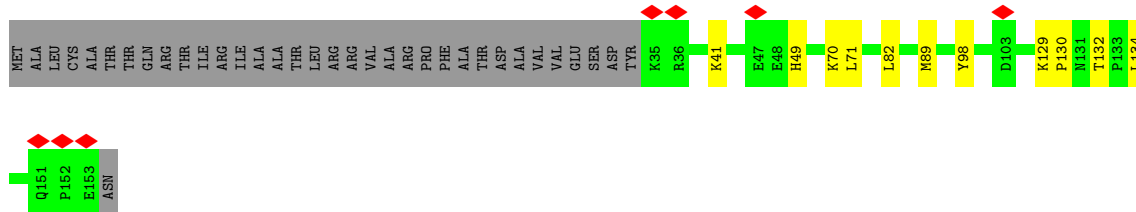


• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

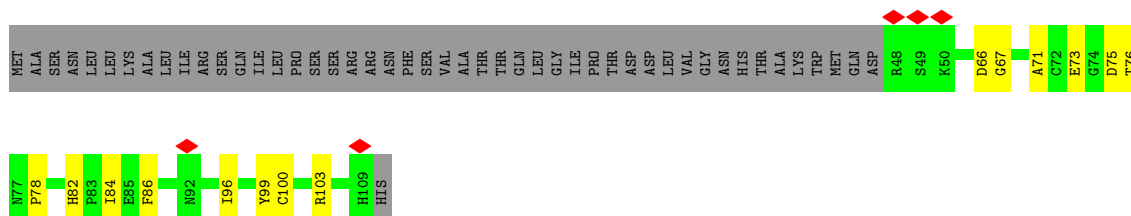
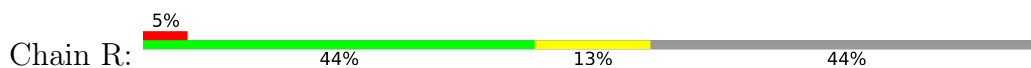
Chain P: 



- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

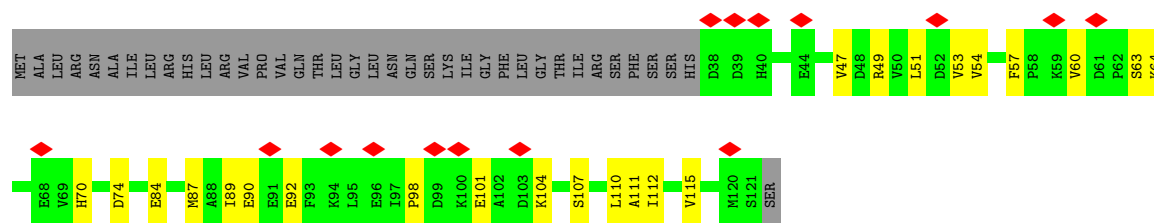


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

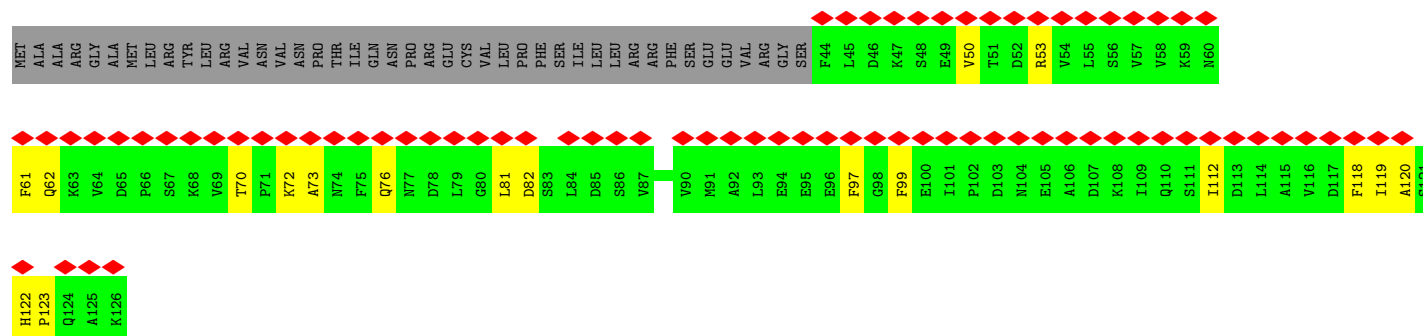


- Molecule 20: Acyl carrier protein 1, mitochondrial

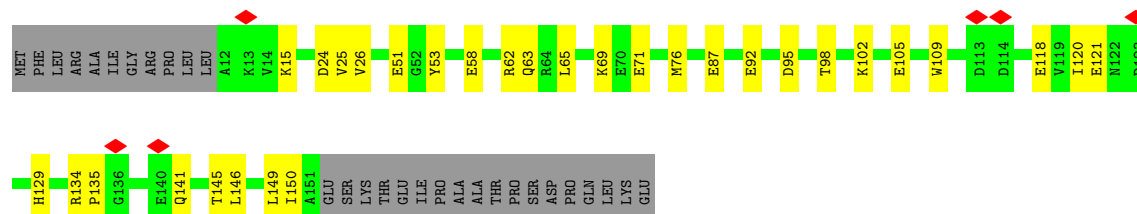




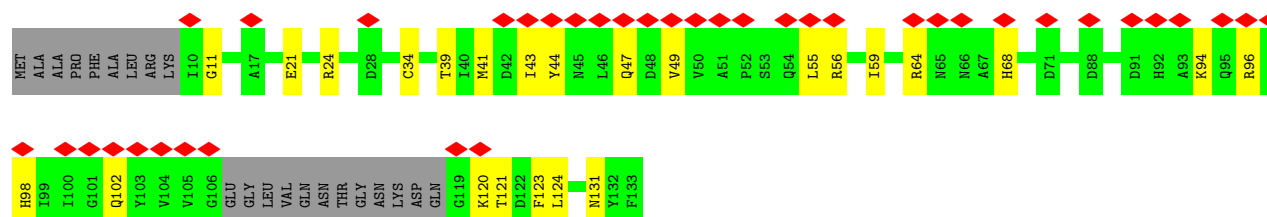
- Molecule 21: Acyl carrier protein 2, mitochondrial



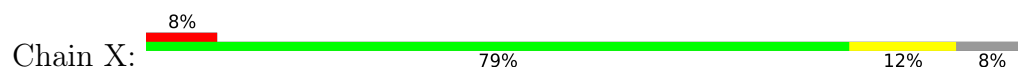
- Molecule 22: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial

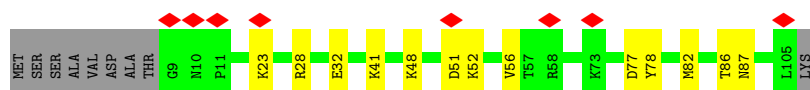


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

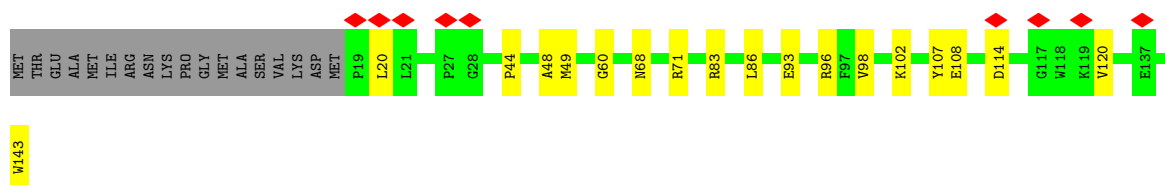
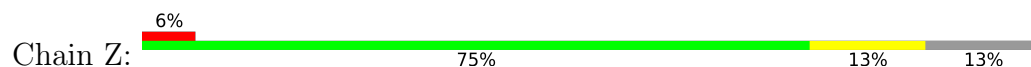


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B





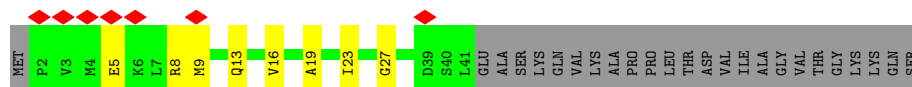
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



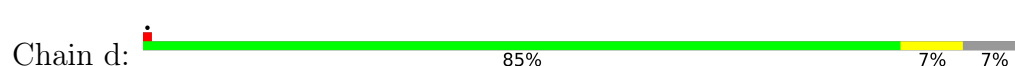
- Molecule 27: At2g46540/F11C10.23



- Molecule 28: Transmembrane protein

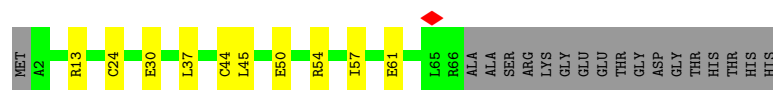


- Molecule 29: Excitatory amino acid transporter

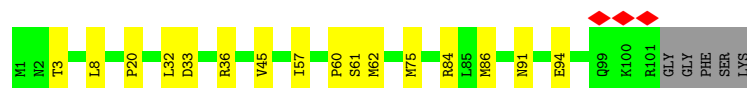
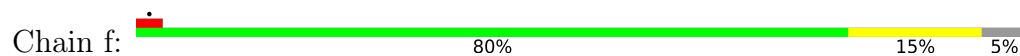


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B

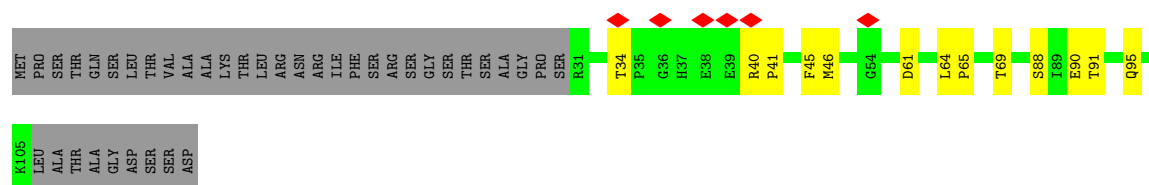




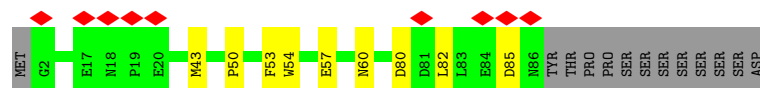
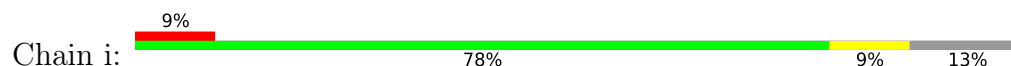
- Molecule 31: At4g16450



- Molecule 32: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein



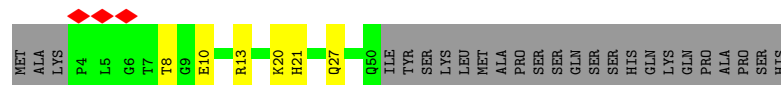
- Molecule 33: P1



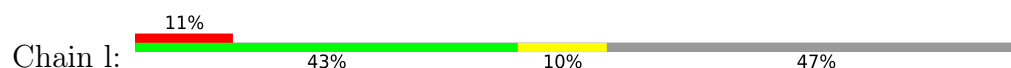
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2

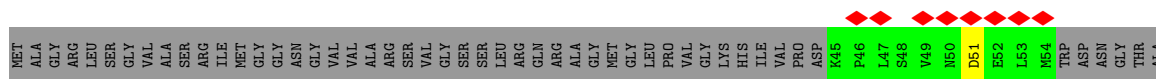


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A

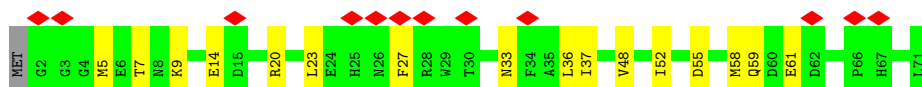
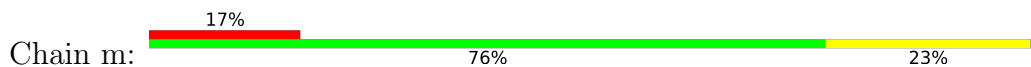


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

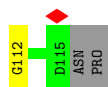




- Molecule 37: B15 – 1 beta subcomplex subunit 4



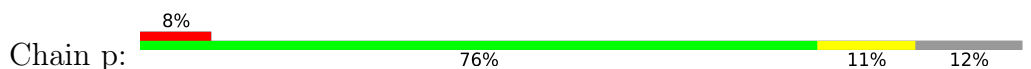
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



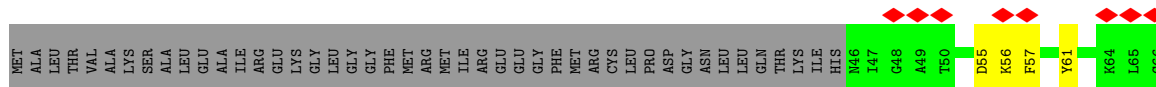
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



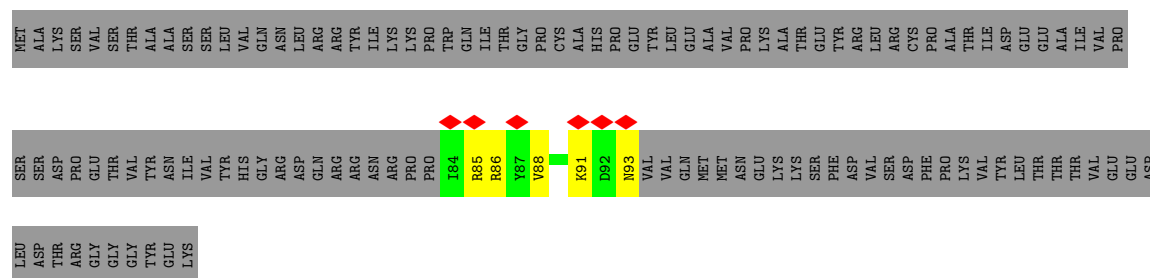
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B



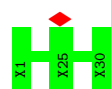
- Molecule 41: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



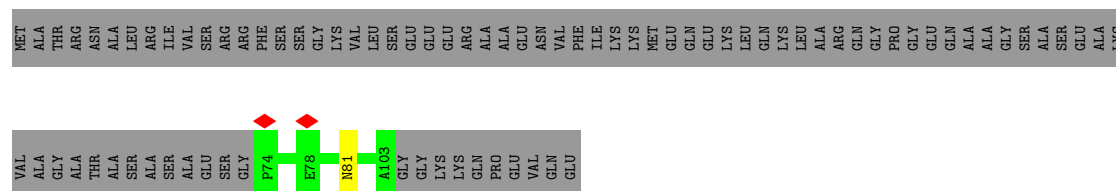
- Molecule 42: Furry



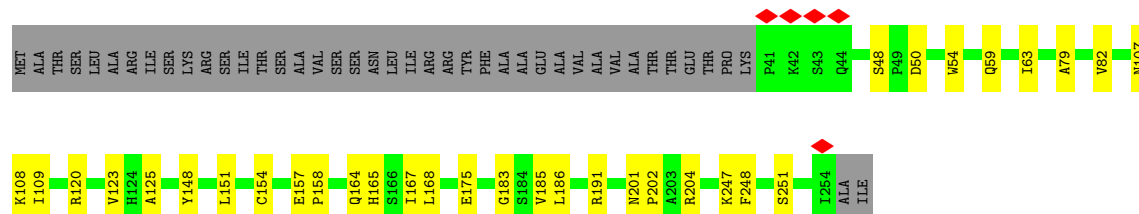
- Molecule 43: unknown



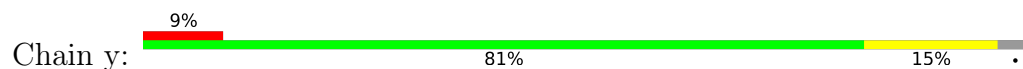
- Molecule 44: Uncharacterized protein At2g27730, mitochondrial

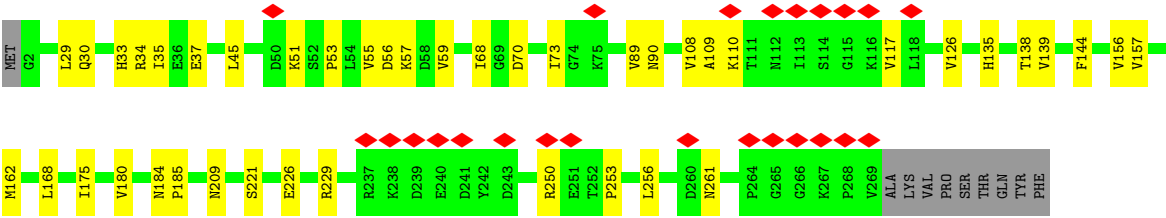


- Molecule 45: Gamma carbonic anhydrase-like 2, mitochondrial

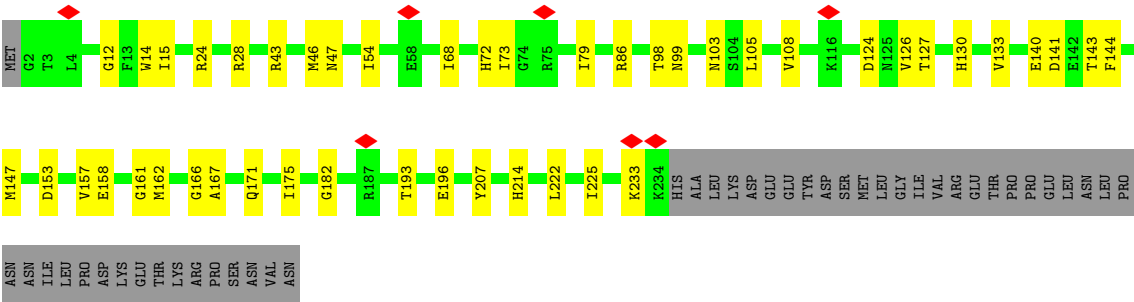


- Molecule 46: Gamma carbonic anhydrase 2, mitochondrial





• Molecule 47: Gamma carbonic anhydrase 1, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	459177	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMN, PC7, 8Q1, ZN, FMN, NDP, UQ9, PTY, FES, PSF, PGT, FE, SF4, T7X

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	0.16	0/807	0.28	0/1096
2	B	0.18	0/1279	0.33	0/1734
3	C	0.15	0/1629	0.29	0/2207
4	D	0.17	0/3147	0.32	0/4256
5	E	0.14	0/1535	0.35	0/2084
6	F	0.14	0/3441	0.31	1/4641 (0.0%)
7	G	0.15	0/5347	0.29	0/7242
8	H	0.19	0/2510	0.37	0/3416
9	I	0.16	0/1378	0.29	0/1862
10	J	0.15	0/1187	0.30	0/1617
11	K	0.16	0/717	0.30	0/969
12	L	0.15	0/4938	0.32	0/6706
13	M	0.14	0/3995	0.27	0/5428
14	N	0.15	0/3924	0.31	0/5327
15	O	0.11	0/971	0.26	0/1314
16	P	0.14	0/2617	0.34	1/3544 (0.0%)
17	Q	0.12	0/966	0.24	0/1305
18	R	0.12	0/493	0.25	0/668
19	S	0.16	0/739	0.32	0/996
20	T	0.14	0/679	0.37	0/922
21	U	0.11	0/660	0.29	0/892
22	V	0.15	0/1146	0.39	0/1555
23	W	0.12	0/923	0.27	0/1249
24	X	0.12	0/781	0.27	0/1049
25	Z	0.16	0/1027	0.36	0/1392
26	a	0.15	0/481	0.35	0/646
27	b	0.13	0/300	0.25	0/407
28	c	0.12	0/637	0.25	0/860
29	d	0.15	0/605	0.28	0/815
30	e	0.13	0/570	0.20	0/759
31	f	0.14	0/779	0.26	0/1052
32	g	0.12	0/635	0.28	0/863

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.13	0/757	0.26	0/1019
34	j	0.10	0/433	0.20	0/592
35	k	0.09	0/384	0.23	0/515
36	l	0.12	0/513	0.26	0/696
37	m	0.13	0/592	0.28	0/793
38	n	0.10	0/938	0.28	0/1273
39	o	0.14	0/666	0.30	0/886
40	p	0.14	0/799	0.31	0/1074
41	q	0.11	0/553	0.32	0/750
42	r	0.11	0/89	0.35	0/118
44	v	0.10	0/230	0.20	0/311
45	x	0.14	0/1700	0.29	0/2320
46	y	0.13	0/2066	0.26	0/2800
47	z	0.13	0/1804	0.23	0/2441
All	All	0.15	0/62367	0.30	2/84461 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	368	VAL	N-CA-C	-6.39	106.22	111.91
16	P	338	ILE	N-CA-C	-5.59	108.40	113.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	779	0	796	23	0
2	B	1244	0	1231	36	0
3	C	1581	0	1529	36	0
4	D	3077	0	3043	61	0
5	E	1500	0	1473	42	0
6	F	3368	0	3352	65	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	5252	0	5241	79	0
8	H	2439	0	2554	70	0
9	I	1349	0	1293	23	0
10	J	1162	0	1238	29	0
11	K	707	0	771	20	0
12	L	4807	0	4847	108	0
13	M	3887	0	4036	83	0
14	N	3820	0	3926	70	0
15	O	956	0	968	19	0
16	P	2560	0	2605	68	0
17	Q	939	0	928	8	0
18	R	482	0	478	8	0
19	S	727	0	759	18	0
20	T	667	0	648	16	0
21	U	650	0	635	13	0
22	V	1123	0	1112	22	0
23	W	904	0	901	15	0
24	X	767	0	766	9	0
25	Z	997	0	979	14	0
26	a	469	0	472	11	0
27	b	295	0	322	8	0
28	c	617	0	619	15	0
29	d	592	0	610	7	0
30	e	557	0	525	7	0
31	f	763	0	767	15	0
32	g	615	0	604	10	0
33	i	737	0	705	7	0
34	j	415	0	406	6	0
35	k	374	0	369	6	0
36	l	502	0	504	10	0
37	m	577	0	564	12	0
38	n	911	0	879	22	0
39	o	657	0	671	14	0
40	p	778	0	766	9	0
41	q	536	0	495	13	0
42	r	89	0	95	4	0
43	u	150	0	34	0	0
44	v	226	0	235	1	0
45	x	1659	0	1673	21	0
46	y	2032	0	2044	30	0
47	z	1772	0	1771	35	0
48	B	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	F	8	0	0	2	0
48	G	16	0	0	0	0
48	I	16	0	0	0	0
49	D	50	0	79	3	0
49	M	50	0	79	2	0
49	N	50	0	79	6	0
50	E	4	0	0	6	0
50	G	4	0	0	0	0
51	F	31	0	19	1	0
52	H	35	0	43	2	0
53	M	69	0	88	1	0
54	O	1	0	0	0	0
55	P	48	0	26	1	0
56	R	1	0	0	0	0
56	y	1	0	0	0	0
57	W	35	0	0	0	0
57	n	35	0	0	1	0
58	c	52	0	84	13	0
58	v	52	0	84	1	0
59	f	41	0	52	3	0
60	f	61	0	0	0	0
61	z	30	0	32	3	0
All	All	61765	0	61904	1023	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 8.

All (1023) 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)
5:E:180:MET:HE3	50:E:500:FES:S2	1.77	1.25
5:E:169:MET:HE1	50:E:500:FES:S2	1.98	1.03
16:P:322:ARG:NH1	16:P:333:LEU:HD23	1.78	0.98
3:C:60:CYS:HB3	4:D:354:LYS:HD2	1.54	0.88
2:B:80:ARG:HA	8:H:57:LYS:HD3	1.56	0.88
5:E:180:MET:CE	50:E:500:FES:S2	2.62	0.87
7:G:507:LYS:HG2	7:G:540:ASN:OD1	1.74	0.86
16:P:322:ARG:NH1	16:P:333:LEU:CD2	2.38	0.86
11:K:76:GLY:HA2	14:N:180:LEU:HD21	1.58	0.85
7:G:176:GLY:O	7:G:182:GLN:NE2	2.11	0.83
11:K:36:GLU:OE1	11:K:73:SER:OG	1.98	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:82:HIS:CD2	18:R:100:CYS:SG	2.73	0.81
13:M:147:GLU:HB2	14:N:402:PRO:HG2	1.64	0.80
3:C:170:GLU:HG2	16:P:64:SER:HB3	1.63	0.79
3:C:21:LYS:HB3	3:C:32:ASP:HB2	1.64	0.78
5:E:135:CYS:SG	50:E:500:FES:S1	2.82	0.78
22:V:63:GLN:OE1	22:V:141:GLN:NE2	2.12	0.78
10:J:37:THR:HG21	11:K:40:LEU:HD11	1.66	0.77
5:E:128:LEU:HB2	5:E:182:THR:HB	1.67	0.77
13:M:142:PHE:O	13:M:146:PHE:HB2	1.86	0.76
23:W:34:CYS:HB3	23:W:56:ARG:HH21	1.51	0.76
12:L:32:THR:HG21	12:L:114:MET:HB3	1.67	0.75
39:o:66:VAL:HG12	39:o:70:MET:HE2	1.67	0.75
2:B:204:LYS:HZ3	41:q:83:ARG:HB3	1.50	0.75
38:n:63:ARG:HH11	38:n:67:LEU:HD11	1.52	0.74
7:G:507:LYS:CG	7:G:540:ASN:OD1	2.34	0.74
13:M:146:PHE:HE1	13:M:259:PHE:HB3	1.52	0.74
3:C:23:GLU:OE1	3:C:30:ARG:NH2	2.20	0.74
13:M:303:ASP:HB3	13:M:306:LYS:HB2	1.68	0.74
16:P:322:ARG:HH12	16:P:333:LEU:HG	1.53	0.74
2:B:204:LYS:HZ3	41:q:83:ARG:HD3	1.52	0.73
38:n:12:ARG:HH12	38:n:61:VAL:HG11	1.53	0.73
2:B:116:ARG:NH2	2:B:121:GLN:OE1	2.21	0.72
7:G:409:TRP:HB2	7:G:414:ALA:HB1	1.70	0.72
14:N:401:ILE:HG22	14:N:403:PRO:HD2	1.68	0.72
32:g:91:THR:O	32:g:95:GLN:NE2	2.22	0.72
4:D:26:LEU:HD21	4:D:382:ILE:HD13	1.70	0.72
46:y:55:VAL:HG22	46:y:73:ILE:HD12	1.72	0.72
14:N:436:GLY:HA2	14:N:439:TYR:CE1	2.24	0.72
14:N:489:VAL:HB	29:d:56:LEU:HD21	1.71	0.71
19:S:13:GLU:OE1	19:S:15:ARG:NH1	2.23	0.71
24:X:41:LYS:NZ	33:i:80:ASP:OD1	2.23	0.71
16:P:322:ARG:HH12	16:P:333:LEU:CG	2.04	0.71
12:L:250:THR:HG21	12:L:353:GLY:HA3	1.72	0.71
16:P:80:LEU:HD22	16:P:222:MET:HE1	1.73	0.71
3:C:4:GLN:O	3:C:8:LYS:NZ	2.23	0.70
16:P:58:LYS:HB3	16:P:66:VAL:HB	1.73	0.70
8:H:95:ASP:OD2	8:H:96:TYR:N	2.18	0.70
7:G:327:TRP:HB2	7:G:453:MET:HE1	1.71	0.70
47:z:98:THR:HG22	47:z:126:VAL:H	1.56	0.70
45:x:148:TYR:OH	47:z:103:ASN:O	2.10	0.70
10:J:150:VAL:HB	14:N:86:LEU:HD12	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HD12	1:A:92:GLY:HA3	1.75	0.69
5:E:133:THR:HG21	6:F:393:LEU:HD22	1.72	0.69
16:P:322:ARG:CZ	16:P:333:LEU:HD23	2.21	0.69
4:D:186:ILE:HG12	4:D:268:MET:HE3	1.75	0.69
8:H:12:ILE:HD12	26:a:26:GLN:HE22	1.57	0.69
14:N:351:ILE:HG22	14:N:355:MET:HE2	1.74	0.69
31:f:33:ASP:OD2	31:f:84:ARG:NH2	2.26	0.69
12:L:567:GLN:NE2	12:L:571:ASP:OD2	2.26	0.68
5:E:169:MET:HE2	5:E:171:CYS:HA	1.75	0.68
12:L:212:ASN:HA	37:m:58:MET:HE1	1.76	0.68
14:N:375:ALA:HB3	15:O:90:ALA:HB2	1.76	0.68
5:E:174:CYS:HA	6:F:146:GLY:HA2	1.75	0.68
16:P:322:ARG:HH12	16:P:333:LEU:CD2	2.07	0.68
8:H:264:PRO:HD2	8:H:267:ILE:HD12	1.75	0.67
23:W:21:GLU:OE1	23:W:24:ARG:NH2	2.27	0.67
36:l:122:GLY:O	40:p:71:ARG:NH1	2.27	0.67
12:L:183:LEU:HD21	13:M:404:LEU:HB3	1.76	0.67
12:L:430:THR:HA	12:L:433:TYR:CE1	2.29	0.67
21:U:73:ALA:H	21:U:112:ILE:HG22	1.59	0.67
5:E:78:ASP:O	5:E:82:GLN:HG3	1.95	0.67
6:F:293:ASN:HD21	6:F:361:ASP:HB3	1.58	0.67
3:C:135:ASP:OD1	3:C:136:TYR:N	2.28	0.67
12:L:377:LEU:O	12:L:381:MET:HG2	1.94	0.67
23:W:120:LYS:HD3	23:W:124:LEU:HD23	1.76	0.67
38:n:47:ASP:OD2	38:n:51:LYS:NZ	2.27	0.67
5:E:132:THR:HG22	5:E:133:THR:H	1.59	0.67
8:H:126:ARG:HD2	10:J:70:MET:HE3	1.77	0.67
2:B:83:SER:O	8:H:57:LYS:NZ	2.28	0.66
25:Z:143:TRP:O	26:a:51:ARG:NH2	2.28	0.66
36:l:105:VAL:O	39:o:77:ARG:NH2	2.29	0.66
13:M:453:ASN:ND2	38:n:112:GLY:O	2.27	0.66
5:E:175:CYS:SG	5:E:180:MET:HE1	2.36	0.66
6:F:385:ASP:OD1	6:F:472:ARG:NH2	2.28	0.66
6:F:334:TRP:NE1	6:F:356:GLU:OE2	2.29	0.66
58:c:101:PC7:H472	58:c:101:PC7:H262	1.78	0.66
39:o:81:ALA:O	39:o:85:GLN:NE2	2.29	0.66
7:G:299:VAL:O	7:G:632:ASN:ND2	2.29	0.65
2:B:83:SER:HB3	8:H:57:LYS:HG3	1.76	0.65
6:F:240:GLU:OE2	6:F:247:ARG:NH2	2.29	0.65
12:L:451:ARG:HD3	20:T:49:ARG:HH22	1.61	0.65
24:X:77:ASP:OD2	24:X:78:TYR:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:168:LEU:HG	45:x:186:LEU:HD21	1.77	0.65
46:y:51:LYS:HD2	46:y:70:ASP:HB2	1.77	0.65
47:z:24:ARG:NH1	61:z:301:PSF:OT2	2.30	0.65
8:H:98:MET:HG2	26:a:27:TYR:HB2	1.79	0.65
2:B:76:MET:HE3	2:B:80:ARG:HH12	1.62	0.65
4:D:74:SER:O	4:D:78:GLN:NE2	2.30	0.65
5:E:128:LEU:HB3	5:E:169:MET:HB3	1.79	0.65
46:y:138:THR:HB	46:y:156:VAL:HG12	1.79	0.65
7:G:429:THR:OG1	7:G:548:ASN:O	2.15	0.64
11:K:53:LEU:HD22	30:e:45:LEU:HD22	1.80	0.64
47:z:143:THR:OG1	47:z:161:GLY:O	2.15	0.64
33:i:50:PRO:HG2	33:i:53:PHE:HB3	1.78	0.64
34:j:32:CYS:SG	34:j:36:TRP:NE1	2.71	0.64
1:A:69:LEU:HD11	11:K:70:ALA:HB1	1.80	0.64
2:B:88:THR:HG23	4:D:20:PRO:HD2	1.78	0.64
10:J:46:LEU:HA	10:J:136:ASN:HD22	1.62	0.64
46:y:89:VAL:HG11	46:y:110:LYS:HA	1.78	0.64
7:G:213:THR:HG23	7:G:215:MET:HE2	1.80	0.64
7:G:236:ASP:O	7:G:250:THR:HG22	1.98	0.64
46:y:56:ASP:OD1	46:y:57:LYS:N	2.30	0.64
31:f:91:ASN:HB2	31:f:94:GLU:HB2	1.78	0.64
3:C:33:THR:HG21	3:C:41:LEU:HD22	1.79	0.63
47:z:157:VAL:HG22	47:z:175:ILE:HD13	1.79	0.63
3:C:132:ILE:HG23	3:C:133:LEU:HG	1.80	0.63
12:L:417:ASN:HD21	36:l:99:ASN:HD22	1.45	0.63
26:a:12:LEU:HA	26:a:15:ILE:HD12	1.81	0.63
46:y:34:ARG:HA	47:z:47:ASN:HD21	1.63	0.63
7:G:556:TYR:HB2	7:G:559:GLN:HG3	1.79	0.63
10:J:127:TYR:HE1	25:Z:93:GLU:HG3	1.64	0.62
12:L:31:MET:HE1	28:c:41:MET:HG3	1.82	0.62
6:F:181:ILE:HD11	6:F:192:LEU:HD23	1.81	0.62
4:D:110:ARG:NH2	4:D:332:GLU:O	2.27	0.62
4:D:299:ARG:NH2	9:I:175:ASP:OD1	2.32	0.62
12:L:596:ILE:HA	12:L:601:GLY:HA3	1.81	0.62
19:S:19:CYS:O	19:S:29:ARG:NH1	2.32	0.62
3:C:83:ASN:HB3	22:V:135:PRO:HG3	1.80	0.62
14:N:370:ARG:O	15:O:84:ARG:NH2	2.32	0.62
8:H:126:ARG:HB3	10:J:70:MET:HE3	1.81	0.62
31:f:84:ARG:NH1	31:f:94:GLU:OE2	2.32	0.62
58:c:101:PC7:H242	58:c:101:PC7:H451	1.82	0.61
25:Z:44:PRO:HG2	25:Z:49:MET:SD	2.39	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:209:VAL:HG22	4:D:260:ARG:NH2	2.15	0.61
11:K:61:PHE:CZ	14:N:191:LEU:HD11	2.36	0.61
16:P:246:ILE:HD13	16:P:344:ILE:HG12	1.81	0.61
12:L:508:GLU:OE2	39:o:69:ARG:NH2	2.31	0.61
13:M:300:ARG:O	37:m:20:ARG:NH2	2.33	0.61
4:D:112:LEU:HD21	4:D:141:LEU:HB2	1.83	0.61
7:G:317:PRO:HG3	7:G:328:ILE:HG12	1.81	0.61
13:M:82:PHE:HD1	13:M:136:MET:HE1	1.66	0.61
14:N:14:ASN:ND2	31:f:20:PRO:O	2.33	0.61
18:R:96:ILE:HG12	18:R:103:ARG:HG2	1.83	0.61
2:B:123:ASP:OD1	8:H:57:LYS:NZ	2.33	0.61
8:H:105:ILE:HG13	8:H:108:LEU:HB3	1.82	0.60
8:H:291:ARG:NH2	8:H:293:ASP:OD2	2.34	0.60
16:P:289:THR:HG22	16:P:292:GLU:HG3	1.83	0.60
34:j:21:LYS:HD2	34:j:23:TRP:HE3	1.66	0.60
1:A:77:PHE:O	10:J:145:TYR:OH	2.19	0.60
8:H:36:ARG:HG2	9:I:92:VAL:HG22	1.83	0.60
46:y:109:ALA:HB3	46:y:117:VAL:HG11	1.84	0.60
12:L:96:VAL:HG21	12:L:255:LEU:HB2	1.82	0.60
41:q:68:THR:HG23	41:q:69:GLN:HG2	1.84	0.60
5:E:135:CYS:HB2	50:E:500:FES:S1	2.42	0.60
7:G:338:GLY:O	7:G:606:HIS:NE2	2.32	0.60
8:H:195:LEU:HD22	8:H:201:ALA:HB2	1.84	0.60
14:N:139:MET:HE1	14:N:155:GLN:HG2	1.83	0.60
16:P:249:GLY:HA2	16:P:290:THR:HB	1.82	0.60
2:B:91:LEU:HB2	2:B:129:GLY:HA3	1.82	0.60
6:F:350:ILE:HG23	6:F:354:ILE:HG13	1.84	0.60
14:N:78:ILE:HD11	31:f:86:MET:HE1	1.83	0.60
14:N:347:ILE:HG13	14:N:490:THR:HG21	1.84	0.60
14:N:390:THR:HG1	29:d:19:TYR:HH	1.50	0.59
20:T:57:PHE:HB3	20:T:60:VAL:HG22	1.82	0.59
7:G:83:VAL:HG21	7:G:98:ALA:HB2	1.84	0.59
16:P:337:GLN:HG2	16:P:338:ILE:HG13	1.83	0.59
4:D:31:GLU:HB3	4:D:39:ARG:HG2	1.84	0.59
45:x:120:ARG:NH2	47:z:103:ASN:OD1	2.35	0.59
46:y:221:SER:HB3	47:z:233:LYS:HB3	1.85	0.59
12:L:47:PHE:HA	12:L:83:VAL:HG11	1.84	0.59
14:N:244:VAL:HG12	14:N:247:HIS:CG	2.37	0.59
14:N:47:TYR:O	46:y:250:ARG:NH2	2.31	0.59
23:W:44:TYR:OH	23:W:94:LYS:O	2.20	0.59
1:A:99:PHE:CD1	10:J:156:SER:HB2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:140:LEU:HD21	11:K:63:LEU:HD22	1.83	0.59
46:y:33:HIS:O	47:z:47:ASN:ND2	2.36	0.59
5:E:135:CYS:CB	50:E:500:FES:S1	2.91	0.59
6:F:257:GLY:HA3	6:F:263:THR:HG22	1.85	0.59
2:B:204:LYS:NZ	41:q:83:ARG:HD3	2.17	0.59
6:F:343:GLY:H	6:F:347:VAL:HG21	1.67	0.59
3:C:114:GLU:OE2	4:D:394:ARG:NH2	2.35	0.59
21:U:70:THR:HG23	21:U:72:LYS:H	1.66	0.59
13:M:50:LEU:HD21	32:g:69:THR:HG23	1.84	0.58
3:C:52:ARG:HD2	22:V:92:GLU:HG2	1.84	0.58
13:M:448:LYS:NZ	38:n:106:GLU:OE2	2.36	0.58
22:V:146:LEU:O	22:V:150:ILE:HG12	2.04	0.58
7:G:629:THR:HG22	7:G:639:GLN:HG2	1.84	0.58
12:L:370:GLY:HA2	35:k:27:GLN:HG3	1.83	0.58
26:a:3:LEU:HD23	26:a:4:VAL:HG23	1.86	0.58
28:c:29:ARG:NH2	32:g:34:THR:O	2.36	0.58
1:A:16:LEU:HA	8:H:83:MET:HE1	1.86	0.58
3:C:161:GLU:HG3	3:C:163:ARG:HG2	1.84	0.58
21:U:50:VAL:HG21	21:U:120:ALA:HB2	1.85	0.58
6:F:331:ARG:O	6:F:336:ASN:ND2	2.36	0.58
1:A:79:PHE:CE2	8:H:108:LEU:HD13	2.39	0.58
13:M:372:SER:HA	58:c:101:PC7:H73	1.86	0.58
16:P:359:LYS:HD2	16:P:361:GLN:HE22	1.67	0.58
39:o:33:LEU:HD13	39:o:57:VAL:HG12	1.85	0.58
6:F:136:LEU:HD13	6:F:172:MET:HE1	1.84	0.58
7:G:171:PRO:O	7:G:283:ARG:NH2	2.37	0.58
13:M:250:VAL:HG13	13:M:346:SER:HB2	1.86	0.58
12:L:230:VAL:HG13	12:L:235:GLN:HB2	1.85	0.58
14:N:461:MET:HE2	14:N:465:LYS:HB3	1.86	0.58
11:K:61:PHE:HZ	14:N:191:LEU:HD11	1.68	0.57
12:L:32:THR:OG1	12:L:118:SER:OG	2.20	0.57
6:F:64:ILE:HG23	6:F:276:THR:HG21	1.86	0.57
9:I:189:THR:HB	9:I:192:GLU:HG3	1.84	0.57
13:M:287:SER:OG	13:M:317:ASN:O	2.21	0.57
11:K:61:PHE:HD1	14:N:146:ILE:HG23	1.69	0.57
16:P:322:ARG:NE	16:P:336:PRO:HD3	2.19	0.57
45:x:48:SER:OG	45:x:50:ASP:OD1	2.22	0.57
25:Z:107:TYR:OH	30:e:61:GLU:OE2	2.16	0.57
8:H:26:ALA:HB2	26:a:11:PRO:HB2	1.85	0.57
8:H:282:TRP:CZ2	9:I:84:LEU:HB2	2.40	0.57
2:B:97:GLU:HG3	2:B:189:PRO:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:l:113:PRO:HG3	39:o:10:MET:HE3	1.87	0.57
13:M:92:PHE:HB3	13:M:339:LEU:HD21	1.86	0.57
14:N:15:LEU:HD21	31:f:3:THR:HB	1.86	0.57
2:B:200:LEU:O	2:B:204:LYS:HG2	2.05	0.57
16:P:218:ARG:NH2	16:P:281:GLU:OE2	2.37	0.57
7:G:145:LYS:HD3	7:G:148:THR:HG21	1.86	0.57
6:F:351:PRO:HD2	6:F:354:ILE:HD11	1.86	0.57
7:G:689:HIS:ND1	19:S:53:CYS:SG	2.78	0.57
8:H:88:ALA:HB2	8:H:113:ILE:HG21	1.87	0.56
10:J:44:LEU:HD11	11:K:48:VAL:HG22	1.86	0.56
19:S:11:MET:HE1	19:S:14:LEU:HD13	1.87	0.56
5:E:148:LEU:HD11	5:E:154:LYS:HA	1.87	0.56
13:M:308:ILE:HD13	13:M:348:LEU:HB3	1.87	0.56
24:X:82:MET:HE3	24:X:87:ASN:HA	1.87	0.56
2:B:93:CYS:HB2	4:D:153:MET:HE1	1.87	0.56
2:B:204:LYS:NZ	41:q:83:ARG:HB3	2.18	0.56
8:H:134:PHE:HE1	10:J:70:MET:HE2	1.70	0.56
14:N:24:PHE:HB2	31:f:75:MET:HE1	1.88	0.56
15:O:51:ILE:HD13	21:U:123:PRO:HG3	1.86	0.56
5:E:78:ASP:OD1	5:E:79:LEU:N	2.39	0.56
6:F:76:LEU:O	6:F:80:MET:HG2	2.05	0.56
8:H:270:SER:O	8:H:274:LEU:HG	2.05	0.56
9:I:130:GLU:HB2	9:I:140:ILE:HD12	1.87	0.56
21:U:119:ILE:HA	21:U:122:HIS:HD1	1.71	0.56
25:Z:44:PRO:O	25:Z:48:ALA:HB3	2.05	0.56
10:J:123:ARG:O	25:Z:96:ARG:NH2	2.38	0.56
14:N:102:LEU:HB3	49:N:501:PTY:H443	1.88	0.56
26:a:46:ASP:O	26:a:50:GLU:HG3	2.06	0.56
12:L:64:TRP:HB3	12:L:72:ALA:O	2.06	0.56
12:L:591:LYS:HE2	37:m:27:PHE:CE1	2.40	0.56
13:M:334:SER:HA	13:M:403:ILE:HD11	1.88	0.56
14:N:396:PHE:HE1	14:N:441:ILE:HG22	1.71	0.55
4:D:28:LEU:HD23	4:D:30:LEU:HD21	1.87	0.55
7:G:345:SER:HB2	7:G:648:GLY:HA3	1.87	0.55
13:M:294:THR:HG21	13:M:313:VAL:HB	1.87	0.55
28:c:30:PRO:HG2	28:c:33:TRP:HB3	1.87	0.55
5:E:136:MET:HA	5:E:140:SER:H	1.71	0.55
7:G:294:ASP:OD2	7:G:332:THR:OG1	2.19	0.55
22:V:121:GLU:HB2	42:r:85:ARG:HB2	1.88	0.55
4:D:13:LEU:HD21	4:D:15:PHE:CE1	2.41	0.55
7:G:529:ILE:HA	7:G:710:MET:HE2	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:296:LEU:HD11	12:L:565:PHE:CZ	2.41	0.55
13:M:163:ARG:HG3	13:M:165:ARG:H	1.70	0.55
14:N:39:PHE:CZ	31:f:60:PRO:HB3	2.42	0.55
14:N:378:GLY:HA2	14:N:446:ARG:HG3	1.89	0.55
25:Z:86:LEU:HD13	33:i:82:LEU:HD21	1.89	0.55
1:A:105:ILE:HD12	14:N:34:ILE:HD11	1.88	0.55
16:P:301:ILE:HD11	16:P:378:LEU:HD22	1.87	0.55
19:S:74:LEU:HD22	19:S:82:ILE:HG12	1.88	0.55
12:L:252:VAL:HG13	12:L:256:ILE:HG13	1.87	0.55
8:H:36:ARG:HH21	9:I:86:TYR:HE2	1.54	0.55
18:R:71:ALA:HB1	18:R:84:ILE:HD11	1.88	0.55
19:S:74:LEU:HA	19:S:77:LEU:HD13	1.89	0.55
47:z:28:ARG:HH12	61:z:301:PSF:H1	1.55	0.55
7:G:96:GLU:OE2	7:G:104:ARG:NH2	2.40	0.55
8:H:277:LEU:HA	8:H:280:TYR:HD2	1.72	0.55
40:p:88:LYS:HG3	40:p:89:ASP:H	1.72	0.55
13:M:55:LEU:HD23	13:M:58:GLN:HE21	1.71	0.54
2:B:120:ARG:NH1	2:B:145:GLN:HB3	2.21	0.54
30:e:50:GLU:OE1	30:e:54:ARG:NH2	2.39	0.54
1:A:76:THR:HG23	10:J:52:ILE:HD12	1.90	0.54
13:M:72:LEU:HB3	13:M:82:PHE:HB2	1.90	0.54
18:R:75:ASP:OD1	18:R:76:THR:N	2.41	0.54
14:N:159:PHE:CE2	14:N:269:PRO:HG3	2.42	0.54
46:y:226:GLU:OE2	46:y:229:ARG:NH2	2.40	0.54
47:z:46:MET:HB3	47:z:68:ILE:HG12	1.89	0.54
11:K:21:ILE:HD11	11:K:35:ILE:HG13	1.90	0.54
39:o:8:LYS:HG2	39:o:29:MET:HE2	1.89	0.54
7:G:110:ARG:NH2	7:G:321:GLU:OE1	2.40	0.54
12:L:41:ILE:O	12:L:45:ILE:HD12	2.07	0.54
15:O:44:ARG:NH1	45:x:175:GLU:OE2	2.41	0.54
5:E:47:TRP:HE1	5:E:84:ASN:HD22	1.55	0.54
12:L:112:ARG:NH1	58:c:101:PC7:O2P	2.37	0.54
38:n:61:VAL:HA	38:n:64:ILE:HG22	1.88	0.54
47:z:86:ARG:NH2	47:z:108:VAL:O	2.39	0.54
6:F:151:ARG:HH11	6:F:155:ARG:HH11	1.54	0.53
21:U:118:PHE:O	21:U:122:HIS:ND1	2.41	0.53
6:F:293:ASN:ND2	6:F:361:ASP:HB3	2.23	0.53
23:W:55:LEU:O	23:W:59:ILE:HD12	2.08	0.53
24:X:86:THR:OG1	26:a:36:ARG:NH2	2.41	0.53
5:E:42:LYS:HE2	5:E:44:ASP:HB2	1.89	0.53
9:I:181:PRO:HG3	9:I:210:GLU:HG2	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:4:ARG:NH2	19:S:35:ASN:OD1	2.36	0.53
4:D:175:ILE:HG22	4:D:279:LEU:HD11	1.91	0.53
8:H:313:SER:HA	27:b:27:GLY:HA3	1.89	0.53
14:N:402:PRO:HA	14:N:407:PHE:CG	2.44	0.53
16:P:186:LEU:HA	16:P:218:ARG:HG2	1.89	0.53
39:o:23:ALA:HA	40:p:64:VAL:HG11	1.90	0.53
2:B:100:HIS:ND1	4:D:139:GLU:OE2	2.42	0.53
12:L:303:LEU:HD12	12:L:559:PHE:HB2	1.89	0.53
5:E:32:LEU:O	5:E:119:ARG:NH1	2.37	0.53
8:H:200:ARG:NH1	8:H:236:MET:SD	2.82	0.53
46:y:35:ILE:O	47:z:43:ARG:NH1	2.36	0.53
1:A:62:TYR:OH	11:K:74:ALA:O	2.26	0.53
4:D:292:ARG:NH1	4:D:296:PRO:O	2.40	0.53
6:F:402:CYS:HA	7:G:242:ARG:HG3	1.91	0.53
8:H:68:SER:O	8:H:129:ASN:ND2	2.32	0.53
12:L:137:PHE:HD1	12:L:178:LEU:HD23	1.73	0.53
16:P:100:ARG:NH2	55:P:500:NDP:O3X	2.42	0.53
16:P:131:ILE:HG22	16:P:170:VAL:HG11	1.91	0.53
20:T:101:GLU:HA	20:T:104:LYS:HG2	1.90	0.53
20:T:111:ALA:O	20:T:115:VAL:HG22	2.09	0.53
38:n:33:ASN:HD21	38:n:84:TYR:H	1.56	0.53
7:G:304:ARG:NH2	7:G:306:ASP:OD2	2.36	0.53
12:L:458:ASP:HB3	34:j:24:HIS:CE1	2.44	0.53
47:z:126:VAL:HG22	47:z:143:THR:HG22	1.90	0.53
6:F:304:HIS:HE1	6:F:384:THR:CG2	2.21	0.52
12:L:82:THR:OG1	12:L:271:ARG:NH2	2.42	0.52
12:L:613:ILE:HG12	14:N:308:ALA:HB2	1.90	0.52
41:q:55:ASP:HB2	41:q:61:TYR:HE1	1.73	0.52
38:n:55:ASN:ND2	57:n:200:8Q1:O4	2.39	0.52
4:D:112:LEU:HD22	4:D:138:ARG:HG3	1.90	0.52
9:I:152:THR:O	9:I:197:LYS:NZ	2.41	0.52
13:M:331:ILE:HG21	13:M:488:LEU:HD23	1.91	0.52
13:M:441:LEU:HD13	38:n:105:ILE:HD13	1.90	0.52
14:N:144:ASP:OD1	14:N:145:LEU:N	2.42	0.52
5:E:32:LEU:HD23	5:E:34:TYR:CZ	2.45	0.52
7:G:607:GLY:HA2	7:G:611:VAL:HG21	1.90	0.52
13:M:231:VAL:HB	13:M:232:PRO:HD3	1.92	0.52
14:N:216:TYR:OH	14:N:221:ALA:N	2.43	0.52
45:x:79:ALA:HB3	45:x:82:VAL:HG23	1.92	0.52
3:C:53:VAL:HG11	3:C:77:LEU:HB3	1.91	0.52
15:O:98:GLN:HB2	15:O:149:ALA:HB3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:89:LYS:HG3	6:F:212:SER:HB3	1.91	0.52
6:F:443:GLU:OE2	6:F:456:TRP:NE1	2.43	0.52
9:I:58:LYS:HB2	27:b:8:ARG:HH21	1.75	0.52
12:L:587:GLU:HA	12:L:591:LYS:HD3	1.91	0.52
23:W:121:THR:HG22	23:W:123:PHE:H	1.74	0.52
24:X:32:GLU:HB3	24:X:56:VAL:HG22	1.92	0.52
37:m:58:MET:HA	37:m:61:GLU:HG2	1.91	0.52
3:C:19:VAL:HA	3:C:33:THR:HG22	1.92	0.52
49:D:401:PTY:H351	8:H:185:PRO:HB3	1.90	0.52
5:E:188:ASN:HB3	5:E:192:GLY:HA3	1.92	0.52
8:H:309:ALA:HB1	27:b:23:ILE:HG13	1.92	0.52
12:L:274:PRO:HA	12:L:498:LEU:HD23	1.91	0.52
14:N:306:ALA:HB2	14:N:432:THR:HG23	1.92	0.52
16:P:76:ALA:HB3	16:P:97:VAL:HG13	1.91	0.52
36:l:77:GLU:OE2	36:l:81:TRP:NE1	2.41	0.52
6:F:63:ARG:NH1	6:F:312:GLU:O	2.42	0.52
2:B:93:CYS:HB3	4:D:72:TYR:CB	2.40	0.52
16:P:98:PRO:HB2	16:P:123:PHE:CD1	2.45	0.52
6:F:341:ILE:HB	6:F:378:ILE:HB	1.92	0.52
6:F:427:ALA:HB1	6:F:431:GLU:HG3	1.92	0.52
12:L:246:MET:HA	12:L:246:MET:HE2	1.91	0.52
14:N:346:LEU:HB2	14:N:490:THR:HG23	1.90	0.52
16:P:254:GLN:NE2	16:P:284:GLY:O	2.43	0.52
13:M:150:LEU:HD11	13:M:177:THR:HG21	1.92	0.51
37:m:55:ASP:OD1	37:m:59:GLN:NE2	2.42	0.51
46:y:126:VAL:HG11	46:y:139:VAL:HG11	1.92	0.51
12:L:586:PHE:HB2	13:M:297:THR:HG23	1.93	0.51
16:P:60:THR:HG22	17:Q:82:LEU:HD21	1.93	0.51
6:F:348:PRO:HG3	6:F:456:TRP:HB3	1.92	0.51
8:H:59:ILE:HG22	8:H:60:LEU:HD12	1.93	0.51
8:H:74:PHE:HB2	8:H:127:SER:HB3	1.92	0.51
8:H:302:VAL:HG13	27:b:16:VAL:HG21	1.91	0.51
16:P:296:ILE:HG12	16:P:371:LYS:HZ2	1.74	0.51
4:D:311:HIS:ND1	7:G:186:MET:SD	2.80	0.51
5:E:50:SER:HB2	5:E:53:ASN:HB2	1.92	0.51
19:S:53:CYS:SG	19:S:54:SER:N	2.82	0.51
3:C:58:ASP:HB2	4:D:354:LYS:HE2	1.93	0.51
3:C:118:MET:HB3	3:C:143:LEU:HB2	1.93	0.51
8:H:139:ARG:HB3	8:H:292:TYR:CE1	2.46	0.51
12:L:3:LEU:HG	12:L:59:LEU:HD21	1.92	0.51
14:N:25:ILE:HD11	14:N:130:LEU:HD22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:245:LEU:HD13	4:D:274:ILE:HG23	1.92	0.51
12:L:565:PHE:HE1	36:l:82:LEU:HD13	1.75	0.51
2:B:83:SER:OG	8:H:54:ASP:OD1	2.26	0.51
12:L:381:MET:HE2	12:L:467:LEU:HB3	1.92	0.51
5:E:49:PHE:O	5:E:83:GLN:NE2	2.44	0.51
5:E:113:PHE:HB2	6:F:243:GLN:HE21	1.76	0.51
8:H:182:PRO:HG3	25:Z:60:GLY:HA3	1.92	0.51
8:H:201:ALA:HB1	8:H:202:PRO:HD2	1.93	0.51
13:M:112:MET:SD	13:M:120:ILE:HD11	2.50	0.51
13:M:136:MET:HE3	13:M:145:PHE:HE2	1.75	0.51
13:M:217:TRP:HH2	13:M:283:ILE:HD11	1.75	0.51
3:C:52:ARG:NH2	22:V:95:ASP:OD2	2.41	0.50
4:D:162:GLY:HA3	4:D:288:LYS:HA	1.92	0.50
13:M:130:MET:HG2	13:M:259:PHE:HZ	1.75	0.50
13:M:299:LEU:HD23	13:M:428:TYR:HB3	1.92	0.50
15:O:58:GLN:HE21	15:O:77:LEU:HD21	1.76	0.50
37:m:48:VAL:O	37:m:52:ILE:HD12	2.10	0.50
8:H:31:MET:HE1	8:H:284:ARG:HE	1.75	0.50
9:I:105:PRO:HB2	9:I:218:GLU:OE2	2.12	0.50
13:M:365:ARG:NH2	36:l:51:ASP:OD1	2.44	0.50
34:j:12:TYR:HB2	35:k:21:HIS:HD2	1.76	0.50
16:P:56:ALA:H	16:P:68:GLY:H	1.59	0.50
46:y:184:ASN:HB3	46:y:185:PRO:HD3	1.92	0.50
14:N:463:ARG:HD2	49:N:501:PTY:HC51	1.93	0.50
15:O:49:SER:HB2	15:O:147:VAL:HG22	1.93	0.50
6:F:185:TYR:HB3	6:F:188:GLU:HB2	1.93	0.50
45:x:107:ASN:OD1	45:x:108:LYS:N	2.41	0.50
5:E:70:GLN:HG3	5:E:102:VAL:HG11	1.94	0.50
12:L:296:LEU:HD11	12:L:565:PHE:HZ	1.76	0.50
12:L:541:GLN:HB2	38:n:40:ILE:HD13	1.93	0.50
38:n:17:LYS:O	38:n:21:ARG:NH1	2.44	0.50
41:q:92:GLU:HA	41:q:108:LEU:HD23	1.94	0.50
25:Z:83:ARG:NH1	33:i:85:ASP:OD2	2.44	0.50
47:z:167:ALA:HB2	47:z:182:GLY:HA2	1.93	0.50
12:L:252:VAL:O	12:L:256:ILE:HB	2.11	0.50
15:O:116:TYR:CZ	15:O:120:ARG:HD3	2.46	0.50
17:Q:41:LYS:HE2	23:W:68:HIS:CE1	2.46	0.50
19:S:77:LEU:HD23	19:S:81:GLN:HB3	1.94	0.50
4:D:292:ARG:HD3	4:D:295:CYS:SG	2.52	0.50
12:L:321:TYR:HA	12:L:324:PHE:CE1	2.46	0.50
13:M:39:LEU:HD21	32:g:61:ASP:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:109:ILE:HD13	45:x:123:VAL:HG12	1.92	0.50
6:F:339:ALA:HB1	6:F:349:LEU:HD21	1.94	0.49
8:H:244:THR:HA	8:H:248:LEU:HB2	1.94	0.49
15:O:110:ARG:HH12	15:O:127:LEU:HD21	1.78	0.49
32:g:40:ARG:HG2	32:g:41:PRO:HD2	1.94	0.49
46:y:209:ASN:HD21	46:y:261:ASN:HB2	1.77	0.49
11:K:31:MET:HE2	14:N:181:ILE:HD13	1.93	0.49
12:L:128:VAL:HG23	12:L:129:THR:HG23	1.93	0.49
12:L:324:PHE:O	12:L:328:ILE:HG12	2.12	0.49
41:q:74:ARG:NH1	41:q:96:TRP:O	2.36	0.49
1:A:78:PHE:CZ	1:A:100:LEU:HD21	2.48	0.49
2:B:69:ILE:HG23	2:B:212:PHE:HD2	1.76	0.49
4:D:209:VAL:HG22	4:D:260:ARG:HH22	1.77	0.49
6:F:249:LYS:N	6:F:250:PRO:HD2	2.27	0.49
14:N:77:THR:HB	31:f:8:LEU:HB3	1.93	0.49
16:P:156:PHE:HD2	16:P:195:ARG:HE	1.59	0.49
24:X:51:ASP:OD1	24:X:52:LYS:N	2.44	0.49
12:L:95:LEU:HD22	12:L:466:PRO:HA	1.94	0.49
7:G:444:GLY:HA3	7:G:520:LEU:HD21	1.95	0.49
8:H:319:VAL:HG22	8:H:324:LEU:HD11	1.93	0.49
16:P:380:GLN:HG3	16:P:381:TYR:CD1	2.48	0.49
8:H:198:THR:HG21	8:H:236:MET:HG3	1.95	0.49
22:V:65:LEU:HG	22:V:69:LYS:HE3	1.95	0.49
45:x:164:GLN:O	45:x:183:GLY:N	2.36	0.49
14:N:390:THR:OG1	29:d:19:TYR:OH	2.25	0.49
7:G:91:VAL:HG13	7:G:144:ILE:HG12	1.94	0.49
33:i:54:TRP:O	33:i:60:ASN:ND2	2.46	0.49
4:D:197:ARG:NE	9:I:75:GLU:OE2	2.35	0.49
12:L:77:LEU:HD22	12:L:271:ARG:HH12	1.77	0.49
14:N:358:ASP:HB2	14:N:472:THR:HG21	1.94	0.49
20:T:51:LEU:HA	20:T:54:VAL:HG12	1.94	0.49
47:z:193:THR:HG23	47:z:196:GLU:H	1.77	0.49
4:D:32:MET:HG2	4:D:37:VAL:HG12	1.95	0.48
5:E:135:CYS:O	5:E:140:SER:HB3	2.12	0.48
9:I:124:ILE:HG22	9:I:151:ARG:HH12	1.77	0.48
26:a:5:TRP:H	26:a:5:TRP:CD1	2.29	0.48
3:C:38:LEU:HD21	3:C:75:TYR:CZ	2.49	0.48
12:L:302:ILE:HA	12:L:433:TYR:HB3	1.94	0.48
16:P:246:ILE:HG21	16:P:344:ILE:HG12	1.95	0.48
21:U:53:ARG:HD2	21:U:119:ILE:HG21	1.95	0.48
38:n:63:ARG:O	38:n:67:LEU:HG	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PHE:CD1	8:H:156:ILE:HD11	2.49	0.48
2:B:107:ASP:OD1	8:H:37:ARG:HB2	2.12	0.48
7:G:584:MET:HE3	7:G:653:ASP:HB3	1.93	0.48
8:H:79:VAL:O	8:H:83:MET:HG2	2.13	0.48
12:L:170:VAL:HG13	12:L:238:LEU:HD23	1.95	0.48
17:Q:129:LYS:HE3	17:Q:130:PRO:HD2	1.96	0.48
12:L:71:ASP:OD2	40:p:49:LYS:HE3	2.13	0.48
14:N:101:LEU:HD11	14:N:137:LEU:HD11	1.95	0.48
32:g:88:SER:OG	32:g:90:GLU:OE2	2.29	0.48
11:K:10:SER:HB2	11:K:44:LEU:HD23	1.95	0.48
13:M:485:VAL:O	13:M:489:VAL:HG23	2.13	0.48
18:R:73:GLU:HG2	18:R:78:PRO:HA	1.96	0.48
8:H:201:ALA:HB1	8:H:202:PRO:CD	2.43	0.48
13:M:301:GLN:HB2	13:M:307:ILE:HG12	1.96	0.48
13:M:446:LEU:HB3	37:m:7:THR:HG22	1.96	0.48
23:W:98:HIS:NE2	23:W:102:GLN:OE1	2.46	0.48
30:e:13:ARG:NH1	30:e:44:CYS:O	2.46	0.48
7:G:146:THR:O	7:G:155:ARG:NH2	2.46	0.48
21:U:82:ASP:HB3	23:W:64:ARG:HH22	1.79	0.48
46:y:144:PHE:HB3	46:y:162:MET:HG3	1.95	0.48
9:I:194:LEU:HB3	17:Q:89:MET:HE2	1.96	0.48
4:D:13:LEU:HD13	4:D:32:MET:SD	2.54	0.48
8:H:14:LEU:HB2	8:H:15:PRO:HD3	1.96	0.48
12:L:413:THR:HG23	12:L:416:GLY:H	1.78	0.48
12:L:592:GLY:HA2	12:L:595:GLU:HB2	1.94	0.48
23:W:41:MET:O	23:W:47:GLN:NE2	2.47	0.48
37:m:33:ASN:O	37:m:37:ILE:HG12	2.14	0.48
46:y:180:VAL:HG12	46:y:180:VAL:O	2.14	0.48
4:D:286:MET:HE2	4:D:288:LYS:O	2.14	0.47
5:E:172:MET:HB2	6:F:185:TYR:HE1	1.79	0.47
6:F:102:GLU:HA	6:F:105:LYS:HE2	1.95	0.47
6:F:164:GLY:HA2	6:F:275:PRO:HD3	1.95	0.47
10:J:46:LEU:HA	10:J:136:ASN:ND2	2.27	0.47
12:L:102:SER:HB3	12:L:463:MET:HG3	1.95	0.47
13:M:136:MET:HE3	13:M:145:PHE:CE2	2.49	0.47
4:D:119:THR:HG21	4:D:134:ALA:HB2	1.96	0.47
4:D:365:GLY:O	4:D:369:MET:HG3	2.14	0.47
8:H:23:LEU:HA	26:a:15:ILE:HD11	1.95	0.47
12:L:553:ASN:ND2	38:n:77:LYS:O	2.47	0.47
13:M:112:MET:HA	13:M:115:TYR:HD2	1.79	0.47
16:P:282:LEU:HD12	16:P:360:PHE:CZ	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:66:ASP:OD1	18:R:67:GLY:N	2.47	0.47
3:C:126:HIS:O	23:W:11:GLY:HA2	2.14	0.47
12:L:180:LEU:HB3	12:L:224:LEU:HD13	1.94	0.47
13:M:101:ILE:HG13	13:M:127:GLU:HB2	1.95	0.47
45:x:148:TYR:HD2	45:x:165:HIS:CE1	2.32	0.47
11:K:68:VAL:HG11	14:N:153:GLU:HG3	1.97	0.47
13:M:452:LEU:HD22	13:M:456:GLU:HB3	1.96	0.47
28:c:13:GLY:N	28:c:16:ARG:HH21	2.12	0.47
5:E:137:ILE:HD11	6:F:392:ARG:NH2	2.30	0.47
12:L:567:GLN:HE22	36:l:75:LYS:HA	1.78	0.47
16:P:184:SER:O	16:P:219:PRO:HD2	2.14	0.47
7:G:172:ILE:HG23	9:I:124:ILE:HD12	1.96	0.47
7:G:385:GLY:HA2	7:G:411:GLU:HG3	1.97	0.47
13:M:228:VAL:HG13	13:M:228:VAL:O	2.15	0.47
13:M:469:TRP:HE1	49:M:501:PTY:H112	1.78	0.47
46:y:29:LEU:HD12	47:z:15:ILE:HD12	1.96	0.47
4:D:256:ASP:C	4:D:260:ARG:NH1	2.72	0.47
49:D:401:PTY:H232	8:H:188:VAL:HG22	1.95	0.47
12:L:3:LEU:HB2	28:c:55:SER:HB2	1.97	0.47
12:L:95:LEU:HB3	12:L:466:PRO:HB3	1.96	0.47
12:L:263:THR:HB	12:L:338:LEU:HD11	1.97	0.47
12:L:451:ARG:NH2	12:L:455:ARG:HH12	2.13	0.47
13:M:103:ILE:O	13:M:107:VAL:HG23	2.14	0.47
13:M:490:GLN:O	13:M:490:GLN:HG3	2.15	0.47
15:O:92:SER:OG	15:O:94:GLU:OE2	2.28	0.47
16:P:223:ILE:HD12	16:P:230:LEU:HD23	1.95	0.47
30:e:24:CYS:HB2	30:e:37:LEU:HD12	1.96	0.47
8:H:78:PRO:HA	8:H:81:THR:HG22	1.96	0.47
8:H:189:MET:HE1	8:H:310:TRP:CD1	2.50	0.47
8:H:230:LEU:HD21	52:H:500:UQ9:H12	1.96	0.47
12:L:147:SER:HB3	12:L:261:MET:SD	2.55	0.47
15:O:107:LEU:HD21	15:O:143:LEU:HD21	1.97	0.47
7:G:591:VAL:HG11	7:G:610:ALA:HA	1.96	0.47
45:x:167:ILE:HB	45:x:185:VAL:HG22	1.97	0.47
2:B:210:LYS:O	2:B:214:HIS:ND1	2.48	0.47
4:D:114:HIS:CD2	4:D:264:ARG:HG3	2.49	0.47
8:H:108:LEU:HG	10:J:51:MET:HB3	1.97	0.47
13:M:77:TYR:OH	29:d:61:ASP:OD1	2.25	0.47
16:P:289:THR:HG23	16:P:291:HIS:H	1.79	0.47
59:f:201:PGT:H142	59:f:201:PGT:H171	1.55	0.47
34:j:12:TYR:HB2	35:k:21:HIS:CD2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:q:100:ILE:HG22	41:q:101:THR:HG23	1.97	0.47
45:x:202:PRO:O	45:x:204:ARG:HG2	2.15	0.47
46:y:90:ASN:HB3	46:y:108:VAL:HG21	1.96	0.47
2:B:189:PRO:HD3	4:D:154:HIS:CD2	2.50	0.46
15:O:50:ALA:HB2	15:O:60:ILE:HD13	1.97	0.46
22:V:26:VAL:HG23	22:V:87:GLU:HG3	1.97	0.46
13:M:252:LEU:HA	13:M:256:LEU:HB2	1.97	0.46
13:M:10:PHE:O	13:M:58:GLN:NE2	2.49	0.46
14:N:149:TYR:CD1	14:N:191:LEU:HD13	2.51	0.46
35:k:10:GLU:OE2	35:k:13:ARG:NH2	2.49	0.46
39:o:10:MET:HE1	39:o:29:MET:HA	1.97	0.46
4:D:51:THR:O	4:D:55:ILE:HG12	2.15	0.46
6:F:91:LEU:HD11	6:F:279:ARG:HG3	1.98	0.46
7:G:489:PRO:HB3	7:G:710:MET:SD	2.56	0.46
11:K:61:PHE:CD1	14:N:146:ILE:HG23	2.51	0.46
12:L:57:CYS:SG	12:L:78:PHE:HB2	2.55	0.46
20:T:47:VAL:HG22	20:T:112:ILE:HD13	1.97	0.46
20:T:87:MET:O	20:T:90:GLU:N	2.49	0.46
28:c:23:THR:OG1	58:c:101:PC7:O3	2.31	0.46
47:z:153:ASP:OD1	47:z:171:GLN:HG2	2.15	0.46
31:f:57:ILE:O	31:f:57:ILE:HG13	2.16	0.46
6:F:304:HIS:HE1	6:F:384:THR:HG23	1.80	0.46
7:G:287:LEU:HB3	7:G:306:ASP:HB3	1.97	0.46
12:L:331:TYR:HB2	12:L:497:LEU:HD13	1.97	0.46
49:N:501:PTY:H381	49:N:501:PTY:H412	1.69	0.46
25:Z:108:GLU:HG3	30:e:57:ILE:HD13	1.98	0.46
33:i:57:GLU:OE2	33:i:57:GLU:N	2.49	0.46
12:L:484:MET:HG3	12:L:485:MET:HG3	1.97	0.46
13:M:56:TRP:HB2	13:M:95:ILE:HD11	1.98	0.46
16:P:243:LEU:HD12	16:P:244:PRO:HD2	1.98	0.46
28:c:15:PHE:CE1	38:n:101:PRO:HB2	2.51	0.46
12:L:68:GLU:HG3	12:L:69:MET:H	1.81	0.46
13:M:15:LEU:HD22	13:M:55:LEU:HD12	1.97	0.46
3:C:10:SER:O	3:C:14:LEU:HB2	2.16	0.46
52:H:500:UQ9:O5	52:H:500:UQ9:H8	2.15	0.46
14:N:191:LEU:HD12	14:N:191:LEU:HA	1.71	0.46
22:V:51:GLU:HG2	22:V:109:TRP:CE3	2.51	0.46
3:C:97:ARG:HG2	3:C:122:SER:HB3	1.98	0.45
4:D:335:LYS:NZ	4:D:388:VAL:HG22	2.31	0.45
6:F:368:VAL:HG12	6:F:368:VAL:O	2.17	0.45
7:G:364:ALA:O	7:G:368:VAL:HG22	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:337:GLN:HG2	16:P:338:ILE:N	2.31	0.45
20:T:49:ARG:NH2	20:T:92:GLU:O	2.49	0.45
26:a:7:GLU:OE1	26:a:7:GLU:N	2.49	0.45
30:e:30:GLU:OE1	30:e:30:GLU:N	2.47	0.45
7:G:376:LYS:HB2	7:G:379:GLU:HG2	1.98	0.45
8:H:91:VAL:HG12	8:H:167:LEU:HD12	1.98	0.45
8:H:256:ASP:OD1	8:H:256:ASP:N	2.49	0.45
13:M:11:ASN:OD1	13:M:13:SER:OG	2.26	0.45
22:V:145:THR:O	22:V:149:LEU:HG	2.16	0.45
3:C:176:ARG:NH2	9:I:138:ILE:O	2.48	0.45
4:D:182:PHE:CE2	4:D:186:ILE:HD11	2.51	0.45
6:F:79:ALA:HB1	6:F:84:ASP:HB2	1.98	0.45
7:G:292:THR:HG22	7:G:293:ILE:N	2.32	0.45
7:G:655:LYS:NZ	23:W:131:ASN:O	2.45	0.45
12:L:223:ILE:O	12:L:227:ILE:HG12	2.16	0.45
14:N:170:GLU:N	14:N:170:GLU:OE2	2.49	0.45
16:P:301:ILE:HD12	16:P:381:TYR:HB2	1.98	0.45
17:Q:49:HIS:HB3	17:Q:98:TYR:HE2	1.80	0.45
29:d:29:MET:HG3	47:z:14:TRP:CZ2	2.51	0.45
4:D:125:VAL:O	8:H:289:ARG:HB2	2.16	0.45
6:F:413:GLY:O	6:F:417:MET:HG3	2.17	0.45
7:G:440:PHE:HB2	7:G:469:VAL:HG22	1.98	0.45
12:L:484:MET:HB3	39:o:46:TYR:HB3	1.97	0.45
15:O:45:ILE:HG23	15:O:61:ILE:HG23	1.98	0.45
19:S:10:SER:HB2	19:S:94:ALA:HB3	1.98	0.45
24:X:48:LYS:HB3	24:X:48:LYS:HE3	1.70	0.45
45:x:107:ASN:HB3	45:x:125:ALA:HB1	1.98	0.45
2:B:85:TRP:CH2	8:H:58:LEU:HD11	2.52	0.45
2:B:120:ARG:HH12	2:B:145:GLN:HB3	1.82	0.45
3:C:126:HIS:HD2	3:C:128:ASP:H	1.64	0.45
6:F:85:TRP:CD2	6:F:204:LEU:HD13	2.52	0.45
8:H:304:LEU:HB3	8:H:305:PRO:HD3	1.97	0.45
12:L:102:SER:HB2	12:L:462:PRO:HB2	1.97	0.45
12:L:168:MET:HG2	13:M:430:LEU:HD12	1.98	0.45
13:M:174:PHE:HE2	14:N:437:CYS:SG	2.39	0.45
16:P:110:LYS:HE3	16:P:110:LYS:HB3	1.77	0.45
25:Z:68:ASN:OD1	25:Z:71:ARG:NH1	2.49	0.45
12:L:545:ALA:HA	12:L:548:THR:HG22	1.97	0.45
14:N:53:ASN:ND2	31:f:61:SER:OG	2.48	0.45
14:N:445:LYS:HE3	14:N:445:LYS:HB3	1.86	0.45
15:O:127:LEU:HD23	15:O:129:LYS:HD2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:107:SER:HB2	20:T:110:LEU:HD13	1.98	0.45
39:o:35:ILE:HG22	39:o:39:LYS:HE3	1.99	0.45
7:G:413:THR:H	7:G:559:GLN:NE2	2.14	0.45
8:H:240:SER:HB3	8:H:280:TYR:HE2	1.82	0.45
12:L:273:SER:HB2	12:L:331:TYR:CE2	2.51	0.45
13:M:151:ILE:HB	13:M:152:PRO:HD3	1.98	0.45
19:S:57:GLN:NE2	19:S:75:ASP:OD2	2.47	0.45
20:T:90:GLU:CD	38:n:25:ARG:HH21	2.21	0.45
10:J:116:GLN:HA	10:J:119:THR:HB	1.99	0.45
23:W:49:VAL:HG21	23:W:96:ARG:HH22	1.82	0.45
28:c:69:ILE:HD11	28:c:78:PHE:CZ	2.52	0.45
12:L:68:GLU:HG3	12:L:69:MET:N	2.31	0.45
12:L:584:VAL:HG13	12:L:585:SER:N	2.31	0.45
13:M:153:MET:HE2	13:M:252:LEU:HD21	1.99	0.45
2:B:153:ILE:HD11	2:B:202:LEU:HD22	1.99	0.45
2:B:218:LYS:HB3	16:P:100:ARG:HH12	1.81	0.45
12:L:591:LYS:HD2	37:m:23:LEU:HB3	1.97	0.45
12:L:607:ARG:HH21	12:L:608:ARG:HD2	1.82	0.45
13:M:120:ILE:H	13:M:120:ILE:HD12	1.82	0.45
20:T:63:SER:C	20:T:64:LYS:HD2	2.42	0.45
4:D:79:GLU:OE1	4:D:156:SER:HA	2.16	0.44
6:F:60:ASP:N	6:F:60:ASP:OD1	2.50	0.44
7:G:445:THR:HG23	7:G:447:PRO:HD3	1.99	0.44
11:K:61:PHE:CD1	14:N:146:ILE:HG12	2.52	0.44
12:L:157:ARG:NH2	12:L:159:GLN:OE1	2.44	0.44
14:N:24:PHE:HB2	31:f:75:MET:CE	2.47	0.44
58:c:101:PC7:H72	58:c:101:PC7:H41	1.72	0.44
58:v:201:PC7:H42	58:v:201:PC7:H83	1.61	0.44
4:D:150:GLY:HA3	9:I:108:ARG:HG3	1.98	0.44
6:F:237:GLU:HG3	6:F:245:LYS:O	2.17	0.44
13:M:150:LEU:HB3	13:M:174:PHE:CE1	2.52	0.44
15:O:41:VAL:HG22	45:x:191:ARG:HB2	1.99	0.44
19:S:11:MET:HE3	19:S:62:ALA:HB1	2.00	0.44
31:f:32:LEU:O	31:f:36:ARG:HG2	2.18	0.44
38:n:59:GLU:OE1	38:n:59:GLU:N	2.51	0.44
47:z:105:LEU:HD23	47:z:133:VAL:HG22	2.00	0.44
4:D:292:ARG:HB2	7:G:191:ASP:OD1	2.18	0.44
4:D:306:MET:HE3	4:D:310:ILE:HG13	1.99	0.44
7:G:64:ARG:NH1	17:Q:132:THR:O	2.50	0.44
12:L:121:THR:O	12:L:125:LEU:HG	2.18	0.44
12:L:584:VAL:HG13	12:L:585:SER:H	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:217:GLU:OE2	14:N:287:GLY:N	2.45	0.44
16:P:169:LEU:O	16:P:172:LYS:N	2.51	0.44
25:Z:114:ASP:OD1	25:Z:114:ASP:N	2.51	0.44
37:m:9:LYS:HD2	37:m:14:GLU:HG3	1.99	0.44
46:y:45:LEU:HD23	46:y:53:PRO:HG2	1.98	0.44
3:C:118:MET:SD	3:C:142:PRO:HG2	2.57	0.44
5:E:180:MET:HG2	5:E:199:GLU:HA	2.00	0.44
7:G:423:TYR:OH	7:G:700:PRO:HA	2.18	0.44
12:L:254:ALA:O	12:L:258:ALA:HB3	2.17	0.44
13:M:108:GLY:O	13:M:112:MET:HB2	2.16	0.44
14:N:160:TYR:OH	14:N:183:GLY:HA3	2.18	0.44
58:c:101:PC7:H122	58:c:101:PC7:H151	1.56	0.44
34:j:54:ARG:HA	34:j:54:ARG:HD2	1.84	0.44
4:D:314:GLU:HG3	7:G:186:MET:HG3	1.99	0.44
16:P:204:GLU:O	16:P:208:LEU:HD23	2.17	0.44
19:S:31:PHE:O	19:S:35:ASN:HB2	2.17	0.44
45:x:248:PHE:O	45:x:251:SER:OG	2.32	0.44
47:z:99:ASN:OD1	47:z:127:THR:HA	2.18	0.44
1:A:14:ILE:HD12	8:H:9:ILE:HD13	1.99	0.44
1:A:78:PHE:HZ	1:A:100:LEU:HD11	1.83	0.44
10:J:48:PHE:CD1	10:J:137:LEU:HD13	2.52	0.44
10:J:66:LEU:HG	10:J:70:MET:SD	2.58	0.44
10:J:143:LEU:HD12	10:J:148:TYR:HE2	1.82	0.44
13:M:46:LEU:HD22	32:g:69:THR:HG21	1.98	0.44
13:M:450:SER:HB2	38:n:108:VAL:HG23	1.98	0.44
14:N:273:ILE:O	14:N:277:ILE:HG13	2.17	0.44
16:P:208:LEU:HD21	16:P:216:ILE:HG13	2.00	0.44
16:P:328:LYS:HD3	16:P:328:LYS:HA	1.88	0.44
12:L:31:MET:HE1	28:c:41:MET:CG	2.48	0.44
13:M:73:ARG:NH2	53:M:502:LMN:O3	2.50	0.44
22:V:15:LYS:HB3	22:V:25:VAL:HG21	1.99	0.44
22:V:71:GLU:OE1	22:V:76:MET:HB3	2.18	0.44
28:c:22:MET:HE3	58:c:101:PC7:H121	1.98	0.44
40:p:36:HIS:NE2	40:p:40:GLU:OE2	2.51	0.44
1:A:81:TRP:CD2	1:A:96:MET:HG2	2.53	0.44
6:F:267:ASN:N	51:F:500:FMN:O1P	2.41	0.44
6:F:306:ASN:HB2	6:F:328:GLY:HA3	1.99	0.44
7:G:198:MET:HG3	18:R:86:PHE:CE1	2.52	0.44
7:G:486:GLY:HA3	7:G:491:THR:OG1	2.18	0.44
10:J:7:SER:O	10:J:11:LEU:HG	2.17	0.44
15:O:140:THR:HG22	15:O:142:GLU:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:64:TYR:HB2	19:S:68:VAL:HB	1.98	0.44
37:m:5:MET:HE2	37:m:5:MET:HB3	1.87	0.44
2:B:186:PRO:HD3	9:I:186:ALA:HA	2.00	0.44
6:F:446:THR:HB	48:F:501:SF4:S3	2.57	0.44
12:L:10:LEU:HB2	12:L:122:PHE:CD1	2.53	0.44
13:M:192:LEU:HD13	13:M:198:THR:HG23	2.00	0.44
14:N:159:PHE:HB3	14:N:179:TYR:HE2	1.83	0.44
16:P:152:ARG:HH21	16:P:326:VAL:HB	1.82	0.44
21:U:76:GLN:HA	21:U:81:LEU:HB2	2.00	0.44
23:W:120:LYS:HG3	23:W:121:THR:H	1.83	0.44
3:C:161:GLU:OE1	16:P:373:TYR:OH	2.28	0.43
4:D:119:THR:HB	4:D:131:PHE:HA	2.00	0.43
10:J:72:PHE:HE2	11:K:84:PHE:CG	2.36	0.43
12:L:395:LEU:HD11	12:L:475:LEU:HD23	2.00	0.43
16:P:337:GLN:OE1	16:P:337:GLN:N	2.50	0.43
38:n:18:GLU:O	38:n:22:ILE:HG12	2.18	0.43
39:o:29:MET:HB3	39:o:65:LEU:HD11	1.99	0.43
1:A:62:TYR:CE1	10:J:64:LEU:HD11	2.53	0.43
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.83	0.43
2:B:130:THR:HA	2:B:158:CYS:HB3	2.00	0.43
4:D:273:ARG:HG2	4:D:277:GLN:HE21	1.82	0.43
19:S:11:MET:HE3	19:S:62:ALA:CB	2.48	0.43
21:U:50:VAL:HG11	21:U:120:ALA:HA	2.00	0.43
45:x:157:GLU:HB3	45:x:158:PRO:HD2	1.99	0.43
47:z:140:GLU:HG3	47:z:158:GLU:HA	2.00	0.43
1:A:2:MET:HE3	1:A:2:MET:HB3	1.85	0.43
16:P:181:ILE:HG12	16:P:215:THR:OG1	2.18	0.43
16:P:321:PRO:HA	16:P:324:PHE:CZ	2.53	0.43
20:T:70:HIS:H	20:T:74:ASP:HB2	1.83	0.43
27:b:19:ALA:O	27:b:23:ILE:HG12	2.18	0.43
36:l:90:VAL:O	36:l:94:LEU:HG	2.18	0.43
2:B:99:MET:HB3	4:D:135:PHE:HE2	1.82	0.43
4:D:98:ALA:O	4:D:102:ARG:HG3	2.18	0.43
4:D:192:MET:SD	9:I:82:LEU:HD23	2.59	0.43
6:F:141:ASP:HB2	6:F:180:TYR:HD1	1.83	0.43
7:G:173:CYS:O	7:G:283:ARG:NH1	2.41	0.43
7:G:324:ASN:OD1	7:G:325:GLU:N	2.51	0.43
8:H:153:LEU:HD23	8:H:153:LEU:HA	1.91	0.43
12:L:367:LYS:HD3	12:L:367:LYS:HA	1.86	0.43
13:M:483:THR:O	13:M:487:ASN:ND2	2.50	0.43
16:P:201:ALA:O	16:P:204:GLU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:291:HIS:CE1	16:P:307:TYR:HE2	2.36	0.43
20:T:84:GLU:OE2	35:k:8:THR:OG1	2.31	0.43
23:W:39:THR:HG22	23:W:43:ILE:HD12	2.00	0.43
47:z:73:ILE:HD12	47:z:79:ILE:HD11	2.00	0.43
2:B:95:ALA:HA	2:B:98:MET:HE3	2.00	0.43
6:F:155:ARG:HB3	6:F:188:GLU:HG3	2.00	0.43
12:L:291:ALA:HB1	12:L:422:LEU:HD12	2.00	0.43
13:M:35:ARG:O	13:M:39:LEU:HD23	2.19	0.43
24:X:28:ARG:HG2	24:X:28:ARG:O	2.17	0.43
1:A:70:ILE:HG13	10:J:163:MET:HG3	2.01	0.43
4:D:73:VAL:HG11	4:D:116:LEU:HD22	1.99	0.43
6:F:55:PHE:HB3	6:F:316:SER:HB3	2.00	0.43
7:G:407:ASN:HB3	7:G:409:TRP:HZ3	1.82	0.43
8:H:57:LYS:O	8:H:61:LYS:HG2	2.17	0.43
9:I:128:LEU:HD23	9:I:173:PRO:HD3	2.01	0.43
16:P:298:TYR:CE2	16:P:305:PRO:HA	2.53	0.43
32:g:45:PHE:CZ	32:g:46:MET:HE3	2.54	0.43
45:x:247:LYS:HB3	45:x:247:LYS:HE2	1.74	0.43
47:z:124:ASP:H	47:z:141:ASP:HB3	1.83	0.43
7:G:518:ALA:HB2	7:G:554:LEU:HA	2.00	0.43
8:H:154:ILE:HG21	8:H:190:PHE:HB2	2.01	0.43
9:I:59:ASP:HB3	9:I:62:THR:HG23	2.01	0.43
9:I:218:GLU:HB2	9:I:222:ARG:HH21	1.83	0.43
22:V:24:ASP:OD1	22:V:24:ASP:N	2.46	0.43
5:E:136:MET:SD	6:F:392:ARG:NH1	2.92	0.43
5:E:176:VAL:HG13	6:F:308:PRO:HG2	2.00	0.43
7:G:409:TRP:HD1	7:G:410:CYS:O	2.01	0.43
13:M:69:VAL:HA	13:M:84:LEU:O	2.19	0.43
14:N:159:PHE:HE1	14:N:264:PHE:HD2	1.66	0.43
16:P:105:SER:OG	16:P:106:PRO:HD3	2.19	0.43
16:P:147:ARG:HD2	16:P:149:TYR:CZ	2.54	0.43
25:Z:98:VAL:O	25:Z:102:LYS:HG2	2.19	0.43
59:f:201:PGT:H122	59:f:201:PGT:H151	1.72	0.43
6:F:338:LEU:HD22	6:F:382:LYS:HA	2.01	0.43
6:F:366:LYS:HA	6:F:370:SER:O	2.19	0.43
7:G:500:HIS:HB3	7:G:503:CYS:SG	2.59	0.43
12:L:31:MET:HE3	28:c:37:THR:HG23	2.00	0.43
12:L:322:MET:HG3	12:L:337:HIS:HD2	1.84	0.43
13:M:184:MET:HE2	13:M:188:ILE:HD11	2.01	0.43
27:b:9:MET:O	27:b:13:GLN:HG2	2.19	0.43
4:D:85:ALA:HA	4:D:329:THR:HG21	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:554:LEU:H	7:G:633:THR:HG22	1.83	0.43
10:J:58:ILE:HA	10:J:62:ALA:HB3	2.01	0.43
16:P:142:ILE:HD11	16:P:269:LEU:HD11	2.01	0.43
42:r:91:LYS:HE3	42:r:93:ASN:HA	2.00	0.43
46:y:157:VAL:HG22	46:y:175:ILE:HD13	2.00	0.43
5:E:128:LEU:HD12	5:E:168:GLU:C	2.43	0.42
5:E:137:ILE:HD12	5:E:137:ILE:H	1.84	0.42
11:K:17:GLY:O	11:K:34:SER:HB3	2.19	0.42
13:M:419:ALA:O	13:M:422:MET:HG2	2.18	0.42
49:N:501:PTY:H431	49:N:501:PTY:H401	1.76	0.42
16:P:282:LEU:HD12	16:P:360:PHE:CE1	2.54	0.42
24:X:23:LYS:HD3	24:X:23:LYS:HA	1.80	0.42
39:o:22:ILE:HD11	39:o:35:ILE:HG12	1.99	0.42
3:C:107:SER:HB3	4:D:217:TRP:HA	2.01	0.42
4:D:107:GLU:OE2	4:D:242:TYR:OH	2.30	0.42
4:D:163:VAL:HG12	4:D:287:ILE:HB	2.00	0.42
8:H:126:ARG:HB3	10:J:70:MET:CE	2.46	0.42
8:H:162:VAL:HG11	8:H:170:ILE:HG12	2.01	0.42
12:L:581:GLY:HA2	13:M:296:LEU:HG	2.01	0.42
19:S:30:THR:O	19:S:34:LYS:HG2	2.18	0.42
4:D:105:PHE:HD1	4:D:145:TYR:HE1	1.68	0.42
7:G:634:GLU:OE1	7:G:693:ARG:NH2	2.53	0.42
7:G:724:MET:SD	7:G:730:ARG:HA	2.59	0.42
12:L:237:GLY:C	12:L:238:LEU:HD12	2.45	0.42
16:P:245:LEU:HD12	16:P:309:LYS:HD3	2.00	0.42
22:V:98:THR:O	22:V:102:LYS:HG3	2.19	0.42
27:b:5:GLU:HG3	27:b:9:MET:HE3	2.00	0.42
28:c:25:GLY:HA2	58:c:101:PC7:H62	2.01	0.42
40:p:11:GLU:OE1	40:p:11:GLU:N	2.53	0.42
46:y:253:PRO:HD2	46:y:256:LEU:HD12	1.99	0.42
4:D:115:LEU:HD23	4:D:115:LEU:HA	1.93	0.42
5:E:137:ILE:HD11	6:F:392:ARG:HH22	1.84	0.42
7:G:653:ASP:O	7:G:657:VAL:HG23	2.19	0.42
12:L:242:LEU:HD11	12:L:257:HIS:HB3	2.01	0.42
13:M:129:LEU:HD22	13:M:148:SER:OG	2.20	0.42
13:M:151:ILE:HD11	14:N:401:ILE:HG21	2.02	0.42
14:N:101:LEU:CD1	14:N:137:LEU:HD11	2.49	0.42
49:N:501:PTY:H202	29:d:16:THR:HG21	2.00	0.42
15:O:103:TRP:CZ3	15:O:143:LEU:HA	2.54	0.42
16:P:233:TRP:HB3	16:P:297:MET:HE1	2.00	0.42
20:T:49:ARG:NE	20:T:92:GLU:OE2	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:c:69:ILE:HD11	28:c:78:PHE:HZ	1.84	0.42
31:f:62:MET:HE1	44:v:81:ASN:O	2.19	0.42
46:y:209:ASN:HD21	46:y:261:ASN:CB	2.31	0.42
1:A:71:PHE:CZ	8:H:304:LEU:HD21	2.54	0.42
3:C:142:PRO:HA	3:C:147:PHE:CD2	2.54	0.42
7:G:411:GLU:OE2	7:G:586:ALA:HA	2.19	0.42
7:G:684:ALA:HB3	7:G:687:LEU:HD12	2.00	0.42
12:L:64:TRP:H	12:L:73:SER:HA	1.83	0.42
12:L:137:PHE:CD1	12:L:178:LEU:HD23	2.53	0.42
14:N:24:PHE:HD2	14:N:65:THR:HB	1.83	0.42
16:P:186:LEU:HD22	16:P:220:ALA:HB2	2.01	0.42
20:T:98:PRO:HG2	20:T:101:GLU:OE2	2.20	0.42
22:V:118:GLU:HG3	42:r:88:VAL:HG22	2.02	0.42
29:d:64:LEU:HD13	33:i:43:MET:HE2	2.00	0.42
46:y:68:ILE:HG21	47:z:214:HIS:HE1	1.85	0.42
47:z:99:ASN:HD22	47:z:207:TYR:CB	2.32	0.42
1:A:15:SER:HA	1:A:18:VAL:HG12	2.01	0.42
4:D:87:GLU:OE2	22:V:129:HIS:NE2	2.46	0.42
5:E:135:CYS:SG	5:E:171:CYS:SG	3.16	0.42
7:G:64:ARG:HH21	17:Q:134:LEU:HD12	1.85	0.42
7:G:422:ARG:HA	7:G:425:TYR:CE2	2.55	0.42
8:H:205:LEU:HG	8:H:206:PRO:HD3	2.01	0.42
12:L:355:VAL:HG23	12:L:378:THR:HG21	2.00	0.42
13:M:318:LEU:HD21	13:M:400:GLU:HG2	2.02	0.42
38:n:30:ASP:OD1	38:n:80:HIS:N	2.49	0.42
46:y:135:HIS:CD2	47:z:130:HIS:NE2	2.87	0.42
3:C:156:ARG:NH1	3:C:167:GLU:OE2	2.43	0.42
5:E:128:LEU:HD12	5:E:168:GLU:O	2.19	0.42
6:F:149:LYS:HD2	6:F:269:GLU:OE2	2.20	0.42
6:F:234:ALA:HB2	6:F:246:PRO:HG3	2.01	0.42
6:F:472:ARG:HA	6:F:475:GLU:HG3	2.01	0.42
7:G:373:HIS:NE2	7:G:664:SER:O	2.49	0.42
7:G:419:ALA:O	19:S:51:ARG:NH2	2.34	0.42
12:L:439:PHE:HD1	12:L:443:LEU:HD12	1.84	0.42
40:p:78:LEU:HA	40:p:81:THR:HG22	2.00	0.42
1:A:68:PHE:CG	8:H:145:VAL:HG13	2.55	0.42
3:C:107:SER:HB2	3:C:111:TRP:HZ3	1.85	0.42
6:F:408:CYS:HB3	48:F:501:SF4:S4	2.59	0.42
7:G:526:LYS:HB3	7:G:526:LYS:HE2	1.89	0.42
14:N:50:LEU:HD23	14:N:50:LEU:H	1.84	0.42
49:N:501:PTY:H331	49:N:501:PTY:H362	1.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:97:PHE:HD2	21:U:99:PHE:HD1	1.67	0.42
22:V:120:ILE:HG13	42:r:86:ARG:HG2	2.01	0.42
61:z:301:PSF:H42	61:z:301:PSF:HB1	2.02	0.42
6:F:137:VAL:HG11	6:F:235:LEU:HD22	2.02	0.42
10:J:143:LEU:HD12	10:J:148:TYR:CE2	2.54	0.42
6:F:161:LEU:HD13	6:F:268:VAL:HG13	2.02	0.42
7:G:169:ASP:HA	18:R:99:TYR:OH	2.20	0.42
7:G:325:GLU:HB2	7:G:457:ARG:HH22	1.85	0.42
11:K:31:MET:HE2	14:N:181:ILE:HG21	2.02	0.42
21:U:72:LYS:HA	21:U:72:LYS:HD3	1.94	0.42
22:V:58:GLU:HG2	22:V:62:ARG:NH1	2.35	0.42
25:Z:20:LEU:H	25:Z:20:LEU:HD23	1.85	0.42
5:E:179:PRO:O	5:E:201:VAL:HG12	2.19	0.41
7:G:310:PRO:HA	7:G:645:PRO:HD2	2.02	0.41
12:L:47:PHE:HD1	12:L:83:VAL:HG12	1.85	0.41
12:L:235:GLN:O	12:L:239:HIS:HB3	2.20	0.41
13:M:36:LEU:O	13:M:40:ILE:HG13	2.19	0.41
13:M:184:MET:HB2	13:M:223:SER:HB3	2.01	0.41
13:M:482:HIS:HA	13:M:485:VAL:HG22	2.02	0.41
14:N:354:LEU:HA	14:N:354:LEU:HD23	1.74	0.41
22:V:102:LYS:HA	22:V:105:GLU:HG2	2.02	0.41
58:c:101:PC7:H172	58:c:101:PC7:H202	1.81	0.41
32:g:64:LEU:HB3	32:g:65:PRO:HD3	2.01	0.41
45:x:54:TRP:CE2	47:z:222:LEU:HD22	2.55	0.41
3:C:60:CYS:SG	3:C:74:VAL:HB	2.60	0.41
5:E:133:THR:HG23	6:F:392:ARG:HE	1.85	0.41
7:G:673:ILE:O	7:G:677:ARG:HG3	2.20	0.41
9:I:141:GLU:HB2	9:I:154:ARG:HB3	2.01	0.41
12:L:157:ARG:NH2	38:n:92:GLY:O	2.52	0.41
14:N:60:LEU:O	14:N:64:ILE:HG13	2.20	0.41
41:q:82:ASP:C	41:q:84:TYR:H	2.28	0.41
3:C:63:ASP:O	4:D:351:TYR:OH	2.37	0.41
7:G:391:GLU:HA	7:G:680:ILE:HD11	2.01	0.41
8:H:61:LYS:HD2	8:H:61:LYS:HA	1.92	0.41
10:J:9:LEU:HB2	10:J:36:ASP:OD2	2.20	0.41
13:M:251:ILE:HG22	13:M:256:LEU:HD23	2.03	0.41
59:f:201:PGT:H191	59:f:201:PGT:H162	1.78	0.41
2:B:76:MET:HE1	2:B:211:ASP:HB2	2.02	0.41
3:C:13:THR:HG23	22:V:53:TYR:HA	2.02	0.41
3:C:143:LEU:HD23	3:C:143:LEU:HA	1.83	0.41
8:H:28:ARG:HH22	8:H:50:GLN:HG2	1.83	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:148:TYR:CD1	12:L:164:ALA:HB1	2.56	0.41
12:L:304:GLN:HB2	12:L:310:VAL:HG22	2.01	0.41
12:L:321:TYR:OH	12:L:423:GLY:O	2.29	0.41
13:M:26:LEU:HD23	13:M:37:ILE:HG23	2.01	0.41
13:M:210:GLU:HA	13:M:213:GLN:CD	2.45	0.41
13:M:433:TYR:OH	58:c:101:PC7:H352	2.21	0.41
14:N:302:MET:SD	14:N:332:ILE:HD11	2.61	0.41
16:P:157:GLU:OE2	16:P:161:HIS:ND1	2.53	0.41
45:x:59:GLN:NE2	45:x:63:ILE:HD11	2.35	0.41
4:D:201:GLN:NE2	49:D:401:PTY:O13	2.54	0.41
5:E:201:VAL:HA	5:E:205:LYS:HD2	2.03	0.41
12:L:606:PHE:HA	12:L:609:LEU:HB3	2.02	0.41
39:o:35:ILE:HB	39:o:36:PRO:HD3	2.03	0.41
41:q:84:TYR:C	41:q:86:ALA:H	2.28	0.41
3:C:38:LEU:HD21	3:C:75:TYR:CE1	2.55	0.41
7:G:377:PRO:O	7:G:405:SER:HB2	2.21	0.41
7:G:693:ARG:HA	7:G:693:ARG:HD3	1.80	0.41
9:I:58:LYS:HB2	27:b:8:ARG:NH2	2.34	0.41
14:N:382:LYS:HA	14:N:382:LYS:HD3	1.79	0.41
32:g:45:PHE:CE2	32:g:46:MET:HE3	2.56	0.41
7:G:304:ARG:CZ	7:G:316:ILE:HD11	2.51	0.41
8:H:57:LYS:HD2	8:H:57:LYS:HA	1.84	0.41
12:L:30:ILE:HG22	12:L:31:MET:HE2	2.03	0.41
13:M:75:LEU:HD12	13:M:79:ASN:HB3	2.02	0.41
45:x:201:ASN:HB3	45:x:202:PRO:HD3	2.02	0.41
5:E:169:MET:HE2	5:E:171:CYS:CA	2.47	0.41
7:G:512:PRO:HB2	7:G:542:VAL:HG12	2.02	0.41
12:L:166:LYS:NZ	12:L:566:ASP:OD1	2.48	0.41
12:L:411:LYS:HG3	12:L:413:THR:HG22	2.03	0.41
13:M:62:SER:C	13:M:483:THR:HG21	2.45	0.41
21:U:61:PHE:O	21:U:62:GLN:HG2	2.21	0.41
31:f:45:VAL:HG13	31:f:62:MET:HG3	2.03	0.41
46:y:30:GLN:HG3	47:z:12:GLY:HA3	2.02	0.41
2:B:90:GLY:H	4:D:20:PRO:HD3	1.85	0.41
2:B:94:CYS:HB3	2:B:128:ALA:HB1	2.01	0.41
2:B:98:MET:HE2	2:B:128:ALA:HB3	2.02	0.41
7:G:431:ILE:O	7:G:457:ARG:HD2	2.20	0.41
8:H:87:VAL:HG22	8:H:109:TYR:OH	2.20	0.41
13:M:146:PHE:CE1	13:M:259:PHE:HB3	2.42	0.41
13:M:383:PHE:CZ	13:M:467:LEU:HD22	2.56	0.41
14:N:218:ILE:HG23	14:N:222:ARG:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:223:ILE:HG13	16:P:370:LEU:HD23	2.03	0.41
41:q:83:ARG:C	41:q:85:ASN:H	2.29	0.41
47:z:54:ILE:HD12	47:z:72:HIS:CD2	2.55	0.41
47:z:147:MET:O	47:z:166:GLY:N	2.49	0.41
5:E:147:LEU:HD11	5:E:210:VAL:HG21	2.03	0.41
6:F:313:GLU:OE1	6:F:326:HIS:NE2	2.53	0.41
7:G:421:LEU:HB3	7:G:423:TYR:CE1	2.55	0.41
7:G:603:GLN:NE2	7:G:653:ASP:HA	2.35	0.41
10:J:108:GLU:OE2	14:N:223:SER:OG	2.27	0.41
13:M:75:LEU:HD11	13:M:80:ILE:HD12	2.03	0.41
49:M:501:PTY:H391	49:M:501:PTY:H422	1.86	0.41
16:P:286:ASP:HB2	16:P:288:PHE:CE1	2.56	0.41
35:k:20:LYS:HB2	35:k:20:LYS:HE3	1.78	0.41
45:x:151:LEU:HB3	45:x:154:CYS:SG	2.61	0.41
46:y:37:GLU:HG3	47:z:43:ARG:HD3	2.03	0.41
3:C:118:MET:HE3	3:C:133:LEU:HD12	2.02	0.40
4:D:94:VAL:HG22	4:D:161:GLY:O	2.21	0.40
4:D:119:THR:HG21	4:D:134:ALA:CB	2.51	0.40
12:L:23:LEU:HB3	12:L:27:GLY:HA3	2.03	0.40
12:L:180:LEU:HD23	12:L:180:LEU:HA	1.88	0.40
12:L:236:ILE:N	12:L:293:THR:OG1	2.54	0.40
12:L:504:GLU:O	36:l:110:ARG:NH1	2.42	0.40
13:M:411:ASN:HB3	13:M:414:VAL:HG12	2.02	0.40
15:O:133:LEU:HD23	15:O:133:LEU:HA	1.94	0.40
16:P:140:VAL:HG22	16:P:179:ARG:HB2	2.03	0.40
16:P:184:SER:OG	16:P:185:CYS:N	2.54	0.40
16:P:285:PRO:HD3	16:P:367:PRO:HB2	2.04	0.40
19:S:79:GLU:HB3	19:S:80:PRO:HD3	2.01	0.40
22:V:134:ARG:HG3	22:V:134:ARG:O	2.21	0.40
58:c:101:PC7:H222	58:c:101:PC7:H191	1.85	0.40
40:p:46:GLU:OE1	40:p:49:LYS:HD3	2.21	0.40
46:y:209:ASN:HD21	46:y:261:ASN:CG	2.29	0.40
1:A:21:ILE:O	1:A:25:VAL:HG23	2.20	0.40
1:A:75:VAL:HG12	1:A:79:PHE:CZ	2.55	0.40
3:C:160:PRO:HG2	16:P:86:GLN:HG2	2.03	0.40
6:F:313:GLU:CD	6:F:326:HIS:HE2	2.28	0.40
6:F:349:LEU:HD23	6:F:350:ILE:N	2.36	0.40
10:J:170:THR:O	10:J:170:THR:OG1	2.39	0.40
12:L:584:VAL:HG23	37:m:36:LEU:HG	2.03	0.40
14:N:73:ALA:HB3	14:N:74:PRO:HD3	2.03	0.40
14:N:107:THR:HG21	14:N:264:PHE:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:70:LYS:C	17:Q:71:LEU:HD12	2.47	0.40
22:V:118:GLU:N	22:V:118:GLU:OE1	2.54	0.40
6:F:443:GLU:OE1	6:F:459:GLN:NE2	2.45	0.40
6:F:466:ARG:N	6:F:467:PRO:HD2	2.36	0.40
7:G:632:ASN:OD1	7:G:636:PHE:HB3	2.20	0.40
12:L:67:SER:HB2	12:L:70:PHE:HB3	2.03	0.40
12:L:284:ILE:HG23	12:L:415:SER:HB2	2.02	0.40
12:L:541:GLN:HB3	38:n:40:ILE:HG21	2.03	0.40
13:M:176:TYR:O	13:M:179:LEU:HG	2.21	0.40
20:T:53:VAL:HG11	20:T:89:ILE:HG13	2.02	0.40
28:c:26:PRO:HD3	58:c:101:PC7:H62	2.03	0.40
41:q:56:LYS:HE3	41:q:57:PHE:CZ	2.56	0.40
47:z:225:ILE:HD12	47:z:225:ILE:H	1.86	0.40
2:B:84:ILE:O	2:B:113:ILE:HA	2.20	0.40
12:L:242:LEU:HB3	12:L:243:PRO:HD3	2.04	0.40
16:P:158:ASP:OD1	16:P:162:HIS:ND1	2.50	0.40
16:P:201:ALA:O	16:P:205:GLU:OE1	2.39	0.40
16:P:343:GLN:HE21	16:P:343:GLN:HB3	1.72	0.40
28:c:81:LYS:HE2	40:p:57:TRP:CE2	2.56	0.40
46:y:168:LEU:HD12	47:z:166:GLY:HA3	2.04	0.40
47:z:144:PHE:HD2	47:z:162:MET:HG3	1.86	0.40
6:F:297:LYS:HE3	6:F:375:ALA:HB3	2.02	0.40
7:G:175:GLN:O	7:G:179:CYS:HB2	2.22	0.40
8:H:275:PHE:O	8:H:279:LEU:HD23	2.21	0.40
14:N:369:THR:HG22	15:O:84:ARG:HH12	1.86	0.40
16:P:328:LYS:HG3	16:P:330:PRO:HD2	2.03	0.40
38:n:25:ARG:HG2	38:n:25:ARG:HH11	1.87	0.40
46:y:56:ASP:HB3	46:y:59:VAL:HG23	2.02	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	88/119 (74%)	86 (98%)	2 (2%)	0	100	100
2	B	155/218 (71%)	147 (95%)	8 (5%)	0	100	100
3	C	183/190 (96%)	179 (98%)	4 (2%)	0	100	100
4	D	383/394 (97%)	368 (96%)	15 (4%)	0	100	100
5	E	190/255 (74%)	182 (96%)	8 (4%)	0	100	100
6	F	432/486 (89%)	421 (98%)	11 (2%)	0	100	100
7	G	686/748 (92%)	654 (95%)	31 (4%)	1 (0%)	48	78
8	H	307/325 (94%)	289 (94%)	17 (6%)	1 (0%)	36	65
9	I	163/222 (73%)	161 (99%)	2 (1%)	0	100	100
10	J	143/205 (70%)	136 (95%)	7 (5%)	0	100	100
11	K	88/100 (88%)	84 (96%)	4 (4%)	0	100	100
12	L	613/669 (92%)	582 (95%)	31 (5%)	0	100	100
13	M	483/495 (98%)	474 (98%)	8 (2%)	1 (0%)	43	71
14	N	486/499 (97%)	474 (98%)	12 (2%)	0	100	100
15	O	120/159 (76%)	115 (96%)	5 (4%)	0	100	100
16	P	330/402 (82%)	318 (96%)	12 (4%)	0	100	100
17	Q	117/154 (76%)	111 (95%)	6 (5%)	0	100	100
18	R	60/110 (54%)	57 (95%)	3 (5%)	0	100	100
19	S	91/97 (94%)	81 (89%)	10 (11%)	0	100	100
20	T	82/122 (67%)	77 (94%)	5 (6%)	0	100	100
21	U	81/126 (64%)	75 (93%)	6 (7%)	0	100	100
22	V	138/169 (82%)	135 (98%)	3 (2%)	0	100	100
23	W	108/133 (81%)	101 (94%)	7 (6%)	0	100	100
24	X	95/106 (90%)	92 (97%)	3 (3%)	0	100	100
25	Z	123/143 (86%)	118 (96%)	4 (3%)	1 (1%)	16	44
26	a	56/65 (86%)	56 (100%)	0	0	100	100
27	b	38/65 (58%)	38 (100%)	0	0	100	100
28	c	74/88 (84%)	74 (100%)	0	0	100	100
29	d	73/81 (90%)	71 (97%)	2 (3%)	0	100	100
30	e	63/83 (76%)	63 (100%)	0	0	100	100
31	f	99/106 (93%)	96 (97%)	3 (3%)	0	100	100
32	g	73/114 (64%)	71 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	i	83/98 (85%)	80 (96%)	3 (4%)	0	100	100
34	j	49/69 (71%)	44 (90%)	5 (10%)	0	100	100
35	k	45/72 (62%)	42 (93%)	3 (7%)	0	100	100
36	l	62/125 (50%)	57 (92%)	5 (8%)	0	100	100
37	m	68/71 (96%)	63 (93%)	5 (7%)	0	100	100
38	n	107/117 (92%)	105 (98%)	2 (2%)	0	100	100
39	o	78/103 (76%)	76 (97%)	2 (3%)	0	100	100
40	p	91/106 (86%)	87 (96%)	4 (4%)	0	100	100
41	q	63/159 (40%)	56 (89%)	7 (11%)	0	100	100
42	r	8/131 (6%)	7 (88%)	1 (12%)	0	100	100
44	v	28/113 (25%)	27 (96%)	1 (4%)	0	100	100
45	x	212/256 (83%)	206 (97%)	6 (3%)	0	100	100
46	y	266/278 (96%)	255 (96%)	11 (4%)	0	100	100
47	z	231/275 (84%)	227 (98%)	4 (2%)	0	100	100
All	All	7612/9221 (83%)	7318 (96%)	290 (4%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	201	ALA
7	G	253	GLU
13	M	231	VAL
25	Z	120	VAL

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	83/106 (78%)	83 (100%)	0	100	100
2	B	132/184 (72%)	132 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	175/179 (98%)	175 (100%)	0	100	100
4	D	331/340 (97%)	331 (100%)	0	100	100
5	E	166/220 (76%)	165 (99%)	1 (1%)	78	80
6	F	353/396 (89%)	353 (100%)	0	100	100
7	G	571/625 (91%)	571 (100%)	0	100	100
8	H	262/272 (96%)	262 (100%)	0	100	100
9	I	147/195 (75%)	147 (100%)	0	100	100
10	J	131/186 (70%)	131 (100%)	0	100	100
11	K	78/86 (91%)	78 (100%)	0	100	100
12	L	518/568 (91%)	518 (100%)	0	100	100
13	M	426/434 (98%)	426 (100%)	0	100	100
14	N	406/416 (98%)	406 (100%)	0	100	100
15	O	107/141 (76%)	107 (100%)	0	100	100
16	P	273/334 (82%)	273 (100%)	0	100	100
17	Q	100/128 (78%)	100 (100%)	0	100	100
18	R	55/97 (57%)	55 (100%)	0	100	100
19	S	82/85 (96%)	82 (100%)	0	100	100
20	T	79/112 (70%)	79 (100%)	0	100	100
21	U	75/113 (66%)	75 (100%)	0	100	100
22	V	123/148 (83%)	123 (100%)	0	100	100
23	W	98/114 (86%)	98 (100%)	0	100	100
24	X	87/94 (93%)	87 (100%)	0	100	100
25	Z	100/115 (87%)	100 (100%)	0	100	100
26	a	48/53 (91%)	48 (100%)	0	100	100
27	b	33/53 (62%)	33 (100%)	0	100	100
28	c	66/71 (93%)	66 (100%)	0	100	100
29	d	60/66 (91%)	60 (100%)	0	100	100
30	e	60/73 (82%)	60 (100%)	0	100	100
31	f	81/84 (96%)	81 (100%)	0	100	100
32	g	65/96 (68%)	65 (100%)	0	100	100
33	i	77/90 (86%)	77 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	j	42/51 (82%)	42 (100%)	0	100	100
35	k	38/60 (63%)	38 (100%)	0	100	100
36	l	53/97 (55%)	53 (100%)	0	100	100
37	m	58/59 (98%)	58 (100%)	0	100	100
38	n	92/99 (93%)	92 (100%)	0	100	100
39	o	70/87 (80%)	70 (100%)	0	100	100
40	p	83/93 (89%)	83 (100%)	0	100	100
41	q	54/133 (41%)	54 (100%)	0	100	100
42	r	10/118 (8%)	10 (100%)	0	100	100
44	v	23/84 (27%)	23 (100%)	0	100	100
45	x	183/216 (85%)	183 (100%)	0	100	100
46	y	223/232 (96%)	223 (100%)	0	100	100
47	z	188/228 (82%)	188 (100%)	0	100	100
All	All	6565/7831 (84%)	6564 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	135	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	212	GLN
4	D	244	GLN
5	E	84	ASN
5	E	94	ASN
6	F	54	HIS
6	F	72	HIS
6	F	159	HIS
6	F	304	HIS
6	F	336	ASN
7	G	93	GLN
7	G	206	ASN
7	G	320	ASN
7	G	386	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	639	GLN
8	H	176	GLN
8	H	322	GLN
9	I	95	ASN
9	I	190	HIS
10	J	118	ASN
10	J	136	ASN
11	K	59	GLN
12	L	109	HIS
12	L	318	GLN
12	L	340	ASN
12	L	363	GLN
12	L	447	ASN
12	L	567	GLN
13	M	58	GLN
13	M	201	GLN
13	M	482	HIS
13	M	490	GLN
14	N	53	ASN
14	N	326	HIS
14	N	464	ASN
14	N	491	HIS
15	O	130	HIS
16	P	117	GLN
16	P	361	GLN
17	Q	149	ASN
18	R	106	GLN
19	S	88	ASN
22	V	85	GLN
22	V	132	GLN
23	W	62	GLN
24	X	87	ASN
25	Z	63	GLN
26	a	26	GLN
26	a	39	HIS
28	c	27	ASN
29	d	47	ASN
29	d	48	GLN
32	g	95	GLN
33	i	34	HIS
36	l	99	ASN
38	n	37	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	o	85	GLN
45	x	61	GLN
45	x	116	ASN
45	x	165	HIS
46	y	42	HIS
46	y	101	GLN
46	y	130	HIS
46	y	171	GLN
46	y	224	GLN
47	z	47	ASN
47	z	101	GLN
47	z	118	HIS
47	z	160	HIS
47	z	172	ASN
47	z	184	ASN
47	z	218	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 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
49	PTY	N	501	-	49,49,49	0.87	4 (8%)	52,54,54	1.12	2 (3%)
48	SF4	I	500	9	0,12,12	-	-	-	-	-
55	NDP	P	500	-	51,52,52	2.37	7 (13%)	71,80,80	1.55	17 (23%)
51	FMN	F	500	-	33,33,33	1.07	2 (6%)	48,50,50	1.24	8 (16%)
60	T7X	f	202	-	61,61,61	0.85	4 (6%)	70,73,73	1.07	2 (2%)
50	FES	E	500	5	0,4,4	-	-	-	-	-
52	UQ9	H	500	-	35,35,58	2.54	14 (40%)	43,45,73	2.05	12 (27%)
53	LMN	M	502	-	72,72,72	1.68	15 (20%)	92,98,98	1.06	4 (4%)
58	PC7	c	101	-	51,51,51	0.99	4 (7%)	57,59,59	1.04	2 (3%)
48	SF4	I	501	9	0,12,12	-	-	-	-	-
49	PTY	M	501	-	49,49,49	0.89	4 (8%)	52,54,54	1.10	2 (3%)
57	8Q1	n	200	-	32,34,34	1.61	5 (15%)	39,43,43	1.59	5 (12%)
49	PTY	D	401	-	49,49,49	0.88	4 (8%)	52,54,54	1.11	2 (3%)
48	SF4	B	500	2	0,12,12	-	-	-	-	-
59	PGT	f	201	-	40,40,50	1.18	4 (10%)	43,46,56	1.12	2 (4%)
58	PC7	v	201	-	51,51,51	0.98	4 (7%)	57,59,59	1.05	2 (3%)
48	SF4	G	803	7	0,12,12	-	-	-	-	-
48	SF4	F	501	6	0,12,12	-	-	-	-	-
50	FES	G	801	7	0,4,4	-	-	-	-	-
48	SF4	G	802	7	0,12,12	-	-	-	-	-
57	8Q1	W	200	-	32,34,34	1.63	6 (18%)	39,43,43	1.59	4 (10%)
61	PSF	z	301	-	28,29,29	1.20	4 (14%)	30,36,36	1.22	2 (6%)

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
49	PTY	N	501	-	-	22/53/53/53	-
48	SF4	I	500	9	-	-	0/6/5/5
55	NDP	P	500	-	-	8/34/77/77	0/5/5/5
51	FMN	F	500	-	-	8/18/18/18	0/3/3/3
60	T7X	f	202	-	-	29/56/80/80	0/1/1/1
50	FES	E	500	5	-	-	0/1/1/1
52	UQ9	H	500	-	-	7/30/54/81	0/1/1/1
53	LMN	M	502	-	-	38/50/130/130	0/4/4/4
58	PC7	c	101	-	-	29/55/55/55	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	SF4	I	501	9	-	-	0/6/5/5
49	PTY	M	501	-	-	25/53/53/53	-
57	8Q1	n	200	-	-	19/41/41/41	-
49	PTY	D	401	-	-	18/53/53/53	-
59	PGT	f	201	-	-	21/45/45/55	-
48	SF4	B	500	2	-	-	0/6/5/5
58	PC7	v	201	-	-	20/55/55/55	-
48	SF4	G	803	7	-	-	0/6/5/5
48	SF4	F	501	6	-	-	0/6/5/5
57	8Q1	W	200	-	-	25/41/41/41	-
48	SF4	G	802	7	-	-	0/6/5/5
50	FES	G	801	7	-	-	0/1/1/1
61	PSF	z	301	-	-	10/35/35/35	-

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	P	500	NDP	P2B-O2B	13.57	1.83	1.59
52	H	500	UQ9	C6-C1	9.96	1.53	1.35
57	W	200	8Q1	C34-N36	5.16	1.45	1.33
57	W	200	8Q1	C39-N41	5.15	1.45	1.33
57	n	200	8Q1	C39-N41	5.08	1.45	1.33
57	n	200	8Q1	C34-N36	5.07	1.45	1.33
52	H	500	UQ9	C4-C3	4.87	1.53	1.36
53	M	502	LMN	O5-C1	4.67	1.53	1.41
55	P	500	NDP	PA-O3	4.51	1.64	1.59
53	M	502	LMN	CBS-CCM	4.28	1.63	1.53
53	M	502	LMN	CBT-CCM	4.16	1.62	1.53
55	P	500	NDP	PN-O5D	3.98	1.75	1.59
53	M	502	LMN	CBR-CCM	3.76	1.61	1.54
53	M	502	LMN	O1-C1	-3.73	1.34	1.40
52	H	500	UQ9	C7-C8	3.63	1.56	1.50
51	F	500	FMN	C4A-N5	3.39	1.38	1.30
55	P	500	NDP	O2B-C2B	-3.24	1.33	1.44
59	f	201	PGT	O2-C31	2.94	1.42	1.34
59	f	201	PGT	O3-C11	2.94	1.41	1.33
58	c	101	PC7	O2-C2	-2.88	1.39	1.46
53	M	502	LMN	O4-C4	2.83	1.51	1.43
53	M	502	LMN	OBY-CCR	2.83	1.49	1.41
53	M	502	LMN	OBZ-CCS	2.79	1.49	1.41
58	v	201	PC7	O2-C2	-2.77	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	M	501	PTY	O7-C6	-2.77	1.40	1.46
61	z	301	PSF	O11-C3	-2.74	1.40	1.46
49	D	401	PTY	O7-C6	-2.70	1.40	1.46
53	M	502	LMN	OBX-CCF	2.60	1.50	1.44
52	H	500	UQ9	C11-C9	2.60	1.56	1.51
52	H	500	UQ9	C6-C5	2.50	1.53	1.46
52	H	500	UQ9	C16-C14	2.49	1.56	1.51
52	H	500	UQ9	C21-C19	2.45	1.56	1.51
52	H	500	UQ9	C7-C6	2.44	1.56	1.51
57	W	200	8Q1	C1-S44	2.43	1.82	1.76
52	H	500	UQ9	O4-C4M	-2.42	1.39	1.45
57	n	200	8Q1	C1-S44	2.41	1.81	1.76
49	M	501	PTY	O4-C30	2.40	1.40	1.33
58	v	201	PC7	O3-C11	2.39	1.40	1.33
51	F	500	FMN	C10-N1	2.38	1.38	1.33
52	H	500	UQ9	C26-C24	2.38	1.56	1.51
57	W	200	8Q1	O40-C39	-2.37	1.18	1.23
57	n	200	8Q1	O35-C34	-2.36	1.18	1.23
49	N	501	PTY	O4-C30	2.36	1.40	1.33
55	P	500	NDP	C5A-C4A	2.36	1.43	1.39
60	f	202	T7X	O16-C10	2.36	1.40	1.34
60	f	202	T7X	O18-C11	2.36	1.40	1.33
53	M	502	LMN	OBX-CCJ	2.35	1.47	1.41
49	N	501	PTY	O7-C6	-2.34	1.41	1.46
61	z	301	PSF	O52-C5	2.34	1.40	1.33
58	c	101	PC7	O3-C11	2.34	1.40	1.33
49	D	401	PTY	O4-C30	2.31	1.40	1.33
57	W	200	8Q1	O35-C34	-2.31	1.19	1.23
60	f	202	T7X	O16-C8	-2.29	1.41	1.46
58	c	101	PC7	O3-C3	-2.28	1.40	1.45
49	D	401	PTY	O4-C1	-2.28	1.40	1.45
57	n	200	8Q1	O40-C39	-2.27	1.18	1.23
49	N	501	PTY	O7-C8	2.25	1.40	1.34
55	P	500	NDP	C2A-N1A	2.25	1.37	1.33
49	M	501	PTY	O4-C1	-2.24	1.40	1.45
61	z	301	PSF	O52-C4	-2.24	1.40	1.45
49	N	501	PTY	O4-C1	-2.23	1.40	1.45
59	f	201	PGT	P-O3P	2.22	1.68	1.59
58	v	201	PC7	O3-C3	-2.21	1.40	1.45
53	M	502	LMN	C3-C4	-2.21	1.46	1.52
60	f	202	T7X	O18-C9	-2.19	1.40	1.45
52	H	500	UQ9	C17-C18	2.14	1.57	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	M	501	PTY	O7-C8	2.13	1.40	1.34
53	M	502	LMN	OCB-CCQ	2.12	1.49	1.43
49	D	401	PTY	O7-C8	2.12	1.40	1.34
59	f	201	PGT	O2-C2	-2.10	1.41	1.46
53	M	502	LMN	CBQ-CCM	2.10	1.58	1.54
58	v	201	PC7	O2-C31	2.10	1.40	1.34
57	W	200	8Q1	C6-C1	2.07	1.53	1.50
55	P	500	NDP	O5D-C5D	-2.07	1.36	1.44
61	z	301	PSF	O11-C1	2.07	1.40	1.34
53	M	502	LMN	O5-C5	2.06	1.49	1.44
52	H	500	UQ9	O2-C2	-2.05	1.18	1.23
58	c	101	PC7	O2-C31	2.05	1.40	1.34
52	H	500	UQ9	O5-C5	-2.05	1.18	1.23
52	H	500	UQ9	O3-C3M	-2.04	1.40	1.45
53	M	502	LMN	CBQ-CBK	2.02	1.59	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	H	500	UQ9	C7-C6-C5	5.61	125.03	118.52
57	n	200	8Q1	C6-C1-S44	5.56	120.03	113.40
57	W	200	8Q1	C6-C1-S44	5.52	119.98	113.40
52	H	500	UQ9	C7-C6-C1	-5.39	115.65	124.89
55	P	500	NDP	P2B-O2B-C2B	-4.43	111.60	123.43
60	f	202	T7X	O16-C10-C12	4.29	120.76	111.48
53	M	502	LMN	CCR-O4-C4	-4.25	107.90	117.98
59	f	201	PGT	O2-C31-C32	4.11	120.36	111.48
49	N	501	PTY	O7-C8-C11	4.10	120.35	111.48
49	M	501	PTY	O7-C8-C11	4.10	120.34	111.48
52	H	500	UQ9	C7-C8-C9	-4.04	119.87	126.83
61	z	301	PSF	O11-C1-C13	4.00	120.14	111.48
49	D	401	PTY	O7-C8-C11	3.93	119.99	111.48
58	v	201	PC7	O2-C31-C32	3.90	119.92	111.48
58	c	101	PC7	O2-C31-C32	3.80	119.69	111.48
52	H	500	UQ9	C12-C13-C14	-3.77	119.00	127.62
57	W	200	8Q1	O4-C1-C6	-3.72	119.69	123.98
55	P	500	NDP	O2B-P2B-O1X	-3.59	96.55	109.33
57	n	200	8Q1	O4-C1-C6	-3.53	119.90	123.98
55	P	500	NDP	O3-PA-O1A	-3.45	100.33	110.70
52	H	500	UQ9	C17-C18-C19	-3.40	119.85	127.62
51	F	500	FMN	C4-N3-C2	-3.37	119.66	125.64
52	H	500	UQ9	C1M-C1-C6	-3.21	119.17	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	H	500	UQ9	C22-C23-C24	-3.14	120.44	127.62
55	P	500	NDP	PA-O5B-C5B	-3.10	103.60	121.35
57	W	200	8Q1	C43-S44-C1	2.97	110.62	101.84
55	P	500	NDP	PN-O5D-C5D	-2.92	104.65	121.35
60	f	202	T7X	O18-C11-C31	2.83	120.45	111.83
49	N	501	PTY	O4-C30-C31	2.81	120.40	111.83
49	M	501	PTY	O4-C30-C31	2.78	120.31	111.83
51	F	500	FMN	C4A-C4-N3	2.76	120.27	113.25
49	D	401	PTY	O4-C30-C31	2.71	120.11	111.83
51	F	500	FMN	O4-C4-C4A	-2.64	119.55	126.53
58	v	201	PC7	O3-C11-C12	2.64	119.89	111.83
58	c	101	PC7	O3-C11-C12	2.63	119.86	111.83
61	z	301	PSF	O52-C5-C6	2.60	119.77	111.83
57	n	200	8Q1	C43-S44-C1	2.59	109.51	101.84
52	H	500	UQ9	C25-C24-C26	2.58	119.71	115.23
52	H	500	UQ9	C20-C19-C21	2.58	119.70	115.23
52	H	500	UQ9	C15-C14-C16	2.56	119.67	115.23
52	H	500	UQ9	C10-C9-C11	2.55	119.66	115.23
55	P	500	NDP	O3X-P2B-O2X	2.55	117.35	107.80
51	F	500	FMN	C4A-C10-N10	2.53	120.10	116.48
52	H	500	UQ9	C6-C1-C2	2.52	121.16	119.17
59	f	201	PGT	O3-C11-C12	2.47	119.36	111.83
55	P	500	NDP	O2N-PN-O1N	2.45	123.86	112.44
55	P	500	NDP	C2A-N1A-C6A	-2.45	114.70	118.73
55	P	500	NDP	O2N-PN-O3	2.44	113.88	107.27
55	P	500	NDP	O4B-C4B-C3B	2.44	110.00	105.15
53	M	502	LMN	CCS-OCB-CCQ	-2.42	112.24	117.98
55	P	500	NDP	O5D-PN-O1N	-2.40	99.41	108.94
57	W	200	8Q1	C38-C39-N41	2.37	120.66	116.34
55	P	500	NDP	C5B-C4B-C3B	-2.35	106.75	115.21
51	F	500	FMN	C5A-C9A-N10	2.32	120.06	117.97
55	P	500	NDP	N3A-C4A-N9A	2.21	130.93	127.17
51	F	500	FMN	C10-C4A-N5	-2.20	120.31	124.81
57	n	200	8Q1	C38-C39-N41	2.20	120.36	116.34
53	M	502	LMN	CBK-CBQ-CCM	-2.19	110.54	117.19
51	F	500	FMN	C9A-C5A-N5	-2.18	120.14	122.45
53	M	502	LMN	CBL-CBR-CCM	-2.09	110.83	117.19
55	P	500	NDP	C5A-C4A-N3A	-2.07	123.87	126.72
57	n	200	8Q1	O4-C1-S44	-2.06	120.06	122.68
51	F	500	FMN	C4A-C10-N1	-2.05	119.56	124.59
55	P	500	NDP	O3X-P2B-O2B	-2.05	97.86	105.85
55	P	500	NDP	C3N-C2N-N1N	-2.04	120.20	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	P	500	NDP	C5D-C4D-C3D	-2.02	107.93	115.21

There are no chirality outliers.

All (279) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	D	401	PTY	N1-C2-C3-O11
49	D	401	PTY	C5-O14-P1-O13
49	M	501	PTY	N1-C2-C3-O11
49	M	501	PTY	O10-C8-O7-C6
49	M	501	PTY	C11-C8-O7-C6
49	N	501	PTY	C2-C3-O11-P1
49	N	501	PTY	C11-C8-O7-C6
49	N	501	PTY	C3-O11-P1-O12
51	F	500	FMN	N10-C1'-C2'-O2'
51	F	500	FMN	N10-C1'-C2'-C3'
51	F	500	FMN	C1'-C2'-C3'-O3'
51	F	500	FMN	C1'-C2'-C3'-C4'
52	H	500	UQ9	C9-C11-C12-C13
52	H	500	UQ9	C1-C6-C7-C8
52	H	500	UQ9	C5-C6-C7-C8
53	M	502	LMN	O1-CBS-CCM-CBR
53	M	502	LMN	CCM-CBT-OBV-CCJ
53	M	502	LMN	OBV-CBT-CCM-CBQ
53	M	502	LMN	OBV-CBT-CCM-CBR
53	M	502	LMN	CCL-CCJ-OBV-CBT
55	P	500	NDP	C5B-O5B-PA-O2A
55	P	500	NDP	C5B-O5B-PA-O3
55	P	500	NDP	O4B-C4B-C5B-O5B
55	P	500	NDP	O4D-C4D-C5D-O5D
57	W	200	8Q1	O4-C1-C6-C7
57	W	200	8Q1	O4-C1-S44-C43
57	W	200	8Q1	C6-C1-S44-C43
57	W	200	8Q1	O27-C28-C29-C30
57	W	200	8Q1	O27-C28-C29-C31
57	W	200	8Q1	O27-C28-C29-C32
57	W	200	8Q1	C28-C29-C32-C34
57	W	200	8Q1	C31-C29-C32-C34
57	W	200	8Q1	C29-C32-C34-O35
57	W	200	8Q1	O33-C32-C34-N36
57	W	200	8Q1	N41-C42-C43-S44
57	W	200	8Q1	C28-O27-P24-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
57	W	200	8Q1	C28-O27-P24-O2
57	W	200	8Q1	C28-O27-P24-O1
57	n	200	8Q1	O4-C1-S44-C43
57	n	200	8Q1	C6-C1-S44-C43
57	n	200	8Q1	C28-C29-C32-C34
57	n	200	8Q1	C28-C29-C32-O33
57	n	200	8Q1	C30-C29-C32-C34
57	n	200	8Q1	C30-C29-C32-O33
57	n	200	8Q1	C31-C29-C32-C34
57	n	200	8Q1	C31-C29-C32-O33
57	n	200	8Q1	C28-O27-P24-O3
57	n	200	8Q1	C28-O27-P24-O2
57	n	200	8Q1	C28-O27-P24-O1
58	c	101	PC7	C1-O3P-P-O1P
58	c	101	PC7	C1-O3P-P-O4P
58	c	101	PC7	C4-O4P-P-O1P
58	v	201	PC7	C32-C31-O2-C2
58	v	201	PC7	O2-C2-C3-O3
58	v	201	PC7	C1-O3P-P-O4P
58	v	201	PC7	C4-O4P-P-O3P
58	v	201	PC7	C4-O4P-P-O1P
59	f	201	PGT	C4-O4P-P-O3P
59	f	201	PGT	C4-O4P-P-O1P
60	f	202	T7X	C1-O1-P1-O13
60	f	202	T7X	C12-C10-O16-C8
61	z	301	PSF	C2-O2-P-O3
61	z	301	PSF	C13-C1-O11-C3
61	z	301	PSF	N-CA-CB-O1
61	z	301	PSF	C-CA-CB-O1
61	z	301	PSF	OT1-C-CA-CB
58	v	201	PC7	C12-C11-O3-C3
49	M	501	PTY	O30-C30-O4-C1
58	v	201	PC7	O11-C11-O3-C3
49	N	501	PTY	O10-C8-O7-C6
58	v	201	PC7	O31-C31-O2-C2
60	f	202	T7X	O17-C10-O16-C8
49	M	501	PTY	C31-C30-O4-C1
52	H	500	UQ9	C15-C14-C16-C17
57	n	200	8Q1	C38-C39-N41-C42
58	c	101	PC7	O11-C11-O3-C3
53	M	502	LMN	OAI-CBM-CCC-OBV
61	z	301	PSF	O12-C1-O11-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	M	502	LMN	CCF-CCQ-OCB-CCS
60	f	202	T7X	C31-C11-O18-C9
51	F	500	FMN	O2'-C2'-C3'-C4'
55	P	500	NDP	C3B-C4B-C5B-O5B
58	c	101	PC7	C12-C11-O3-C3
60	f	202	T7X	O19-C11-O18-C9
53	M	502	LMN	OAI-CBM-CCC-CCN
53	M	502	LMN	OAL-CBP-CCF-CCQ
53	M	502	LMN	O5-C1-O1-CBS
53	M	502	LMN	OBX-CCJ-OBV-CBT
57	n	200	8Q1	O40-C39-N41-C42
53	M	502	LMN	OBV-CBT-CCM-CBS
52	H	500	UQ9	C13-C14-C16-C17
59	f	201	PGT	C14-C15-C16-C17
53	M	502	LMN	C4-C5-C6-O6
52	H	500	UQ9	C24-C26-C27-C28
53	M	502	LMN	OAL-CBP-CCF-OBX
49	M	501	PTY	C30-C31-C32-C33
53	M	502	LMN	CCW-CCS-OCB-CCQ
60	f	202	T7X	C11-C31-C32-C33
53	M	502	LMN	OBZ-CCS-OCB-CCQ
51	F	500	FMN	O2'-C2'-C3'-O3'
53	M	502	LMN	O5-C5-C6-O6
49	D	401	PTY	C8-C11-C12-C13
55	P	500	NDP	C3D-C4D-C5D-O5D
49	D	401	PTY	C31-C30-O4-C1
53	M	502	LMN	CCH-CCQ-OCB-CCS
53	M	502	LMN	CBD-CBF-CBH-CBJ
59	f	201	PGT	C38-C39-C40-C41
53	M	502	LMN	CAY-CBA-CBC-CBE
58	c	101	PC7	C32-C31-O2-C2
53	M	502	LMN	CBE-CBG-CBI-CBK
53	M	502	LMN	CBG-CBI-CBK-CBQ
53	M	502	LMN	OAJ-CBN-CCD-CCO
58	v	201	PC7	C21-C22-C23-C24
60	f	202	T7X	C33-C34-C35-C36
49	D	401	PTY	O30-C30-O4-C1
59	f	201	PGT	C32-C31-O2-C2
53	M	502	LMN	CBB-CBD-CBF-CBH
58	c	101	PC7	O31-C31-O2-C2
58	v	201	PC7	C12-C13-C14-C15
60	f	202	T7X	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	v	201	PC7	C40-C41-C42-C43
58	c	101	PC7	C20-C21-C22-C23
59	f	201	PGT	C15-C16-C17-C18
53	M	502	LMN	CBC-CBE-CBG-CBI
59	f	201	PGT	C16-C17-C18-C19
59	f	201	PGT	C17-C18-C19-C20
58	v	201	PC7	C18-C19-C20-C21
59	f	201	PGT	C33-C34-C35-C36
58	c	101	PC7	C36-C37-C38-C39
57	W	200	8Q1	O33-C32-C34-O35
58	c	101	PC7	C31-C32-C33-C34
59	f	201	PGT	C37-C38-C39-C40
60	f	202	T7X	C38-C39-C40-C41
60	f	202	T7X	C36-C37-C38-C39
59	f	201	PGT	O31-C31-O2-C2
49	N	501	PTY	C8-C11-C12-C13
49	D	401	PTY	O4-C1-C6-C5
49	N	501	PTY	O4-C1-C6-C5
59	f	201	PGT	C1-C2-C3-O3
60	f	202	T7X	C7-C8-C9-O18
59	f	201	PGT	C18-C19-C20-C21
58	c	101	PC7	C15-C16-C17-C18
49	D	401	PTY	C39-C40-C41-C42
59	f	201	PGT	C13-C14-C15-C16
51	F	500	FMN	C5'-O5'-P-O1P
58	c	101	PC7	C11-C12-C13-C14
49	N	501	PTY	C5-C6-O7-C8
60	f	202	T7X	C12-C13-C14-C15
49	M	501	PTY	C31-C32-C33-C34
53	M	502	LMN	CAX-CAZ-CBB-CBD
49	N	501	PTY	C12-C13-C14-C15
58	c	101	PC7	C38-C39-C40-C41
49	D	401	PTY	O4-C1-C6-O7
49	N	501	PTY	O4-C1-C6-O7
53	M	502	LMN	CBK-CBQ-CCM-CBR
60	f	202	T7X	O18-C11-C31-C32
60	f	202	T7X	C44-C45-C46-C47
49	D	401	PTY	C11-C12-C13-C14
57	W	200	8Q1	C30-C29-C32-O33
57	W	200	8Q1	C31-C29-C32-O33
59	f	201	PGT	C32-C33-C34-C35
57	n	200	8Q1	N41-C42-C43-S44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	c	101	PC7	O3P-C1-C2-C3
57	W	200	8Q1	C29-C32-C34-N36
58	c	101	PC7	C35-C36-C37-C38
53	M	502	LMN	CAW-CAY-CBA-CBC
58	c	101	PC7	C32-C33-C34-C35
52	H	500	UQ9	C19-C21-C22-C23
58	v	201	PC7	C1-C2-C3-O3
49	N	501	PTY	C13-C14-C15-C16
49	N	501	PTY	C37-C38-C39-C40
58	c	101	PC7	O3P-C1-C2-O2
60	f	202	T7X	O13-C7-C8-O16
49	D	401	PTY	C12-C13-C14-C15
60	f	202	T7X	C15-C16-C17-C18
60	f	202	T7X	C19-C20-C21-C22
49	M	501	PTY	C16-C17-C18-C19
57	W	200	8Q1	S44-C1-C6-C7
49	M	501	PTY	C15-C16-C17-C18
53	M	502	LMN	OAJ-CBN-CCD-OBZ
53	M	502	LMN	CBJ-CBL-CBR-CCM
60	f	202	T7X	C31-C32-C33-C34
49	N	501	PTY	C16-C17-C18-C19
49	M	501	PTY	C8-C11-C12-C13
60	f	202	T7X	C9-C8-O16-C10
49	N	501	PTY	C11-C12-C13-C14
49	D	401	PTY	C14-C15-C16-C17
58	c	101	PC7	C18-C19-C20-C21
49	D	401	PTY	C11-C8-O7-C6
58	c	101	PC7	O4P-C4-C5-N
58	v	201	PC7	C15-C16-C17-C18
58	v	201	PC7	C14-C15-C16-C17
53	M	502	LMN	O1-CBS-CCM-CBQ
49	N	501	PTY	C33-C34-C35-C36
58	v	201	PC7	O3P-C1-C2-C3
60	f	202	T7X	O13-C7-C8-C9
49	D	401	PTY	C37-C38-C39-C40
57	n	200	8Q1	O27-C28-C29-C31
49	N	501	PTY	C24-C25-C26-C27
58	v	201	PC7	C32-C33-C34-C35
49	D	401	PTY	O10-C8-O7-C6
58	v	201	PC7	O3P-C1-C2-O2
53	M	502	LMN	CAA-CAW-CAY-CBA
59	f	201	PGT	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
60	f	202	T7X	O16-C8-C9-O18
53	M	502	LMN	O1-CBS-CCM-CBT
49	M	501	PTY	C25-C26-C27-C28
49	N	501	PTY	C21-C22-C23-C24
49	M	501	PTY	C3-O11-P1-O12
49	M	501	PTY	C3-O11-P1-O13
49	M	501	PTY	C3-O11-P1-O14
49	M	501	PTY	C5-O14-P1-O13
49	N	501	PTY	N1-C2-C3-O11
49	N	501	PTY	C3-O11-P1-O13
49	N	501	PTY	C3-O11-P1-O14
49	N	501	PTY	C5-O14-P1-O13
57	W	200	8Q1	C28-C29-C32-O33
58	c	101	PC7	C4-O4P-P-O3P
58	c	101	PC7	C4-O4P-P-O2P
61	z	301	PSF	C2-O2-P-O1
61	z	301	PSF	C2-O2-P-O4
49	M	501	PTY	C13-C14-C15-C16
59	f	201	PGT	C5-C4-O4P-P
49	M	501	PTY	C11-C12-C13-C14
49	M	501	PTY	C18-C19-C20-C21
57	W	200	8Q1	C11-C10-C9-C8
49	D	401	PTY	C35-C36-C37-C38
49	N	501	PTY	C39-C40-C41-C42
49	D	401	PTY	C13-C14-C15-C16
49	M	501	PTY	C19-C20-C21-C22
58	c	101	PC7	C13-C14-C15-C16
53	M	502	LMN	CBK-CBQ-CCM-CBT
58	c	101	PC7	C12-C13-C14-C15
60	f	202	T7X	O19-C11-C31-C32
53	M	502	LMN	CAZ-CBB-CBD-CBF
57	n	200	8Q1	C11-C10-C9-C8
57	n	200	8Q1	C13-C14-C15-C16
49	D	401	PTY	C33-C34-C35-C36
55	P	500	NDP	O4D-C1D-N1N-C6N
53	M	502	LMN	CBH-CBJ-CBL-CBR
57	W	200	8Q1	C6-C7-C8-C9
49	M	501	PTY	O4-C1-C6-O7
49	D	401	PTY	C31-C32-C33-C34
49	M	501	PTY	C41-C42-C43-C44
60	f	202	T7X	C18-C19-C20-C21
60	f	202	T7X	C22-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	N	501	PTY	C15-C16-C17-C18
59	f	201	PGT	O11-C11-O3-C3
60	f	202	T7X	C24-C25-C26-C27
59	f	201	PGT	C12-C11-O3-C3
59	f	201	PGT	C12-C13-C14-C15
58	c	101	PC7	C19-C20-C21-C22
49	M	501	PTY	C36-C37-C38-C39
59	f	201	PGT	C35-C36-C37-C38
57	W	200	8Q1	C12-C13-C14-C15
51	F	500	FMN	C5'-O5'-P-O2P
53	M	502	LMN	CBK-CBQ-CCM-CBS
49	M	501	PTY	C22-C23-C24-C25
55	P	500	NDP	C2D-C1D-N1N-C6N
57	n	200	8Q1	C6-C7-C8-C9
57	W	200	8Q1	C30-C29-C32-C34
49	M	501	PTY	C21-C22-C23-C24
60	f	202	T7X	C13-C14-C15-C16
60	f	202	T7X	C41-C42-C43-C44
58	c	101	PC7	C41-C42-C43-C44
49	M	501	PTY	C37-C38-C39-C40
58	v	201	PC7	C16-C17-C18-C19
58	c	101	PC7	O2-C31-C32-C33
60	f	202	T7X	O16-C10-C12-C13
58	c	101	PC7	C17-C18-C19-C20
57	W	200	8Q1	C29-C28-O27-P24
61	z	301	PSF	O11-C1-C13-C14
58	v	201	PC7	C19-C20-C21-C22
57	n	200	8Q1	O27-C28-C29-C30
61	z	301	PSF	O12-C1-C13-C14
60	f	202	T7X	O17-C10-C12-C13
58	c	101	PC7	C21-C22-C23-C24
53	M	502	LMN	CBF-CBH-CBJ-CBL
58	c	101	PC7	O31-C31-C32-C33

There are no ring outliers.

14 monomers are involved in 45 short contacts:

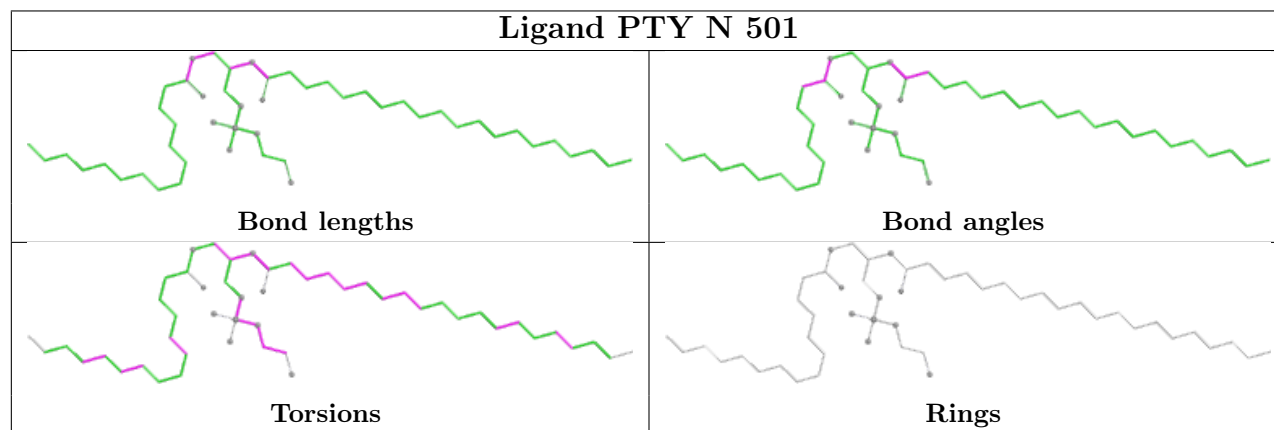
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	N	501	PTY	6	0
55	P	500	NDP	1	0
51	F	500	FMN	1	0
50	E	500	FES	6	0

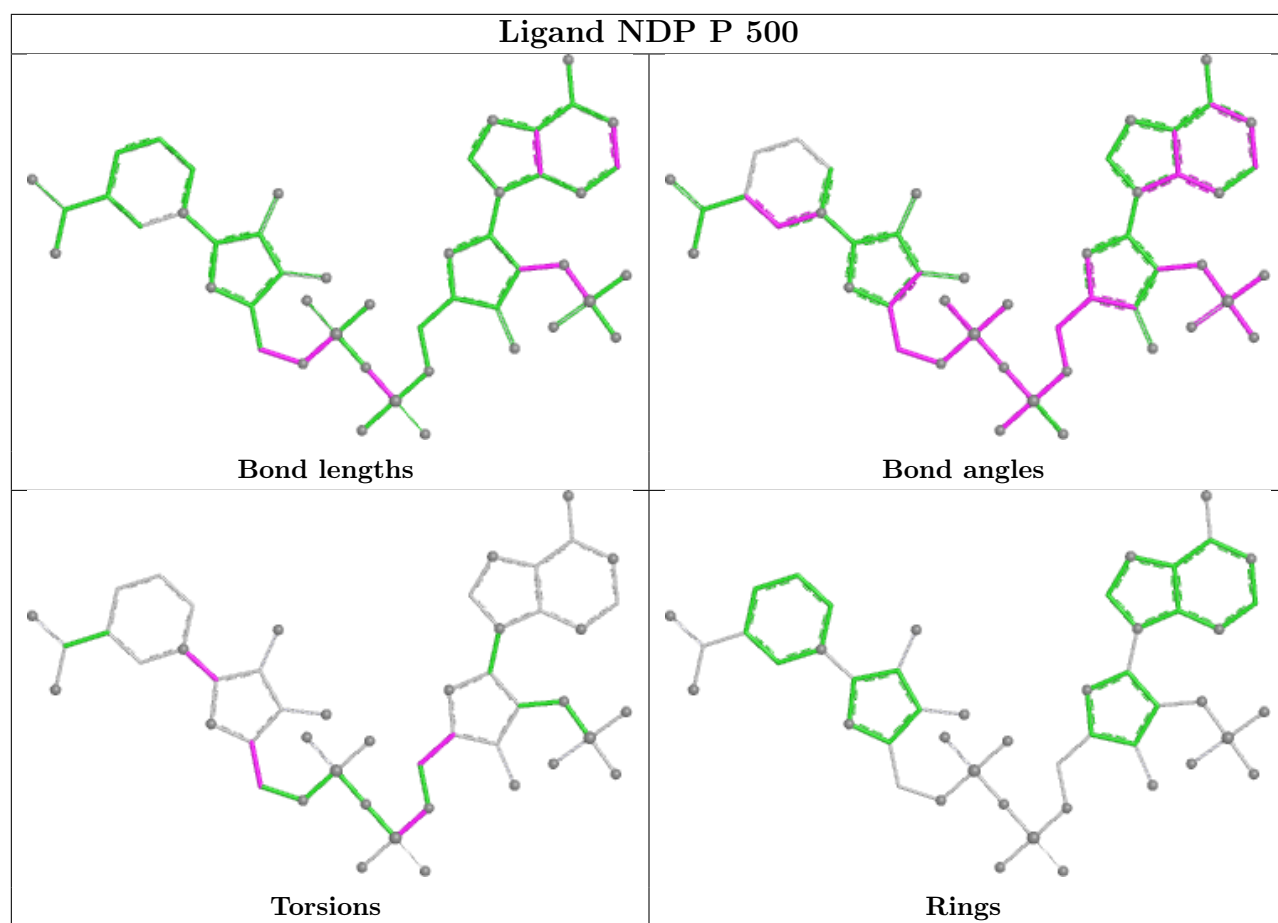
Continued on next page...

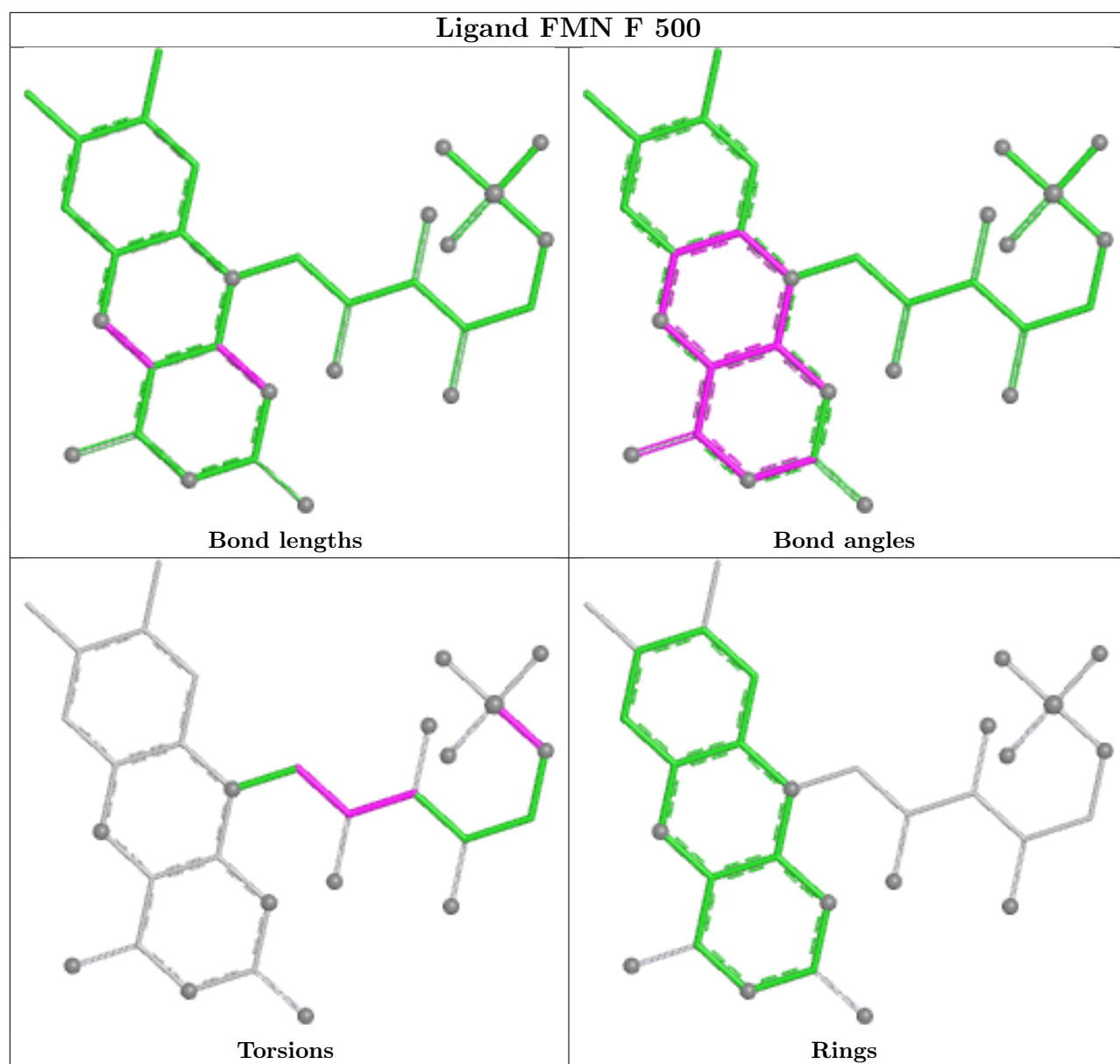
Continued from previous page...

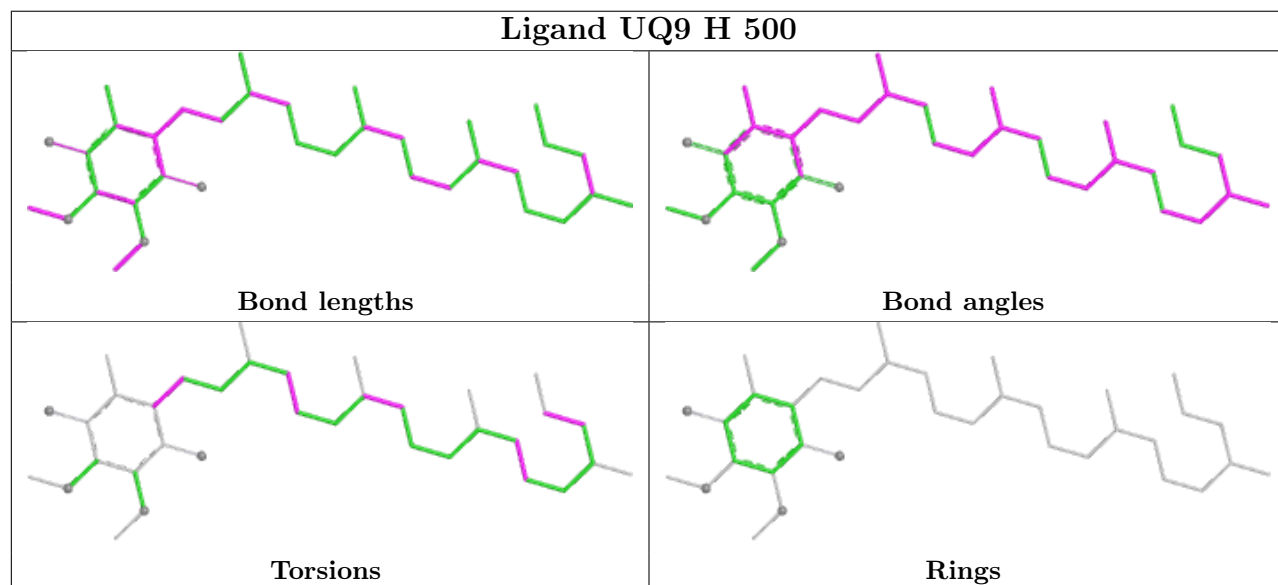
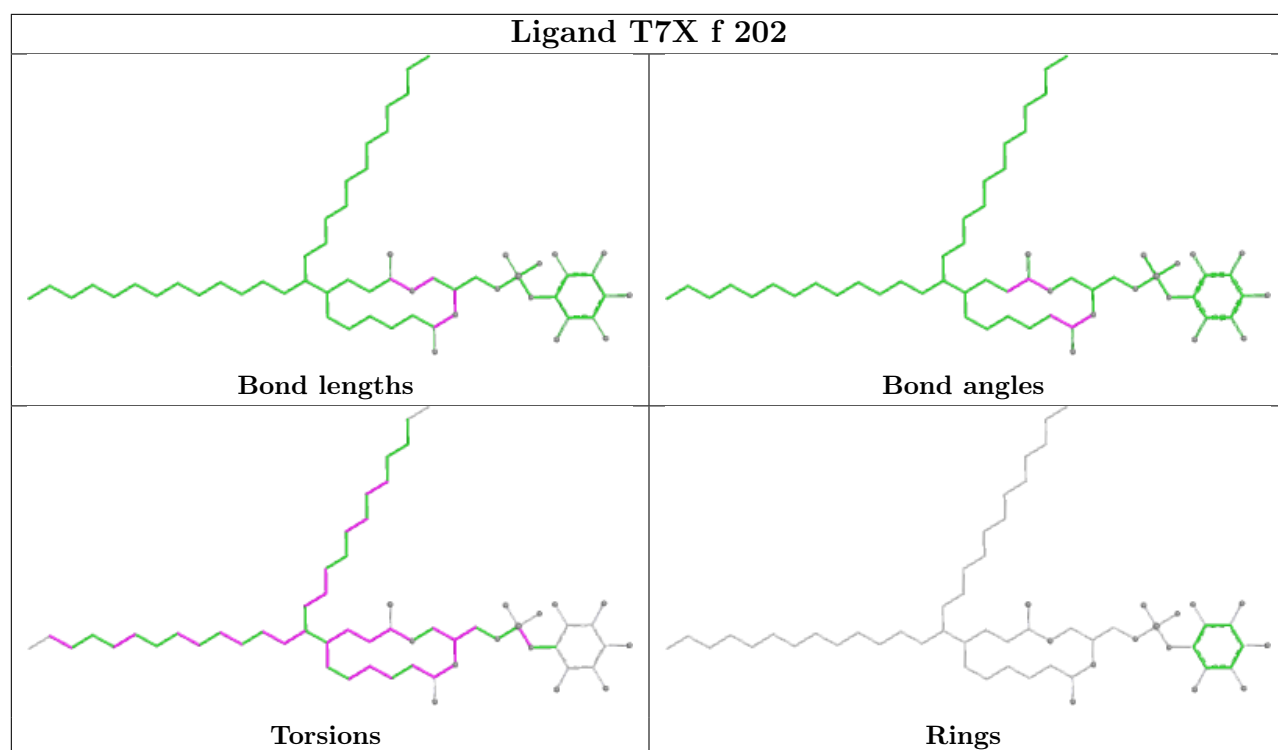
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	H	500	UQ9	2	0
53	M	502	LMN	1	0
58	c	101	PC7	13	0
49	M	501	PTY	2	0
57	n	200	8Q1	1	0
49	D	401	PTY	3	0
59	f	201	PGT	3	0
58	v	201	PC7	1	0
48	F	501	SF4	2	0
61	z	301	PSF	3	0

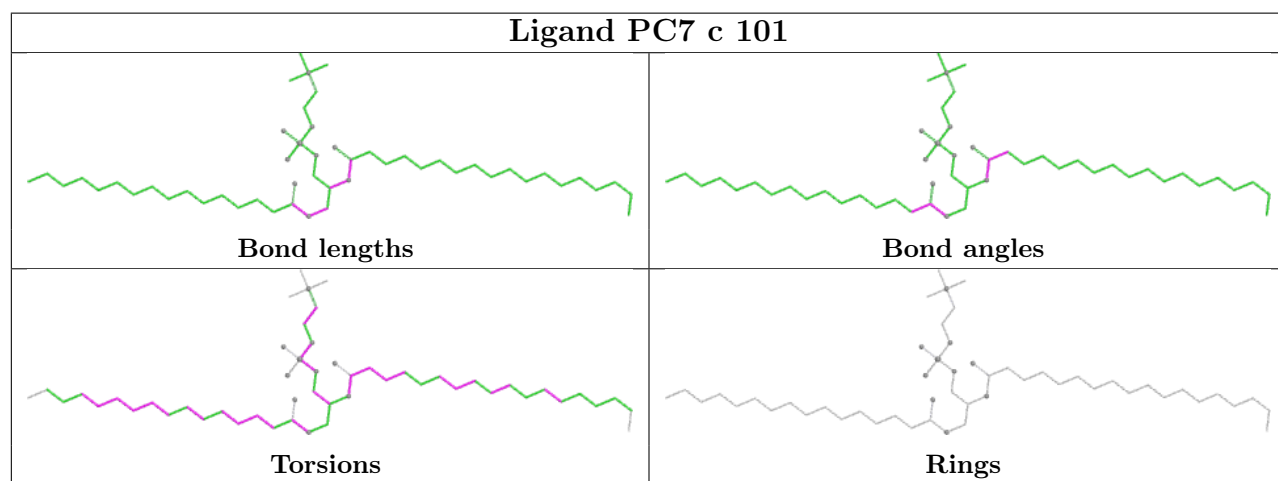
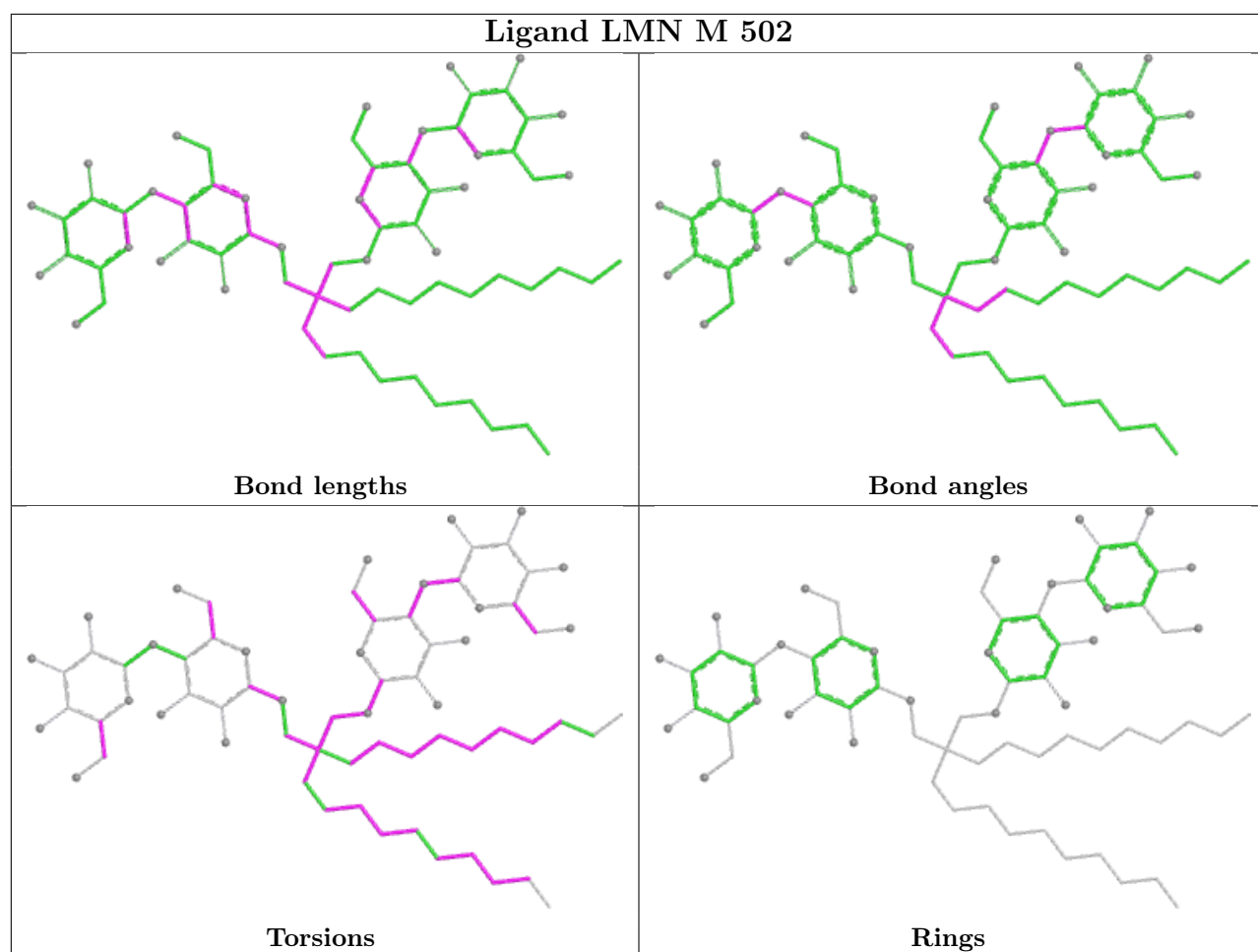
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

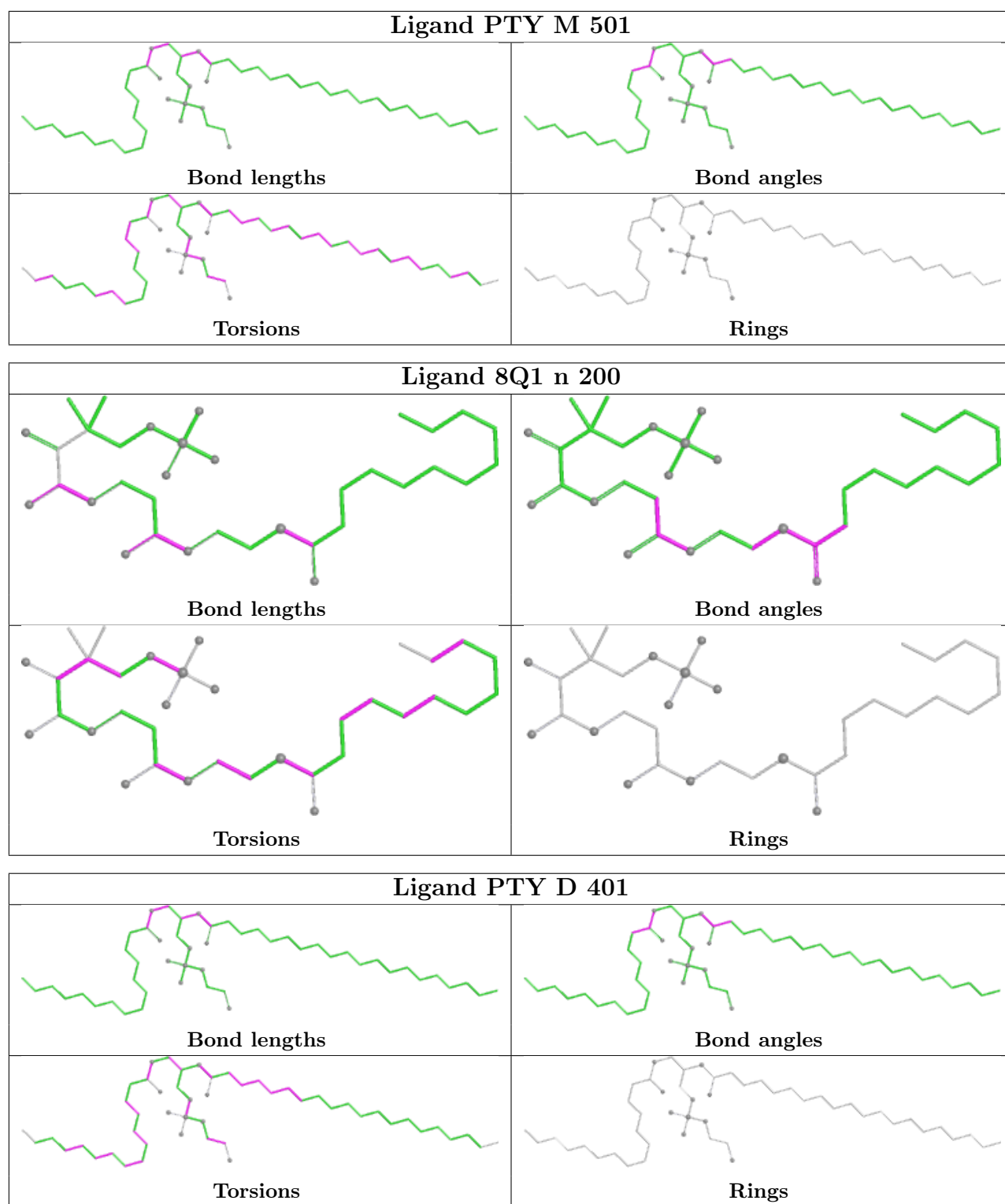


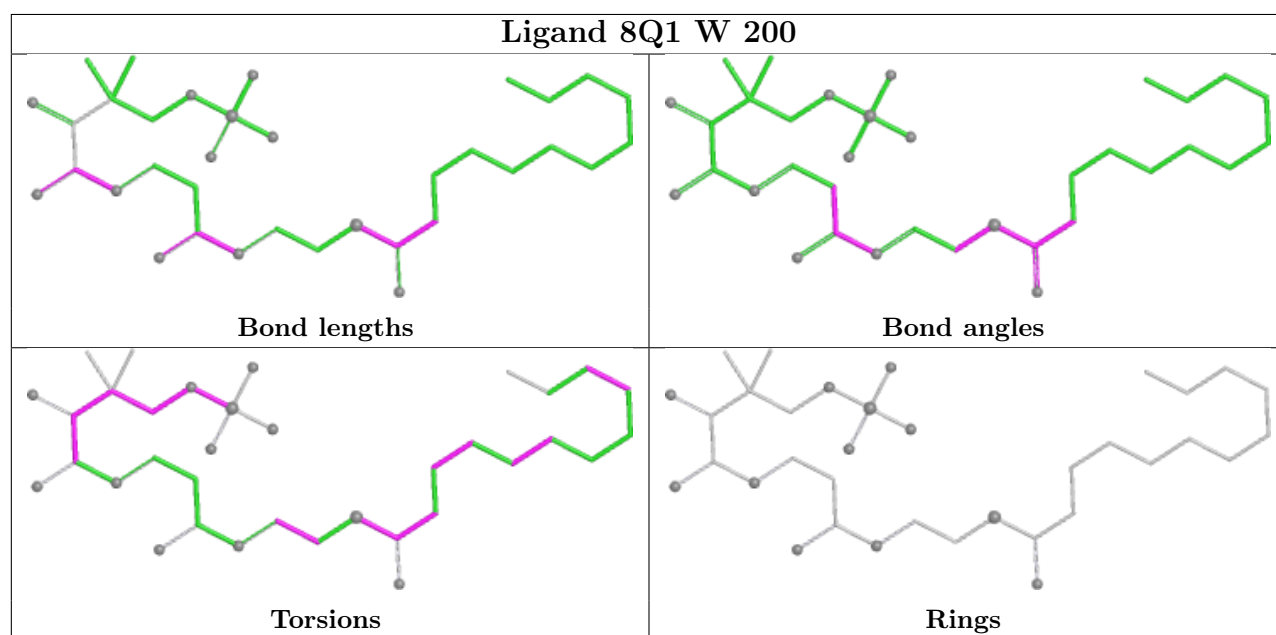
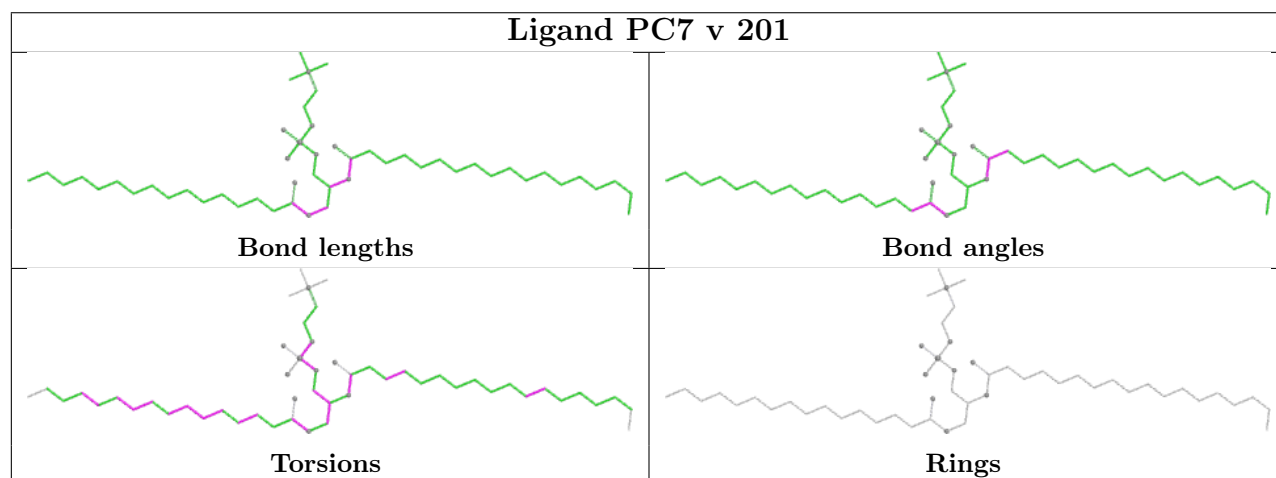
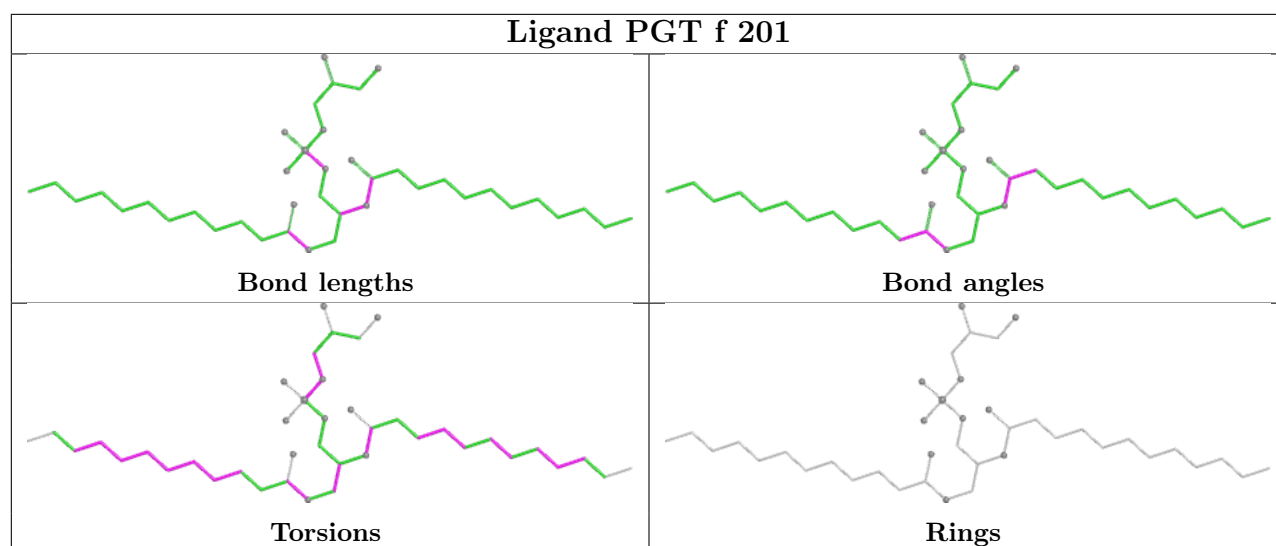


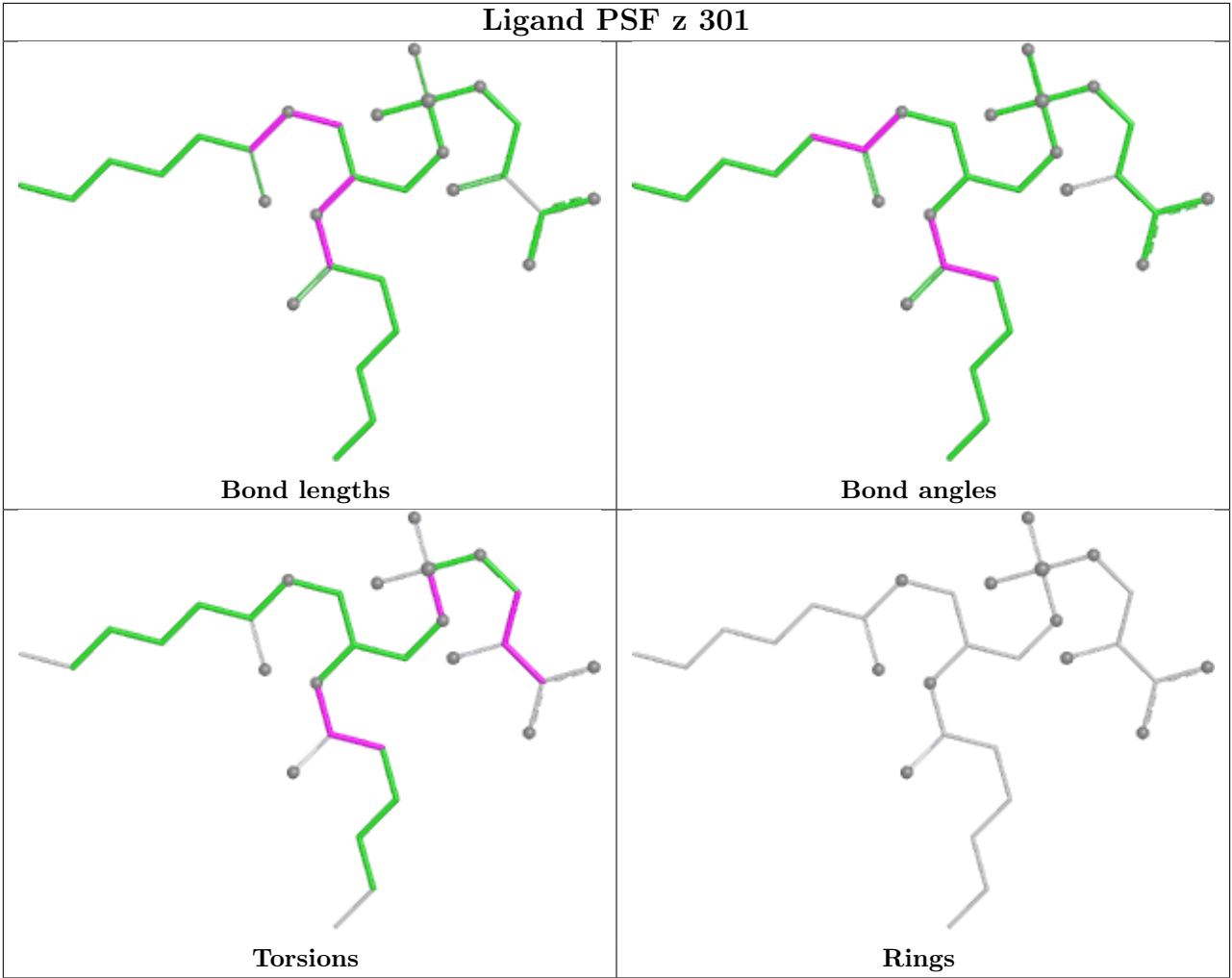












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	270:PRO	C	271:MET	N	3.13

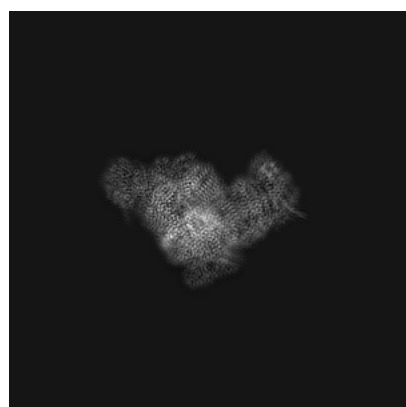
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11878. These allow visual inspection of the internal detail of the map and identification of artifacts.

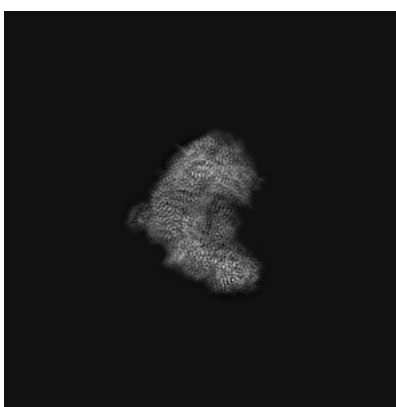
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

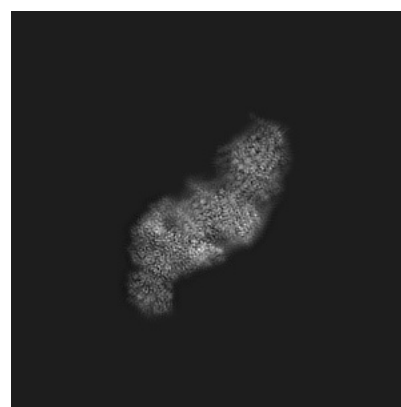
6.1.1 Primary map



X



Y

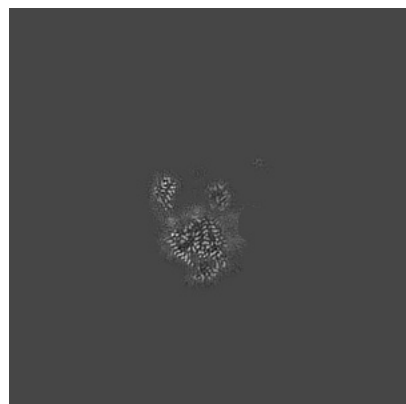


Z

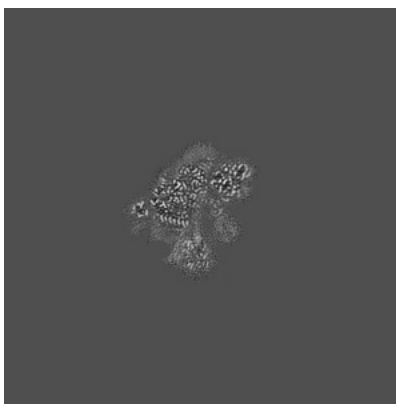
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

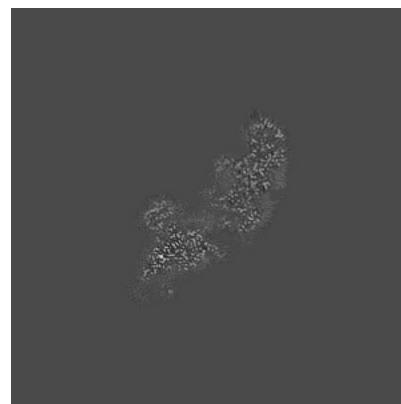
6.2.1 Primary map



X Index: 300



Y Index: 300

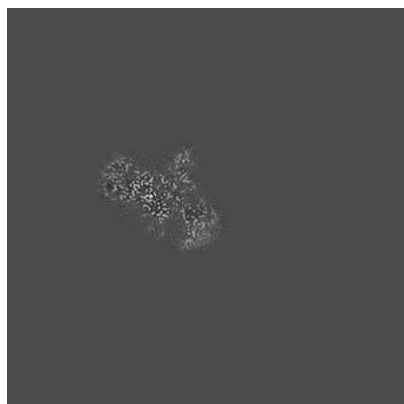


Z Index: 300

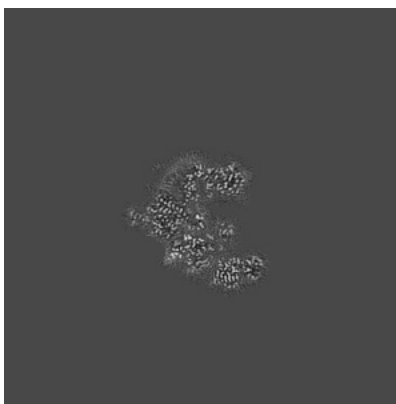
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

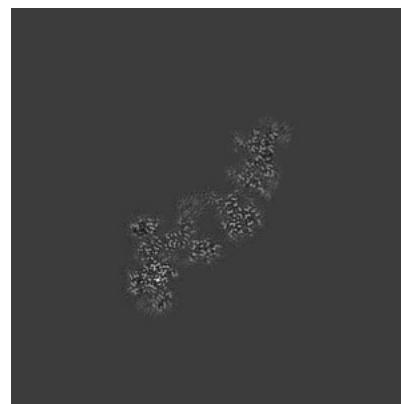
6.3.1 Primary map



X Index: 222



Y Index: 268

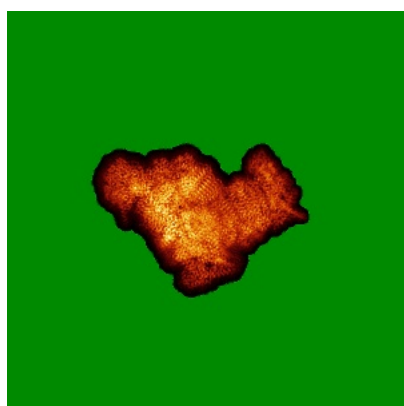


Z Index: 334

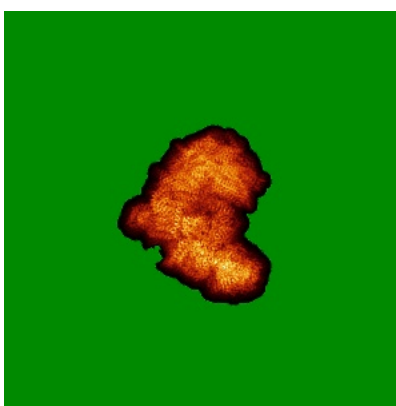
The images above show the largest variance slices of the map in three orthogonal directions.

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

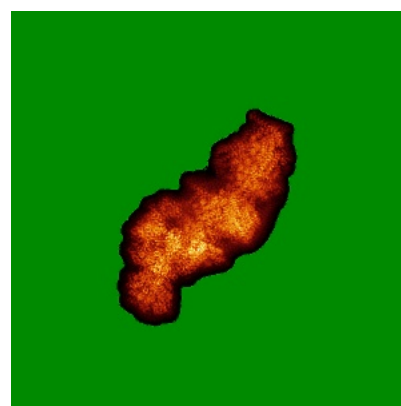
6.4.1 Primary map



X



Y

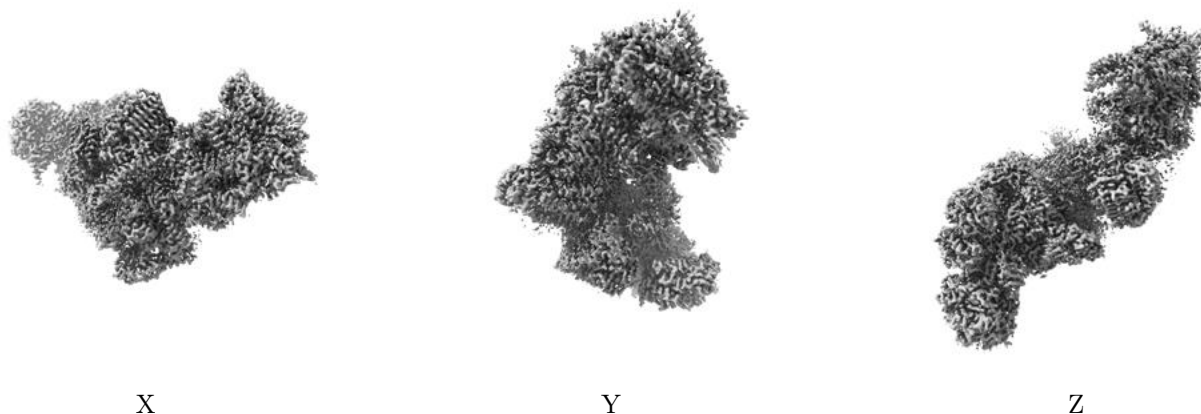


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

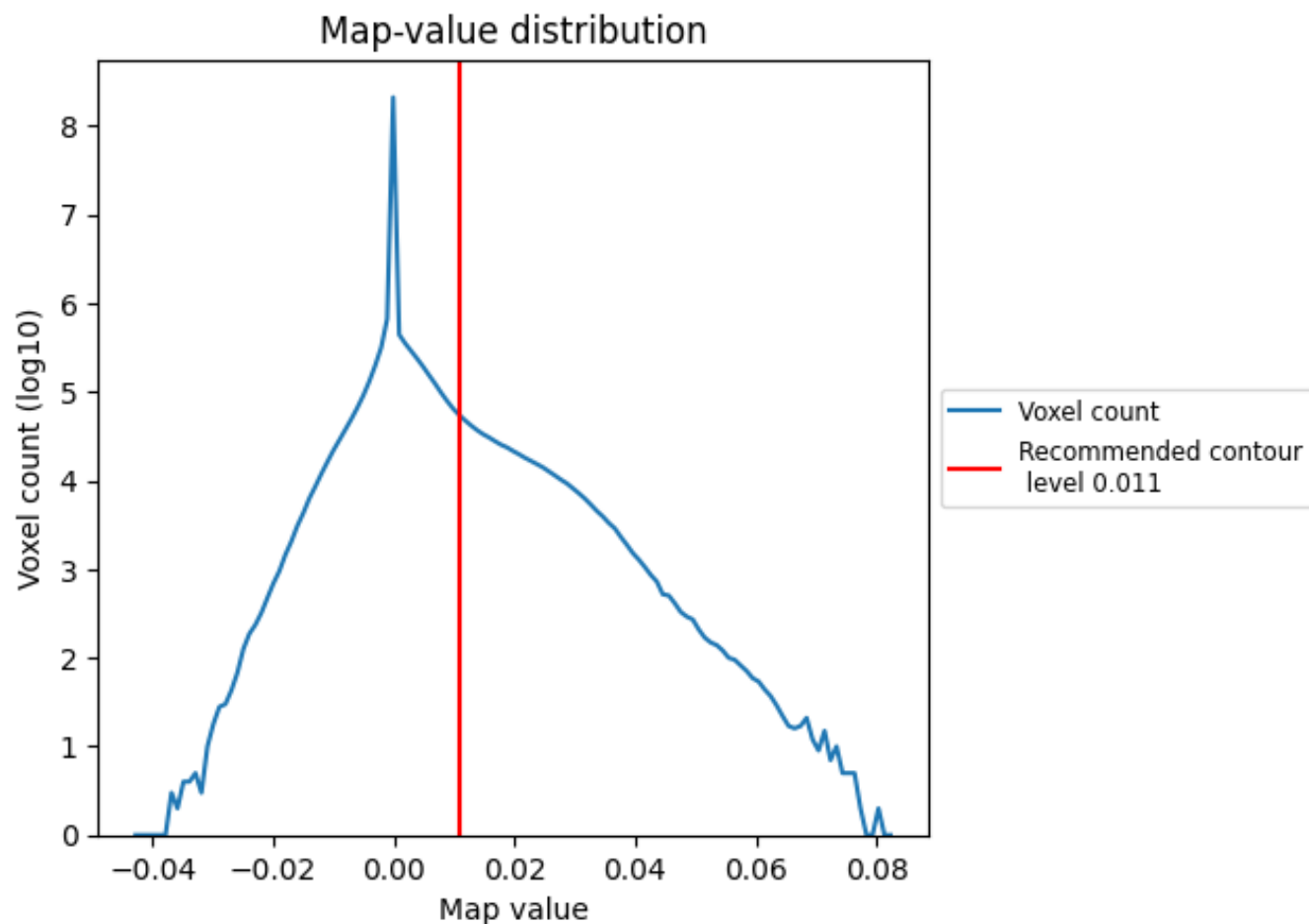
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

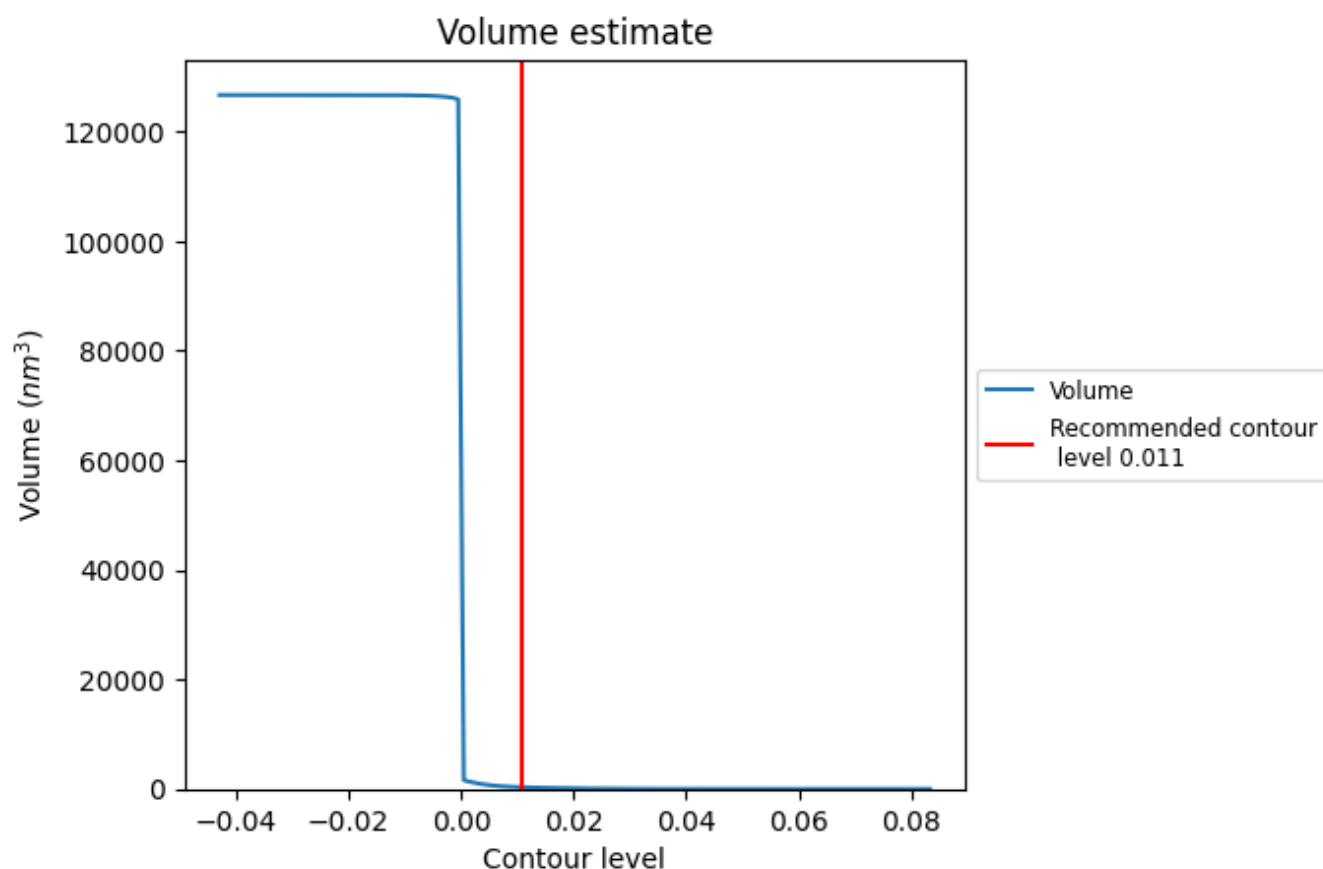
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

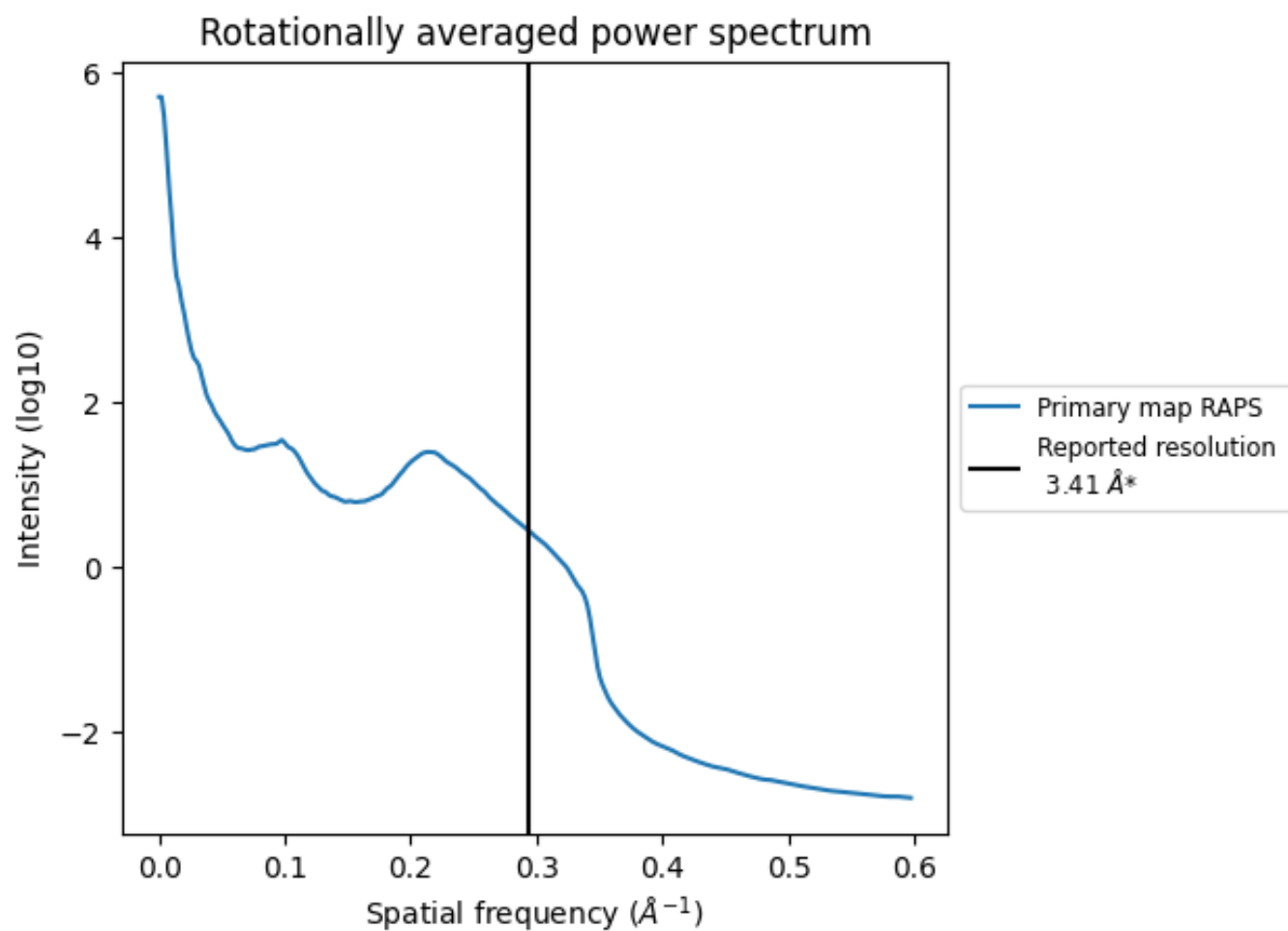
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 303 nm³; this corresponds to an approximate mass of 274 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 ⓘ

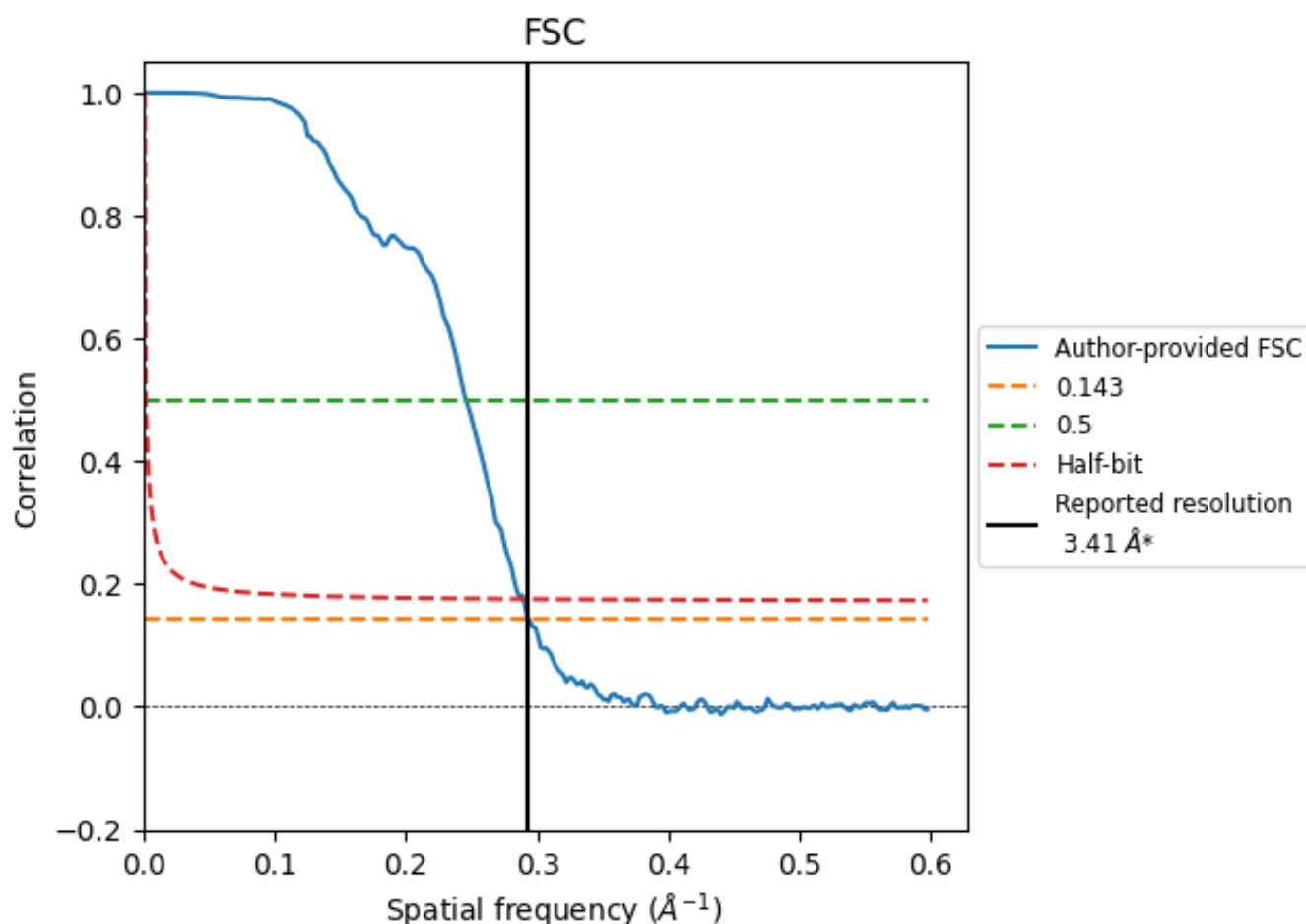


*Reported resolution corresponds to spatial frequency of 0.293 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.293 Å⁻¹

8.2 Resolution estimates [i](#)

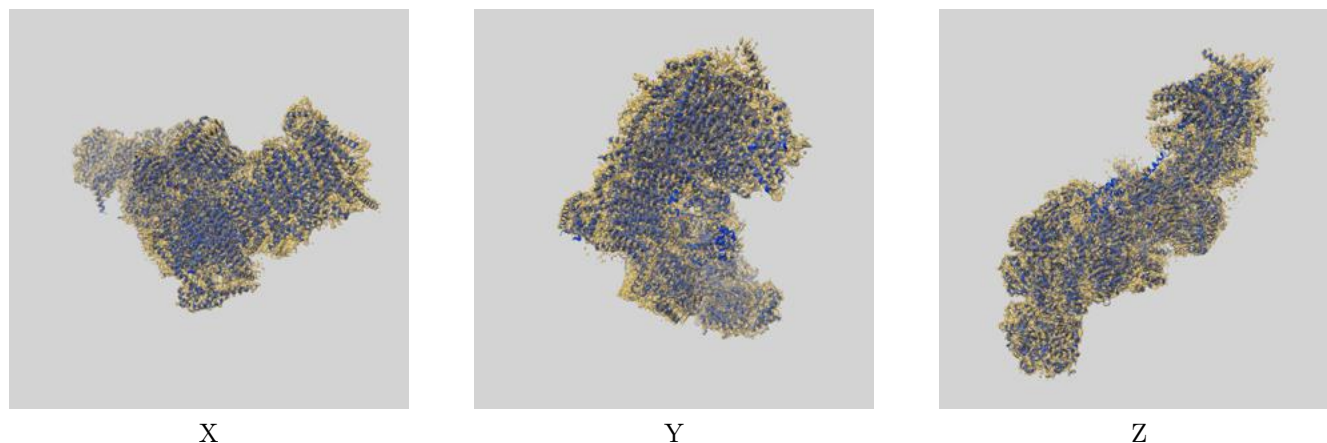
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.41	-	-
Author-provided FSC curve	3.40	4.07	3.45
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

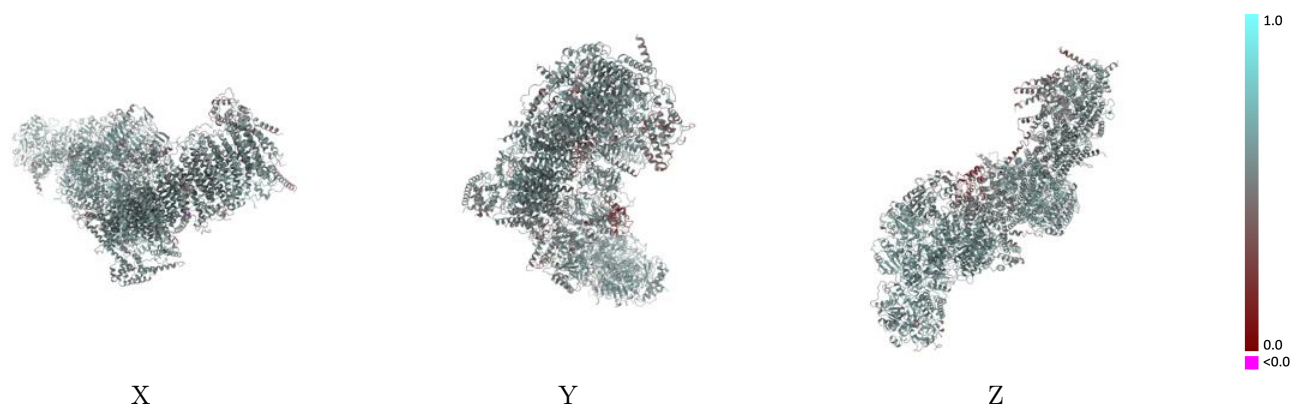
This section contains information regarding the fit between EMDB map EMD-11878 and PDB model 7ARB. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



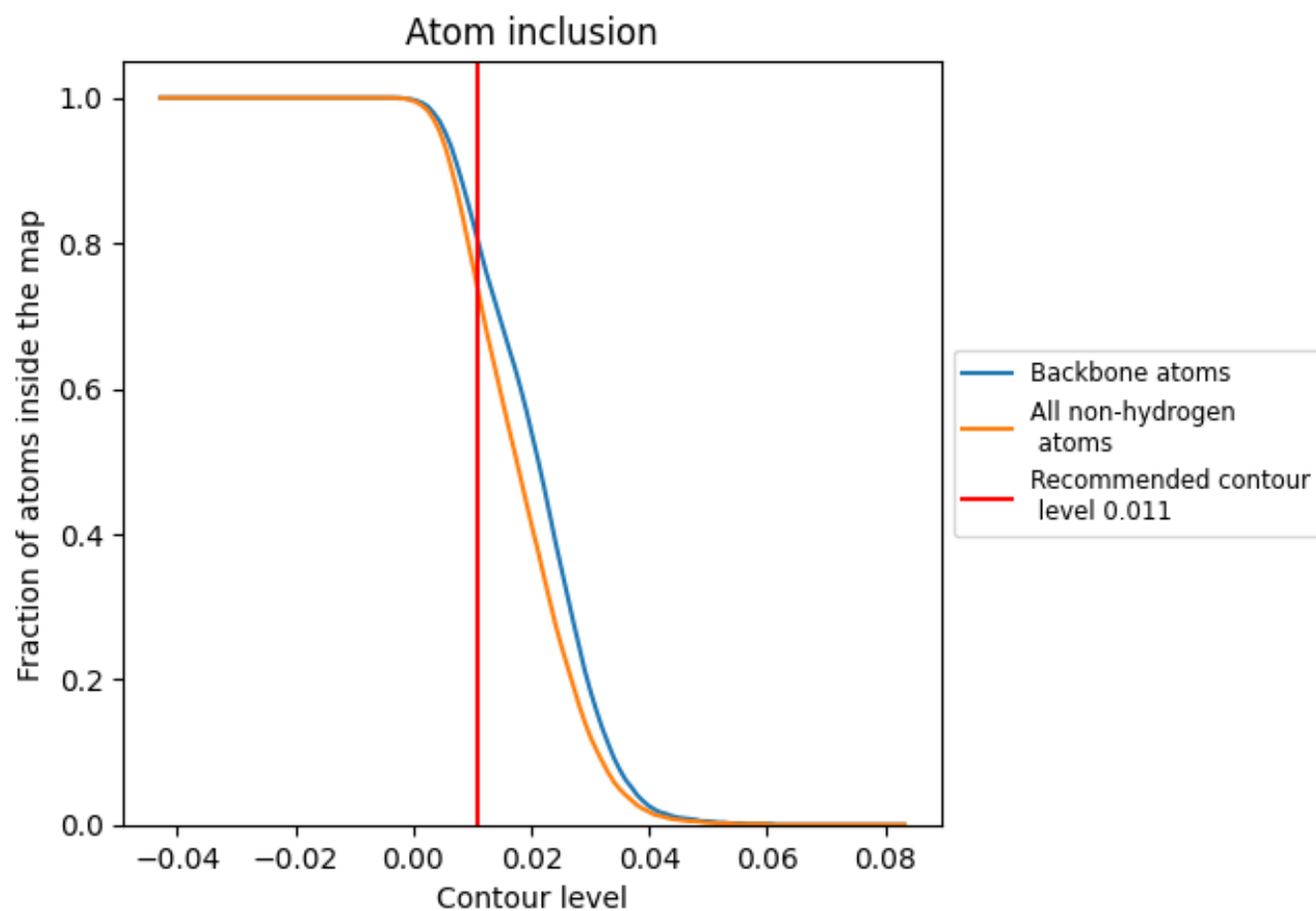
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7370	 0.5440
A	 0.6970	 0.5420
B	 0.9140	 0.5780
C	 0.8390	 0.5960
D	 0.8460	 0.5850
E	 0.7070	 0.5280
F	 0.7550	 0.5610
G	 0.7960	 0.5810
H	 0.7350	 0.5350
I	 0.8800	 0.5820
J	 0.6910	 0.5410
K	 0.6770	 0.5450
L	 0.7070	 0.5370
M	 0.7450	 0.5480
N	 0.7580	 0.5680
O	 0.4740	 0.5190
P	 0.7480	 0.5180
Q	 0.7550	 0.5930
R	 0.7680	 0.5860
S	 0.7690	 0.5600
T	 0.6220	 0.4570
U	 0.1300	 0.2530
V	 0.7480	 0.5390
W	 0.5240	 0.4890
X	 0.6700	 0.5170
Z	 0.7280	 0.5220
a	 0.7010	 0.5150
b	 0.6600	 0.5300
c	 0.7600	 0.5430
d	 0.7660	 0.5520
e	 0.7930	 0.5590
f	 0.7830	 0.5690
g	 0.7160	 0.5160
i	 0.7260	 0.5190
j	 0.7400	 0.5170



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	 0.7020	 0.5040
l	 0.5850	 0.4970
m	 0.6070	 0.4680
n	 0.6590	 0.4890
o	 0.7430	 0.5130
p	 0.7480	 0.4980
q	 0.4920	 0.4870
r	 0.3810	 0.4860
u	 0.7270	 0.4840
v	 0.6780	 0.5540
x	 0.7900	 0.5640
y	 0.7300	 0.5450
z	 0.7780	 0.5580