Full wwPDB EM Validation Report

Mar 23, 2026 – 10:28 AM UTC

PDB ID	:	7DGZ / pdb_00007dgz
EMDB ID	:	EMD-30676
Title	:	Activity optimized complex I (closed form)
Authors	:	Jeon, T.J.; Lee, S.G.; Yoo, S.H.; Ryu, J.H.; Kim, D.S.; Hyun, J.K.; Kim, H.M.; Ryu, S.E.
Deposited on	:	2020-11-12
Resolution	:	3.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

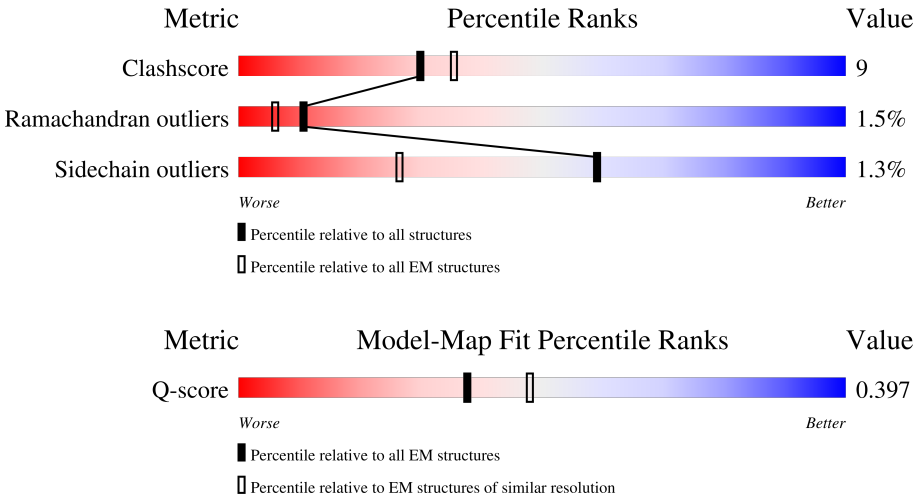
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	2	347	86% 12%
2	3	115	32% 62% 24% 7%
3	4	459	9% 82% 17%
4	5	98	7% 78% 20%

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Mol	Chain	Length	Quality of chain
5	7	175	30% 86% 10%
6	8	444	80% 16%
7	9	217	8% 71% 23% 5%
8	A	704	78% 18%
9	B	430	12% 83% 15%
10	C	228	75% 15% 9%
11	D	179	68% 17% 15%
12	E	176	80% 20%
13	F	75	12% 27% 11% 63%
14	G	133	9% 76% 17% 8%
15	H	105	7% 71% 17% 9%
16	I	96	28% 59% 10% 26%
17	J	70	90% 9%
18	K	98	76% 10% 14%
19	L	83	28% 88% 8%
20	N	115	8% 82% 15%
21	O	127	11% 77% 13% 10%
22	P	112	25% 62% 18% 20%
23	Q	171	8% 80% 17%
24	R	345	19% 70% 22% 8%
25	S	320	50% 82% 17%
26	T	140	49% 91% 6%
27	U	145	57% 81% 10% 9%
28	V	143	6% 83% 13%
29	M	88	49% 68% 23% 9%

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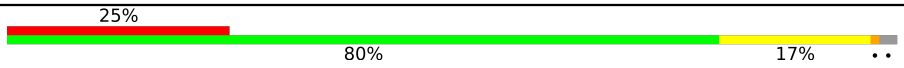
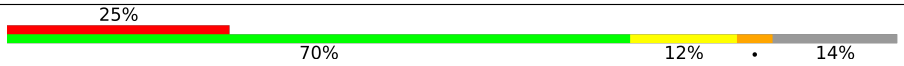
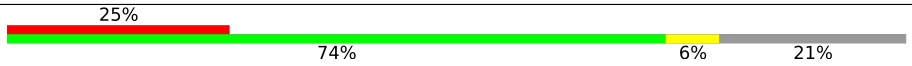
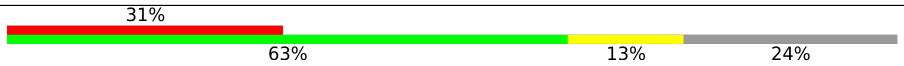
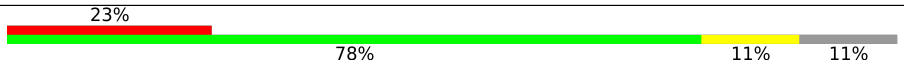
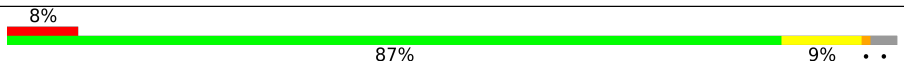
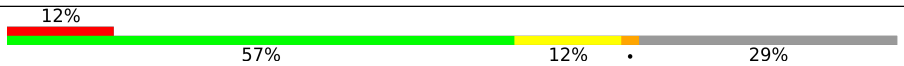
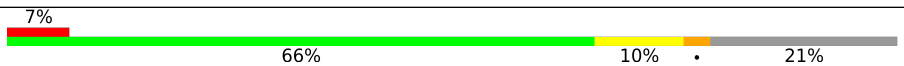
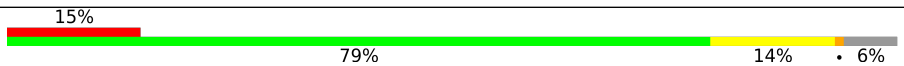
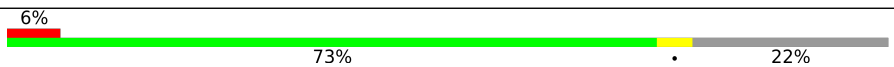
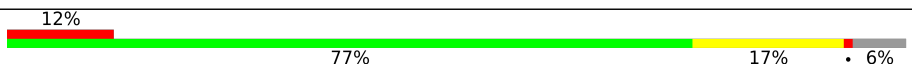
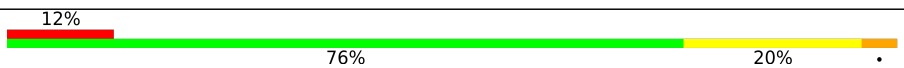
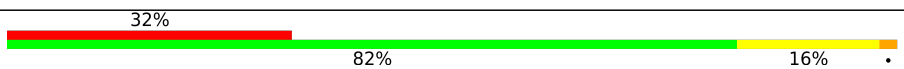
Mol	Chain	Length	Quality of chain
29	W	88	
30	X	57	
31	Y	72	
32	Z	97	
33	a	128	
34	b	143	
35	c	127	
36	d	136	
37	f	178	
38	h	125	
39	i	49	
40	j	120	
41	1	318	
42	6	606	
43	g	176	
44	e	158	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 60921 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	344	2582	1707	404	437	34	0	0

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	112	864	582	127	150	5	0	0

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	458	3447	2293	548	574	32	1	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	5	96	697	454	109	124	10	0	0

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	7	172	1186	798	179	202	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	8	427	2965	1864	552	534	15	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	207	Total	C	N	O	S	0	0
			1535	978	261	286	10		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	688	Total	C	N	O	S	0	0
			5183	3254	915	978	36		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	430	Total	C	N	O	S	0	0
			3410	2178	587	620	25		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	208	Total	C	N	O	S	0	0
			1705	1102	294	306	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	152	Total	C	N	O	S	0	0
			1200	769	209	208	14		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	176	Total	C	N	O	S	0	0
			1388	874	239	264	11		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	F	28	Total	C	N	O	0	0
			183	116	32	35		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	123	Total	C	N	O	S	0	0
			981	619	177	182	3		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	96	Total	C	N	O	S	0	0
			780	494	147	134	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	71	Total	C	N	O	S	0	0
			530	331	99	97	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	69	Total	C	N	O	S	0	0
			530	344	96	88	2		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	K	84	Total	C	N	O	0	0
			652	409	125	118		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	80	Total	C	N	O	S	0	0
			602	398	97	105	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	111	Total	C	N	O	S	0	0
			862	559	149	152	2		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	114	Total	C	N	O	S	0	0
			925	595	170	156	4		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	90	Total	C	N	O	S	0	0
			698	442	128	126	2		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	168	Total	C	N	O	S	0	0
			1345	851	242	243	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	319	Total	C	N	O	S	0	0
			2407	1548	431	425	3		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	319	Total	C	N	O	S	0	0
			2299	1457	395	438	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	138	Total	C	N	O	S	0	0
			942	599	165	172	6		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	132	Total	C	N	O	S	0	0
			1019	659	179	178	3		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	138	Total	C	N	O	S	0	0
			1093	702	189	193	9		

- Molecule 29 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	86	Total	C	N	O	S	0	0
			616	400	98	114	4		
29	M	80	Total	C	N	O	S	0	0
			642	413	96	128	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
30	X	49	Total	C	N	O	0	0
			372	243	64	65		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	57	Total	C	N	O	S	0	0
			409	277	65	66	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	74	Total	C	N	O	S	0	0
			493	320	89	82	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	a	114	Total	C	N	O	0	0
			857	550	159	148		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	139	Total	C	N	O	S	0	0
			1032	672	190	168	2		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	c	90	Total	C	N	O	0	0
			617	391	119	107		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	107	Total	C	N	O	S	0	0
			708	445	134	125	4		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	167	Total	C	N	O	S	0	0
			1156	739	205	208	4		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	91	Total	C	N	O	S	0	0
			721	461	123	135	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	i	38	Total	C	N	O	0	0
			277	185	46	46		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	113	Total	C	N	O	S	0	0
			892	587	149	153	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1	317	Total	C	N	O	S	0	0
			2500	1676	384	417	23		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	6	606	Total	C	N	O	S	0	0
			4765	3172	732	819	42		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

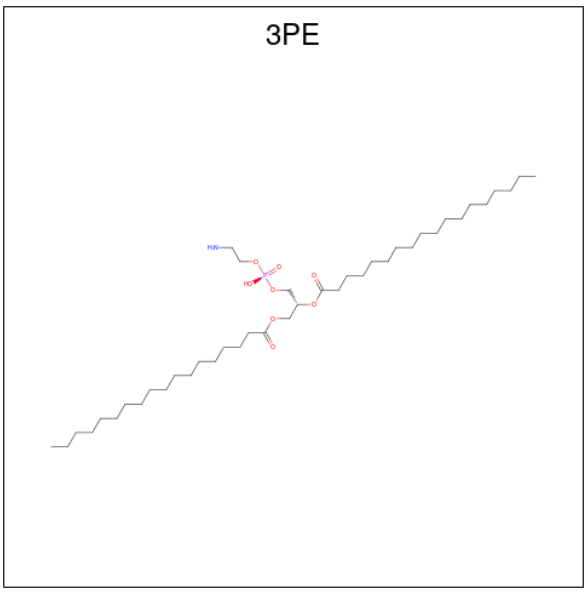
Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	173	Total	C	N	O	S	0	0
			1351	849	246	248	8		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	e	141	Total	C	N	O	S	0	0
			864	539	161	160	4		

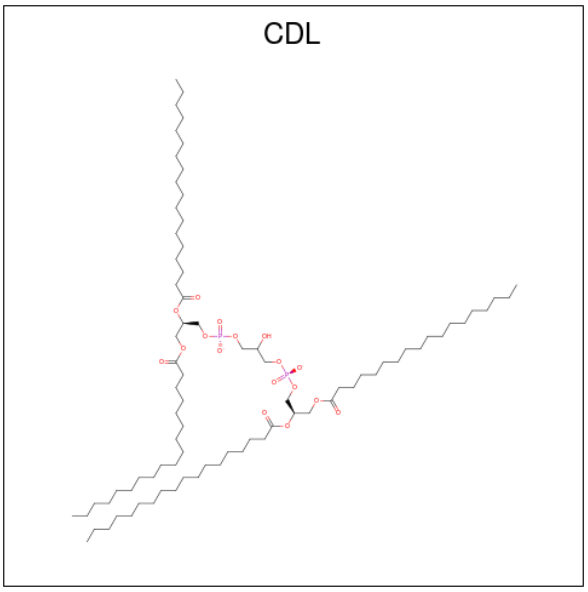
- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:

$C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



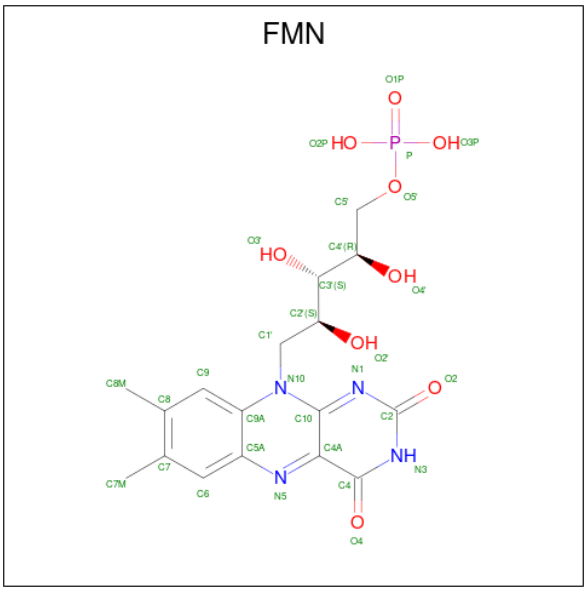
Mol	Chain	Residues	Atoms					AltConf
45	2	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	V	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 46 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



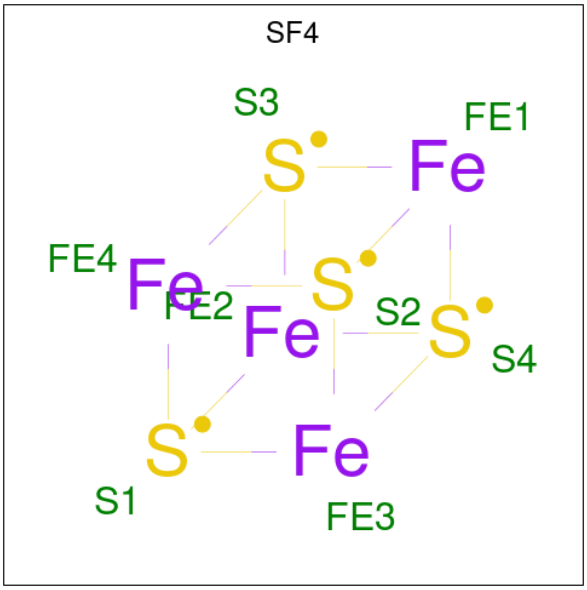
Mol	Chain	Residues	Atoms				AltConf
46	4	1	Total	C	O	P	0
			82	63	17	2	
46	J	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 47 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$) (labeled as "Ligand of Interest" by depositor).



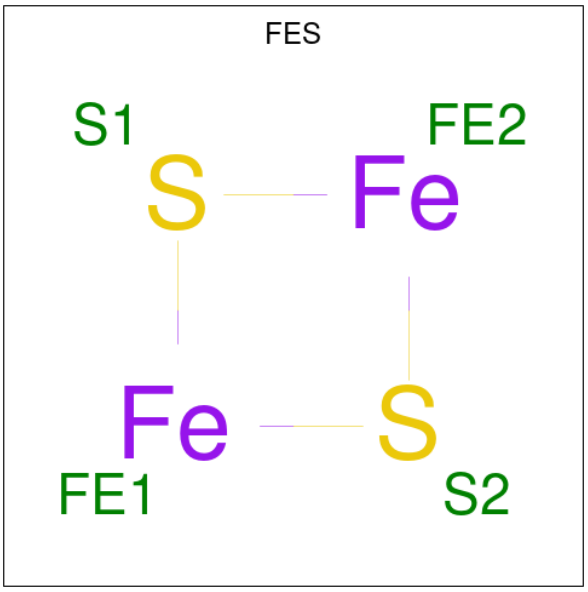
Mol	Chain	Residues	Atoms					AltConf
47	8	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
48	8	1	Total Fe S 8 4 4	0
48	A	1	Total Fe S 8 4 4	0
48	A	1	Total Fe S 8 4 4	0
48	D	1	Total Fe S 8 4 4	0
48	E	1	Total Fe S 8 4 4	0
48	E	1	Total Fe S 8 4 4	0

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

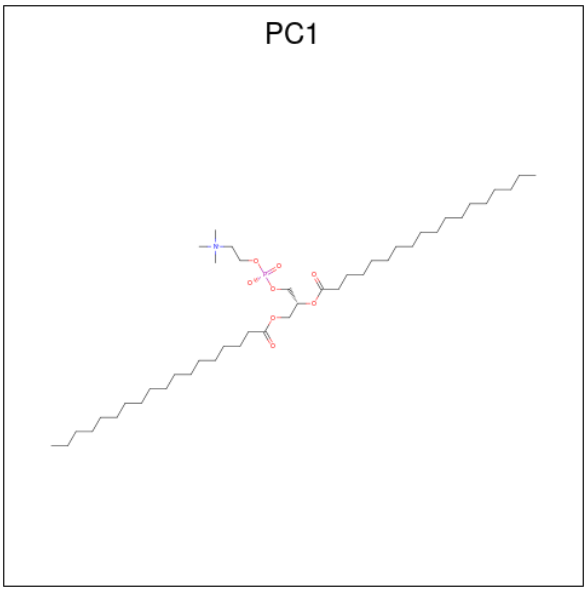


Mol	Chain	Residues	Atoms			AltConf
49	9	1	Total	Fe	S	0
			4	2	2	
49	A	1	Total	Fe	S	0
			4	2	2	

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

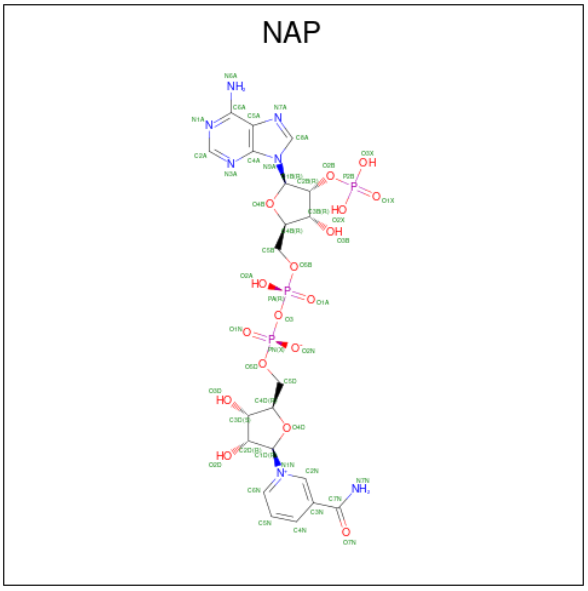
Mol	Chain	Residues	Atoms		AltConf
50	I	1	Total	Zn	0
			1	1	

- Molecule 51 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
51	L	1	Total	C	N	O	P	0
			47	37	1	8	1	
51	Q	1	Total	C	N	O	P	0
			46	36	1	8	1	
51	S	1	Total	C	N	O	P	0
			47	37	1	8	1	
51	j	1	Total	C	N	O	P	0
			39	29	1	8	1	

- Molecule 52 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



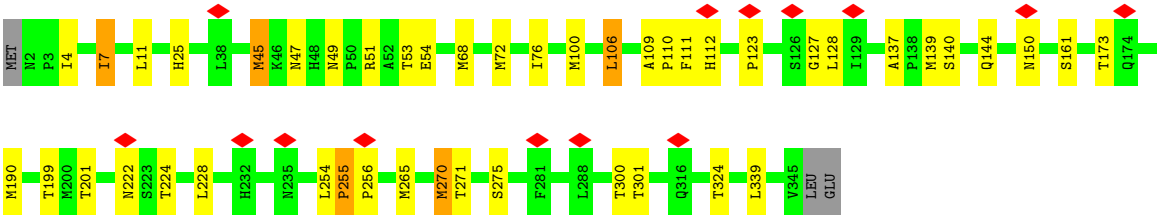
Mol	Chain	Residues	Atoms					AltConf
52	R	1	Total	C	N	O	P	0
			48	21	7	17	3	

3 Residue-property plots (i)

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

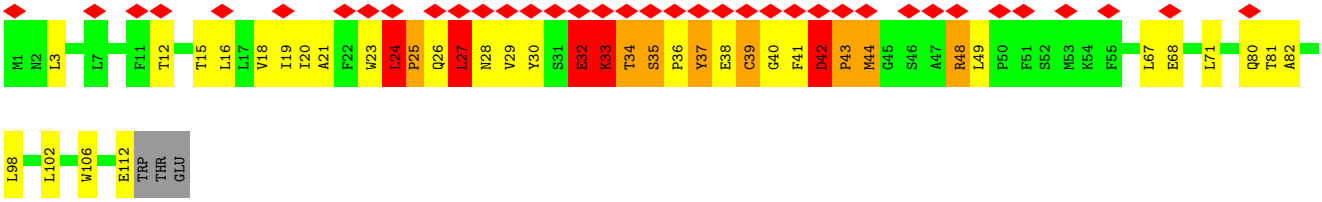
• Molecule 1: NADH-ubiquinone oxidoreductase chain 2

Chain 2:



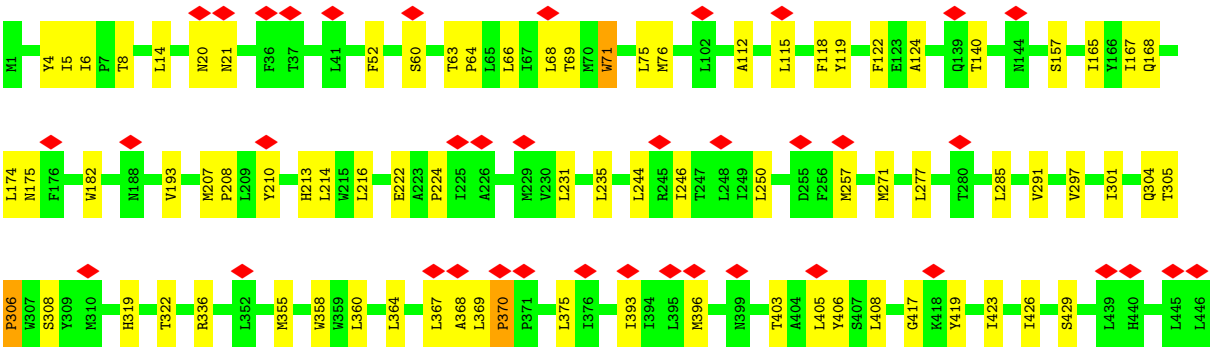
• Molecule 2: NADH-ubiquinone oxidoreductase chain 3

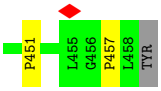
Chain 3:



• Molecule 3: NADH-ubiquinone oxidoreductase chain 4

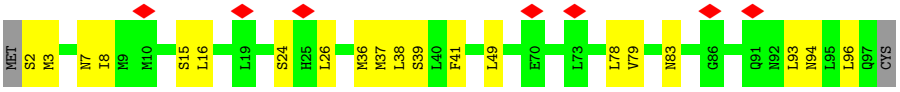
Chain 4:





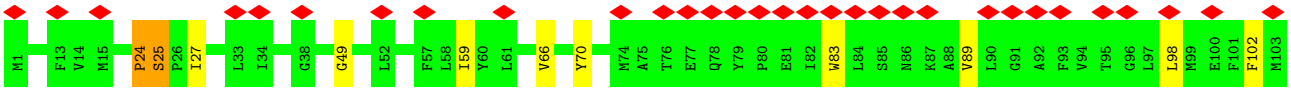
• Molecule 4: NADH-ubiquinone oxidoreductase chain 4L

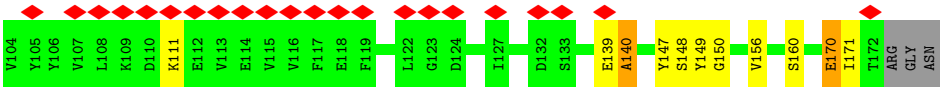
Chain 5:



• Molecule 5: NADH-ubiquinone oxidoreductase chain 6

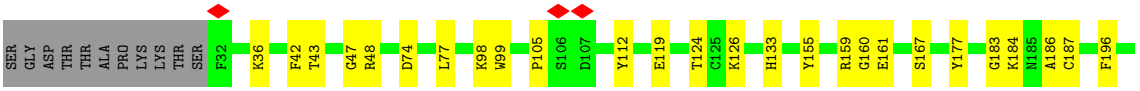
Chain 7:

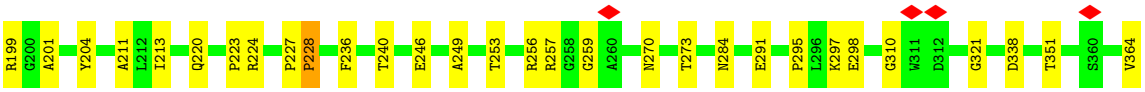


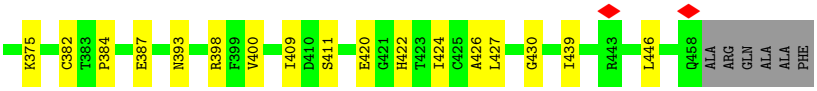


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 8:

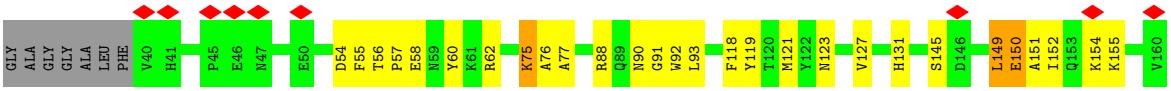


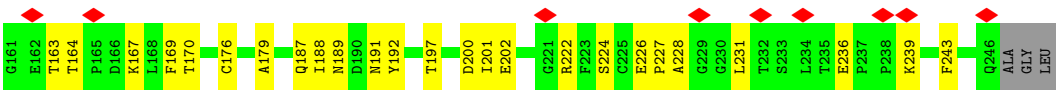




• Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

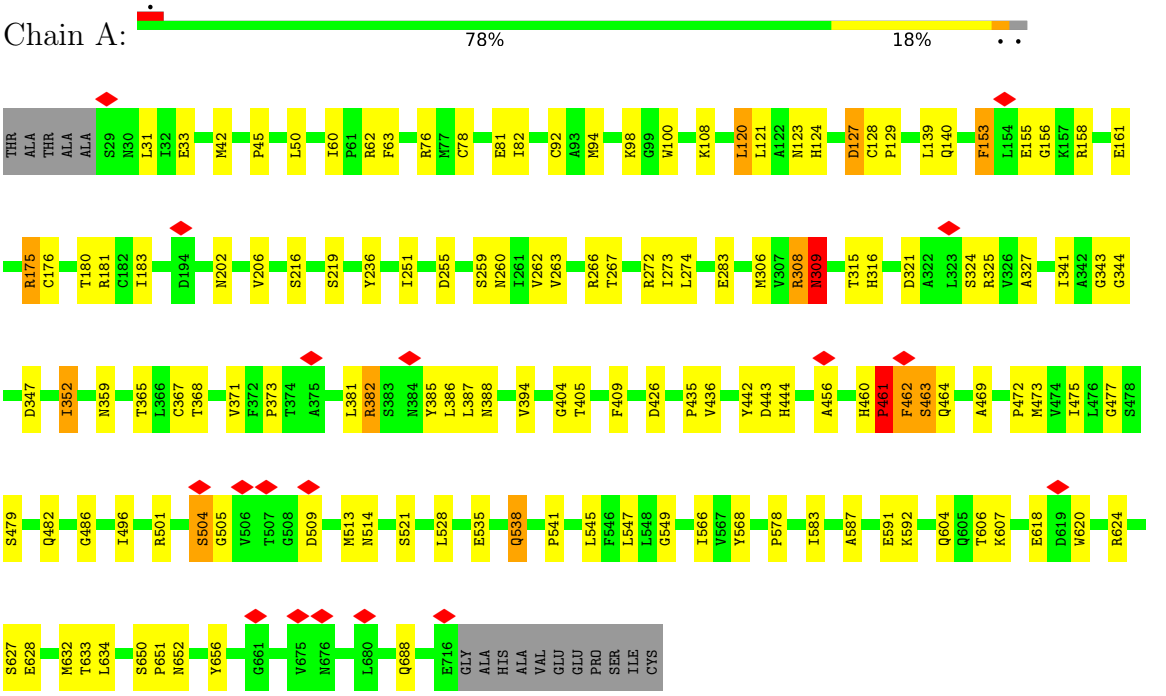
Chain 9:





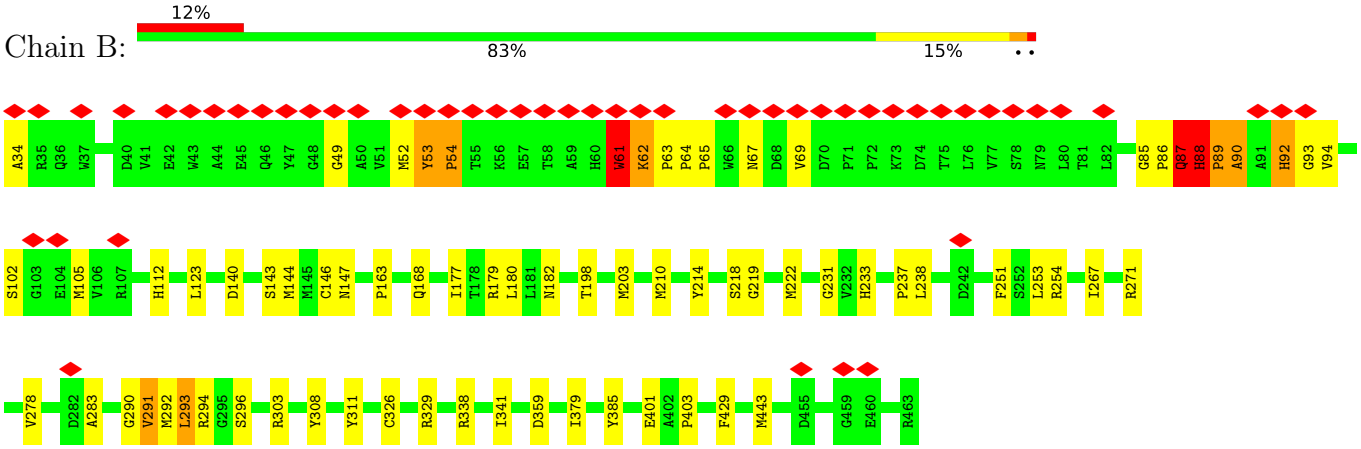
• Molecule 8: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain A:



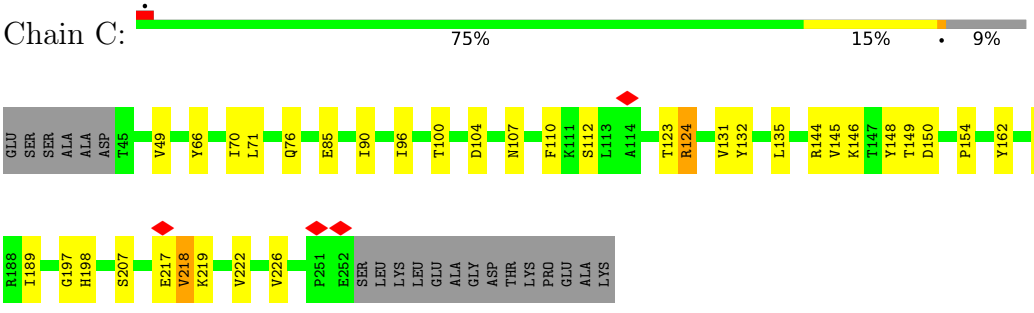
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain B:



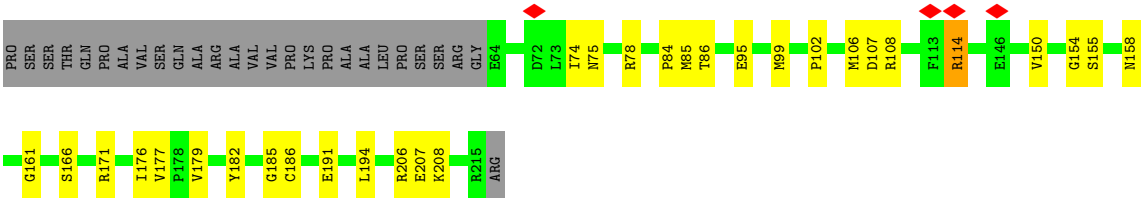
• Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:

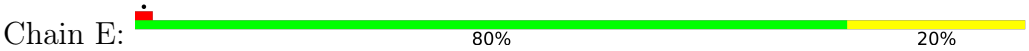


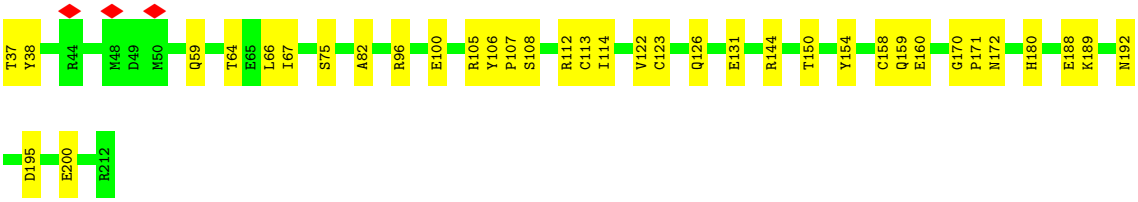
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain D:

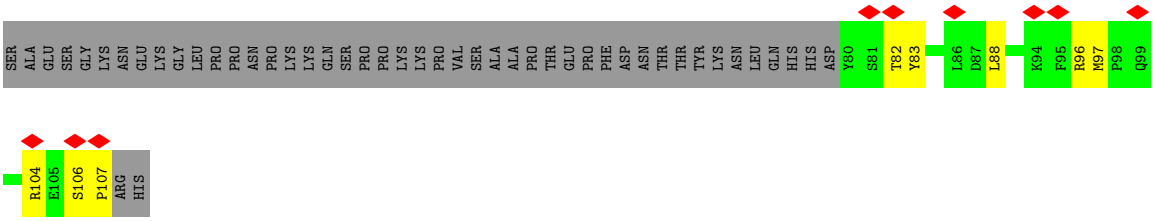


• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

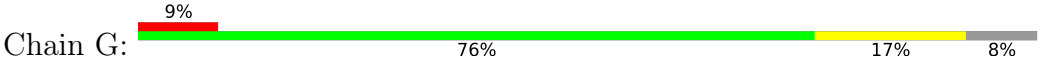




• Molecule 13: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

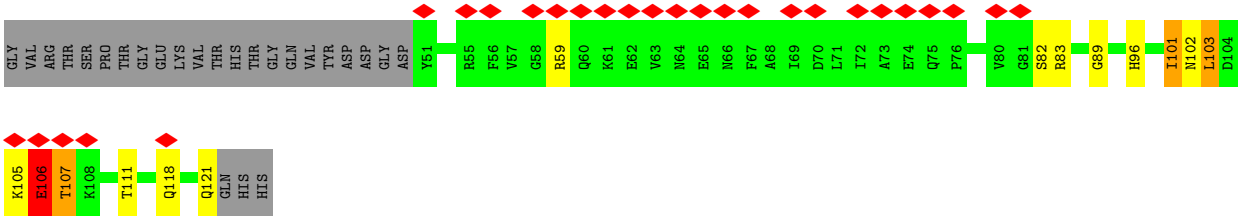


• Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

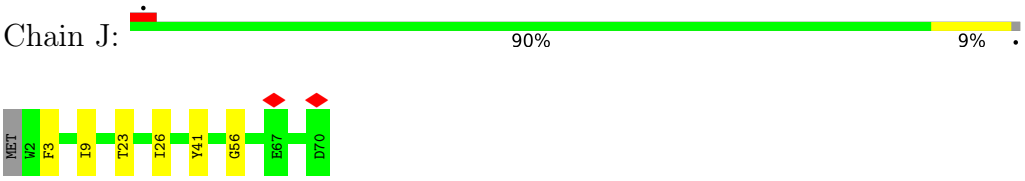


• Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

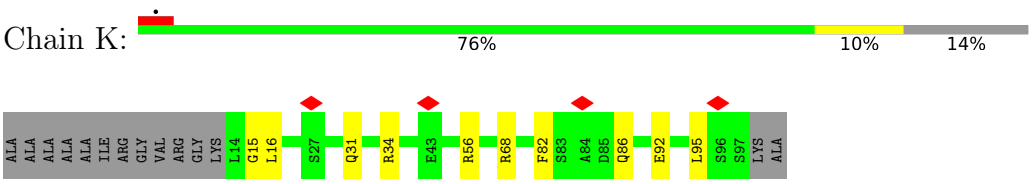
• Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



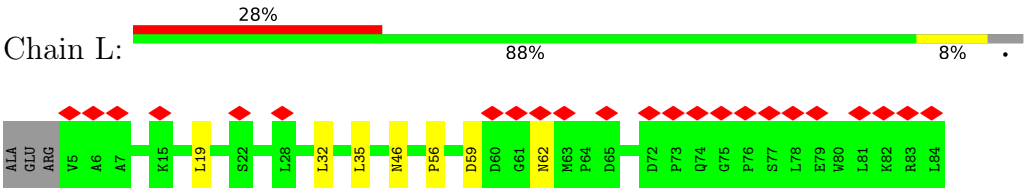
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



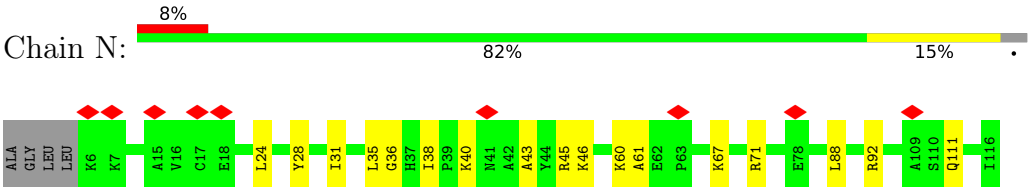
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



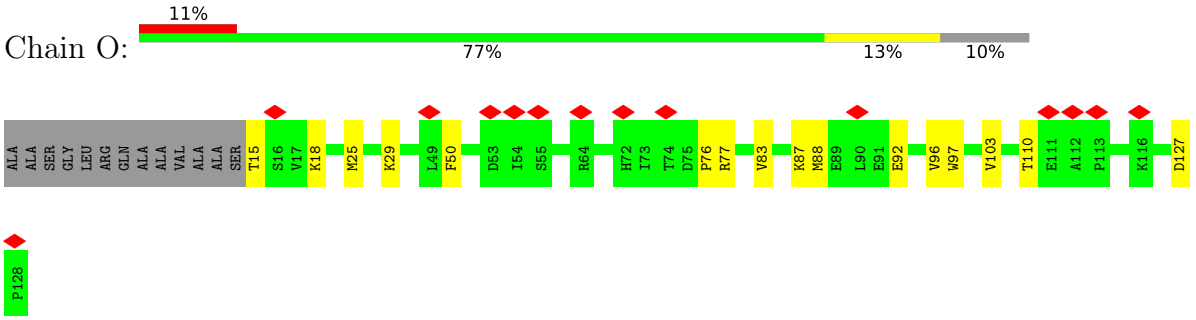
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

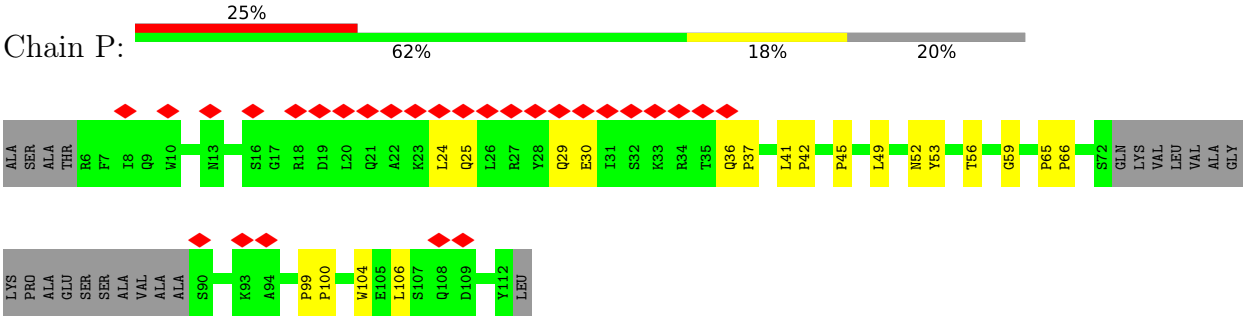


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



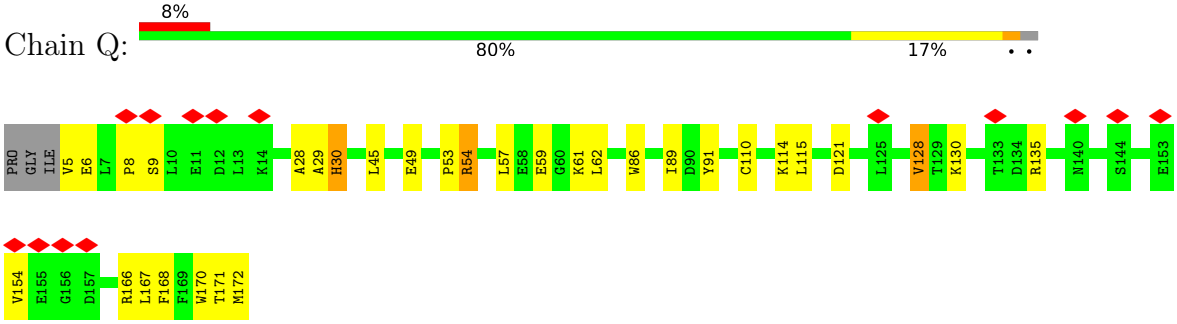
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain P:



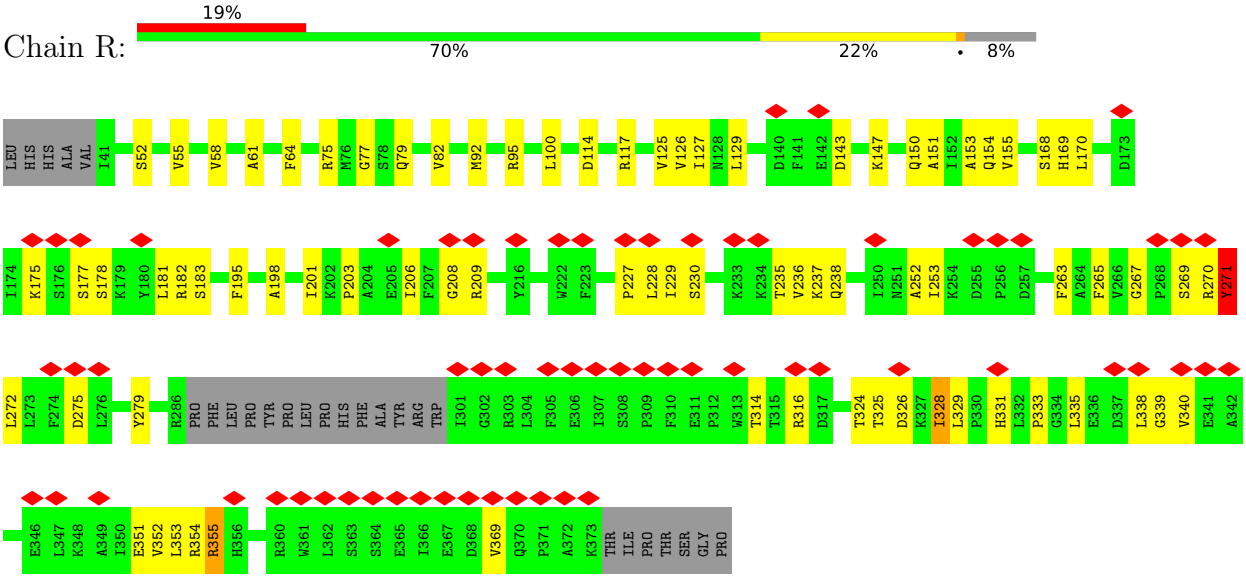
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Q:



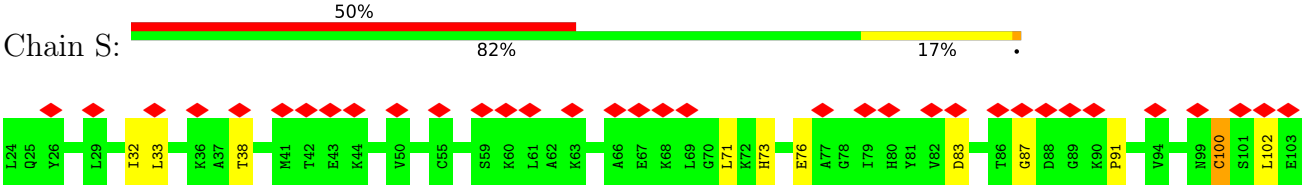
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

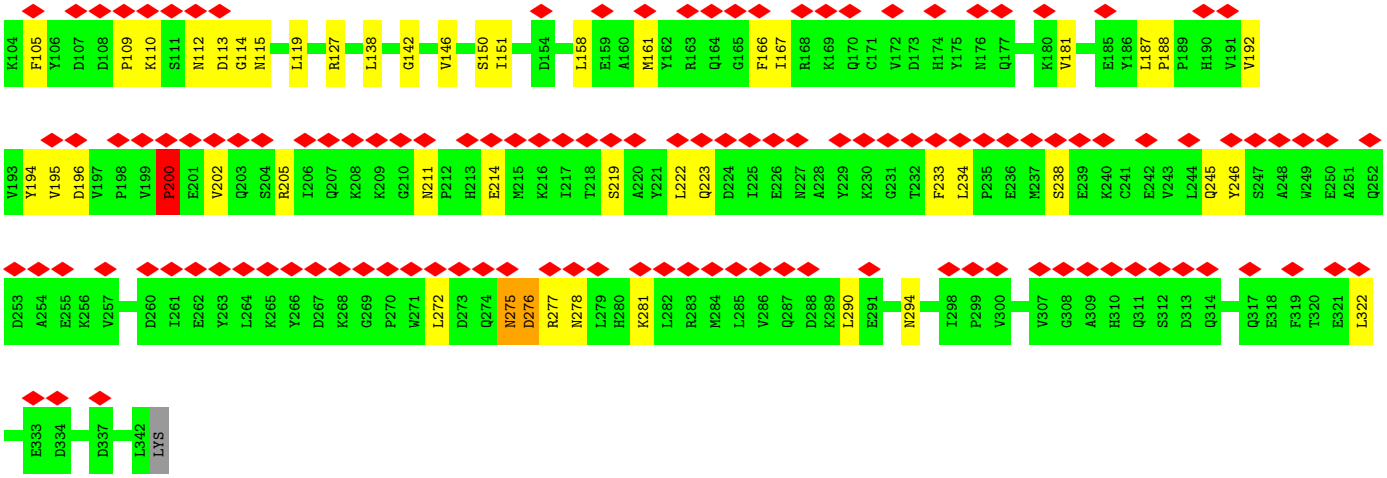
Chain R:



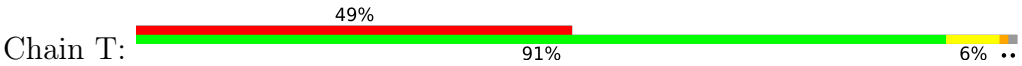
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

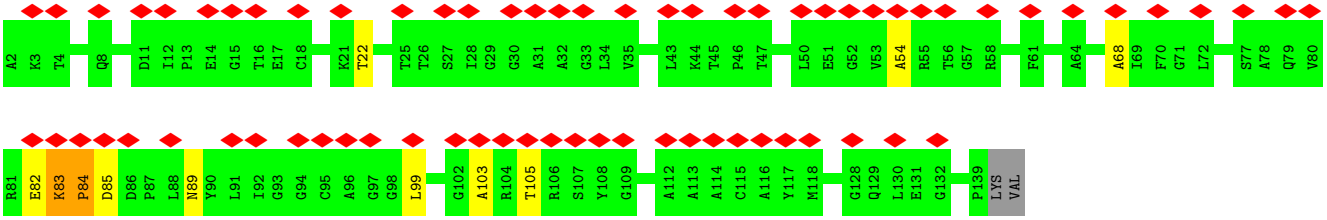
Chain S:



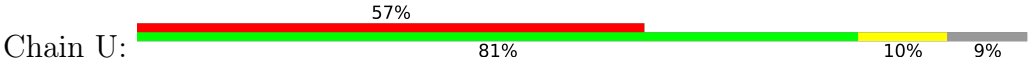


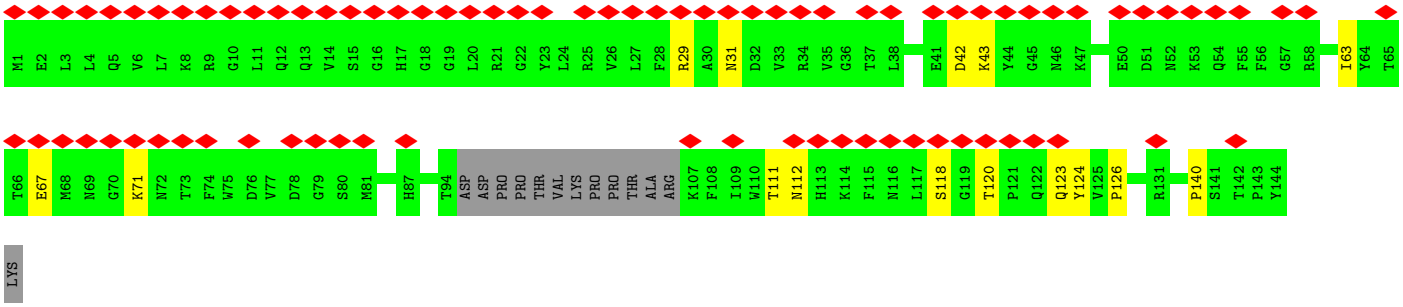
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



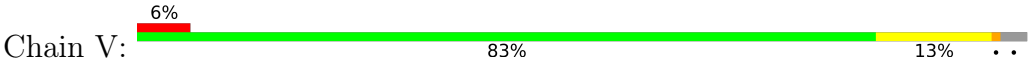


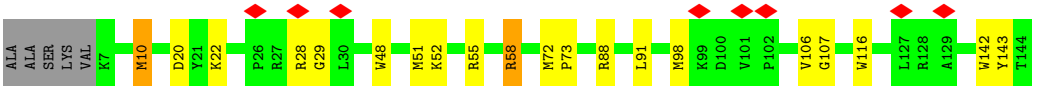
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



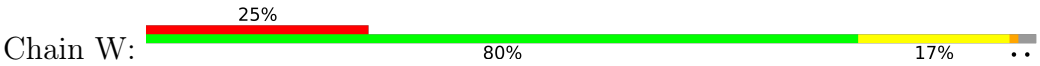


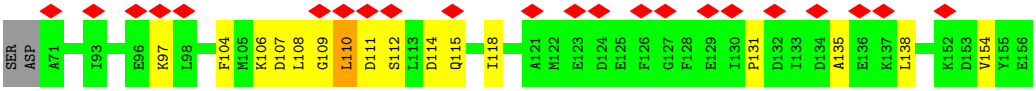
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13





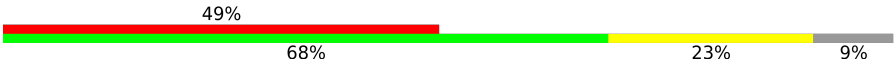
• Molecule 29: Acyl carrier protein, mitochondrial

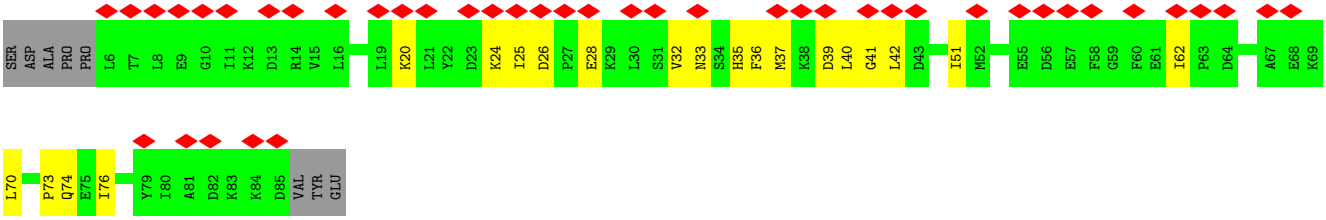




• Molecule 29: Acyl carrier protein, mitochondrial

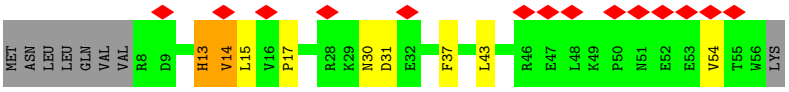
Chain M:





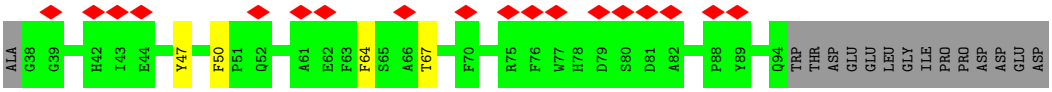
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain X:



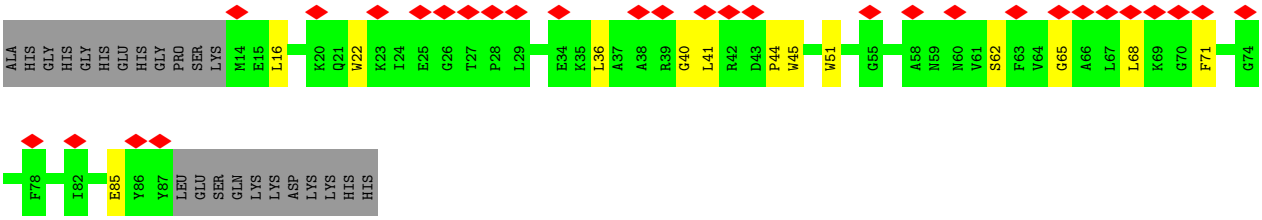
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y:



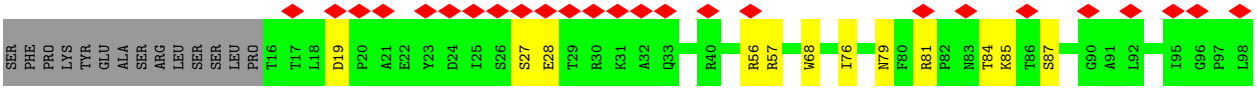
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

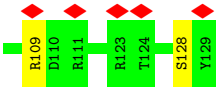
Chain Z:



• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

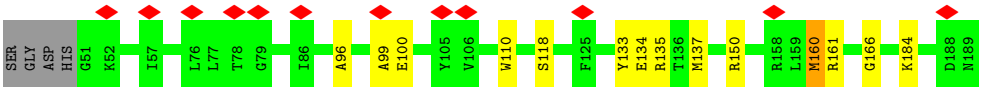
Chain a:





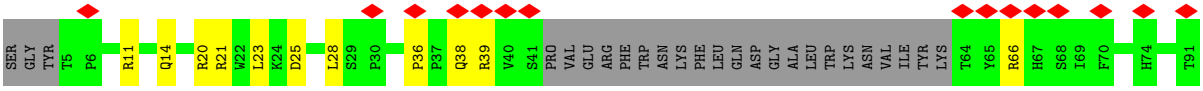
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

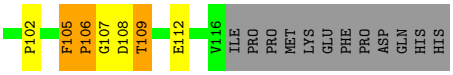
Chain b:



• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

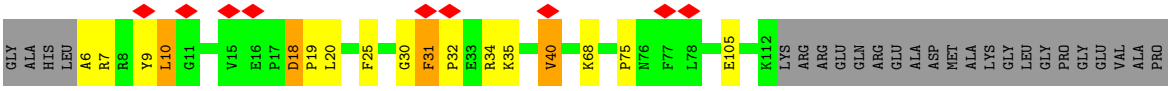
Chain c:





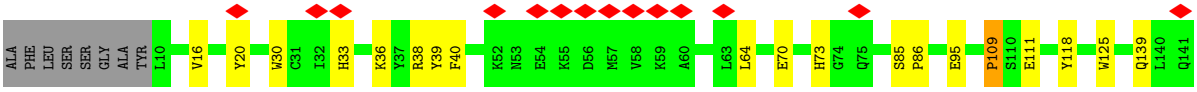
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

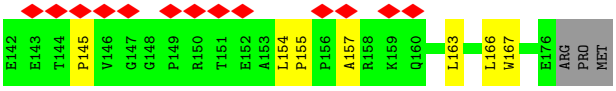
Chain d:



• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

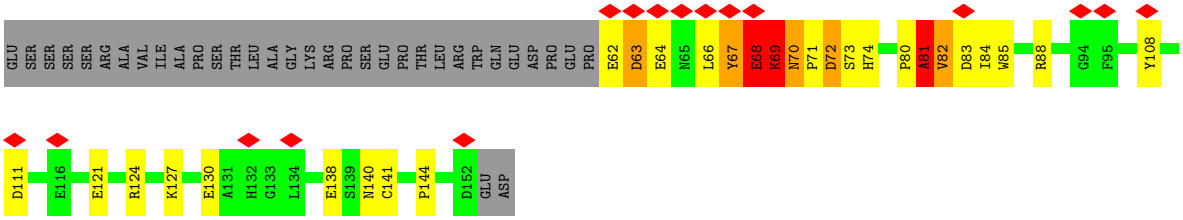
Chain f:



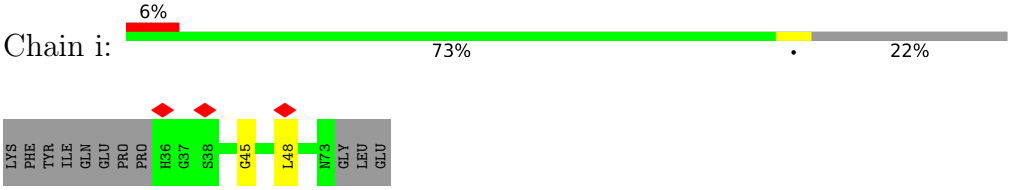


• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

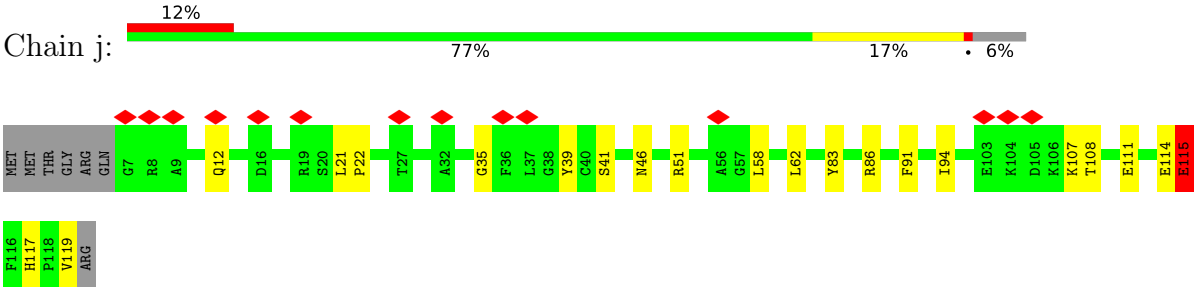
Chain h:



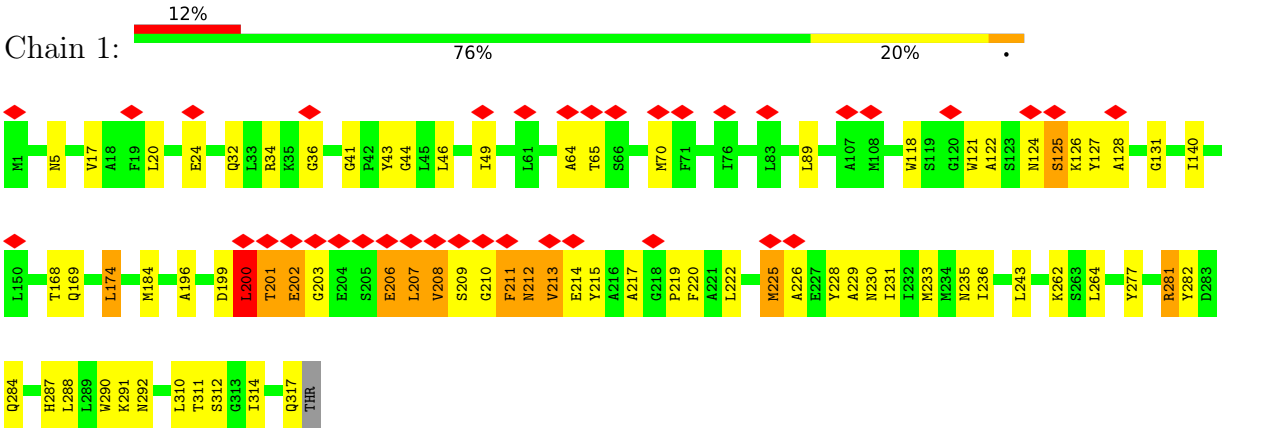
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



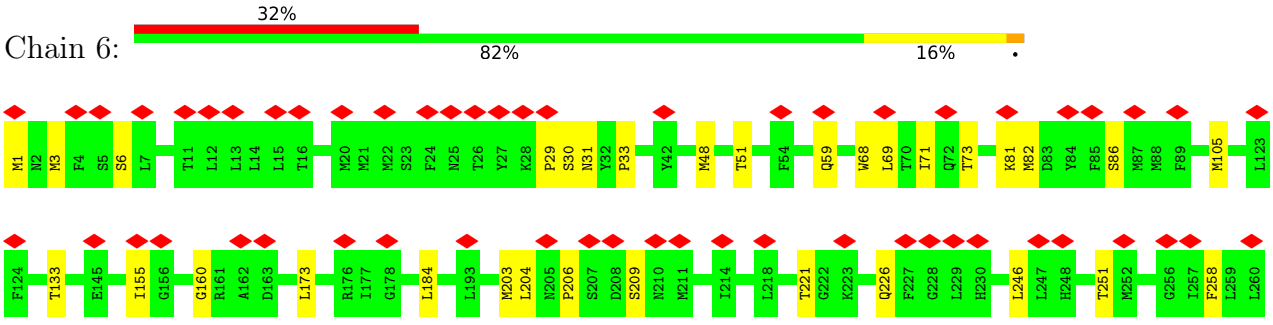
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 subunit C2

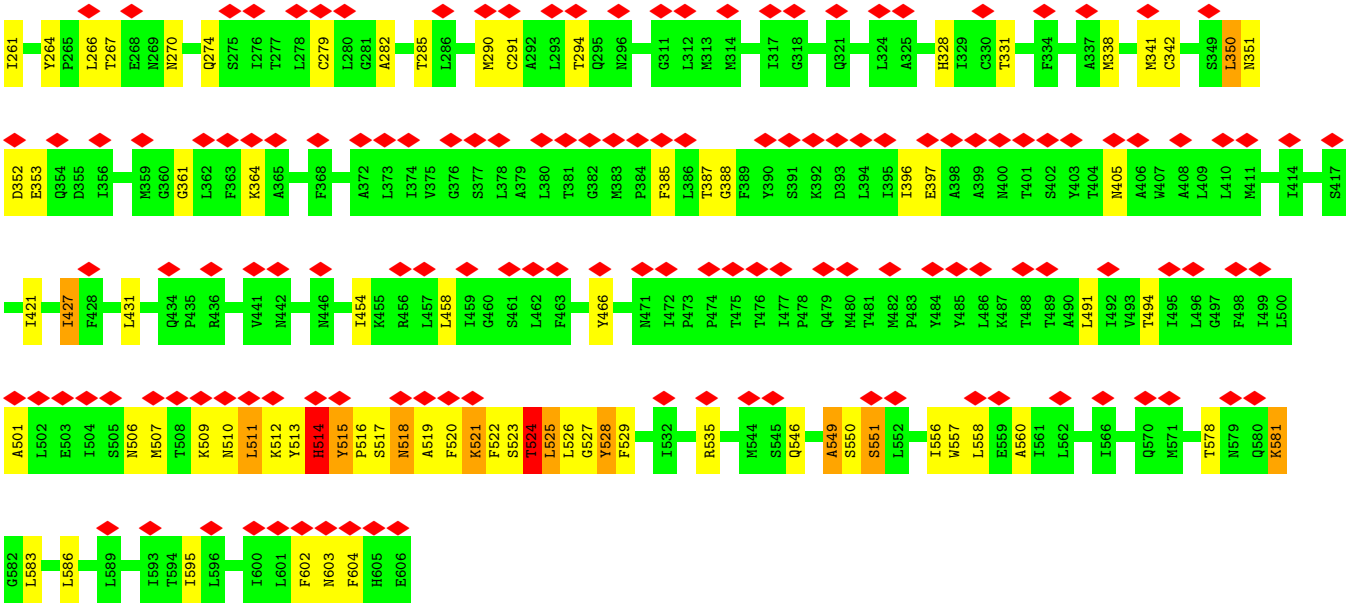


• Molecule 41: NADH-ubiquinone oxidoreductase chain 1



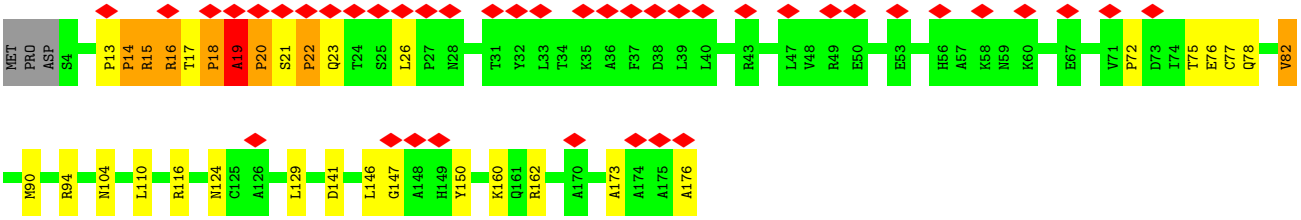
• Molecule 42: NADH-ubiquinone oxidoreductase chain 5





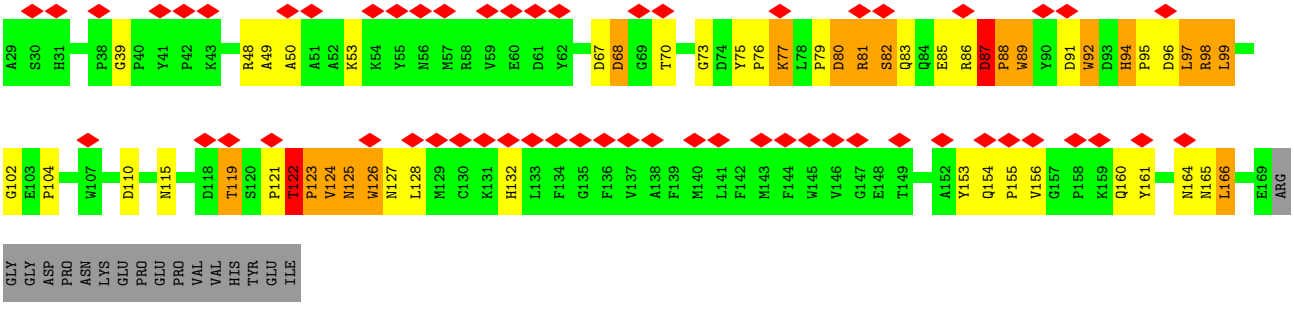
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain g:



• Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain e:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.143	Depositor
Minimum map value	-0.274	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.111	Depositor
Map size (Å)	391.244, 391.244, 391.244	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3973, 1.3973, 1.3973	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, NAP, FES, 3PE, FMN, ZN, PC1, CDL

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	2	0.41	0/2646	0.85	3/3618 (0.1%)
2	3	0.51	0/887	0.99	5/1216 (0.4%)
3	4	0.38	0/3538	0.86	10/4845 (0.2%)
4	5	0.36	0/706	0.84	0/960
5	7	0.34	0/1213	0.83	4/1659 (0.2%)
6	8	0.31	0/3035	0.76	6/4130 (0.1%)
7	9	0.29	0/1572	0.76	0/2150
8	A	0.37	0/5269	0.79	12/7152 (0.2%)
9	B	0.46	0/3500	0.88	11/4748 (0.2%)
10	C	0.39	0/1756	0.74	2/2394 (0.1%)
11	D	0.49	0/1231	0.87	1/1669 (0.1%)
12	E	0.45	0/1418	0.83	3/1922 (0.2%)
13	F	0.37	0/188	1.27	5/259 (1.9%)
14	G	0.40	0/1004	0.85	2/1359 (0.1%)
15	H	0.34	0/800	0.82	2/1076 (0.2%)
16	I	0.35	0/538	0.84	1/722 (0.1%)
17	J	0.29	0/545	0.63	0/740
18	K	0.28	0/663	0.72	0/896
19	L	0.33	0/623	0.81	2/862 (0.2%)
20	N	0.27	0/882	0.72	0/1203
21	O	0.31	0/948	0.68	2/1279 (0.2%)
22	P	0.32	0/719	0.80	0/981
23	Q	0.29	0/1381	0.84	2/1869 (0.1%)
24	R	0.32	0/2465	0.85	4/3349 (0.1%)
25	S	0.31	0/2348	0.85	5/3198 (0.2%)
26	T	0.31	0/959	0.83	1/1305 (0.1%)
27	U	0.27	0/1053	0.79	3/1439 (0.2%)
28	V	0.31	0/1121	0.70	0/1515
29	M	0.27	0/651	0.77	2/876 (0.2%)
29	W	0.25	0/624	0.84	0/847
30	X	0.31	0/383	0.94	4/523 (0.8%)
31	Y	0.26	0/428	0.60	0/592

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	Z	0.37	0/506	1.04	6/688 (0.9%)
33	a	0.29	0/878	0.82	5/1195 (0.4%)
34	b	0.32	0/1058	0.83	5/1434 (0.3%)
35	c	0.34	0/632	1.03	6/871 (0.7%)
36	d	0.31	0/724	0.79	2/989 (0.2%)
37	f	0.24	0/1191	0.77	2/1639 (0.1%)
38	h	0.34	0/743	0.87	0/1013
39	i	0.22	0/286	0.48	0/392
40	j	0.31	0/922	0.83	5/1254 (0.4%)
41	1	0.40	0/2572	0.86	7/3513 (0.2%)
42	6	0.30	0/4892	0.74	6/6660 (0.1%)
43	g	0.27	0/1380	0.88	7/1872 (0.4%)
44	e	0.36	0/888	1.22	19/1234 (1.5%)
All	All	0.35	0/61766	0.83	162/84107 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	9
3	4	0	6
4	5	0	3
5	7	0	5
6	8	0	1
7	9	0	4
8	A	0	12
9	B	0	3
10	C	0	1
11	D	0	3
12	E	0	1
15	H	0	1
16	I	0	1
20	N	0	1
22	P	0	2
23	Q	0	1
24	R	0	4
25	S	0	4
26	T	0	3
27	U	0	1
28	V	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	M	0	1
29	W	0	1
34	b	0	3
36	d	0	1
37	f	0	1
38	h	0	2
40	j	0	2
41	1	0	1
42	6	0	5
43	g	0	1
44	e	0	3
All	All	0	90

There are no bond length outliers.

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	g	19	ALA	CA-C-N	11.74	134.52	119.84
43	g	19	ALA	C-N-CA	11.74	134.52	119.84
8	A	176	CYS	N-CA-C	8.82	122.05	111.02
37	f	163	LEU	CA-C-N	8.70	147.89	127.00
37	f	163	LEU	C-N-CA	8.70	147.89	127.00
2	3	42	ASP	C-N-CD	-8.67	89.45	125.00
6	8	228	PRO	CA-C-N	8.18	136.42	121.70
6	8	228	PRO	C-N-CA	8.18	136.42	121.70
9	B	88	HIS	CA-C-N	7.94	129.76	119.84
9	B	88	HIS	C-N-CA	7.94	129.76	119.84
23	Q	54	ARG	N-CA-C	-7.72	105.02	114.75
2	3	3	LEU	CA-C-N	7.71	135.58	121.70
2	3	3	LEU	C-N-CA	7.71	135.58	121.70
35	c	66	ARG	CA-C-N	7.67	135.51	121.70
35	c	66	ARG	C-N-CA	7.67	135.51	121.70
3	4	4	TYR	N-CA-C	-7.50	104.75	114.04
6	8	36	LYS	CA-C-N	7.34	134.91	121.70
6	8	36	LYS	C-N-CA	7.34	134.91	121.70
35	c	36	PRO	CA-C-N	7.32	144.58	127.00
35	c	36	PRO	C-N-CA	7.32	144.58	127.00
32	Z	85	GLU	CA-C-N	7.21	134.68	121.70
32	Z	85	GLU	C-N-CA	7.21	134.68	121.70
6	8	259	GLY	CA-C-N	7.21	134.68	121.70
6	8	259	GLY	C-N-CA	7.21	134.68	121.70
44	e	87	ASP	N-CA-C	7.02	125.33	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	F	104	ARG	CA-C-N	6.93	134.18	121.70
13	F	104	ARG	C-N-CA	6.93	134.18	121.70
19	L	62	ASN	CA-C-N	6.88	134.09	121.70
19	L	62	ASN	C-N-CA	6.88	134.09	121.70
41	1	311	THR	N-CA-C	-6.88	104.18	114.64
8	A	461	PRO	CA-C-N	6.85	134.63	121.54
8	A	461	PRO	C-N-CA	6.85	134.63	121.54
35	c	36	PRO	C-N-CD	-6.84	105.55	120.60
34	b	99	ALA	N-CA-C	6.84	119.56	111.02
44	e	161	TYR	CA-C-N	6.79	128.33	119.84
44	e	161	TYR	C-N-CA	6.79	128.33	119.84
30	X	43	LEU	CA-C-N	6.76	133.87	121.70
30	X	43	LEU	C-N-CA	6.76	133.87	121.70
15	H	58	ILE	N-CA-C	-6.72	106.48	112.12
33	a	128	SER	CA-C-N	6.72	133.80	121.70
33	a	128	SER	C-N-CA	6.72	133.80	121.70
44	e	154	GLN	CA-C-N	6.72	128.24	119.84
44	e	154	GLN	C-N-CA	6.72	128.24	119.84
11	D	191	GLU	N-CA-C	-6.68	104.29	113.18
5	7	140	ALA	CA-C-N	6.68	133.73	121.70
5	7	140	ALA	C-N-CA	6.68	133.73	121.70
5	7	139	GLU	CA-C-N	6.61	133.59	121.70
5	7	139	GLU	C-N-CA	6.61	133.59	121.70
35	c	109	THR	CB-CA-C	-6.58	108.97	116.54
12	E	75	SER	CA-C-N	6.58	133.55	121.70
12	E	75	SER	C-N-CA	6.58	133.55	121.70
24	R	271	TYR	CA-C-N	6.49	133.94	121.54
24	R	271	TYR	C-N-CA	6.49	133.94	121.54
14	G	155	PRO	CA-C-N	6.47	133.34	121.70
14	G	155	PRO	C-N-CA	6.47	133.34	121.70
44	e	119	THR	N-CA-C	6.45	119.84	109.79
25	S	87	GLY	CA-C-N	6.43	133.27	121.70
25	S	87	GLY	C-N-CA	6.43	133.27	121.70
40	j	22	PRO	CA-C-N	6.42	142.40	127.00
40	j	22	PRO	C-N-CA	6.42	142.40	127.00
36	d	31	PHE	CA-C-N	6.35	142.23	127.00
36	d	31	PHE	C-N-CA	6.35	142.23	127.00
9	B	293	LEU	N-CA-C	-6.34	97.29	110.80
23	Q	30	HIS	N-CA-C	-6.34	104.75	113.18
9	B	292	MET	CA-C-N	6.34	133.65	121.54
9	B	292	MET	C-N-CA	6.34	133.65	121.54
24	R	369	VAL	CA-C-N	6.33	133.09	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	369	VAL	C-N-CA	6.33	133.09	121.70
8	A	381	LEU	CA-C-N	6.24	133.46	121.54
8	A	381	LEU	C-N-CA	6.24	133.46	121.54
1	2	127	GLY	CA-C-N	6.16	132.79	121.70
1	2	127	GLY	C-N-CA	6.16	132.79	121.70
41	1	125	SER	CA-C-N	6.12	129.32	120.38
41	1	125	SER	C-N-CA	6.12	129.32	120.38
44	e	122	THR	CA-C-N	6.11	127.48	119.84
44	e	122	THR	C-N-CA	6.11	127.48	119.84
44	e	85	GLU	CA-C-N	6.04	133.08	121.54
44	e	85	GLU	C-N-CA	6.04	133.08	121.54
27	U	120	THR	CA-C-N	6.04	141.49	127.00
27	U	120	THR	C-N-CA	6.04	141.49	127.00
33	a	19	ASP	CA-C-N	6.02	141.45	127.00
33	a	19	ASP	C-N-CA	6.02	141.45	127.00
16	I	105	LYS	O-C-N	5.99	128.96	121.95
41	1	126	LYS	N-CA-C	5.95	119.37	111.75
12	E	67	ILE	N-CA-C	-5.92	106.94	111.62
3	4	457	PRO	CA-C-N	5.92	132.35	121.70
3	4	457	PRO	C-N-CA	5.92	132.35	121.70
42	6	509	LYS	N-CA-C	-5.89	105.34	113.18
9	B	87	GLN	N-CA-C	-5.87	104.74	112.72
41	1	212	ASN	N-CA-C	-5.87	105.38	113.18
40	j	22	PRO	C-N-CD	-5.81	107.81	120.60
30	X	54	VAL	CA-C-N	5.79	132.60	121.54
30	X	54	VAL	C-N-CA	5.79	132.60	121.54
42	6	350	LEU	CA-C-N	5.78	132.58	121.54
42	6	350	LEU	C-N-CA	5.78	132.58	121.54
25	S	113	ASP	CA-C-N	5.72	132.00	121.70
25	S	113	ASP	C-N-CA	5.72	132.00	121.70
9	B	53	TYR	CA-C-N	5.71	126.97	119.84
9	B	53	TYR	C-N-CA	5.71	126.97	119.84
13	F	97	MET	C-N-CD	-5.67	108.11	120.60
3	4	224	PRO	CA-C-N	5.67	128.20	120.77
3	4	224	PRO	C-N-CA	5.67	128.20	120.77
44	e	99	LEU	N-CA-C	5.59	122.71	110.80
29	M	36	PHE	CA-C-N	5.58	132.19	121.54
29	M	36	PHE	C-N-CA	5.58	132.19	121.54
44	e	88	PRO	N-CA-C	-5.57	100.99	112.47
27	U	120	THR	C-N-CD	-5.52	108.45	120.60
2	3	39	CYS	N-CA-C	-5.48	99.13	110.80
3	4	14	LEU	N-CA-C	-5.47	107.26	114.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	76	ILE	N-CA-C	-5.45	107.54	112.12
44	e	50	ALA	N-CA-C	-5.42	105.01	111.03
44	e	82	SER	N-CA-C	5.41	122.33	110.80
41	1	212	ASN	CA-C-N	5.34	131.59	121.97
41	1	212	ASN	C-N-CA	5.34	131.59	121.97
8	A	352	ILE	N-CA-C	-5.34	107.64	112.12
42	6	602	PHE	CA-C-N	5.33	131.72	121.54
42	6	602	PHE	C-N-CA	5.33	131.72	121.54
15	H	15	ASP	O-C-N	5.29	124.74	120.83
40	j	115	GLU	CA-C-N	5.29	131.22	121.70
40	j	115	GLU	C-N-CA	5.29	131.22	121.70
9	B	231	GLY	CA-C-N	5.28	127.77	120.49
9	B	231	GLY	C-N-CA	5.28	127.77	120.49
3	4	417	GLY	CA-C-N	5.27	131.60	121.54
3	4	417	GLY	C-N-CA	5.27	131.60	121.54
21	O	76	PRO	CA-C-N	5.25	131.58	121.54
21	O	76	PRO	C-N-CA	5.25	131.58	121.54
25	S	276	ASP	N-CA-C	5.25	121.98	110.80
3	4	370	PRO	N-CA-C	5.25	117.11	110.70
32	Z	41	LEU	CA-C-N	5.22	131.10	121.70
32	Z	41	LEU	C-N-CA	5.22	131.10	121.70
10	C	124	ARG	CA-C-N	5.20	131.48	121.54
10	C	124	ARG	C-N-CA	5.20	131.48	121.54
8	A	504	SER	CA-C-N	5.19	131.05	121.70
8	A	504	SER	C-N-CA	5.19	131.05	121.70
3	4	75	LEU	N-CA-C	-5.18	108.22	114.75
43	g	82	VAL	N-CA-C	-5.18	107.53	111.62
43	g	124	ASN	CA-C-N	5.17	131.41	121.54
43	g	124	ASN	C-N-CA	5.17	131.41	121.54
26	T	83	LYS	N-CA-C	5.16	121.22	109.81
32	Z	62	SER	CA-C-N	5.16	131.40	121.54
32	Z	62	SER	C-N-CA	5.16	131.40	121.54
34	b	160	MET	CA-C-N	5.10	130.88	121.70
34	b	160	MET	C-N-CA	5.10	130.88	121.70
8	A	656	TYR	CA-C-N	5.09	131.27	121.54
8	A	656	TYR	C-N-CA	5.09	131.27	121.54
44	e	80	ASP	CA-C-N	5.09	131.26	121.54
44	e	80	ASP	C-N-CA	5.09	131.26	121.54
44	e	97	LEU	N-CA-C	-5.08	105.82	111.36
9	B	92	HIS	N-CA-C	5.08	121.61	110.80
1	2	255	PRO	N-CA-C	5.07	116.88	110.70
42	6	524	THR	N-CA-C	-5.06	108.13	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	F	97	MET	CA-C-N	5.06	139.14	127.00
13	F	97	MET	C-N-CA	5.06	139.14	127.00
44	e	115	ASN	N-CA-C	-5.06	106.95	113.02
34	b	100	GLU	CA-C-N	5.05	130.79	121.70
34	b	100	GLU	C-N-CA	5.05	130.79	121.70
43	g	72	PRO	CA-C-N	-5.04	115.55	121.90
43	g	72	PRO	C-N-CA	-5.04	115.55	121.90
44	e	164	ASN	N-CA-C	5.04	117.03	110.43
2	3	3	LEU	N-CA-C	5.04	119.88	113.18
8	A	153	PHE	CA-C-N	5.03	130.75	121.70
8	A	153	PHE	C-N-CA	5.03	130.75	121.70

There are no chirality outliers.

All (90) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	1	281	ARG	Peptide
1	2	106	LEU	Peptide
1	2	111	PHE	Peptide
1	2	128	LEU	Peptide
1	2	199	THR	Peptide
1	2	222	ASN	Peptide
1	2	270	MET	Peptide
1	2	271	THR	Peptide
1	2	339	LEU	Peptide
1	2	45	MET	Peptide
3	4	140	THR	Peptide
3	4	222	GLU	Peptide
3	4	306	PRO	Peptide
3	4	368	ALA	Peptide
3	4	369	LEU	Peptide
3	4	71	TRP	Peptide
4	5	15	SER	Peptide
4	5	16	LEU	Peptide
4	5	24	SER	Peptide
42	6	29	PRO	Peptide
42	6	351	ASN	Peptide
42	6	352	ASP	Peptide
42	6	549	ALA	Peptide
42	6	71	ILE	Peptide
5	7	140	ALA	Peptide
5	7	148	SER	Peptide

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Mol	Chain	Res	Type	Group
5	7	170	GLU	Peptide
5	7	24	PRO	Peptide
5	7	25	SER	Peptide
6	8	228	PRO	Peptide
7	9	150	GLU	Peptide
7	9	167	LYS	Peptide
7	9	179	ALA	Peptide
7	9	75	LYS	Peptide
8	A	127	ASP	Peptide
8	A	128	CYS	Peptide
8	A	175	ARG	Peptide
8	A	236	TYR	Peptide
8	A	283	GLU	Peptide
8	A	308	ARG	Peptide
8	A	309	ASN	Peptide
8	A	382	ARG	Peptide
8	A	460	HIS	Peptide
8	A	461	PRO	Peptide
8	A	462	PHE	Peptide
8	A	98	LYS	Peptide
9	B	218	SER	Peptide
9	B	290	GLY	Peptide
9	B	291	VAL	Peptide
10	C	198	HIS	Peptide
11	D	161	GLY	Peptide
11	D	186	CYS	Peptide
11	D	84	PRO	Peptide
12	E	107	PRO	Peptide
15	H	84	GLU	Peptide
16	I	106	GLU	Peptide
29	M	24	LYS	Peptide
20	N	40	LYS	Peptide
22	P	36	GLN	Peptide
22	P	52	ASN	Peptide
23	Q	91	TYR	Peptide
24	R	271	TYR	Peptide
24	R	324	THR	Peptide
24	R	333	PRO	Peptide
24	R	355	ARG	Peptide
25	S	100	CYS	Peptide
25	S	275	ASN	Peptide
25	S	278	ASN	Peptide

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Mol	Chain	Res	Type	Group
25	S	38	THR	Peptide
26	T	105	THR	Peptide
26	T	54	ALA	Peptide
26	T	83	LYS	Peptide
27	U	118	SER	Peptide
28	V	10	MET	Peptide
28	V	142	TRP	Peptide
28	V	72	MET	Peptide
29	W	154	VAL	Peptide
34	b	110	TRP	Peptide
34	b	134	GLU	Peptide
34	b	96	ALA	Peptide
36	d	18	ASP	Peptide
44	e	77	LYS	Peptide
44	e	79	PRO	Peptide
44	e	81	ARG	Peptide
37	f	109	PRO	Peptide
43	g	160	LYS	Peptide
38	h	80	PRO	Peptide
38	h	81	ALA	Peptide
40	j	115	GLU	Peptide
40	j	21	LEU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2582	0	2612	30	0
2	3	864	0	866	65	0
3	4	3447	0	3442	46	0
4	5	697	0	708	13	0
5	7	1186	0	1123	14	0
6	8	2965	0	2596	46	0
7	9	1535	0	1491	34	0
8	A	5183	0	5179	77	0
9	B	3410	0	3318	86	0
10	C	1705	0	1645	27	0
11	D	1200	0	1195	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	E	1388	0	1340	22	0
13	F	183	0	132	5	0
14	G	981	0	965	14	0
15	H	780	0	753	21	0
16	I	530	0	508	8	0
17	J	530	0	503	5	0
18	K	652	0	636	6	0
19	L	602	0	592	5	0
20	N	862	0	868	10	0
21	O	925	0	907	16	0
22	P	698	0	659	13	0
23	Q	1345	0	1282	19	0
24	R	2407	0	2296	52	0
25	S	2299	0	2028	34	0
26	T	942	0	890	4	0
27	U	1019	0	900	9	0
28	V	1093	0	1048	28	0
29	M	642	0	642	13	0
29	W	616	0	579	22	0
30	X	372	0	314	4	0
31	Y	409	0	318	3	0
32	Z	493	0	395	6	0
33	a	857	0	765	29	0
34	b	1032	0	954	8	0
35	c	617	0	492	28	0
36	d	708	0	513	30	0
37	f	1156	0	892	45	0
38	h	721	0	632	60	0
39	i	277	0	240	1	0
40	j	892	0	835	12	0
41	1	2500	0	2615	119	0
42	6	4765	0	4893	109	0
43	g	1351	0	1262	48	0
44	e	864	0	567	56	0
45	2	41	0	59	1	0
45	4	41	0	59	1	0
45	B	51	0	82	2	0
45	V	51	0	82	0	0
46	4	82	0	114	1	0
46	J	58	0	60	1	0
47	8	31	0	19	2	0
48	8	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	A	16	0	0	1	0
48	D	8	0	0	0	0
48	E	16	0	0	0	0
49	9	4	0	0	0	0
49	A	4	0	0	0	0
50	I	1	0	0	0	0
51	L	47	0	71	2	0
51	Q	46	0	66	1	0
51	S	47	0	71	2	0
51	j	39	0	55	0	0
52	R	48	0	23	3	0
All	All	60921	0	58151	1081	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 9.

All (1081) 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)
41:1:17:VAL:HG21	41:1:225:MET:CE	1.21	1.61
41:1:131:GLY:CA	41:1:207:LEU:CD1	1.75	1.58
36:d:6:ALA:CB	36:d:31:PHE:N	1.68	1.54
35:c:109:THR:CB	43:g:18:PRO:HA	1.15	1.53
41:1:200:LEU:CD1	41:1:206:GLU:HG2	1.37	1.51
9:B:88:HIS:CD2	11:D:114:ARG:HH11	1.27	1.51
28:V:58:ARG:HH22	41:1:314:ILE:CG2	1.22	1.50
28:V:58:ARG:HH22	41:1:314:ILE:CB	1.22	1.49
41:1:17:VAL:CG2	41:1:225:MET:CE	1.78	1.48
36:d:6:ALA:HB2	36:d:30:GLY:C	1.36	1.48
41:1:202:GLU:O	41:1:209:SER:CB	1.63	1.42
35:c:106:PRO:HG3	36:d:68:LYS:NZ	1.34	1.41
2:3:24:LEU:HB3	2:3:25:PRO:CD	1.45	1.40
9:B:88:HIS:CD2	11:D:114:ARG:NH1	1.88	1.40
43:g:19:ALA:CB	43:g:20:PRO:HD2	1.38	1.40
33:a:57:ARG:NH1	38:h:67:TYR:HD1	1.17	1.37
37:f:86:PRO:N	44:e:92:TRP:HZ3	1.18	1.37
35:c:109:THR:CB	43:g:18:PRO:CA	2.01	1.36
41:1:200:LEU:HD12	41:1:206:GLU:CD	1.46	1.36
43:g:19:ALA:CB	43:g:20:PRO:CD	2.02	1.35
36:d:25:PHE:HD2	36:d:40:VAL:CB	1.39	1.34
41:1:131:GLY:O	41:1:207:LEU:HD12	1.22	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1:200:LEU:HD12	41:1:206:GLU:CG	1.58	1.33
37:f:39:TYR:CD2	42:6:513:TYR:CE2	2.17	1.32
35:c:106:PRO:CG	36:d:68:LYS:NZ	1.92	1.32
41:1:131:GLY:CA	41:1:207:LEU:HD11	1.42	1.31
2:3:28:ASN:HD22	2:3:32:GLU:CB	1.43	1.30
28:V:58:ARG:NH2	41:1:314:ILE:HG22	1.43	1.29
41:1:200:LEU:CD1	41:1:206:GLU:CG	2.10	1.29
2:3:41:PHE:CE1	9:B:87:GLN:NE2	2.00	1.29
36:d:25:PHE:CD2	36:d:40:VAL:CB	2.16	1.29
41:1:17:VAL:CG2	41:1:225:MET:HE1	0.81	1.28
41:1:131:GLY:C	41:1:207:LEU:CD1	2.04	1.28
28:V:58:ARG:NH2	41:1:314:ILE:CB	1.95	1.28
41:1:200:LEU:HA	41:1:206:GLU:OE2	1.28	1.26
33:a:57:ARG:NH1	38:h:67:TYR:CD1	2.01	1.25
9:B:34:ALA:HA	38:h:62:GLU:O	1.34	1.24
2:3:28:ASN:ND2	2:3:32:GLU:HB2	1.53	1.24
38:h:69:LYS:HZ1	38:h:71:PRO:CD	1.50	1.24
35:c:106:PRO:CG	36:d:68:LYS:HZ1	1.48	1.23
41:1:131:GLY:HA3	41:1:207:LEU:CD1	1.48	1.23
52:R:601:NAP:O4D	52:R:601:NAP:C1D	1.63	1.22
37:f:86:PRO:N	44:e:92:TRP:CZ3	2.07	1.22
42:6:507:MET:O	42:6:514:HIS:NE2	1.72	1.22
28:V:58:ARG:HH21	41:1:314:ILE:C	1.49	1.21
41:1:131:GLY:CA	41:1:207:LEU:HD13	1.48	1.20
43:g:19:ALA:HB3	43:g:20:PRO:CD	1.69	1.19
37:f:39:TYR:CE2	42:6:513:TYR:CE2	2.30	1.19
38:h:68:GLU:O	38:h:70:ASN:N	1.75	1.18
41:1:196:ALA:HA	41:1:199:ASP:OD2	1.41	1.18
25:S:196:ASP:OD1	25:S:246:TYR:HB3	1.39	1.18
42:6:507:MET:O	42:6:514:HIS:CE1	1.96	1.18
33:a:57:ARG:NH2	38:h:67:TYR:HB3	1.60	1.17
9:B:88:HIS:CB	9:B:89:PRO:HD2	1.75	1.17
37:f:39:TYR:CD2	42:6:513:TYR:OH	1.97	1.17
41:1:131:GLY:O	41:1:207:LEU:CD1	1.92	1.14
36:d:6:ALA:HB2	36:d:31:PHE:N	0.81	1.13
37:f:39:TYR:CD2	42:6:513:TYR:CZ	2.37	1.13
28:V:58:ARG:NH2	41:1:314:ILE:CG2	1.94	1.13
2:3:35:SER:HB3	2:3:36:PRO:HD2	1.29	1.12
2:3:41:PHE:CZ	9:B:87:GLN:NE2	2.15	1.12
24:R:328:ILE:HG22	24:R:329:LEU:H	1.05	1.10
38:h:69:LYS:HZ1	38:h:71:PRO:HD3	0.97	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:57:ARG:HH22	38:h:67:TYR:HB3	1.11	1.09
28:V:58:ARG:NH2	41:1:314:ILE:HB	1.63	1.08
29:W:131:PRO:HB3	44:e:92:TRP:HE1	1.09	1.08
42:6:528:TYR:OH	44:e:125:ASN:O	1.69	1.08
43:g:19:ALA:HB1	43:g:20:PRO:CD	1.79	1.07
2:3:24:LEU:HB3	2:3:25:PRO:HD2	1.17	1.06
2:3:28:ASN:ND2	2:3:32:GLU:CB	2.12	1.06
9:B:88:HIS:HB2	9:B:89:PRO:HD2	1.10	1.06
37:f:39:TYR:CD2	42:6:513:TYR:HE2	1.61	1.06
9:B:88:HIS:CB	9:B:89:PRO:CD	2.34	1.05
41:1:17:VAL:HG23	41:1:225:MET:HE1	1.06	1.05
38:h:69:LYS:NZ	38:h:71:PRO:HD3	1.70	1.05
28:V:58:ARG:NH2	41:1:314:ILE:C	2.15	1.04
28:V:58:ARG:NH2	41:1:314:ILE:O	1.90	1.04
37:f:40:PHE:HE1	42:6:513:TYR:CE2	1.75	1.04
38:h:69:LYS:NZ	38:h:71:PRO:CD	2.21	1.04
1:2:25:HIS:NE2	15:H:18:MET:O	1.91	1.03
25:S:196:ASP:OD1	25:S:246:TYR:CB	2.08	1.01
44:e:86:ARG:O	44:e:87:ASP:CB	2.04	1.01
2:3:28:ASN:HD22	2:3:32:GLU:HB3	1.21	1.01
2:3:24:LEU:HB3	2:3:25:PRO:HD3	1.42	1.00
44:e:122:THR:CB	44:e:123:PRO:CD	2.39	0.99
29:W:108:LEU:HD11	29:W:114:ASP:CB	1.93	0.99
33:a:57:ARG:NH2	38:h:68:GLU:HG2	1.76	0.99
37:f:40:PHE:CE1	42:6:513:TYR:CE2	2.51	0.99
2:3:24:LEU:CB	2:3:25:PRO:CD	2.39	0.99
41:1:202:GLU:O	41:1:209:SER:HB2	0.81	0.98
44:e:122:THR:CB	44:e:123:PRO:HD3	1.93	0.98
29:W:108:LEU:CD1	29:W:114:ASP:CB	2.42	0.97
41:1:17:VAL:HG22	41:1:225:MET:HE1	1.43	0.97
33:a:57:ARG:HH21	38:h:68:GLU:HG2	1.26	0.97
41:1:200:LEU:HD11	41:1:206:GLU:HG2	1.01	0.97
41:1:200:LEU:CA	41:1:206:GLU:OE2	2.13	0.97
29:W:110:LEU:HD12	29:W:110:LEU:H	1.28	0.97
41:1:212:ASN:O	41:1:214:GLU:N	1.97	0.97
24:R:328:ILE:CG2	24:R:329:LEU:H	1.75	0.97
29:W:131:PRO:HB3	44:e:92:TRP:NE1	1.78	0.96
43:g:19:ALA:HB1	43:g:20:PRO:HD3	1.48	0.96
36:d:6:ALA:HB2	36:d:31:PHE:CA	1.96	0.96
33:a:57:ARG:HH12	38:h:67:TYR:HD1	1.05	0.96
44:e:97:LEU:CB	44:e:102:GLY:C	2.39	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:V:58:ARG:HH22	41:1:314:ILE:HB	1.16	0.95
37:f:39:TYR:HD2	42:6:513:TYR:CE2	1.64	0.95
43:g:14:PRO:O	43:g:116:ARG:NH2	1.99	0.95
41:1:196:ALA:CA	41:1:199:ASP:OD2	2.14	0.94
41:1:131:GLY:HA2	41:1:207:LEU:HD11	0.95	0.94
41:1:17:VAL:HG21	41:1:225:MET:HE3	1.50	0.94
2:3:39:CYS:SG	2:3:43:PRO:O	2.26	0.94
33:a:57:ARG:HH21	38:h:68:GLU:CG	1.81	0.94
2:3:38:GLU:OE2	41:1:64:ALA:N	2.00	0.93
33:a:81:ARG:NH2	44:e:70:THR:CG2	2.31	0.93
37:f:86:PRO:CB	44:e:92:TRP:CE3	2.52	0.93
24:R:328:ILE:HG22	24:R:329:LEU:N	1.77	0.92
2:3:48:ARG:HH11	2:3:48:ARG:HG3	1.33	0.92
36:d:6:ALA:CB	36:d:31:PHE:CA	2.47	0.92
2:3:35:SER:HB3	2:3:36:PRO:CD	1.99	0.92
36:d:6:ALA:CB	36:d:30:GLY:C	2.25	0.92
38:h:71:PRO:O	38:h:73:SER:N	2.02	0.92
42:6:528:TYR:OH	44:e:125:ASN:C	2.13	0.92
35:c:106:PRO:CD	36:d:68:LYS:NZ	2.32	0.92
35:c:109:THR:CB	43:g:18:PRO:C	2.43	0.91
15:H:19:THR:HG22	15:H:20:ILE:HG23	1.50	0.91
2:3:28:ASN:ND2	2:3:32:GLU:OE1	2.02	0.91
2:3:44:MET:HE2	21:O:50:PHE:HA	1.52	0.91
42:6:528:TYR:HH	44:e:125:ASN:C	1.78	0.91
9:B:34:ALA:CA	38:h:62:GLU:O	2.18	0.91
2:3:35:SER:CB	2:3:36:PRO:HD2	2.01	0.90
35:c:106:PRO:CD	36:d:68:LYS:HZ1	1.85	0.89
44:e:125:ASN:O	44:e:126:TRP:C	2.15	0.89
35:c:106:PRO:HG3	36:d:68:LYS:HZ2	1.28	0.89
41:1:200:LEU:CD1	41:1:206:GLU:CD	2.37	0.88
1:2:25:HIS:CD2	15:H:18:MET:O	2.28	0.87
9:B:88:HIS:HB2	9:B:89:PRO:CD	1.98	0.86
11:D:86:THR:O	11:D:114:ARG:NH2	2.09	0.86
35:c:106:PRO:HG3	36:d:68:LYS:HZ3	1.34	0.86
2:3:24:LEU:CB	2:3:25:PRO:HD2	2.05	0.84
37:f:40:PHE:HE1	42:6:513:TYR:CD2	1.94	0.84
42:6:535:ARG:NH1	44:e:119:THR:O	2.10	0.84
43:g:22:PRO:HG2	43:g:23:GLN:H	1.39	0.84
2:3:33:LYS:O	2:3:37:TYR:CZ	2.32	0.83
38:h:69:LYS:NZ	38:h:71:PRO:HD2	1.93	0.82
44:e:97:LEU:CB	44:e:102:GLY:O	2.27	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1:131:GLY:C	41:1:207:LEU:HD12	1.84	0.82
33:a:81:ARG:NH2	44:e:70:THR:HG22	1.93	0.82
41:1:131:GLY:HA2	41:1:207:LEU:CD1	1.75	0.82
2:3:33:LYS:O	2:3:35:SER:N	2.13	0.82
28:V:58:ARG:NH2	41:1:314:ILE:CA	2.43	0.81
2:3:35:SER:CB	2:3:36:PRO:CD	2.54	0.81
33:a:57:ARG:NH2	38:h:67:TYR:CB	2.42	0.81
35:c:106:PRO:HG2	36:d:68:LYS:HZ1	1.46	0.81
41:1:207:LEU:O	41:1:208:VAL:C	2.23	0.81
42:6:535:ARG:NH2	44:e:119:THR:O	2.15	0.80
9:B:88:HIS:HB3	9:B:89:PRO:CD	2.10	0.80
9:B:88:HIS:CG	11:D:114:ARG:HH11	1.98	0.80
9:B:88:HIS:HD2	11:D:114:ARG:HH11	0.85	0.80
42:6:507:MET:HA	42:6:510:ASN:O	1.81	0.79
33:a:81:ARG:NH2	44:e:70:THR:HG21	1.97	0.79
37:f:86:PRO:CB	44:e:92:TRP:HE3	1.96	0.79
37:f:39:TYR:HE2	42:6:513:TYR:CE2	1.93	0.78
41:1:128:ALA:HB2	41:1:210:GLY:O	1.84	0.78
37:f:39:TYR:CE2	42:6:513:TYR:HE2	1.85	0.78
3:4:426:ILE:HB	38:h:68:GLU:OE1	1.83	0.77
37:f:86:PRO:CB	44:e:92:TRP:CZ3	2.68	0.77
37:f:40:PHE:CE1	42:6:513:TYR:CD2	2.70	0.77
41:1:131:GLY:HA3	41:1:207:LEU:HD13	0.78	0.77
33:a:57:ARG:CZ	38:h:67:TYR:HB3	2.14	0.77
41:1:17:VAL:HG23	41:1:225:MET:CE	1.76	0.77
15:H:15:ASP:O	15:H:17:TRP:CD1	2.37	0.76
41:1:199:ASP:O	41:1:206:GLU:OE1	2.03	0.76
9:B:88:HIS:HD2	11:D:114:ARG:NH1	1.51	0.76
33:a:81:ARG:HH22	44:e:70:THR:CG2	1.97	0.76
9:B:88:HIS:CD2	11:D:114:ARG:HH12	1.99	0.76
36:d:25:PHE:CE2	36:d:40:VAL:CB	2.68	0.76
37:f:39:TYR:HD2	42:6:513:TYR:CZ	1.90	0.75
33:a:81:ARG:HH22	44:e:70:THR:HG21	1.52	0.75
41:1:212:ASN:C	41:1:214:GLU:H	1.95	0.74
43:g:19:ALA:HB3	43:g:20:PRO:HD2	0.77	0.74
43:g:15:ARG:O	43:g:15:ARG:NH1	2.21	0.74
29:W:108:LEU:HD13	29:W:114:ASP:CB	2.16	0.73
43:g:22:PRO:CG	43:g:23:GLN:H	1.94	0.73
42:6:525:LEU:HD13	42:6:525:LEU:C	2.14	0.73
37:f:86:PRO:CA	44:e:92:TRP:HZ3	2.01	0.72
42:6:514:HIS:CD2	42:6:514:HIS:H	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:6:527:GLY:C	42:6:529:PHE:H	1.96	0.72
2:3:28:ASN:HD21	2:3:32:GLU:HB2	1.51	0.72
2:3:32:GLU:O	2:3:34:THR:N	2.23	0.72
36:d:6:ALA:CB	36:d:31:PHE:CB	2.67	0.72
35:c:105:PHE:CB	35:c:106:PRO:HD3	2.20	0.71
41:1:202:GLU:O	41:1:209:SER:CA	2.39	0.71
29:M:35:HIS:H	29:M:39:ASP:HB3	1.54	0.71
29:W:110:LEU:H	29:W:110:LEU:CD1	2.03	0.71
44:e:98:ARG:O	44:e:104:PRO:HG3	1.90	0.71
42:6:294:THR:O	42:6:525:LEU:HD23	1.90	0.71
5:7:150:GLY:HA2	15:H:17:TRP:CZ2	2.26	0.70
7:9:131:HIS:H	7:9:189:ASN:HD21	1.38	0.70
41:1:41:GLY:HA3	41:1:44:GLY:H	1.57	0.70
35:c:105:PHE:CB	35:c:106:PRO:CD	2.69	0.70
41:1:200:LEU:HD12	41:1:206:GLU:HG2	1.27	0.69
41:1:206:GLU:C	41:1:208:VAL:H	1.99	0.69
43:g:14:PRO:HB2	43:g:16:ARG:HD3	1.74	0.69
7:9:224:SER:OG	7:9:226:GLU:HG2	1.92	0.69
2:3:44:MET:CE	21:O:50:PHE:HA	2.23	0.69
44:e:97:LEU:CB	44:e:102:GLY:HA3	2.23	0.69
2:3:81:THR:H	19:L:46:ASN:HD21	1.38	0.69
4:5:94:ASN:O	9:B:62:LYS:NZ	2.25	0.69
41:1:128:ALA:CB	41:1:210:GLY:O	2.41	0.69
36:d:6:ALA:HB1	36:d:31:PHE:N	1.98	0.68
9:B:52:MET:O	9:B:54:PRO:HD3	1.93	0.68
26:T:82:GLU:HG3	26:T:84:PRO:HD2	1.75	0.68
42:6:535:ARG:CZ	44:e:119:THR:O	2.40	0.68
19:L:59:ASP:HB3	23:Q:130:LYS:HD2	1.75	0.68
28:V:58:ARG:CZ	41:1:314:ILE:HG22	2.23	0.68
2:3:19:ILE:HG23	2:3:23:TRP:HB2	1.75	0.68
35:c:102:PRO:CB	43:g:18:PRO:HD2	2.24	0.68
41:1:210:GLY:HA2	41:1:213:VAL:HB	1.76	0.68
29:W:104:PHE:CE2	29:W:138:LEU:O	2.47	0.68
9:B:88:HIS:HB3	9:B:89:PRO:HD3	1.77	0.67
3:4:355:MET:HA	3:4:358:TRP:HD1	1.57	0.67
42:6:506:ASN:O	42:6:510:ASN:O	2.05	0.67
29:W:131:PRO:CB	44:e:92:TRP:HE1	1.98	0.67
10:C:132:TYR:HB2	10:C:145:VAL:HB	1.77	0.67
24:R:170:LEU:O	24:R:328:ILE:HD11	1.94	0.66
24:R:238:GLN:HB3	24:R:267:GLY:HA3	1.77	0.66
42:6:525:LEU:O	42:6:525:LEU:HD22	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:109:ALA:HB2	1:2:161:SER:HA	1.76	0.66
2:3:33:LYS:O	2:3:37:TYR:CE1	2.47	0.66
38:h:71:PRO:C	38:h:73:SER:H	2.03	0.66
41:1:200:LEU:HD11	41:1:206:GLU:CG	1.95	0.66
41:1:17:VAL:HG21	41:1:225:MET:SD	2.33	0.66
35:c:106:PRO:CD	36:d:68:LYS:HZ2	2.05	0.66
8:A:343:GLY:H	8:A:549:GLY:HA2	1.61	0.65
24:R:170:LEU:O	24:R:328:ILE:CD1	2.44	0.65
41:1:200:LEU:HD12	41:1:206:GLU:OE1	1.96	0.65
35:c:109:THR:CB	43:g:19:ALA:N	2.59	0.65
41:1:196:ALA:C	41:1:199:ASP:OD2	2.39	0.65
42:6:267:THR:O	42:6:274:GLN:NE2	2.29	0.65
44:e:97:LEU:CB	44:e:102:GLY:CA	2.74	0.65
8:A:367:CYS:SG	8:A:368:THR:N	2.69	0.65
41:1:206:GLU:O	41:1:208:VAL:N	2.29	0.65
42:6:527:GLY:O	42:6:529:PHE:N	2.29	0.65
11:D:99:MET:HG2	11:D:106:MET:HB2	1.79	0.65
2:3:33:LYS:O	2:3:37:TYR:OH	2.14	0.65
41:1:169:GLN:HE21	41:1:174:LEU:HD13	1.62	0.65
4:5:96:LEU:HG	9:B:61:TRP:CD2	2.31	0.64
25:S:71:LEU:HD23	25:S:146:VAL:HG13	1.79	0.64
26:T:85:ASP:HA	26:T:89:ASN:HD22	1.63	0.64
38:h:141:CYS:HA	43:g:162:ARG:HD3	1.79	0.64
10:C:170:ARG:HD3	10:C:187:ARG:HB2	1.79	0.64
11:D:86:THR:H	11:D:114:ARG:NH2	1.97	0.63
43:g:15:ARG:HH11	43:g:15:ARG:HA	1.63	0.63
6:8:420:GLU:H	6:8:422:HIS:HD2	1.47	0.63
20:N:67:LYS:HG3	20:N:71:ARG:HH11	1.61	0.63
38:h:69:LYS:NZ	38:h:69:LYS:O	2.31	0.63
43:g:13:PRO:O	43:g:14:PRO:O	2.16	0.63
44:e:67:ASP:O	44:e:68:ASP:C	2.41	0.63
9:B:182:ASN:HD22	9:B:403:PRO:HG2	1.63	0.63
38:h:69:LYS:HZ1	38:h:71:PRO:HD2	1.47	0.63
2:3:48:ARG:HG3	2:3:48:ARG:NH1	2.07	0.63
29:W:104:PHE:CE2	29:W:118:ILE:HD12	2.32	0.63
33:a:57:ARG:HH22	38:h:67:TYR:CB	1.99	0.63
25:S:322:LEU:CB	38:h:62:GLU:N	2.62	0.63
8:A:81:GLU:HG3	8:A:108:LYS:HB3	1.81	0.63
29:W:108:LEU:HD13	29:W:109:GLY:N	2.13	0.63
6:8:211:ALA:HB2	6:8:223:PRO:HB3	1.80	0.62
34:b:160:MET:HE2	34:b:166:GLY:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:82:GLN:HE21	28:V:98:MET:HB2	1.64	0.62
3:4:451:PRO:HG2	42:6:69:LEU:HD23	1.82	0.62
24:R:92:MET:HG3	24:R:95:ARG:HH21	1.63	0.62
25:S:219:SER:HA	25:S:222:LEU:HB2	1.82	0.62
38:h:68:GLU:C	38:h:70:ASN:N	2.57	0.62
2:3:28:ASN:O	2:3:32:GLU:HG2	2.00	0.62
40:j:114:GLU:HG3	40:j:115:GLU:HG2	1.81	0.62
42:6:514:HIS:O	42:6:515:TYR:C	2.43	0.62
1:2:68:MET:HE2	4:5:37:MET:HE2	1.80	0.62
24:R:201:ILE:HG23	24:R:203:PRO:HD3	1.82	0.61
33:a:57:ARG:HH11	38:h:67:TYR:HD1	1.34	0.61
41:1:17:VAL:HG21	41:1:225:MET:HE1	0.63	0.61
27:U:29:ARG:HH12	27:U:63:ILE:HG23	1.65	0.61
36:d:9:TYR:O	36:d:10:LEU:CB	2.48	0.61
6:8:98:LYS:NZ	47:8:501:FMN:O3P	2.34	0.61
8:A:124:HIS:NE2	48:A:801:SF4:S3	2.74	0.61
9:B:62:LYS:O	9:B:64:PRO:CD	2.49	0.61
10:C:112:SER:HB2	10:C:135:LEU:HB3	1.83	0.61
36:d:6:ALA:HB1	36:d:31:PHE:CB	2.31	0.61
6:8:297:LYS:NZ	6:8:310:GLY:O	2.34	0.61
2:3:48:ARG:NH1	2:3:49:LEU:O	2.34	0.61
2:3:28:ASN:O	2:3:32:GLU:CG	2.49	0.60
8:A:127:ASP:OD2	8:A:175:ARG:NH1	2.34	0.60
2:3:20:ILE:O	2:3:20:ILE:HG22	2.00	0.60
6:8:382:CYS:HB3	6:8:384:PRO:HD2	1.83	0.60
15:H:17:TRP:CD1	15:H:17:TRP:H	2.20	0.60
3:4:52:PHE:O	34:b:135:ARG:NH1	2.31	0.60
41:1:131:GLY:C	41:1:207:LEU:HD11	1.97	0.60
3:4:246:ILE:HG23	3:4:250:LEU:HD23	1.83	0.60
20:N:38:ILE:O	20:N:45:ARG:NH2	2.34	0.60
37:f:16:VAL:HG22	37:f:64:LEU:HD21	1.83	0.60
44:e:125:ASN:O	44:e:127:ASN:N	2.34	0.60
23:Q:45:LEU:O	23:Q:135:ARG:NH2	2.35	0.59
29:W:97:LYS:NZ	29:W:107:ASP:CB	2.64	0.59
8:A:501:ARG:NH2	8:A:509:ASP:OD1	2.34	0.59
24:R:178:SER:H	24:R:182:ARG:H	1.50	0.59
4:5:93:LEU:HD22	42:6:583:LEU:H	1.67	0.59
6:8:167:SER:HA	13:F:88:LEU:HD21	1.82	0.59
10:C:90:ILE:HD12	10:C:145:VAL:HG13	1.83	0.59
41:1:131:GLY:C	41:1:207:LEU:HD13	2.03	0.59
42:6:513:TYR:O	42:6:515:TYR:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Q:49:GLU:OE1	23:Q:135:ARG:NH2	2.36	0.59
41:1:222:LEU:O	41:1:226:ALA:N	2.22	0.59
7:9:163:THR:HA	7:9:170:THR:HA	1.85	0.59
7:9:222:ARG:HD3	7:9:228:ALA:HB2	1.84	0.59
8:A:183:ILE:HD11	8:A:206:VAL:HG13	1.84	0.59
12:E:105:ARG:NH1	12:E:195:ASP:OD2	2.36	0.59
3:4:175:ASN:ND2	23:Q:168:PHE:O	2.35	0.59
29:M:33:ASN:OD1	29:M:74:GLN:NE2	2.36	0.59
6:8:424:ILE:HG12	8:A:76:ARG:HH21	1.68	0.59
9:B:88:HIS:CG	11:D:114:ARG:NH1	2.61	0.59
6:8:284:ASN:HD22	7:9:228:ALA:HB3	1.68	0.58
9:B:179:ARG:HH22	9:B:303:ARG:HD3	1.68	0.58
24:R:227:PRO:HG2	24:R:230:SER:HA	1.85	0.58
28:V:48:TRP:O	28:V:52:LYS:NZ	2.34	0.58
6:8:411:SER:HB3	22:P:49:LEU:HD13	1.84	0.58
41:1:65:THR:OG1	41:1:124:ASN:ND2	2.35	0.58
3:4:271:MET:HE2	42:6:549:ALA:HB3	1.85	0.58
3:4:193:VAL:HG22	3:4:257:MET:HE1	1.85	0.58
6:8:220:GLN:HE21	7:9:118:PHE:HB2	1.67	0.58
41:1:127:TYR:O	41:1:210:GLY:HA3	2.02	0.58
42:6:454:ILE:HG22	42:6:458:LEU:HD23	1.85	0.58
1:2:173:THR:HG21	9:B:49:GLY:HA2	1.85	0.58
2:3:42:ASP:CB	2:3:43:PRO:CD	2.80	0.58
3:4:214:LEU:HD11	42:6:558:LEU:HB3	1.86	0.58
6:8:257:ARG:HA	7:9:243:PHE:HB2	1.85	0.58
29:W:110:LEU:HD12	29:W:110:LEU:N	2.09	0.58
38:h:141:CYS:HB2	38:h:144:PRO:HG3	1.86	0.58
1:2:150:ASN:HD22	42:6:604:PHE:HA	1.68	0.58
21:O:92:GLU:HG3	21:O:97:TRP:HE3	1.67	0.58
44:e:124:VAL:O	44:e:126:TRP:N	2.36	0.58
7:9:228:ALA:HA	7:9:231:LEU:HD23	1.85	0.58
3:4:115:LEU:HB2	3:4:174:LEU:HD13	1.85	0.58
8:A:50:LEU:HD21	8:A:62:ARG:HE	1.69	0.58
25:S:211:ASN:HB3	25:S:214:GLU:HB2	1.86	0.58
2:3:41:PHE:CD1	9:B:87:GLN:NE2	2.65	0.58
1:2:144:GLN:HE21	15:H:3:PHE:HB2	1.69	0.58
5:7:83:TRP:HB2	5:7:89:VAL:HG11	1.86	0.58
3:4:336:ARG:HH22	3:4:429:SER:HA	1.69	0.57
1:2:47:ASN:HD21	1:2:123:PRO:HB2	1.69	0.57
3:4:60:SER:OG	3:4:63:THR:O	2.20	0.57
7:9:224:SER:OG	7:9:226:GLU:CG	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:266:ARG:HG3	8:A:267:THR:HG23	1.86	0.57
42:6:525:LEU:HD13	42:6:526:LEU:HG	1.85	0.57
9:B:88:HIS:N	9:B:88:HIS:HD1	2.02	0.57
9:B:163:PRO:HG2	9:B:168:GLN:HE21	1.70	0.57
33:a:79:ASN:ND2	44:e:73:GLY:O	2.38	0.57
7:9:197:THR:HG23	7:9:200:ASP:H	1.68	0.57
43:g:16:ARG:HH11	43:g:16:ARG:HB3	1.68	0.57
7:9:56:THR:HG22	7:9:58:GLU:H	1.70	0.57
23:Q:168:PHE:H	23:Q:170:TRP:HD1	1.53	0.57
17:J:41:TYR:OH	41:1:317:GLN:NE2	2.36	0.57
41:1:199:ASP:O	41:1:206:GLU:CD	2.48	0.57
36:d:18:ASP:O	36:d:20:LEU:N	2.38	0.57
15:H:9:ARG:NH2	40:j:12:GLN:OE1	2.37	0.56
23:Q:5:VAL:N	28:V:107:GLY:O	2.38	0.56
41:1:209:SER:O	41:1:209:SER:OG	2.20	0.56
6:8:398:ARG:NH2	8:A:155:GLU:OE2	2.37	0.56
7:9:90:ASN:ND2	7:9:92:TRP:O	2.39	0.56
9:B:278:VAL:HG12	9:B:283:ALA:HB2	1.88	0.56
10:C:197:GLY:HA2	14:G:67:VAL:HG13	1.88	0.56
33:a:57:ARG:CZ	38:h:67:TYR:CD1	2.87	0.56
36:d:6:ALA:CA	36:d:30:GLY:C	2.79	0.56
38:h:81:ALA:O	38:h:83:ASP:N	2.37	0.56
3:4:285:LEU:O	3:4:406:TYR:OH	2.23	0.56
8:A:324:SER:HA	8:A:327:ALA:HB3	1.88	0.56
38:h:71:PRO:C	38:h:73:SER:N	2.60	0.56
42:6:514:HIS:CD2	42:6:514:HIS:N	2.72	0.56
43:g:13:PRO:O	43:g:116:ARG:NH2	2.39	0.56
9:B:179:ARG:NH2	9:B:401:GLU:O	2.37	0.56
38:h:67:TYR:N	38:h:67:TYR:CD2	2.73	0.56
42:6:361:GLY:O	42:6:364:LYS:NZ	2.39	0.56
42:6:387:THR:OG1	42:6:388:GLY:N	2.38	0.56
12:E:131:GLU:OE1	12:E:144:ARG:NH1	2.39	0.56
41:1:70:MET:HG3	41:1:121:TRP:HZ3	1.70	0.56
1:2:173:THR:HG22	9:B:52:MET:HE2	1.88	0.56
8:A:382:ARG:HD2	8:A:386:LEU:HD23	1.88	0.56
8:A:587:ALA:HB1	8:A:591:GLU:HB2	1.88	0.56
29:W:108:LEU:HD13	29:W:108:LEU:C	2.31	0.55
35:c:106:PRO:CG	36:d:68:LYS:HZ2	1.90	0.55
36:d:105:GLU:OE1	44:e:165:ASN:N	2.39	0.55
2:3:44:MET:CE	21:O:50:PHE:C	2.79	0.55
24:R:209:ARG:NH1	24:R:351:GLU:OE2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:387:LEU:HD12	8:A:514:ASN:HB2	1.88	0.55
34:b:133:TYR:HE2	43:g:90:MET:HG3	1.71	0.55
35:c:14:GLN:NE2	37:f:155:PRO:O	2.38	0.55
29:M:70:LEU:HD13	29:M:76:ILE:HG12	1.87	0.55
37:f:39:TYR:CG	42:6:513:TYR:OH	2.39	0.55
8:A:82:ILE:HD11	8:A:100:TRP:HB3	1.87	0.55
25:S:100:CYS:HB3	25:S:119:LEU:HB2	1.89	0.55
41:1:207:LEU:O	41:1:209:SER:N	2.39	0.55
8:A:388:ASN:ND2	8:A:513:MET:O	2.35	0.55
24:R:275:ASP:O	24:R:279:TYR:N	2.39	0.55
6:8:159:ARG:HG2	6:8:161:GLU:H	1.72	0.55
8:A:263:VAL:HA	8:A:273:ILE:HG22	1.89	0.55
8:A:568:TYR:HB3	8:A:583:ILE:HG22	1.88	0.55
9:B:86:PRO:C	9:B:88:HIS:H	2.15	0.55
14:G:111:LEU:HD13	24:R:100:LEU:HD23	1.87	0.55
41:1:230:ASN:HA	41:1:233:MET:HE2	1.89	0.55
42:6:290:MET:O	42:6:524:THR:O	2.24	0.55
3:4:69:THR:HG22	3:4:235:LEU:HD11	1.89	0.55
42:6:523:SER:O	42:6:523:SER:OG	2.22	0.55
44:e:125:ASN:OD1	44:e:126:TRP:N	2.40	0.55
44:e:166:LEU:HD23	44:e:166:LEU:H	1.72	0.54
10:C:66:TYR:OH	10:C:107:ASN:ND2	2.39	0.54
2:3:71:LEU:O	5:7:147:TYR:OH	2.24	0.54
4:5:49:LEU:HD21	5:7:49:GLY:H	1.72	0.54
38:h:69:LYS:CE	38:h:71:PRO:HD3	2.38	0.54
44:e:89:TRP:CD2	44:e:89:TRP:N	2.73	0.54
6:8:74:ASP:HA	6:8:77:LEU:HB2	1.89	0.54
8:A:426:ASP:HA	14:G:169:ARG:HH12	1.73	0.54
23:Q:8:PRO:O	28:V:88:ARG:NH2	2.40	0.54
28:V:58:ARG:HG3	28:V:58:ARG:O	2.07	0.54
29:M:26:ASP:HB3	29:M:40:LEU:HD21	1.89	0.54
8:A:161:GLU:OE1	16:I:102:ASN:ND2	2.40	0.54
2:3:41:PHE:CZ	9:B:87:GLN:CD	2.85	0.54
3:4:216:LEU:HD23	3:4:291:VAL:HG22	1.90	0.54
8:A:473:MET:HE2	8:A:475:ILE:HD11	1.89	0.54
9:B:237:PRO:HD3	12:E:96:ARG:HH22	1.73	0.54
24:R:114:ASP:HA	24:R:117:ARG:HB2	1.88	0.54
24:R:154:GLN:HG3	24:R:155:VAL:HG23	1.90	0.54
44:e:39:GLY:HA3	44:e:77:LYS:HB3	1.90	0.54
5:7:111:LYS:HA	15:H:81:ARG:HH21	1.71	0.54
8:A:251:ILE:HG13	8:A:604:GLN:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1:207:LEU:C	41:1:209:SER:N	2.65	0.54
35:c:21:ARG:HG3	37:f:125:TRP:HH2	1.72	0.54
2:3:29:VAL:HG12	2:3:29:VAL:O	2.07	0.54
5:7:150:GLY:HA2	15:H:17:TRP:HZ2	1.73	0.54
15:H:19:THR:CG2	15:H:20:ILE:HG23	2.31	0.54
42:6:515:TYR:N	42:6:515:TYR:CD1	2.73	0.54
43:g:77:CYS:SG	43:g:78:GLN:N	2.74	0.54
44:e:92:TRP:CE3	44:e:92:TRP:HA	2.41	0.54
42:6:583:LEU:HD23	42:6:586:LEU:HD22	1.90	0.53
3:4:301:ILE:O	3:4:304:GLN:NE2	2.41	0.53
6:8:426:ALA:O	6:8:430:GLY:N	2.42	0.53
38:h:121:GLU:OE2	38:h:124:ARG:NH2	2.41	0.53
42:6:73:THR:O	43:g:104:ASN:ND2	2.41	0.53
42:6:515:TYR:HD1	42:6:515:TYR:O	1.91	0.53
24:R:252:ALA:HB2	24:R:338:LEU:HD11	1.91	0.53
6:8:159:ARG:NH1	7:9:176:CYS:O	2.40	0.53
9:B:443:MET:SD	41:1:281:ARG:NH1	2.82	0.53
16:I:107:THR:CB	16:I:121:GLN:HG2	2.39	0.53
26:T:22:THR:OG1	26:T:68:ALA:O	2.26	0.53
28:V:58:ARG:CZ	41:1:314:ILE:CG2	2.81	0.53
37:f:86:PRO:CA	44:e:92:TRP:CZ3	2.83	0.53
40:j:108:THR:OG1	43:g:75:THR:O	2.26	0.53
10:C:70:ILE:HG13	10:C:71:LEU:HD12	1.91	0.53
21:O:50:PHE:HE1	21:O:96:VAL:HG12	1.73	0.53
43:g:141:ASP:OD1	43:g:141:ASP:N	2.41	0.53
4:5:79:VAL:O	4:5:83:ASN:N	2.40	0.53
11:D:150:VAL:HG12	11:D:179:VAL:HG13	1.90	0.53
37:f:85:SER:HA	44:e:92:TRP:HH2	1.72	0.53
40:j:35:GLY:O	40:j:39:TYR:N	2.41	0.53
12:E:188:GLU:O	12:E:192:ASN:ND2	2.41	0.53
6:8:201:ALA:HB3	7:9:119:TYR:HB3	1.90	0.53
41:1:200:LEU:HG	41:1:206:GLU:HB3	1.90	0.53
7:9:149:LEU:HD23	7:9:150:GLU:H	1.74	0.53
10:C:207:SER:OG	11:D:171:ARG:NH2	2.42	0.53
24:R:147:LYS:O	24:R:151:ALA:N	2.39	0.53
6:8:160:GLY:HA2	6:8:199:ARG:HD2	1.89	0.52
24:R:329:LEU:HG	24:R:331:HIS:H	1.73	0.52
42:6:583:LEU:HB3	42:6:586:LEU:HB2	1.90	0.52
14:G:57:GLU:OE1	21:O:15:THR:N	2.42	0.52
18:K:31:GLN:HB3	18:K:34:ARG:HH21	1.74	0.52
19:L:56:PRO:HA	23:Q:128:VAL:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:28:LEU:HD13	37:f:118:TYR:HD1	1.74	0.52
5:7:66:VAL:O	5:7:70:TYR:N	2.42	0.52
9:B:62:LYS:O	9:B:64:PRO:HD3	2.09	0.52
10:C:149:THR:OG1	10:C:150:ASP:N	2.42	0.52
37:f:154:LEU:HB2	37:f:157:ALA:HA	1.92	0.52
4:5:36:MET:O	4:5:39:SER:OG	2.25	0.52
9:B:385:TYR:HD2	12:E:122:VAL:HG11	1.75	0.52
16:I:59:ARG:NH1	27:U:123:GLN:OE1	2.43	0.52
20:N:36:GLY:O	20:N:45:ARG:NH2	2.43	0.52
42:6:204:LEU:HD12	43:g:129:LEU:HD11	1.91	0.52
11:D:154:GLY:O	11:D:158:ASN:ND2	2.42	0.52
37:f:40:PHE:HE1	42:6:513:TYR:HE2	1.46	0.52
38:h:70:ASN:ND2	38:h:74:HIS:O	2.38	0.52
15:H:22:SER:HA	15:H:25:GLN:HE22	1.75	0.52
24:R:64:PHE:HZ	24:R:208:GLY:HA3	1.74	0.52
35:c:106:PRO:HD3	36:d:68:LYS:HZ2	1.73	0.52
37:f:139:GLN:HE22	37:f:157:ALA:HB1	1.74	0.52
43:g:22:PRO:CG	43:g:23:GLN:N	2.61	0.52
2:3:39:CYS:O	2:3:41:PHE:N	2.43	0.51
32:Z:22:TRP:NE1	32:Z:51:TRP:O	2.43	0.51
10:C:154:PRO:HG2	21:O:18:LYS:HE2	1.92	0.51
24:R:354:ARG:O	24:R:355:ARG:NH2	2.38	0.51
29:W:97:LYS:HZ1	29:W:107:ASP:CB	2.23	0.51
6:8:204:TYR:HE1	6:8:427:LEU:HD13	1.75	0.51
8:A:352:ILE:HD11	8:A:528:LEU:HD22	1.93	0.51
9:B:198:THR:HG22	41:1:32:GLN:HE22	1.75	0.51
14:G:128:PHE:HD2	14:G:134:ALA:HA	1.74	0.51
44:e:122:THR:CB	44:e:123:PRO:HD2	2.35	0.51
6:8:119:GLU:O	6:8:159:ARG:NH2	2.42	0.51
42:6:427:ILE:HG13	42:6:431:LEU:HD12	1.91	0.51
2:3:44:MET:HE1	21:O:50:PHE:O	2.11	0.51
8:A:33:GLU:HG2	8:A:42:MET:HG2	1.93	0.51
25:S:83:ASP:HB3	25:S:91:PRO:HA	1.93	0.51
41:1:17:VAL:CG2	41:1:225:MET:SD	2.92	0.51
2:3:112:GLU:OE2	41:1:290:TRP:NE1	2.44	0.51
3:4:68:LEU:HA	3:4:71:TRP:HD1	1.75	0.51
3:4:118:PHE:O	3:4:122:PHE:N	2.40	0.51
6:8:409:ILE:HG23	6:8:439:ILE:HD12	1.93	0.51
8:A:255:ASP:N	8:A:255:ASP:OD1	2.43	0.51
8:A:382:ARG:HB2	8:A:385:TYR:HB3	1.93	0.51
28:V:55:ARG:HH22	41:1:312:SER:HG	1.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:102:PRO:CB	43:g:18:PRO:CD	2.89	0.51
42:6:291:CYS:HA	42:6:524:THR:O	2.11	0.51
1:2:265:MET:HE1	23:Q:167:LEU:HD11	1.93	0.51
2:3:24:LEU:CD1	2:3:25:PRO:HD3	2.41	0.51
2:3:68:GLU:HG3	2:3:98:LEU:HD12	1.92	0.51
12:E:59:GLN:HA	12:E:64:THR:HG22	1.92	0.51
24:R:143:ASP:O	24:R:147:LYS:N	2.41	0.51
24:R:314:THR:HG22	24:R:316:ARG:HB2	1.93	0.51
33:a:109:ARG:HH22	40:j:119:VAL:HG13	1.75	0.51
4:5:2:SER:OG	4:5:3:MET:N	2.43	0.50
9:B:62:LYS:O	9:B:64:PRO:N	2.44	0.50
15:H:13:ASP:OD1	15:H:16:ARG:CZ	2.59	0.50
27:U:67:GLU:HA	27:U:71:LYS:HB2	1.92	0.50
42:6:528:TYR:OH	44:e:125:ASN:CA	2.58	0.50
8:A:306:MET:HG2	8:A:316:HIS:HA	1.94	0.50
8:A:462:PHE:O	8:A:464:GLN:N	2.44	0.50
17:J:3:PHE:HZ	46:J:101:CDL:HA21	1.76	0.50
1:2:45:MET:HE1	1:2:53:THR:HA	1.93	0.50
2:3:80:GLN:HE22	28:V:58:ARG:NH1	2.09	0.50
7:9:54:ASP:OD1	7:9:60:TYR:OH	2.29	0.50
24:R:182:ARG:O	24:R:183:SER:OG	2.27	0.50
41:1:212:ASN:C	41:1:214:GLU:N	2.60	0.50
42:6:525:LEU:C	42:6:525:LEU:CD1	2.85	0.50
8:A:50:LEU:HG	8:A:60:ILE:HD11	1.93	0.50
9:B:251:PHE:HD2	9:B:341:ILE:HD11	1.77	0.50
10:C:226:VAL:HG11	14:G:120:PRO:HB3	1.92	0.50
43:g:16:ARG:HH11	43:g:16:ARG:CG	2.24	0.50
6:8:177:TYR:O	13:F:96:ARG:NH1	2.44	0.50
9:B:303:ARG:HB3	9:B:311:TYR:HE2	1.75	0.50
9:B:338:ARG:NH1	28:V:22:LYS:O	2.44	0.50
7:9:151:ALA:HA	7:9:154:LYS:HB2	1.94	0.50
8:A:309:ASN:ND2	8:A:315:THR:OG1	2.45	0.50
8:A:461:PRO:HA	8:A:463:SER:HB3	1.94	0.50
23:Q:110:CYS:O	23:Q:114:LYS:N	2.41	0.50
41:1:225:MET:SD	41:1:225:MET:C	2.94	0.50
3:4:208:PRO:HG2	3:4:216:LEU:HD22	1.94	0.50
3:4:370:PRO:HA	3:4:375:LEU:HB2	1.94	0.50
6:8:364:VAL:HG12	6:8:400:VAL:HG22	1.94	0.50
9:B:326:CYS:HA	9:B:329:ARG:HG2	1.92	0.50
21:O:25:MET:SD	21:O:29:LYS:NZ	2.85	0.50
29:W:131:PRO:HB3	44:e:92:TRP:CD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:87:GLN:NE2	9:B:87:GLN:HA	2.21	0.50
44:e:89:TRP:N	44:e:89:TRP:CE3	2.79	0.50
5:7:66:VAL:HG11	41:1:140:ILE:HG21	1.94	0.49
9:B:88:HIS:HD1	9:B:88:HIS:H	1.59	0.49
23:Q:57:LEU:O	23:Q:61:LYS:NZ	2.42	0.49
25:S:32:ILE:HG13	25:S:33:LEU:HD12	1.94	0.49
10:C:123:THR:HG21	14:G:129:SER:H	1.76	0.49
33:a:57:ARG:NH1	38:h:67:TYR:HB3	2.27	0.49
33:a:87:SER:O	42:6:557:TRP:NE1	2.40	0.49
46:4:501:CDL:H321	46:4:501:CDL:H171	1.94	0.49
7:9:75:LYS:O	7:9:77:ALA:N	2.41	0.49
24:R:265:PHE:HA	24:R:335:LEU:HB2	1.94	0.49
9:B:238:LEU:HD23	28:V:10:MET:HE1	1.93	0.49
24:R:237:LYS:HG2	24:R:325:THR:HG23	1.94	0.49
6:8:48:ARG:HA	6:8:133:HIS:CG	2.47	0.49
8:A:251:ILE:HB	8:A:606:THR:HG22	1.94	0.49
40:j:58:LEU:O	40:j:62:LEU:N	2.43	0.49
42:6:511:LEU:CB	42:6:514:HIS:NE2	2.75	0.49
9:B:203:MET:HE1	9:B:254:ARG:HB3	1.94	0.49
15:H:21:GLN:HB3	15:H:37:GLU:HG3	1.95	0.49
24:R:125:VAL:HG21	24:R:253:ILE:HD11	1.94	0.49
28:V:51:MET:HG3	28:V:55:ARG:HH21	1.77	0.49
24:R:55:VAL:HG13	24:R:79:GLN:HB3	1.95	0.49
25:S:200:PRO:HG2	25:S:223:GLN:HE22	1.76	0.49
29:W:115:GLN:HE21	29:W:135:ALA:HB1	1.77	0.49
35:c:25:ASP:OD2	37:f:125:TRP:NE1	2.46	0.49
10:C:222:VAL:HG21	21:O:110:THR:HG21	1.94	0.49
12:E:38:TYR:HB2	22:P:106:LEU:HA	1.95	0.49
24:R:328:ILE:CG2	24:R:329:LEU:N	2.46	0.49
29:W:108:LEU:HD21	29:W:114:ASP:O	2.12	0.49
37:f:39:TYR:CE2	42:6:513:TYR:CZ	2.83	0.49
42:6:511:LEU:CB	42:6:514:HIS:CE1	2.96	0.49
8:A:627:SER:OG	8:A:632:MET:O	2.25	0.49
12:E:66:LEU:O	41:1:277:TYR:OH	2.31	0.49
25:S:234:LEU:O	25:S:238:SER:N	2.45	0.49
42:6:350:LEU:HD22	42:6:353:GLU:HB2	1.94	0.49
18:K:92:GLU:HA	18:K:95:LEU:HB3	1.95	0.48
25:S:196:ASP:OD1	25:S:246:TYR:HB2	2.06	0.48
25:S:202:VAL:HA	25:S:205:ARG:HB2	1.95	0.48
38:h:69:LYS:CE	38:h:69:LYS:C	2.86	0.48
1:2:324:THR:O	40:j:41:SER:OG	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:578:PRO:HB3	27:U:140:PRO:HG3	1.95	0.48
9:B:267:ILE:HD11	45:B:501:3PE:H271	1.95	0.48
29:W:104:PHE:HB3	29:W:108:LEU:HG	1.95	0.48
3:4:119:TYR:HE1	3:4:157:SER:HB2	1.78	0.48
18:K:82:PHE:HB3	18:K:86:GLN:HB2	1.95	0.48
2:3:16:LEU:O	2:3:20:ILE:HD13	2.13	0.48
24:R:203:PRO:HG2	52:R:601:NAP:H72N	1.79	0.48
25:S:275:ASN:O	25:S:277:ARG:N	2.40	0.48
42:6:258:PHE:HA	42:6:261:ILE:HD12	1.95	0.48
9:B:52:MET:O	9:B:54:PRO:CD	2.61	0.48
9:B:61:TRP:HA	9:B:61:TRP:CE3	2.48	0.48
23:Q:59:GLU:HA	23:Q:62:LEU:HB2	1.95	0.48
2:3:42:ASP:HA	2:3:43:PRO:HD3	1.64	0.48
8:A:371:VAL:HB	8:A:482:GLN:HG3	1.96	0.48
8:A:545:LEU:H	8:A:566:ILE:HG22	1.78	0.48
8:A:587:ALA:O	8:A:592:LYS:NZ	2.38	0.48
8:A:650:SER:OG	8:A:652:ASN:OD1	2.31	0.48
6:8:409:ILE:HD11	6:8:446:LEU:HD11	1.95	0.48
25:S:109:PRO:HB2	25:S:112:ASN:HB3	1.96	0.48
38:h:67:TYR:O	38:h:69:LYS:N	2.47	0.48
1:2:109:ALA:O	1:2:112:HIS:ND1	2.47	0.48
2:3:19:ILE:HG22	2:3:19:ILE:O	2.13	0.48
6:8:213:ILE:HD11	6:8:236:PHE:HB2	1.94	0.48
7:9:236:GLU:OE1	7:9:239:LYS:NZ	2.45	0.48
9:B:123:LEU:HD22	11:D:166:SER:HB3	1.96	0.48
1:2:224:THR:H	1:2:228:LEU:HD23	1.79	0.47
2:3:28:ASN:ND2	2:3:28:ASN:O	2.47	0.47
3:4:76:MET:HG2	3:4:231:LEU:HD12	1.96	0.47
6:8:201:ALA:HB1	7:9:121:MET:HB2	1.95	0.47
11:D:155:SER:OG	12:E:150:THR:O	2.31	0.47
21:O:83:VAL:O	21:O:87:LYS:N	2.44	0.47
2:3:44:MET:CE	21:O:50:PHE:CA	2.91	0.47
10:C:85:GLU:OE1	10:C:144:ARG:NH1	2.43	0.47
8:A:535:GLU:HA	8:A:538:GLN:HB2	1.95	0.47
9:B:308:TYR:OH	9:B:401:GLU:N	2.46	0.47
42:6:550:SER:OG	42:6:551:SER:N	2.39	0.47
52:R:601:NAP:O4D	52:R:601:NAP:C2N	2.63	0.47
41:1:46:LEU:HG	41:1:49:ILE:HD11	1.96	0.47
41:1:168:THR:HG23	41:1:169:GLN:HG3	1.96	0.47
41:1:196:ALA:O	41:1:199:ASP:OD2	2.33	0.47
3:4:167:ILE:HD13	3:4:250:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:G:79:ILE:HD13	14:G:134:ALA:HB1	1.94	0.47
14:G:154:LYS:HB2	14:G:156:LYS:HE2	1.97	0.47
37:f:40:PHE:CE1	42:6:513:TYR:HE2	2.21	0.47
2:3:48:ARG:HG3	2:3:49:LEU:N	2.30	0.47
6:8:273:THR:HA	6:8:291:GLU:HA	1.96	0.47
7:9:164:THR:N	7:9:169:PHE:O	2.38	0.47
8:A:31:LEU:HA	8:A:45:PRO:HD3	1.97	0.47
23:Q:53:PRO:HD2	28:V:116:TRP:CD1	2.49	0.47
38:h:69:LYS:NZ	38:h:69:LYS:C	2.73	0.47
7:9:91:GLY:O	7:9:123:ASN:ND2	2.47	0.47
9:B:61:TRP:HA	9:B:61:TRP:HE3	1.79	0.47
9:B:112:HIS:CD2	10:C:187:ARG:HH22	2.33	0.47
42:6:507:MET:O	42:6:514:HIS:HE1	1.80	0.47
1:2:7:ILE:O	1:2:11:LEU:N	2.41	0.47
3:4:306:PRO:HD3	43:g:150:TYR:HA	1.96	0.47
7:9:123:ASN:HD22	7:9:127:VAL:HG11	1.79	0.47
34:b:118:SER:OG	38:h:108:TYR:O	2.31	0.47
38:h:138:GLU:OE1	38:h:140:ASN:ND2	2.48	0.47
8:A:120:LEU:HD12	8:A:121:LEU:HG	1.97	0.47
8:A:394:VAL:HG22	8:A:473:MET:HE1	1.96	0.47
9:B:88:HIS:O	9:B:90:ALA:N	2.47	0.47
9:B:140:ASP:OD2	9:B:143:SER:OG	2.33	0.47
20:N:31:ILE:O	20:N:35:LEU:N	2.45	0.47
24:R:150:GLN:HA	24:R:153:ALA:HB3	1.97	0.47
42:6:264:TYR:HA	42:6:267:THR:HG22	1.97	0.47
10:C:49:VAL:HG22	22:P:59:GLY:HA2	1.97	0.47
42:6:203:MET:HG2	43:g:110:LEU:HD11	1.97	0.47
6:8:270:ASN:HD21	6:8:338:ASP:HA	1.79	0.46
7:9:57:PRO:HA	7:9:60:TYR:HD2	1.80	0.46
8:A:259:SER:OG	8:A:260:ASN:N	2.48	0.46
9:B:88:HIS:NE2	11:D:85:MET:HE3	2.30	0.46
42:6:506:ASN:C	42:6:510:ASN:O	2.58	0.46
3:4:367:LEU:HD11	3:4:408:LEU:HD11	1.97	0.46
3:4:403:THR:HA	3:4:406:TYR:HB3	1.97	0.46
5:7:25:SER:O	5:7:27:ILE:N	2.43	0.46
6:8:321:GLY:N	6:8:351:THR:OG1	2.46	0.46
9:B:88:HIS:N	9:B:88:HIS:ND1	2.59	0.46
24:R:235:THR:HA	24:R:236:VAL:HA	1.58	0.46
41:1:200:LEU:HG	41:1:206:GLU:CB	2.46	0.46
42:6:421:ILE:HG22	42:6:501:ALA:HB2	1.97	0.46
43:g:173:ALA:HB3	43:g:176:ALA:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:9:55:PHE:HB2	7:9:60:TYR:CZ	2.51	0.46
12:E:123:CYS:SG	12:E:126:GLN:N	2.89	0.46
24:R:168:SER:OG	24:R:169:HIS:N	2.47	0.46
37:f:95:GLU:HG2	42:6:160:GLY:HA3	1.97	0.46
42:6:68:TRP:CD1	42:6:69:LEU:HG	2.49	0.46
3:4:119:TYR:HA	3:4:122:PHE:HB3	1.97	0.46
3:4:277:LEU:HB2	42:6:546:GLN:HE22	1.80	0.46
4:5:96:LEU:N	4:5:96:LEU:HD22	2.30	0.46
9:B:143:SER:HB2	9:B:146:CYS:HB3	1.97	0.46
24:R:52:SER:OG	24:R:77:GLY:O	2.27	0.46
42:6:3:MET:HA	42:6:6:SER:HB2	1.98	0.46
9:B:67:ASN:ND2	25:S:181:VAL:O	2.49	0.46
9:B:238:LEU:HD13	22:P:37:PRO:HD2	1.97	0.46
38:h:84:ILE:HG22	38:h:88:ARG:HH12	1.80	0.46
8:A:443:ASP:N	8:A:443:ASP:OD1	2.48	0.46
32:Z:68:LEU:HD22	32:Z:71:PHE:HD1	1.79	0.46
33:a:57:ARG:CZ	38:h:67:TYR:CB	2.90	0.46
42:6:521:LYS:HE2	42:6:521:LYS:HB2	1.59	0.46
6:8:124:THR:HG22	6:8:126:LYS:H	1.81	0.46
7:9:62:ARG:NH1	13:F:83:TYR:OH	2.39	0.46
8:A:341:ILE:HD11	8:A:547:LEU:HG	1.97	0.46
16:I:89:GLY:H	16:I:96:HIS:CE1	2.34	0.46
51:L:200:PC1:H141	41:1:291:LYS:HB3	1.97	0.46
25:S:114:GLY:HA3	25:S:115:ASN:HA	1.70	0.46
32:Z:65:GLY:HA2	32:Z:68:LEU:HB2	1.97	0.46
36:d:75:PRO:HG2	43:g:26:LEU:HB3	1.98	0.46
41:1:284:GLN:HA	41:1:287:HIS:HB3	1.96	0.46
29:M:20:LYS:HD3	29:M:28:GLU:H	1.80	0.46
2:3:24:LEU:CB	2:3:25:PRO:HD3	2.25	0.46
12:E:189:LYS:HB2	27:U:124:TYR:CZ	2.51	0.46
23:Q:9:SER:HA	28:V:88:ARG:HH12	1.81	0.46
32:Z:36:LEU:O	32:Z:40:GLY:N	2.40	0.46
33:a:84:THR:OG1	33:a:85:LYS:N	2.49	0.46
10:C:96:ILE:O	10:C:100:THR:OG1	2.32	0.46
12:E:158:CYS:SG	12:E:159:GLN:N	2.88	0.46
42:6:1:MET:HG2	42:6:59:GLN:HE22	1.81	0.46
42:6:427:ILE:HA	42:6:431:LEU:HB2	1.98	0.46
42:6:512:LYS:O	42:6:513:TYR:C	2.59	0.46
10:C:110:PHE:O	10:C:162:TYR:OH	2.34	0.45
17:J:9:ILE:HG23	41:1:264:LEU:HD21	1.97	0.45
24:R:329:LEU:HD11	24:R:331:HIS:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:S:401:PC1:H292	51:S:401:PC1:H262	1.78	0.45
10:C:131:VAL:HG22	10:C:146:LYS:HG2	1.98	0.45
42:6:33:PRO:HB2	42:6:105:MET:HE2	1.98	0.45
42:6:385:PHE:O	42:6:466:TYR:OH	2.32	0.45
2:3:67:LEU:HA	5:7:59:ILE:HD11	1.98	0.45
4:5:7:ASN:HA	4:5:8:ILE:HA	1.70	0.45
12:E:82:ALA:HB2	22:P:25:GLN:HE21	1.82	0.45
35:c:109:THR:HA	43:g:19:ALA:HB3	1.99	0.45
38:h:69:LYS:HZ2	38:h:71:PRO:CD	2.24	0.45
42:6:507:MET:C	42:6:514:HIS:CE1	2.89	0.45
43:g:15:ARG:NH1	43:g:15:ARG:HA	2.30	0.45
2:3:102:LEU:O	2:3:106:TRP:N	2.48	0.45
7:9:187:GLN:HA	7:9:192:TYR:HA	1.99	0.45
8:A:153:PHE:HE2	8:A:156:GLY:HA3	1.81	0.45
42:6:528:TYR:OH	44:e:125:ASN:HA	2.16	0.45
44:e:67:ASP:O	44:e:68:ASP:O	2.35	0.45
38:h:69:LYS:O	38:h:69:LYS:HD3	2.17	0.45
40:j:115:GLU:HB3	40:j:117:HIS:ND1	2.31	0.45
3:4:426:ILE:HD12	38:h:68:GLU:OE1	2.16	0.45
8:A:504:SER:H	8:A:505:GLY:HA2	1.81	0.45
9:B:293:LEU:O	9:B:296:SER:N	2.34	0.45
14:G:121:LEU:O	14:G:123:ASN:N	2.45	0.45
24:R:269:SER:HA	24:R:270:ARG:HA	1.60	0.45
41:1:206:GLU:C	41:1:208:VAL:N	2.60	0.45
41:1:211:PHE:CD2	41:1:211:PHE:O	2.70	0.45
41:1:231:ILE:O	41:1:235:ASN:ND2	2.50	0.45
43:g:90:MET:HB3	43:g:94:ARG:HH12	1.82	0.45
43:g:146:LEU:HA	43:g:147:GLY:HA2	1.65	0.45
8:A:121:LEU:HD21	8:A:139:LEU:HB3	1.99	0.45
8:A:140:GLN:HG3	9:B:379:ILE:HG23	1.98	0.45
11:D:75:ASN:OD1	11:D:78:ARG:NH2	2.49	0.45
22:P:99:PRO:HA	22:P:100:PRO:HD3	1.88	0.45
25:S:187:LEU:HD13	25:S:277:ARG:HB2	1.97	0.45
37:f:109:PRO:CD	38:h:72:ASP:OD1	2.64	0.45
9:B:61:TRP:HH2	42:6:581:LYS:HG2	1.82	0.45
10:C:104:ASP:OD1	10:C:104:ASP:N	2.50	0.45
1:2:110:PRO:HA	1:2:112:HIS:CE1	2.52	0.45
4:5:26:LEU:HD23	4:5:78:LEU:HD13	1.98	0.45
5:7:150:GLY:CA	15:H:17:TRP:CZ2	2.96	0.45
6:8:42:PHE:HB2	7:9:239:LYS:HG3	1.99	0.45
11:D:108:ARG:HD3	41:1:36:GLY:HA2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:12:THR:HA	2:3:15:THR:HG22	1.98	0.45
6:8:183:GLY:HA2	6:8:184:LYS:HA	1.73	0.45
8:A:628:GLU:HA	8:A:633:THR:HG22	1.99	0.45
16:I:103:LEU:HD13	16:I:121:GLN:HB3	1.99	0.45
25:S:158:LEU:HA	25:S:161:MET:HB3	1.99	0.45
38:h:69:LYS:CA	38:h:69:LYS:HE2	2.47	0.45
1:2:270:MET:O	1:2:275:SER:OG	2.34	0.44
45:2:401:3PE:H331	45:2:401:3PE:H362	1.81	0.44
8:A:31:LEU:HD13	8:A:42:MET:HB3	1.99	0.44
9:B:102:SER:N	9:B:105:MET:O	2.50	0.44
23:Q:86:TRP:HA	23:Q:89:ILE:HG22	1.98	0.44
24:R:238:GLN:HE22	24:R:271:TYR:HA	1.82	0.44
33:a:84:THR:HG23	33:a:87:SER:H	1.82	0.44
2:3:41:PHE:O	2:3:41:PHE:CD2	2.70	0.44
42:6:206:PRO:HD2	42:6:266:LEU:HD13	2.00	0.44
42:6:515:TYR:CD1	42:6:515:TYR:O	2.70	0.44
43:g:13:PRO:C	43:g:14:PRO:O	2.59	0.44
45:4:502:3PE:H2B1	45:4:502:3PE:H2E1	1.75	0.44
28:V:91:LEU:HD11	28:V:106:VAL:HG13	1.99	0.44
30:X:37:PHE:HD2	34:b:137:MET:HB3	1.83	0.44
32:Z:44:PRO:HA	32:Z:45:TRP:HA	1.76	0.44
42:6:221:THR:HG22	42:6:226:GLN:HG3	2.00	0.44
6:8:213:ILE:HG23	6:8:224:ARG:HH12	1.83	0.44
6:8:387:GLU:HG2	8:A:123:ASN:HD22	1.82	0.44
8:A:373:PRO:HG3	8:A:486:GLY:HA3	1.98	0.44
9:B:143:SER:HB3	9:B:182:ASN:HD21	1.83	0.44
9:B:293:LEU:HD23	9:B:293:LEU:HA	1.74	0.44
10:C:187:ARG:HG2	21:O:88:MET:HE1	1.99	0.44
19:L:19:LEU:HD22	51:L:200:PC1:H232	1.99	0.44
23:Q:121:ASP:OD1	23:Q:121:ASP:N	2.50	0.44
25:S:73:HIS:HA	25:S:146:VAL:HG23	1.99	0.44
25:S:138:LEU:O	25:S:142:GLY:N	2.51	0.44
5:7:150:GLY:CA	15:H:17:TRP:CH2	3.01	0.44
6:8:246:GLU:HA	6:8:249:ALA:HB3	2.00	0.44
20:N:67:LYS:HE3	20:N:71:ARG:HE	1.83	0.44
22:P:29:GLN:HG3	22:P:30:GLU:H	1.82	0.44
24:R:178:SER:H	24:R:181:LEU:HB3	1.82	0.44
28:V:20:ASP:HB2	28:V:22:LYS:HG2	1.98	0.44
1:2:25:HIS:HD2	15:H:19:THR:OG1	2.01	0.44
2:3:27:LEU:HD13	2:3:27:LEU:HA	1.84	0.44
8:A:78:CYS:SG	8:A:92:CYS:N	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:404:GLY:O	8:A:479:SER:OG	2.36	0.44
9:B:85:GLY:C	9:B:87:GLN:H	2.26	0.44
27:U:111:THR:OG1	27:U:112:ASN:N	2.51	0.44
8:A:321:ASP:OD2	8:A:325:ARG:NH2	2.50	0.44
43:g:16:ARG:HH11	43:g:16:ARG:CB	2.30	0.44
3:4:423:ILE:HD12	33:a:56:ARG:HB3	2.00	0.44
7:9:155:LYS:HE3	7:9:202:GLU:HA	2.00	0.44
8:A:308:ARG:HA	8:A:308:ARG:HD2	1.85	0.44
14:G:104:ARG:NH1	21:O:127:ASP:O	2.51	0.44
23:Q:171:THR:OG1	23:Q:172:MET:N	2.50	0.44
44:e:128:LEU:O	44:e:132:HIS:N	2.50	0.44
29:M:20:LYS:HE3	29:M:28:GLU:HG2	2.00	0.44
1:2:254:LEU:HA	1:2:255:PRO:HD3	1.88	0.44
3:4:405:LEU:HD11	42:6:173:LEU:HG	1.99	0.44
9:B:67:ASN:HB2	25:S:181:VAL:HG13	1.99	0.44
11:D:85:MET:HE2	11:D:85:MET:HB3	1.86	0.44
24:R:326:ASP:O	24:R:328:ILE:HG13	2.18	0.44
2:3:24:LEU:HD22	2:3:24:LEU:HA	1.84	0.43
8:A:409:PHE:HB2	8:A:688:GLN:HG2	2.00	0.43
8:A:456:ALA:HA	8:A:496:ILE:HD13	2.00	0.43
13:F:106:SER:OG	13:F:107:PRO:O	2.31	0.43
22:P:41:LEU:HD12	22:P:42:PRO:HD2	2.00	0.43
28:V:28:ARG:HA	28:V:29:GLY:HA3	1.66	0.43
41:1:118:TRP:O	41:1:122:ALA:N	2.49	0.43
41:1:288:LEU:HA	41:1:292:ASN:HD22	1.81	0.43
42:6:209:SER:OG	42:6:270:ASN:ND2	2.51	0.43
43:g:76:GLU:HA	43:g:77:CYS:HA	1.77	0.43
1:2:300:THR:HG23	1:2:301:THR:HG23	2.00	0.43
6:8:155:TYR:HE1	6:8:196:PHE:HD2	1.65	0.43
25:S:290:LEU:O	25:S:294:ASN:N	2.50	0.43
30:X:30:ASN:OD1	30:X:31:ASP:N	2.52	0.43
40:j:83:TYR:HD1	40:j:86:ARG:HE	1.64	0.43
41:1:215:TYR:HD1	41:1:219:PRO:HB2	1.83	0.43
41:1:226:ALA:O	41:1:229:ALA:HB3	2.18	0.43
42:6:279:CYS:SG	42:6:405:ASN:ND2	2.91	0.43
42:6:578:THR:O	42:6:581:LYS:HE2	2.18	0.43
1:2:54:GLU:OE1	4:5:94:ASN:ND2	2.51	0.43
1:2:137:ALA:O	1:2:140:SER:OG	2.29	0.43
3:4:210:TYR:O	3:4:213:HIS:ND1	2.44	0.43
4:5:38:LEU:HA	4:5:41:PHE:HB3	1.99	0.43
42:6:518:ASN:OD1	42:6:518:ASN:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4:207:MET:HA	3:4:208:PRO:HD3	1.86	0.43
3:4:396:MET:HE2	3:4:396:MET:HB3	1.87	0.43
7:9:227:PRO:HD2	7:9:231:LEU:HA	1.99	0.43
29:W:109:GLY:HA2	29:W:110:LEU:HA	1.70	0.43
40:j:46:ASN:HA	40:j:51:ARG:HH21	1.84	0.43
44:e:87:ASP:HA	44:e:88:PRO:HD2	1.92	0.43
44:e:123:PRO:HB2	44:e:124:VAL:H	1.59	0.43
29:M:37:MET:HA	29:M:41:GLY:HA2	2.01	0.43
6:8:295:PRO:HG2	6:8:298:GLU:HG2	1.99	0.43
12:E:170:GLY:HA2	12:E:171:PRO:HD3	1.78	0.43
16:I:101:ILE:H	16:I:101:ILE:HG13	1.68	0.43
38:h:70:ASN:HD22	38:h:70:ASN:HA	1.58	0.43
41:1:200:LEU:CG	41:1:206:GLU:CG	2.92	0.43
8:A:272:ARG:HH12	8:A:274:LEU:HD11	1.84	0.43
8:A:347:ASP:N	8:A:347:ASP:OD1	2.50	0.43
11:D:102:PRO:HB3	41:1:34:ARG:HD3	2.01	0.43
11:D:182:TYR:HE2	12:E:180:HIS:HB2	1.84	0.43
24:R:58:VAL:HG13	24:R:127:ILE:HD11	2.00	0.43
24:R:178:SER:N	24:R:182:ARG:H	2.14	0.43
25:S:194:TYR:HB3	25:S:245:GLN:HG3	1.99	0.43
38:h:111:ASP:OD1	38:h:111:ASP:N	2.52	0.43
40:j:91:PHE:HD1	40:j:94:ILE:HD12	1.84	0.43
42:6:82:MET:HA	42:6:86:SER:HB3	2.00	0.43
7:9:152:ILE:HG12	7:9:201:ILE:HD12	2.00	0.43
9:B:64:PRO:HA	9:B:65:PRO:HD3	1.89	0.43
12:E:37:THR:HA	22:P:104:TRP:HB3	2.00	0.43
24:R:64:PHE:CZ	24:R:208:GLY:HA3	2.53	0.43
41:1:281:ARG:HH21	41:1:284:GLN:HE21	1.65	0.43
42:6:81:LYS:N	42:6:133:THR:O	2.52	0.43
44:e:68:ASP:O	44:e:75:TYR:CE2	2.72	0.43
2:3:38:GLU:OE2	41:1:64:ALA:CB	2.67	0.43
3:4:66:LEU:O	3:4:69:THR:OG1	2.27	0.43
3:4:168:GLN:HE21	34:b:150:ARG:NH1	2.17	0.43
8:A:344:GLY:O	8:A:521:SER:OG	2.28	0.43
11:D:155:SER:OG	11:D:155:SER:O	2.36	0.43
16:I:111:THR:HG22	16:I:118:GLN:HA	2.00	0.43
20:N:60:LYS:HA	20:N:61:ALA:HA	1.78	0.43
31:Y:47:TYR:HD2	32:Z:16:LEU:HD12	1.84	0.43
33:a:57:ARG:HH21	38:h:68:GLU:CD	2.24	0.43
35:c:38:GLN:HA	35:c:39:ARG:HA	1.88	0.43
42:6:491:LEU:O	42:6:494:THR:OG1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3:38:GLU:OE2	41:1:64:ALA:HB2	2.19	0.43
6:8:43:THR:O	6:8:257:ARG:NH2	2.49	0.43
11:D:75:ASN:HD21	11:D:207:GLU:HA	1.84	0.43
11:D:194:LEU:HD23	11:D:194:LEU:HA	1.84	0.43
24:R:154:GLN:HG3	24:R:155:VAL:H	1.83	0.43
25:S:192:VAL:HG11	25:S:233:PHE:HZ	1.83	0.43
6:8:375:LYS:HD3	6:8:393:ASN:HD22	1.84	0.43
8:A:607:LYS:HE2	14:G:78:ARG:HE	1.83	0.43
21:O:18:LYS:O	21:O:77:ARG:NH2	2.52	0.43
37:f:16:VAL:O	37:f:20:TYR:N	2.52	0.43
39:i:45:GLY:HA2	39:i:48:LEU:HB2	2.01	0.43
1:2:256:PRO:HD3	3:4:124:ALA:HA	2.01	0.42
24:R:201:ILE:HD12	24:R:263:PHE:HB2	2.01	0.42
27:U:42:ASP:HA	27:U:43:LYS:HA	1.76	0.42
38:h:69:LYS:HE2	38:h:69:LYS:HA	2.00	0.42
43:g:16:ARG:NH1	43:g:16:ARG:HG3	2.34	0.42
44:e:166:LEU:HD23	44:e:166:LEU:N	2.34	0.42
1:2:4:ILE:HB	51:S:401:PC1:H241	2.01	0.42
2:3:20:ILE:HD12	2:3:20:ILE:N	2.34	0.42
6:8:112:TYR:HB2	6:8:240:THR:HG22	2.01	0.42
9:B:254:ARG:HH21	22:P:24:LEU:HA	1.83	0.42
11:D:107:ASP:OD1	11:D:108:ARG:N	2.52	0.42
22:P:53:TYR:O	22:P:56:THR:OG1	2.36	0.42
24:R:195:PHE:HD2	24:R:198:ALA:HB2	1.83	0.42
25:S:102:LEU:HA	25:S:105:PHE:HE1	1.83	0.42
25:S:110:LYS:HA	25:S:166:PHE:HA	2.01	0.42
25:S:200:PRO:CG	25:S:223:GLN:HE22	2.32	0.42
41:1:207:LEU:O	41:1:210:GLY:N	2.52	0.42
42:6:525:LEU:HD13	42:6:525:LEU:O	2.18	0.42
42:6:556:ILE:O	42:6:560:ALA:N	2.52	0.42
29:M:26:ASP:OD1	29:M:26:ASP:N	2.52	0.42
29:M:32:VAL:HG23	29:M:74:GLN:HE21	1.83	0.42
2:3:48:ARG:NH1	2:3:48:ARG:CG	2.73	0.42
11:D:75:ASN:ND2	11:D:206:ARG:O	2.52	0.42
23:Q:28:ALA:O	23:Q:30:HIS:N	2.51	0.42
24:R:203:PRO:HA	24:R:265:PHE:HB2	2.01	0.42
33:a:68:TRP:CH2	44:e:110:ASP:HA	2.55	0.42
42:6:396:ILE:HD12	42:6:397:GLU:HG3	2.01	0.42
2:3:28:ASN:ND2	2:3:32:GLU:CD	2.77	0.42
3:4:306:PRO:HA	3:4:308:SER:H	1.83	0.42
8:A:405:THR:HB	8:A:477:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:253:LEU:HD23	9:B:254:ARG:HH12	1.83	0.42
9:B:359:ASP:HB2	22:P:45:PRO:HG2	2.01	0.42
20:N:43:ALA:HA	20:N:46:LYS:HD3	2.00	0.42
38:h:82:VAL:HA	38:h:85:TRP:HD1	1.84	0.42
43:g:22:PRO:CD	43:g:23:GLN:N	2.83	0.42
9:B:105:MET:SD	9:B:105:MET:N	2.93	0.42
14:G:130:THR:HG23	14:G:133:ASP:H	1.84	0.42
30:X:13:HIS:O	30:X:15:LEU:N	2.52	0.42
34:b:161:ARG:HA	34:b:161:ARG:HD2	1.87	0.42
38:h:68:GLU:HG2	38:h:68:GLU:H	1.36	0.42
41:1:20:LEU:O	41:1:24:GLU:N	2.51	0.42
41:1:222:LEU:HA	41:1:225:MET:HB3	2.02	0.42
43:g:15:ARG:HA	43:g:15:ARG:HD2	1.33	0.42
3:4:244:LEU:HD21	3:4:301:ILE:HD12	2.02	0.42
6:8:47:GLY:O	6:8:133:HIS:ND1	2.52	0.42
6:8:253:THR:HA	6:8:256:ARG:HB3	2.02	0.42
25:S:187:LEU:HA	25:S:188:PRO:HD3	1.86	0.42
30:X:14:VAL:HA	30:X:17:PRO:HD2	2.01	0.42
3:4:5:ILE:HA	3:4:8:THR:HG22	2.01	0.42
3:4:319:HIS:HA	3:4:322:THR:HB	2.02	0.42
3:4:360:LEU:O	3:4:364:LEU:N	2.48	0.42
8:A:216:SER:N	8:A:219:SER:OG	2.48	0.42
8:A:624:ARG:NH1	8:A:634:LEU:O	2.35	0.42
43:g:16:ARG:CG	43:g:16:ARG:NH1	2.80	0.42
10:C:124:ARG:HD2	20:N:111:GLN:HG3	2.02	0.42
14:G:163:ASN:HB3	14:G:172:VAL:HG22	2.01	0.42
17:J:23:THR:HG23	41:1:5:ASN:HD21	1.84	0.42
24:R:61:ALA:H	24:R:129:LEU:HD11	1.83	0.42
35:c:106:PRO:HB2	35:c:107:GLY:H	1.66	0.42
38:h:127:LYS:HA	38:h:130:GLU:HB3	2.01	0.42
2:3:41:PHE:CD2	2:3:41:PHE:C	2.98	0.42
3:4:182:TRP:HZ3	43:g:82:VAL:HG22	1.85	0.42
7:9:188:ILE:HG13	7:9:191:ASN:H	1.84	0.42
8:A:651:PRO:HD2	18:K:56:ARG:HB3	2.02	0.42
33:a:27:SER:HA	33:a:28:GLU:HA	1.81	0.42
29:M:25:ILE:HD12	29:M:42:LEU:HG	2.01	0.42
29:M:51:ILE:HD12	29:M:70:LEU:HD12	2.02	0.42
1:2:106:LEU:HD13	1:2:139:MET:HE2	2.02	0.42
9:B:326:CYS:SG	9:B:329:ARG:NH1	2.93	0.42
15:H:96:PRO:HA	15:H:97:HIS:HA	1.82	0.42
51:Q:201:PC1:H341	51:Q:201:PC1:H372	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:S:102:LEU:HD23	25:S:105:PHE:HE1	1.84	0.42
29:W:111:ASP:O	29:W:112:SER:C	2.62	0.42
37:f:70:GLU:H	37:f:73:HIS:HB3	1.84	0.42
41:1:202:GLU:O	41:1:209:SER:HA	2.16	0.42
41:1:203:GLY:HA3	41:1:209:SER:CA	2.49	0.42
41:1:243:LEU:HB3	41:1:262:LYS:HZ1	1.85	0.42
42:6:246:LEU:O	42:6:251:THR:OG1	2.27	0.42
8:A:94:MET:HE3	8:A:94:MET:HB2	1.90	0.41
15:H:28:LYS:HB3	34:b:184:LYS:HA	2.01	0.41
20:N:88:LEU:HD11	20:N:92:ARG:HH21	1.84	0.41
37:f:109:PRO:HA	37:f:111:GLU:H	1.85	0.41
41:1:201:THR:O	41:1:202:GLU:C	2.63	0.41
1:2:72:MET:HE3	1:2:76:ILE:HD11	2.01	0.41
8:A:180:THR:HG23	8:A:183:ILE:HD12	2.02	0.41
9:B:177:ILE:HG12	9:B:210:MET:HE3	2.02	0.41
11:D:185:GLY:HA2	12:E:154:TYR:CE2	2.55	0.41
35:c:11:ARG:HB2	37:f:155:PRO:HB3	2.02	0.41
41:1:233:MET:HA	41:1:236:ILE:HG22	2.01	0.41
42:6:341:MET:HE3	42:6:454:ILE:HD13	2.02	0.41
43:g:20:PRO:HB2	43:g:21:SER:H	1.61	0.41
1:2:49:ASN:HD22	1:2:123:PRO:HG2	1.85	0.41
1:2:51:ARG:HG3	9:B:69:VAL:HB	2.01	0.41
1:2:100:MET:HE2	42:6:595:ILE:HD12	2.00	0.41
8:A:618:GLU:OE2	8:A:620:TRP:NE1	2.53	0.41
10:C:189:ILE:HD13	10:C:189:ILE:HA	1.93	0.41
21:O:50:PHE:HE2	21:O:103:VAL:HG21	1.84	0.41
24:R:175:LYS:O	24:R:177:SER:N	2.49	0.41
24:R:352:VAL:HG13	24:R:353:LEU:HD12	2.02	0.41
27:U:31:ASN:HD21	41:1:43:TYR:HA	1.85	0.41
35:c:20:ARG:HA	35:c:23:LEU:HB3	2.01	0.41
36:d:6:ALA:N	36:d:30:GLY:C	2.78	0.41
37:f:166:LEU:HA	37:f:167:TRP:HA	1.62	0.41
42:6:527:GLY:C	42:6:529:PHE:N	2.60	0.41
6:8:420:GLU:H	6:8:422:HIS:CD2	2.31	0.41
7:9:88:ARG:NH1	13:F:82:THR:O	2.53	0.41
7:9:145:SER:O	7:9:149:LEU:N	2.53	0.41
8:A:436:VAL:O	8:A:442:TYR:OH	2.31	0.41
10:C:76:GLN:HE22	10:C:148:TYR:HE1	1.67	0.41
12:E:113:CYS:SG	12:E:114:ILE:N	2.94	0.41
18:K:15:GLY:HA2	18:K:16:LEU:HA	1.76	0.41
24:R:228:LEU:HA	24:R:229:ILE:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:f:109:PRO:HD2	38:h:72:ASP:OD1	2.20	0.41
42:6:48:MET:O	42:6:51:THR:OG1	2.28	0.41
42:6:525:LEU:CD1	42:6:526:LEU:HG	2.49	0.41
43:g:17:THR:HG22	43:g:18:PRO:O	2.21	0.41
8:A:359:ASN:ND2	18:K:68:ARG:HH12	2.19	0.41
11:D:206:ARG:HH21	11:D:208:LYS:HE2	1.84	0.41
12:E:100:GLU:O	12:E:170:GLY:N	2.49	0.41
12:E:106:TYR:CE1	12:E:112:ARG:HG3	2.55	0.41
40:j:107:LYS:HD3	40:j:111:GLU:HG2	2.02	0.41
41:1:217:ALA:HA	41:1:220:PHE:HB3	2.02	0.41
44:e:94:HIS:N	44:e:95:PRO:CD	2.84	0.41
9:B:222:MET:HE2	11:D:95:GLU:HB2	2.02	0.41
11:D:108:ARG:HH12	41:1:34:ARG:CZ	2.34	0.41
20:N:24:LEU:HB3	20:N:28:TYR:HE2	1.85	0.41
27:U:124:TYR:CE2	27:U:126:PRO:HG3	2.56	0.41
37:f:40:PHE:CZ	42:6:513:TYR:CD2	3.07	0.41
44:e:49:ALA:HB2	44:e:53:LYS:HA	2.01	0.41
10:C:217:GLU:OE1	24:R:75:ARG:NH2	2.47	0.41
10:C:218:VAL:HG13	10:C:219:LYS:H	1.85	0.41
24:R:253:ILE:HD12	24:R:253:ILE:HA	1.98	0.41
3:4:297:VAL:O	3:4:301:ILE:HG12	2.20	0.41
5:7:98:LEU:O	5:7:102:PHE:N	2.48	0.41
16:I:82:SER:OG	16:I:83:ARG:N	2.53	0.41
25:S:272:LEU:HB3	25:S:275:ASN:HA	2.03	0.41
37:f:38:ARG:HA	37:f:38:ARG:HD2	1.90	0.41
38:h:68:GLU:O	38:h:69:LYS:C	2.52	0.41
29:M:32:VAL:HA	29:M:73:PRO:HG2	2.03	0.41
3:4:393:ILE:HG21	42:6:184:LEU:HD13	2.02	0.41
8:A:435:PRO:HG3	8:A:444:HIS:ND1	2.35	0.41
9:B:443:MET:HE2	9:B:443:MET:HB3	1.99	0.41
45:B:501:3PE:H351	41:1:184:MET:HE3	2.03	0.41
26:T:99:LEU:O	26:T:103:ALA:N	2.51	0.41
37:f:33:HIS:HB2	37:f:36:LYS:HB2	2.03	0.41
37:f:39:TYR:CB	42:6:513:TYR:OH	2.69	0.41
42:6:338:MET:O	42:6:342:CYS:N	2.52	0.41
3:4:5:ILE:HG13	3:4:6:ILE:HG13	2.01	0.41
9:B:143:SER:OG	9:B:147:ASN:OD1	2.38	0.41
9:B:180:LEU:HB2	9:B:210:MET:HE1	2.01	0.41
10:C:170:ARG:HH11	10:C:170:ARG:HD2	1.75	0.41
22:P:65:PRO:HA	22:P:66:PRO:HD3	1.89	0.41
36:d:34:ARG:HA	36:d:35:LYS:HA	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:6:282:ALA:O	42:6:285:THR:OG1	2.31	0.41
9:B:53:TYR:HA	9:B:54:PRO:HD3	1.78	0.40
9:B:271:ARG:HA	9:B:271:ARG:HD2	1.90	0.40
15:H:74:LYS:HD2	15:H:74:LYS:HA	1.92	0.40
25:S:76:GLU:O	25:S:127:ARG:NH1	2.54	0.40
25:S:150:SER:OG	25:S:151:ILE:N	2.54	0.40
29:W:97:LYS:HZ3	29:W:107:ASP:CB	2.32	0.40
8:A:158:ARG:NE	8:A:202:ASN:OD1	2.54	0.40
9:B:144:MET:HG3	9:B:214:TYR:HE2	1.86	0.40
12:E:172:ASN:ND2	12:E:200:GLU:OE1	2.54	0.40
17:J:26:ILE:HD13	17:J:26:ILE:HA	1.94	0.40
23:Q:6:GLU:O	23:Q:54:ARG:NH1	2.54	0.40
31:Y:50:PHE:HE1	42:6:364:LYS:HA	1.87	0.40
31:Y:64:PHE:HA	31:Y:67:THR:HG22	2.03	0.40
41:1:225:MET:SD	41:1:225:MET:O	2.79	0.40
1:2:190:MET:HB2	1:2:201:THR:HG23	2.03	0.40
6:8:98:LYS:HG3	6:8:99:TRP:CD1	2.57	0.40
8:A:469:ALA:HB3	8:A:472:PRO:HG3	2.03	0.40
24:R:339:GLY:HA2	24:R:340:VAL:HA	1.94	0.40
41:1:124:ASN:HB3	41:1:125:SER:H	1.72	0.40
5:7:156:VAL:O	5:7:160:SER:N	2.46	0.40
8:A:63:PHE:O	8:A:181:ARG:NH2	2.54	0.40
9:B:34:ALA:HB1	38:h:63:ASP:HA	2.03	0.40
9:B:233:HIS:NE2	12:E:160:GLU:OE1	2.54	0.40
9:B:303:ARG:HH11	9:B:303:ARG:HD2	1.74	0.40
11:D:176:ILE:HG22	11:D:177:VAL:HG13	2.03	0.40
25:S:161:MET:HE3	25:S:167:ILE:HG12	2.04	0.40
42:6:328:HIS:O	42:6:331:THR:OG1	2.37	0.40
44:e:48:ARG:HA	44:e:49:ALA:HA	1.66	0.40
6:8:186:ALA:HA	6:8:187:CYS:HA	1.60	0.40
47:8:501:FMN:H9	47:8:501:FMN:H1'1	1.58	0.40
19:L:32:LEU:HA	19:L:35:LEU:HD12	2.04	0.40
37:f:109:PRO:HD3	38:h:72:ASP:OD1	2.21	0.40
29:M:51:ILE:HG22	29:M:62:ILE:HG12	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	2	342/347 (99%)	298 (87%)	44 (13%)	0	100 100
2	3	110/115 (96%)	78 (71%)	18 (16%)	14 (13%)	0 4
3	4	457/459 (100%)	374 (82%)	77 (17%)	6 (1%)	9 38
4	5	94/98 (96%)	80 (85%)	14 (15%)	0	100 100
5	7	170/175 (97%)	135 (79%)	31 (18%)	4 (2%)	4 29
6	8	425/444 (96%)	344 (81%)	79 (19%)	2 (0%)	24 57
7	9	205/217 (94%)	165 (80%)	39 (19%)	1 (0%)	24 57
8	A	686/704 (97%)	563 (82%)	118 (17%)	5 (1%)	18 51
9	B	428/430 (100%)	353 (82%)	65 (15%)	10 (2%)	5 30
10	C	206/228 (90%)	175 (85%)	31 (15%)	0	100 100
11	D	150/179 (84%)	131 (87%)	19 (13%)	0	100 100
12	E	174/176 (99%)	148 (85%)	25 (14%)	1 (1%)	21 54
13	F	26/75 (35%)	17 (65%)	9 (35%)	0	100 100
14	G	121/133 (91%)	99 (82%)	20 (16%)	2 (2%)	7 34
15	H	94/105 (90%)	73 (78%)	21 (22%)	0	100 100
16	I	69/96 (72%)	56 (81%)	11 (16%)	2 (3%)	3 25
17	J	67/70 (96%)	63 (94%)	3 (4%)	1 (2%)	8 36
18	K	82/98 (84%)	62 (76%)	20 (24%)	0	100 100
19	L	78/83 (94%)	68 (87%)	10 (13%)	0	100 100
20	N	109/115 (95%)	91 (84%)	18 (16%)	0	100 100
21	O	112/127 (88%)	98 (88%)	14 (12%)	0	100 100
22	P	86/112 (77%)	66 (77%)	20 (23%)	0	100 100
23	Q	166/171 (97%)	117 (70%)	47 (28%)	2 (1%)	10 40
24	R	315/345 (91%)	249 (79%)	64 (20%)	2 (1%)	21 54
25	S	317/320 (99%)	249 (78%)	65 (20%)	3 (1%)	14 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	T	136/140 (97%)	113 (83%)	22 (16%)	1 (1%)	18 51
27	U	128/145 (88%)	101 (79%)	27 (21%)	0	100 100
28	V	136/143 (95%)	119 (88%)	15 (11%)	2 (2%)	8 36
29	M	78/88 (89%)	62 (80%)	16 (20%)	0	100 100
29	W	84/88 (96%)	65 (77%)	19 (23%)	0	100 100
30	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2 19
31	Y	55/72 (76%)	44 (80%)	11 (20%)	0	100 100
32	Z	72/97 (74%)	49 (68%)	23 (32%)	0	100 100
33	a	112/128 (88%)	87 (78%)	25 (22%)	0	100 100
34	b	137/143 (96%)	117 (85%)	20 (15%)	0	100 100
35	c	86/127 (68%)	63 (73%)	19 (22%)	4 (5%)	2 18
36	d	105/136 (77%)	74 (70%)	26 (25%)	5 (5%)	2 17
37	f	165/178 (93%)	126 (76%)	38 (23%)	1 (1%)	21 54
38	h	89/125 (71%)	60 (67%)	24 (27%)	5 (6%)	1 15
39	i	36/49 (74%)	34 (94%)	2 (6%)	0	100 100
40	j	111/120 (92%)	95 (86%)	16 (14%)	0	100 100
41	1	315/318 (99%)	267 (85%)	42 (13%)	6 (2%)	6 32
42	6	604/606 (100%)	513 (85%)	81 (13%)	10 (2%)	7 34
43	g	171/176 (97%)	138 (81%)	28 (16%)	5 (3%)	3 25
44	e	139/158 (88%)	74 (53%)	45 (32%)	20 (14%)	0 3
All	All	7895/8516 (93%)	6390 (81%)	1389 (18%)	116 (2%)	11 36

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	3	24	LEU
2	3	30	TYR
2	3	33	LYS
2	3	34	THR
2	3	35	SER
2	3	40	GLY
2	3	42	ASP
2	3	43	PRO
5	7	171	ILE
8	A	463	SER

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Mol	Chain	Res	Type
9	B	88	HIS
9	B	89	PRO
9	B	294	ARG
16	I	106	GLU
16	I	107	THR
25	S	200	PRO
25	S	276	ASP
36	d	10	LEU
38	h	68	GLU
38	h	69	LYS
38	h	72	ASP
38	h	81	ALA
38	h	82	VAL
41	1	213	VAL
42	6	528	TYR
43	g	14	PRO
43	g	19	ALA
43	g	20	PRO
43	g	22	PRO
44	e	81	ARG
44	e	82	SER
44	e	87	ASP
44	e	99	LEU
44	e	125	ASN
44	e	126	TRP
44	e	153	TYR
2	3	26	GLN
2	3	27	LEU
3	4	20	ASN
3	4	419	TYR
8	A	365	THR
14	G	122	SER
24	R	272	LEU
28	V	143	TYR
30	X	14	VAL
35	c	106	PRO
36	d	40	VAL
41	1	200	LEU
41	1	282	TYR
42	6	31	ASN
42	6	603	ASN
44	e	68	ASP

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Mol	Chain	Res	Type
44	e	96	ASP
44	e	98	ARG
44	e	155	PRO
44	e	156	VAL
3	4	21	ASN
5	7	149	TYR
7	9	76	ALA
8	A	129	PRO
8	A	309	ASN
8	A	541	PRO
9	B	54	PRO
9	B	93	GLY
35	c	108	ASP
36	d	19	PRO
42	6	514	HIS
42	6	516	PRO
42	6	519	ALA
44	e	76	PRO
44	e	123	PRO
2	3	21	ALA
2	3	82	ALA
3	4	64	PRO
3	4	112	ALA
5	7	170	GLU
9	B	63	PRO
9	B	291	VAL
12	E	108	SER
36	d	7	ARG
41	1	174	LEU
41	1	207	LEU
42	6	511	LEU
42	6	551	SER
42	6	581	LYS
43	g	18	PRO
44	e	80	ASP
44	e	83	GLN
2	3	25	PRO
2	3	32	GLU
9	B	61	TRP
9	B	90	ALA
9	B	219	GLY
23	Q	29	ALA

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Mol	Chain	Res	Type
23	Q	166	ARG
35	c	105	PHE
35	c	112	GLU
41	1	206	GLU
42	6	30	SER
44	e	91	ASP
44	e	121	PRO
44	e	122	THR
6	8	227	PRO
14	G	84	ARG
25	S	281	LYS
30	X	13	HIS
44	e	94	HIS
37	f	145	PRO
3	4	305	THR
5	7	24	PRO
6	8	105	PRO
17	J	56	GLY
26	T	84	PRO
24	R	328	ILE
28	V	73	PRO
36	d	32	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	2	274/316 (87%)	273 (100%)	1 (0%)	84 83
2	3	90/101 (89%)	81 (90%)	9 (10%)	7 28
3	4	351/413 (85%)	350 (100%)	1 (0%)	86 84
4	5	75/86 (87%)	75 (100%)	0	100 100
5	7	104/142 (73%)	104 (100%)	0	100 100
6	8	236/353 (67%)	236 (100%)	0	100 100
7	9	160/183 (87%)	158 (99%)	2 (1%)	61 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	A	551/588 (94%)	548 (100%)	3 (0%)	81 81
9	B	359/371 (97%)	352 (98%)	7 (2%)	50 66
10	C	183/204 (90%)	182 (100%)	1 (0%)	81 81
11	D	126/150 (84%)	124 (98%)	2 (2%)	55 68
12	E	145/151 (96%)	145 (100%)	0	100 100
13	F	13/69 (19%)	13 (100%)	0	100 100
14	G	105/119 (88%)	105 (100%)	0	100 100
15	H	80/95 (84%)	78 (98%)	2 (2%)	42 61
16	I	52/79 (66%)	49 (94%)	3 (6%)	18 44
17	J	50/59 (85%)	50 (100%)	0	100 100
18	K	66/81 (82%)	66 (100%)	0	100 100
19	L	63/71 (89%)	63 (100%)	0	100 100
20	N	88/101 (87%)	88 (100%)	0	100 100
21	O	95/113 (84%)	95 (100%)	0	100 100
22	P	72/96 (75%)	72 (100%)	0	100 100
23	Q	142/154 (92%)	139 (98%)	3 (2%)	47 64
24	R	232/298 (78%)	229 (99%)	3 (1%)	61 71
25	S	205/283 (72%)	203 (99%)	2 (1%)	68 74
26	T	79/101 (78%)	79 (100%)	0	100 100
27	U	95/131 (72%)	95 (100%)	0	100 100
28	V	107/120 (89%)	106 (99%)	1 (1%)	70 74
29	M	73/81 (90%)	73 (100%)	0	100 100
29	W	57/81 (70%)	55 (96%)	2 (4%)	32 54
30	X	32/54 (59%)	32 (100%)	0	100 100
31	Y	29/62 (47%)	29 (100%)	0	100 100
32	Z	28/75 (37%)	28 (100%)	0	100 100
33	a	70/114 (61%)	70 (100%)	0	100 100
34	b	85/124 (68%)	85 (100%)	0	100 100
35	c	45/121 (37%)	45 (100%)	0	100 100
36	d	42/119 (35%)	42 (100%)	0	100 100
37	f	80/160 (50%)	79 (99%)	1 (1%)	61 71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
38	h	70/112 (62%)	63 (90%)	7 (10%)	7 28
39	i	23/45 (51%)	23 (100%)	0	100 100
40	j	88/106 (83%)	88 (100%)	0	100 100
41	1	274/275 (100%)	265 (97%)	9 (3%)	33 56
42	6	523/534 (98%)	512 (98%)	11 (2%)	47 64
43	g	130/157 (83%)	128 (98%)	2 (2%)	57 69
44	e	44/141 (31%)	39 (89%)	5 (11%)	5 23
All	All	5891/7389 (80%)	5814 (99%)	77 (1%)	59 71

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	7	ILE
2	3	18	VAL
2	3	24	LEU
2	3	27	LEU
2	3	32	GLU
2	3	33	LYS
2	3	37	TYR
2	3	42	ASP
2	3	44	MET
2	3	48	ARG
3	4	165	ILE
7	9	93	LEU
7	9	149	LEU
8	A	120	LEU
8	A	262	VAL
8	A	538	GLN
9	B	61	TRP
9	B	62	LYS
9	B	87	GLN
9	B	88	HIS
9	B	92	HIS
9	B	94	VAL
9	B	429	PHE
10	C	218	VAL
11	D	74	ILE
11	D	114	ARG
15	H	16	ARG
15	H	19	THR

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Mol	Chain	Res	Type
16	I	101	ILE
16	I	103	LEU
16	I	106	GLU
23	Q	115	LEU
23	Q	128	VAL
23	Q	154	VAL
24	R	82	VAL
24	R	126	VAL
24	R	206	ILE
25	S	195	VAL
25	S	200	PRO
28	V	58	ARG
29	W	106	LYS
29	W	110	LEU
37	f	30	TRP
38	h	63	ASP
38	h	64	GLU
38	h	66	LEU
38	h	67	TYR
38	h	68	GLU
38	h	69	LYS
38	h	70	ASN
41	1	89	LEU
41	1	200	LEU
41	1	201	THR
41	1	202	GLU
41	1	208	VAL
41	1	211	PHE
41	1	225	MET
41	1	228	TYR
41	1	310	LEU
42	6	155	ILE
42	6	427	ILE
42	6	514	HIS
42	6	515	TYR
42	6	517	SER
42	6	518	ASN
42	6	520	PHE
42	6	521	LYS
42	6	522	PHE
42	6	524	THR
42	6	525	LEU

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Mol	Chain	Res	Type
43	g	15	ARG
43	g	16	ARG
44	e	89	TRP
44	e	92	TRP
44	e	124	VAL
44	e	160	GLN
44	e	166	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	49	ASN
2	3	10	ASN
2	3	28	ASN
2	3	80	GLN
3	4	26	ASN
3	4	30	HIS
3	4	168	GLN
3	4	304	GLN
3	4	374	ASN
4	5	25	HIS
5	7	46	ASN
6	8	281	HIS
6	8	346	GLN
6	8	422	HIS
8	A	142	GLN
8	A	309	ASN
8	A	334	GLN
8	A	359	ASN
8	A	571	HIS
9	B	38	GLN
9	B	87	GLN
9	B	112	HIS
9	B	182	ASN
9	B	183	HIS
9	B	250	ASN
9	B	339	GLN
10	C	84	ASN
10	C	249	GLN
11	D	98	HIS
11	D	158	ASN
12	E	192	ASN

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Mol	Chain	Res	Type
15	H	25	GLN
15	H	27	HIS
15	H	70	GLN
15	H	82	GLN
18	K	25	GLN
19	L	46	ASN
20	N	53	ASN
20	N	83	GLN
20	N	111	GLN
21	O	126	HIS
24	R	43	HIS
24	R	79	GLN
24	R	323	HIS
24	R	331	HIS
25	S	223	GLN
26	T	89	ASN
27	U	31	ASN
28	V	112	HIS
29	W	115	GLN
30	X	13	HIS
34	b	141	GLN
34	b	170	HIS
34	b	181	HIS
35	c	14	GLN
35	c	83	HIS
37	f	139	GLN
38	h	70	ASN
39	i	62	HIS
40	j	88	HIS
40	j	97	HIS
41	1	5	ASN
41	1	97	ASN
41	1	124	ASN
41	1	284	GLN
41	1	292	ASN
41	1	317	GLN
42	6	59	GLN
42	6	113	ASN
42	6	139	GLN
42	6	192	ASN
42	6	226	GLN
42	6	270	ASN

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Mol	Chain	Res	Type
42	6	332	HIS
42	6	405	ASN
42	6	479	GLN
42	6	546	GLN
43	g	55	GLN
43	g	161	GLN
44	e	160	GLN
29	M	74	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
48	SF4	8	502	-	0,12,12	-	-	-		
45	3PE	V	201	-	50,50,50	0.87	4 (8%)	53,55,55	1.11	2 (3%)
46	CDL	J	101	-	57,57,99	1.15	8 (14%)	63,69,111	1.20	4 (6%)
48	SF4	E	301	-	0,12,12	-	-	-		
47	FMN	8	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.64	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	3PE	B	501	-	50,50,50	0.86	4 (8%)	53,55,55	1.13	2 (3%)
52	NAP	R	601	-	50,52,52	4.21	24 (48%)	71,80,80	1.83	16 (22%)
51	PC1	j	201	-	38,38,53	1.14	4 (10%)	44,46,61	1.05	2 (4%)
51	PC1	L	200	-	46,46,53	1.03	4 (8%)	52,54,61	1.07	2 (3%)
48	SF4	D	301	-	0,12,12	-	-	-		
51	PC1	Q	201	-	45,45,53	1.02	4 (8%)	51,53,61	1.08	2 (3%)
45	3PE	4	502	-	40,40,50	0.93	3 (7%)	43,45,55	1.39	3 (6%)
49	FES	9	301	-	0,4,4	-	-	-		
48	SF4	A	801	-	0,12,12	-	-	-		
48	SF4	E	302	-	0,12,12	-	-	-		
49	FES	A	803	-	0,4,4	-	-	-		
48	SF4	A	802	-	0,12,12	-	-	-		
46	CDL	4	501	-	81,81,99	0.98	7 (8%)	87,93,111	1.12	5 (5%)
51	PC1	S	401	-	46,46,53	1.01	4 (8%)	52,54,61	1.00	2 (3%)
45	3PE	2	401	-	40,40,50	0.96	4 (10%)	43,45,55	1.19	2 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	SF4	8	502	-	-	-	0/6/5/5
45	3PE	V	201	-	-	20/54/54/54	-
46	CDL	J	101	-	-	29/68/68/110	-
48	SF4	E	301	-	-	-	0/6/5/5
47	FMN	8	501	-	-	10/18/18/18	0/3/3/3
45	3PE	B	501	-	-	25/54/54/54	-
52	NAP	R	601	-	-	17/35/67/67	0/5/5/5
51	PC1	j	201	-	-	20/42/42/57	-
51	PC1	L	200	-	-	23/50/50/57	-
48	SF4	D	301	-	-	-	0/6/5/5
51	PC1	Q	201	-	-	20/49/49/57	-
45	3PE	4	502	-	-	23/44/44/54	-
49	FES	9	301	-	-	-	0/1/1/1
48	SF4	A	801	-	-	-	0/6/5/5
48	SF4	E	302	-	-	-	0/6/5/5
49	FES	A	803	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	SF4	A	802	-	-	-	0/6/5/5
46	CDL	4	501	-	-	39/92/92/110	-
51	PC1	S	401	-	-	32/50/50/57	-
45	3PE	2	401	-	-	20/44/44/54	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	R	601	NAP	O4D-C1D	17.26	1.63	1.40
52	R	601	NAP	C2B-C1B	-9.55	1.29	1.53
52	R	601	NAP	O4B-C1B	8.48	1.61	1.42
52	R	601	NAP	PN-O3	8.42	1.68	1.59
52	R	601	NAP	C7N-N7N	7.16	1.46	1.33
52	R	601	NAP	O4D-C4D	-6.75	1.30	1.45
52	R	601	NAP	O4B-C4B	-5.85	1.32	1.45
52	R	601	NAP	PA-O3	5.43	1.65	1.59
52	R	601	NAP	C3N-C7N	5.40	1.58	1.50
52	R	601	NAP	C5A-N7A	-4.33	1.31	1.39
52	R	601	NAP	C6A-N6A	4.10	1.44	1.34
52	R	601	NAP	O3D-C3D	-4.04	1.32	1.43
52	R	601	NAP	O2D-C2D	3.63	1.51	1.43
52	R	601	NAP	O7N-C7N	-3.55	1.17	1.24
47	8	501	FMN	C4A-N5	3.04	1.37	1.30
46	4	501	CDL	OB6-CB5	2.80	1.42	1.34
45	V	201	3PE	O21-C2	-2.79	1.40	1.46
51	Q	201	PC1	O21-C2	-2.73	1.40	1.46
51	S	401	PC1	O21-C2	-2.71	1.40	1.46
46	4	501	CDL	OA6-CA4	-2.68	1.40	1.46
52	R	601	NAP	C4A-N9A	-2.64	1.32	1.37
51	j	201	PC1	O21-C2	-2.63	1.40	1.46
46	J	101	CDL	OB6-CB4	-2.63	1.40	1.46
46	J	101	CDL	OA6-CA4	-2.59	1.40	1.46
46	4	501	CDL	OB8-CB7	2.57	1.40	1.33
52	R	601	NAP	O3B-C3B	-2.55	1.36	1.43
45	B	501	3PE	O21-C2	-2.54	1.40	1.46
52	R	601	NAP	C8A-N9A	-2.52	1.33	1.37
52	R	601	NAP	C4N-C3N	-2.51	1.35	1.39
52	R	601	NAP	PA-O5B	2.50	1.69	1.59
46	4	501	CDL	OA8-CA7	2.50	1.40	1.33
46	J	101	CDL	OB8-CB7	2.49	1.40	1.33
51	L	200	PC1	O21-C2	-2.46	1.40	1.46
45	4	502	3PE	O31-C3	-2.44	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	R	601	NAP	C5A-C4A	-2.44	1.34	1.39
45	4	502	3PE	O21-C21	2.44	1.41	1.34
46	J	101	CDL	OA8-CA7	2.42	1.40	1.33
47	8	501	FMN	C10-N1	2.40	1.38	1.33
51	L	200	PC1	O31-C31	2.39	1.40	1.33
45	V	201	3PE	O31-C31	2.38	1.40	1.33
45	2	401	3PE	O31-C3	-2.36	1.39	1.45
45	2	401	3PE	O21-C21	2.36	1.40	1.34
45	B	501	3PE	O31-C3	-2.36	1.39	1.45
51	Q	201	PC1	O31-C3	-2.35	1.39	1.45
51	L	200	PC1	O31-C3	-2.35	1.39	1.45
51	j	201	PC1	O31-C31	2.35	1.40	1.33
52	R	601	NAP	P2B-O2B	2.34	1.63	1.59
51	S	401	PC1	O31-C31	2.33	1.40	1.33
45	V	201	3PE	O31-C3	-2.32	1.40	1.45
51	j	201	PC1	O31-C3	-2.32	1.40	1.45
51	j	201	PC1	O21-C21	2.26	1.40	1.34
52	R	601	NAP	C5N-C4N	-2.25	1.35	1.38
45	2	401	3PE	O21-C2	-2.23	1.41	1.46
45	2	401	3PE	O31-C31	2.23	1.39	1.33
51	S	401	PC1	O21-C21	2.23	1.40	1.34
45	B	501	3PE	O21-C21	2.22	1.40	1.34
46	J	101	CDL	OB6-CB5	2.19	1.40	1.34
46	J	101	CDL	OB8-CB6	-2.17	1.40	1.45
51	L	200	PC1	O21-C21	2.17	1.40	1.34
52	R	601	NAP	O2B-C2B	2.15	1.51	1.44
45	4	502	3PE	O31-C31	2.13	1.39	1.33
51	S	401	PC1	O31-C3	-2.13	1.40	1.45
52	R	601	NAP	PN-O5D	2.12	1.67	1.59
45	B	501	3PE	O31-C31	2.11	1.39	1.33
46	4	501	CDL	OA6-CA5	2.11	1.40	1.34
46	J	101	CDL	OA6-CA5	2.10	1.40	1.34
46	4	501	CDL	OA8-CA6	-2.09	1.40	1.45
46	4	501	CDL	OB8-CB6	-2.06	1.40	1.45
51	Q	201	PC1	O21-C21	2.05	1.40	1.34
46	J	101	CDL	OA8-CA6	-2.04	1.40	1.45
51	Q	201	PC1	O31-C31	2.02	1.39	1.33
45	V	201	3PE	O21-C21	2.02	1.40	1.34

All (54) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	R	601	NAP	N3A-C2A-N1A	-6.22	119.17	128.58
45	4	502	3PE	O21-C21-C22	4.87	122.02	111.48
52	R	601	NAP	C5A-C4A-N3A	-4.85	120.04	126.72
52	R	601	NAP	N6A-C6A-N1A	-4.73	107.84	118.38
51	L	200	PC1	O21-C21-C22	4.59	121.42	111.48
45	B	501	3PE	O21-C21-C22	4.52	121.26	111.48
45	2	401	3PE	O21-C21-C22	4.37	120.94	111.48
52	R	601	NAP	N9A-C8A-N7A	-4.35	107.77	113.94
46	4	501	CDL	OA6-CA5-C11	4.30	120.78	111.48
46	J	101	CDL	OA6-CA5-C11	4.17	120.50	111.48
45	V	201	3PE	O21-C21-C22	4.16	120.48	111.48
46	J	101	CDL	OB6-CB5-C51	4.08	120.30	111.48
47	8	501	FMN	C4-N3-C2	-4.02	118.50	125.64
52	R	601	NAP	C4D-O4D-C1D	-4.00	106.26	109.92
51	S	401	PC1	O21-C21-C22	3.84	119.78	111.48
51	Q	201	PC1	O21-C21-C22	3.82	119.75	111.48
52	R	601	NAP	C2A-N3A-C4A	3.63	120.69	111.83
47	8	501	FMN	C4A-C10-N1	-3.56	115.87	124.59
46	4	501	CDL	CB4-OB6-CB5	3.29	125.67	117.80
52	R	601	NAP	C5A-C6A-N6A	3.28	131.40	123.29
47	8	501	FMN	C5A-C9A-N10	3.19	120.85	117.97
46	4	501	CDL	OB6-CB5-C51	3.05	118.08	111.48
47	8	501	FMN	C10-N1-C2	2.99	123.33	116.85
51	j	201	PC1	O31-C31-C32	2.97	120.89	111.83
47	8	501	FMN	C4A-C4-N3	2.97	120.81	113.25
46	4	501	CDL	OA8-CA7-C31	2.95	120.83	111.83
46	J	101	CDL	OA8-CA7-C31	2.90	120.69	111.83
52	R	601	NAP	C5A-N7A-C8A	2.88	107.98	103.45
45	2	401	3PE	O31-C31-C32	2.86	120.56	111.83
52	R	601	NAP	N3A-C4A-N9A	2.80	131.93	127.17
46	J	101	CDL	OB8-CB7-C71	2.76	120.25	111.83
45	4	502	3PE	O31-C31-C32	2.73	120.17	111.83
51	S	401	PC1	O31-C31-C32	2.73	120.16	111.83
51	L	200	PC1	O31-C31-C32	2.70	120.08	111.83
47	8	501	FMN	O4-C4-C4A	-2.70	119.40	126.53
45	B	501	3PE	O31-C31-C32	2.66	119.94	111.83
47	8	501	FMN	C1'-N10-C9A	-2.65	115.47	120.63
51	j	201	PC1	O21-C21-C22	2.65	120.68	110.93
47	8	501	FMN	C4A-C10-N10	2.64	120.27	116.48
47	8	501	FMN	C4-C4A-C10	2.62	121.43	116.93
52	R	601	NAP	C4A-N9A-C1B	-2.61	120.52	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	V	201	3PE	O31-C31-C32	2.58	119.70	111.83
46	4	501	CDL	OB8-CB7-C71	2.49	119.44	111.83
47	8	501	FMN	C2'-C1'-N10	2.41	121.59	110.20
47	8	501	FMN	C5'-C4'-C3'	-2.36	107.76	112.22
51	Q	201	PC1	O31-C31-C32	2.35	119.01	111.83
52	R	601	NAP	C4A-N9A-C8A	2.20	108.05	105.74
45	4	502	3PE	C2-O21-C21	2.18	123.01	117.80
47	8	501	FMN	C9A-C5A-N5	-2.15	120.18	122.45
52	R	601	NAP	C4B-O4B-C1B	-2.12	104.78	109.47
52	R	601	NAP	C4A-C5A-N7A	-2.10	108.18	110.58
52	R	601	NAP	C6N-N1N-C2N	-2.09	120.10	121.88
52	R	601	NAP	C5A-C4A-N9A	2.03	108.03	105.81
52	R	601	NAP	O4B-C1B-C2B	-2.01	103.13	106.59

There are no chirality outliers.

All (278) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	2	401	3PE	C11-O13-P-O11
45	2	401	3PE	C11-O13-P-O12
45	2	401	3PE	C11-O13-P-O14
45	2	401	3PE	C22-C21-O21-C2
45	4	502	3PE	C1-O11-P-O12
45	4	502	3PE	C1-O11-P-O13
45	4	502	3PE	C1-O11-P-O14
45	4	502	3PE	C22-C21-O21-C2
45	B	501	3PE	C1-O11-P-O12
45	B	501	3PE	C1-O11-P-O13
45	B	501	3PE	C1-O11-P-O14
45	B	501	3PE	O13-C11-C12-N
45	B	501	3PE	O22-C21-O21-C2
45	B	501	3PE	C22-C21-O21-C2
45	V	201	3PE	C1-O11-P-O12
45	V	201	3PE	C1-O11-P-O13
45	V	201	3PE	C1-O11-P-O14
45	V	201	3PE	O21-C2-C3-O31
46	4	501	CDL	C1-CA2-OA2-PA1
46	4	501	CDL	CA2-OA2-PA1-OA4
46	4	501	CDL	CA2-OA2-PA1-OA5
46	J	101	CDL	CB2-C1-CA2-OA2
46	J	101	CDL	CA2-OA2-PA1-OA3
46	J	101	CDL	CA2-OA2-PA1-OA5

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Mol	Chain	Res	Type	Atoms
46	J	101	CDL	OA7-CA5-OA6-CA4
47	8	501	FMN	C2'-C1'-N10-C10
47	8	501	FMN	N10-C1'-C2'-O2'
47	8	501	FMN	N10-C1'-C2'-C3'
47	8	501	FMN	C1'-C2'-C3'-O3'
47	8	501	FMN	C1'-C2'-C3'-C4'
47	8	501	FMN	C5'-O5'-P-O2P
47	8	501	FMN	C5'-O5'-P-O3P
51	L	200	PC1	C11-O13-P-O14
51	L	200	PC1	C11-O13-P-O11
51	L	200	PC1	C1-O11-P-O12
51	L	200	PC1	C1-O11-P-O14
51	L	200	PC1	O13-C11-C12-N
51	Q	201	PC1	C1-O11-P-O12
51	Q	201	PC1	C1-O11-P-O14
51	Q	201	PC1	C1-O11-P-O13
51	Q	201	PC1	O22-C21-O21-C2
51	S	401	PC1	C11-O13-P-O12
51	S	401	PC1	C1-O11-P-O14
51	S	401	PC1	C1-O11-P-O13
51	S	401	PC1	O13-C11-C12-N
51	j	201	PC1	C11-O13-P-O12
51	j	201	PC1	C11-O13-P-O14
51	j	201	PC1	C1-O11-P-O14
51	j	201	PC1	C22-C21-O21-C2
52	R	601	NAP	C5B-O5B-PA-O1A
52	R	601	NAP	C5B-O5B-PA-O2A
52	R	601	NAP	C5B-O5B-PA-O3
52	R	601	NAP	C1B-C2B-O2B-P2B
52	R	601	NAP	C5D-O5D-PN-O3
52	R	601	NAP	C5D-O5D-PN-O1N
52	R	601	NAP	C5D-O5D-PN-O2N
52	R	601	NAP	C2D-C1D-N1N-C2N
52	R	601	NAP	C2D-C1D-N1N-C6N
46	4	501	CDL	OB9-CB7-OB8-CB6
45	2	401	3PE	O22-C21-O21-C2
51	j	201	PC1	O22-C21-O21-C2
46	4	501	CDL	C71-CB7-OB8-CB6
46	J	101	CDL	C11-CA5-OA6-CA4
51	Q	201	PC1	C22-C21-O21-C2
45	4	502	3PE	C32-C31-O31-C3
46	J	101	CDL	C31-CA7-OA8-CA6

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Mol	Chain	Res	Type	Atoms
46	J	101	CDL	C71-CB7-OB8-CB6
51	S	401	PC1	C32-C31-O31-C3
46	J	101	CDL	OB9-CB7-OB8-CB6
51	S	401	PC1	O32-C31-O31-C3
51	j	201	PC1	O32-C31-O31-C3
45	4	502	3PE	O22-C21-O21-C2
46	J	101	CDL	O1-C1-CA2-OA2
46	J	101	CDL	OA9-CA7-OA8-CA6
51	j	201	PC1	C32-C31-O31-C3
45	4	502	3PE	O32-C31-O31-C3
45	2	401	3PE	C32-C31-O31-C3
46	J	101	CDL	CA2-C1-CB2-OB2
51	L	200	PC1	C32-C31-O31-C3
51	L	200	PC1	C31-C32-C33-C34
45	2	401	3PE	O32-C31-O31-C3
47	8	501	FMN	O2'-C2'-C3'-O3'
45	B	501	3PE	O11-C1-C2-O21
46	4	501	CDL	C11-CA5-OA6-CA4
47	8	501	FMN	O2'-C2'-C3'-C4'
51	L	200	PC1	O32-C31-O31-C3
52	R	601	NAP	O4B-C4B-C5B-O5B
46	4	501	CDL	CA5-C11-C12-C13
51	Q	201	PC1	C31-C32-C33-C34
46	4	501	CDL	OA7-CA5-OA6-CA4
51	j	201	PC1	C31-C32-C33-C34
46	J	101	CDL	O1-C1-CB2-OB2
45	2	401	3PE	C3-C2-O21-C21
51	S	401	PC1	C23-C24-C25-C26
45	2	401	3PE	C27-C28-C29-C2A
45	B	501	3PE	C32-C33-C34-C35
46	J	101	CDL	C54-C55-C56-C57
51	S	401	PC1	C31-C32-C33-C34
51	S	401	PC1	C3E-C3F-C3G-C3H
51	j	201	PC1	C36-C37-C38-C39
46	4	501	CDL	CA7-C31-C32-C33
52	R	601	NAP	O4D-C4D-C5D-O5D
46	4	501	CDL	C77-C78-C79-C80
46	4	501	CDL	CA2-C1-CB2-OB2
45	4	502	3PE	C32-C33-C34-C35
46	4	501	CDL	C78-C79-C80-C81
46	4	501	CDL	C62-C63-C64-C65
45	B	501	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
51	S	401	PC1	C25-C26-C27-C28
45	B	501	3PE	C31-C32-C33-C34
51	L	200	PC1	C39-C3A-C3B-C3C
51	S	401	PC1	C32-C33-C34-C35
45	B	501	3PE	C2C-C2D-C2E-C2F
45	B	501	3PE	C2D-C2E-C2F-C2G
46	4	501	CDL	C54-C55-C56-C57
51	L	200	PC1	C34-C35-C36-C37
45	4	502	3PE	C31-C32-C33-C34
51	j	201	PC1	C3B-C3C-C3D-C3E
45	4	502	3PE	C28-C29-C2A-C2B
45	V	201	3PE	C32-C33-C34-C35
46	J	101	CDL	C15-C16-C17-C18
45	2	401	3PE	C26-C27-C28-C29
45	B	501	3PE	C21-C22-C23-C24
51	Q	201	PC1	C2B-C2C-C2D-C2E
46	J	101	CDL	C53-C54-C55-C56
46	4	501	CDL	OA6-CA4-CA6-OA8
45	B	501	3PE	C26-C27-C28-C29
46	4	501	CDL	C75-C76-C77-C78
51	S	401	PC1	C39-C3A-C3B-C3C
51	j	201	PC1	C32-C33-C34-C35
45	4	502	3PE	C24-C25-C26-C27
45	B	501	3PE	C35-C36-C37-C38
51	S	401	PC1	C24-C25-C26-C27
45	4	502	3PE	C2E-C2F-C2G-C2H
45	2	401	3PE	C25-C26-C27-C28
45	V	201	3PE	C26-C27-C28-C29
46	4	501	CDL	C80-C81-C82-C83
46	4	501	CDL	C13-C14-C15-C16
45	V	201	3PE	C2B-C2C-C2D-C2E
45	B	501	3PE	O11-C1-C2-C3
45	V	201	3PE	C2A-C2B-C2C-C2D
52	R	601	NAP	C3B-C4B-C5B-O5B
46	J	101	CDL	CA7-C31-C32-C33
45	V	201	3PE	C36-C37-C38-C39
46	4	501	CDL	C34-C35-C36-C37
51	L	200	PC1	C27-C28-C29-C2A
45	V	201	3PE	C2E-C2F-C2G-C2H
46	4	501	CDL	O1-C1-CB2-OB2
51	L	200	PC1	C25-C26-C27-C28
51	L	200	PC1	C3C-C3D-C3E-C3F

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Mol	Chain	Res	Type	Atoms
45	B	501	3PE	C23-C24-C25-C26
47	8	501	FMN	C5'-O5'-P-O1P
45	B	501	3PE	C34-C35-C36-C37
46	4	501	CDL	C73-C74-C75-C76
51	S	401	PC1	C22-C23-C24-C25
46	4	501	CDL	C74-C75-C76-C77
45	4	502	3PE	C21-C22-C23-C24
51	L	200	PC1	O21-C2-C3-O31
51	S	401	PC1	O21-C2-C3-O31
46	4	501	CDL	C84-C85-C86-C87
51	L	200	PC1	C26-C27-C28-C29
51	S	401	PC1	C21-C22-C23-C24
46	4	501	CDL	C52-C53-C54-C55
45	2	401	3PE	C28-C29-C2A-C2B
51	L	200	PC1	O11-C1-C2-C3
45	4	502	3PE	C35-C36-C37-C38
45	B	501	3PE	C3E-C3F-C3G-C3H
46	4	501	CDL	C15-C16-C17-C18
51	S	401	PC1	C3F-C3G-C3H-C3I
45	2	401	3PE	C1-C2-C3-O31
45	V	201	3PE	C1-C2-C3-O31
46	4	501	CDL	CA3-CA4-CA6-OA8
51	j	201	PC1	C1-C2-C3-O31
45	V	201	3PE	C38-C39-C3A-C3B
45	2	401	3PE	O11-C1-C2-O21
51	L	200	PC1	O11-C1-C2-O21
51	Q	201	PC1	C2A-C2B-C2C-C2D
46	J	101	CDL	OA6-CA4-CA6-OA8
45	4	502	3PE	C23-C24-C25-C26
51	S	401	PC1	C3D-C3E-C3F-C3G
51	Q	201	PC1	C21-C22-C23-C24
45	4	502	3PE	C2C-C2D-C2E-C2F
52	R	601	NAP	PN-O3-PA-O5B
52	R	601	NAP	PA-O3-PN-O5D
51	L	200	PC1	C35-C36-C37-C38
46	4	501	CDL	C81-C82-C83-C84
46	J	101	CDL	C12-C13-C14-C15
46	4	501	CDL	OA5-CA3-CA4-CA6
51	S	401	PC1	O11-C1-C2-C3
45	V	201	3PE	C3F-C3G-C3H-C3I
45	V	201	3PE	O21-C21-C22-C23
46	J	101	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
46	J	101	CDL	C16-C17-C18-C19
51	S	401	PC1	O11-C1-C2-O21
46	J	101	CDL	CA3-CA4-CA6-OA8
51	Q	201	PC1	C1-C2-C3-O31
46	4	501	CDL	OB6-CB4-CB6-OB8
51	Q	201	PC1	O21-C2-C3-O31
51	j	201	PC1	O21-C2-C3-O31
46	J	101	CDL	C11-C12-C13-C14
51	j	201	PC1	C35-C36-C37-C38
51	Q	201	PC1	O13-C11-C12-N
51	j	201	PC1	O13-C11-C12-N
45	2	401	3PE	O11-C1-C2-C3
45	4	502	3PE	O11-C1-C2-C3
46	4	501	CDL	OB5-CB3-CB4-CB6
51	Q	201	PC1	C32-C33-C34-C35
46	J	101	CDL	C31-C32-C33-C34
46	4	501	CDL	OA5-CA3-CA4-OA6
45	2	401	3PE	O21-C2-C3-O31
46	4	501	CDL	CB3-CB4-CB6-OB8
45	B	501	3PE	C3B-C3C-C3D-C3E
45	V	201	3PE	C23-C24-C25-C26
45	V	201	3PE	C2C-C2D-C2E-C2F
51	Q	201	PC1	C35-C36-C37-C38
45	4	502	3PE	C11-O13-P-O14
45	4	502	3PE	O13-C11-C12-N
45	V	201	3PE	C11-O13-P-O14
51	L	200	PC1	C11-O13-P-O12
51	L	200	PC1	C1-O11-P-O13
51	S	401	PC1	C11-O13-P-O14
51	S	401	PC1	C11-O13-P-O11
51	S	401	PC1	C1-O11-P-O12
51	j	201	PC1	C11-O13-P-O11
45	4	502	3PE	C2-C1-O11-P
45	V	201	3PE	C2-C1-O11-P
46	4	501	CDL	C14-C15-C16-C17
46	J	101	CDL	OB5-CB3-CB4-CB6
45	B	501	3PE	C2-C1-O11-P
51	L	200	PC1	C1-C2-C3-O31
51	S	401	PC1	C1-C2-C3-O31
46	4	501	CDL	C35-C36-C37-C38
45	4	502	3PE	C34-C35-C36-C37
52	R	601	NAP	C2B-C1B-N9A-C8A

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Mol	Chain	Res	Type	Atoms
45	2	401	3PE	C33-C34-C35-C36
45	B	501	3PE	C37-C38-C39-C3A
45	B	501	3PE	C36-C37-C38-C39
45	V	201	3PE	C3E-C3F-C3G-C3H
51	S	401	PC1	C2-C1-O11-P
45	B	501	3PE	C38-C39-C3A-C3B
51	j	201	PC1	C3A-C3B-C3C-C3D
45	4	502	3PE	C1-C2-O21-C21
46	4	501	CDL	CB3-CB4-OB6-CB5
51	Q	201	PC1	C2-C1-O11-P
51	j	201	PC1	C37-C38-C39-C3A
46	4	501	CDL	CA4-CA3-OA5-PA1
51	L	200	PC1	C32-C33-C34-C35
51	L	200	PC1	C22-C23-C24-C25
46	4	501	CDL	C71-C72-C73-C74
51	S	401	PC1	C34-C35-C36-C37
46	J	101	CDL	OB7-CB5-OB6-CB4
46	J	101	CDL	C14-C15-C16-C17
45	2	401	3PE	C29-C2A-C2B-C2C
51	Q	201	PC1	C26-C27-C28-C29
46	4	501	CDL	C52-C51-CB5-OB6
51	Q	201	PC1	O21-C21-C22-C23
46	J	101	CDL	C51-CB5-OB6-CB4
45	2	401	3PE	C21-C22-C23-C24
51	S	401	PC1	C38-C39-C3A-C3B
45	4	502	3PE	C2D-C2E-C2F-C2G
52	R	601	NAP	C2B-O2B-P2B-O3X
51	j	201	PC1	O31-C31-C32-C33
51	S	401	PC1	O31-C31-C32-C33
51	S	401	PC1	O21-C21-C22-C23
51	S	401	PC1	C27-C28-C29-C2A
45	V	201	3PE	O22-C21-C22-C23
51	Q	201	PC1	C22-C23-C24-C25
46	4	501	CDL	C52-C51-CB5-OB7
46	J	101	CDL	C13-C14-C15-C16
51	Q	201	PC1	O22-C21-C22-C23
51	S	401	PC1	O32-C31-C32-C33
51	j	201	PC1	O32-C31-C32-C33
46	J	101	CDL	CB3-CB4-CB6-OB8
45	B	501	3PE	C22-C23-C24-C25
45	2	401	3PE	O31-C31-C32-C33
52	R	601	NAP	PN-O3-PA-O1A

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Mol	Chain	Res	Type	Atoms
51	S	401	PC1	O22-C21-C22-C23
51	Q	201	PC1	O31-C31-C32-C33

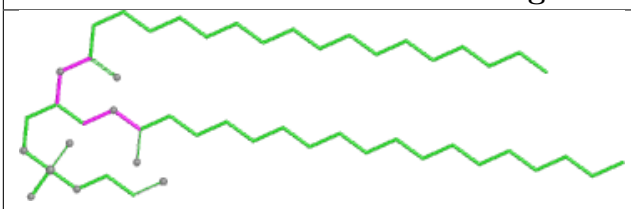
There are no ring outliers.

11 monomers are involved in 17 short contacts:

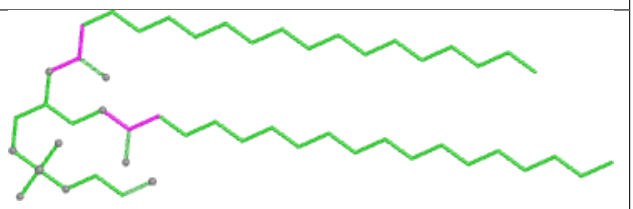
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	J	101	CDL	1	0
47	8	501	FMN	2	0
45	B	501	3PE	2	0
52	R	601	NAP	3	0
51	L	200	PC1	2	0
51	Q	201	PC1	1	0
45	4	502	3PE	1	0
48	A	801	SF4	1	0
46	4	501	CDL	1	0
51	S	401	PC1	2	0
45	2	401	3PE	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

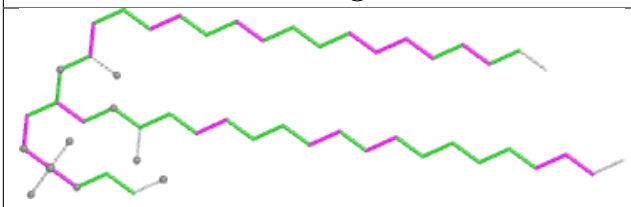
Ligand 3PE V 201



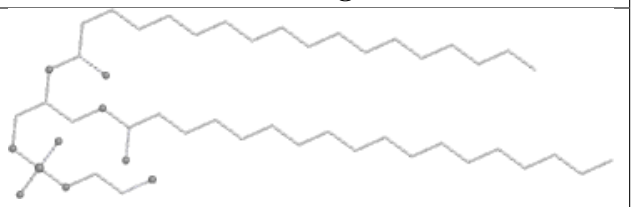
Bond lengths



Bond angles

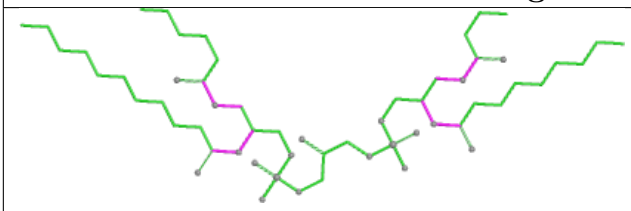


Torsions

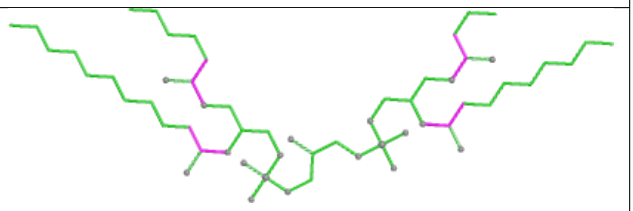


Rings

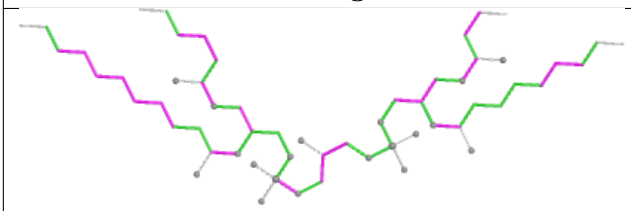
Ligand CDL J 101



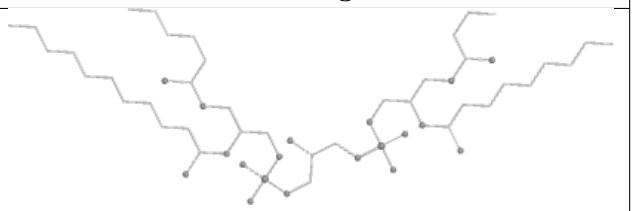
Bond lengths



Bond angles

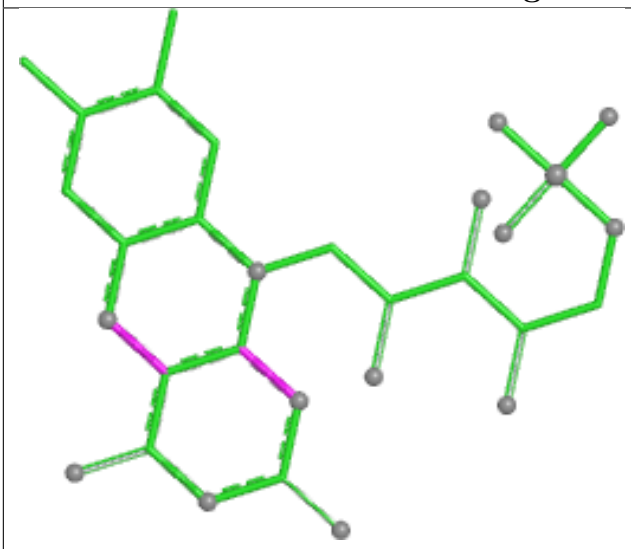


Torsions

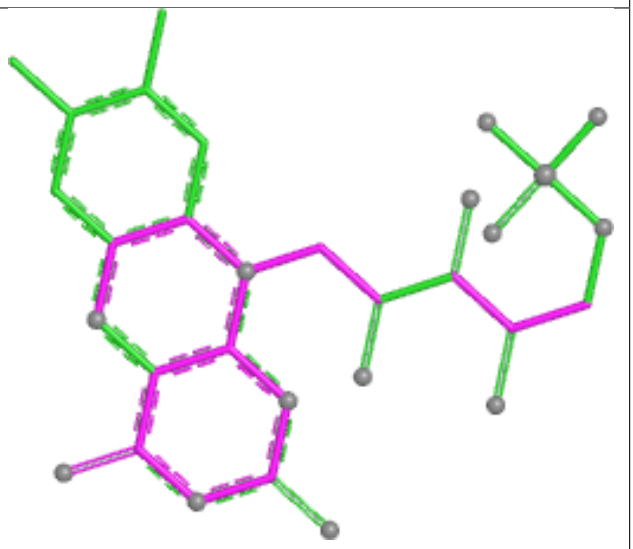


Rings

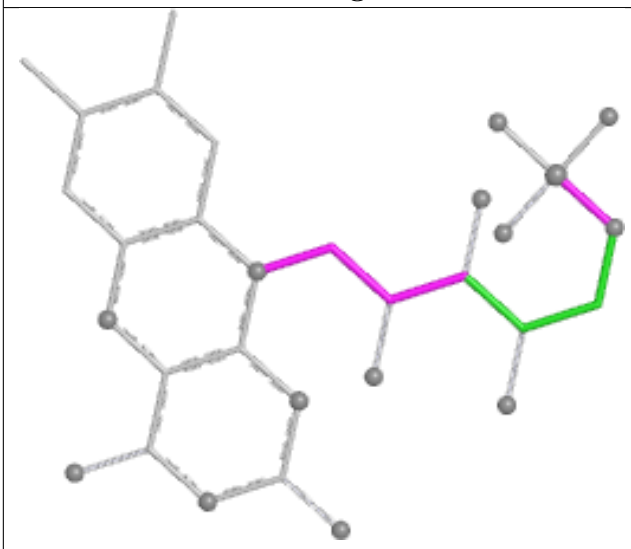
Ligand FMN 8 501



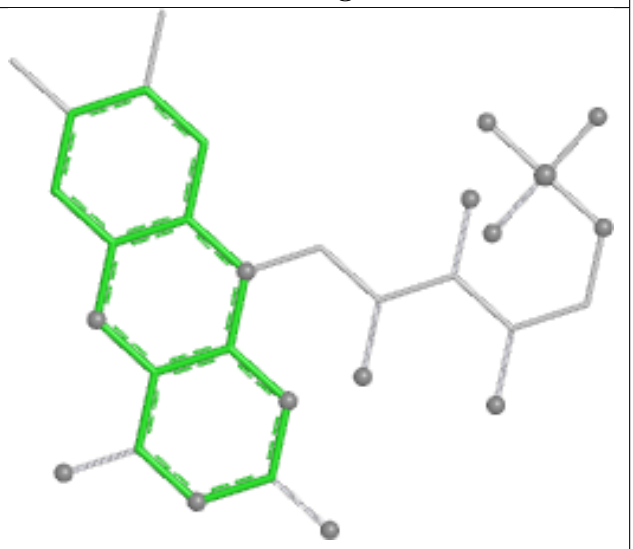
Bond lengths



Bond angles

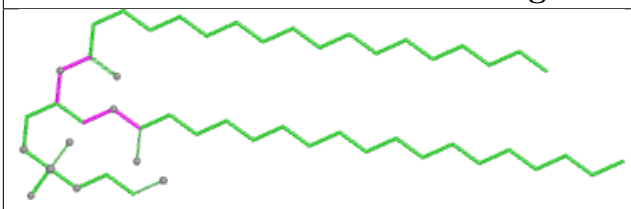


Torsions

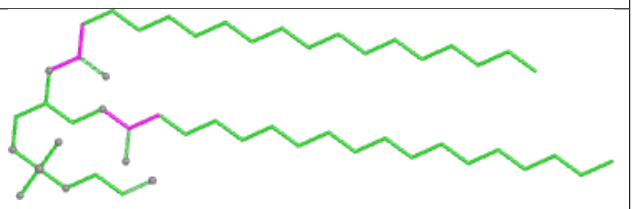


Rings

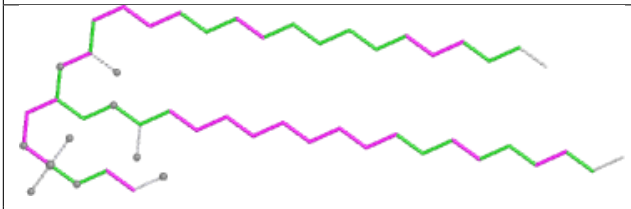
Ligand 3PE B 501



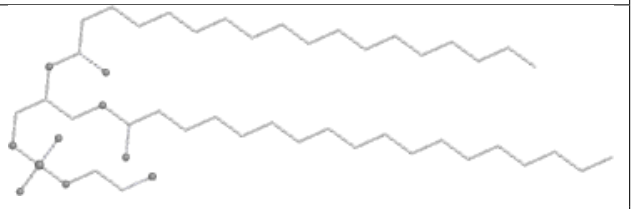
Bond lengths



Bond angles

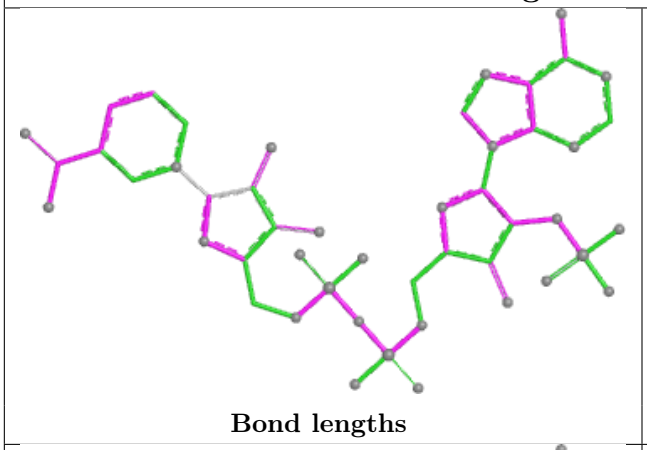


Torsions

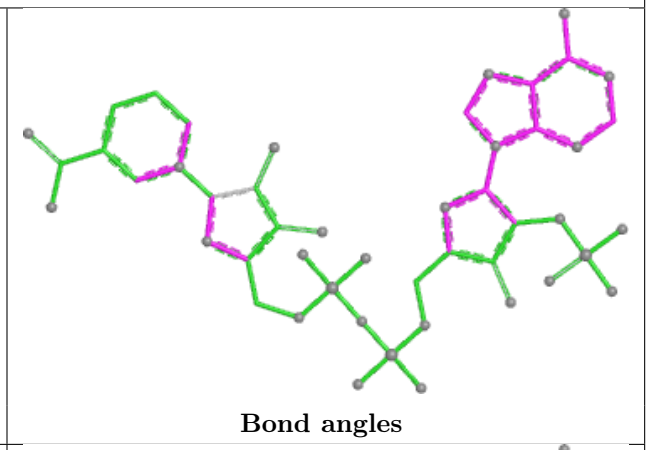


Rings

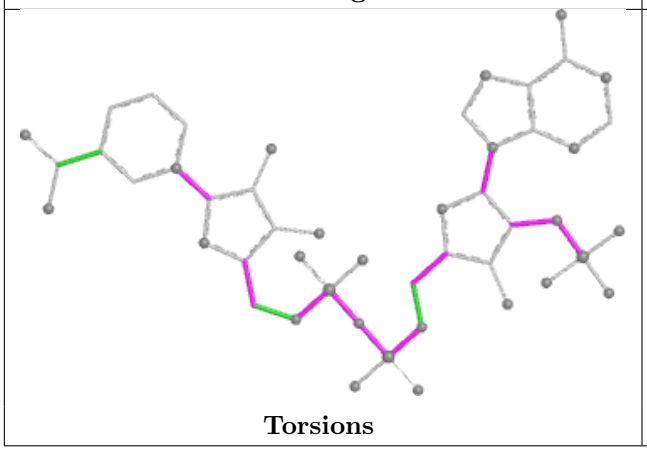
Ligand NAP R 601



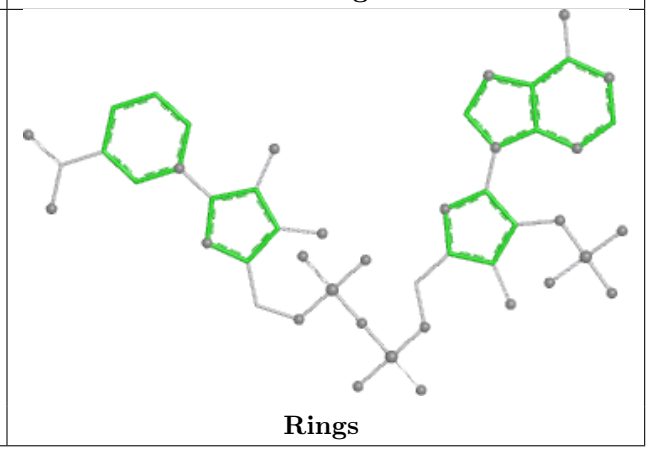
Bond lengths



Bond angles

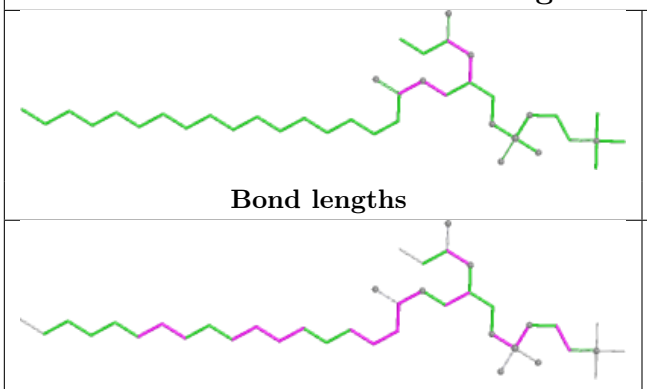


Torsions

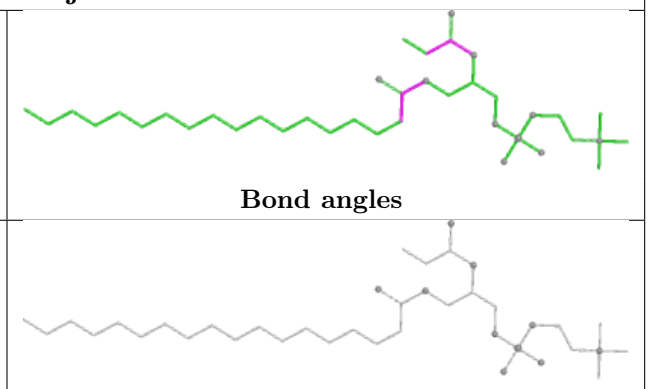


Rings

Ligand PC1 j 201



Bond lengths

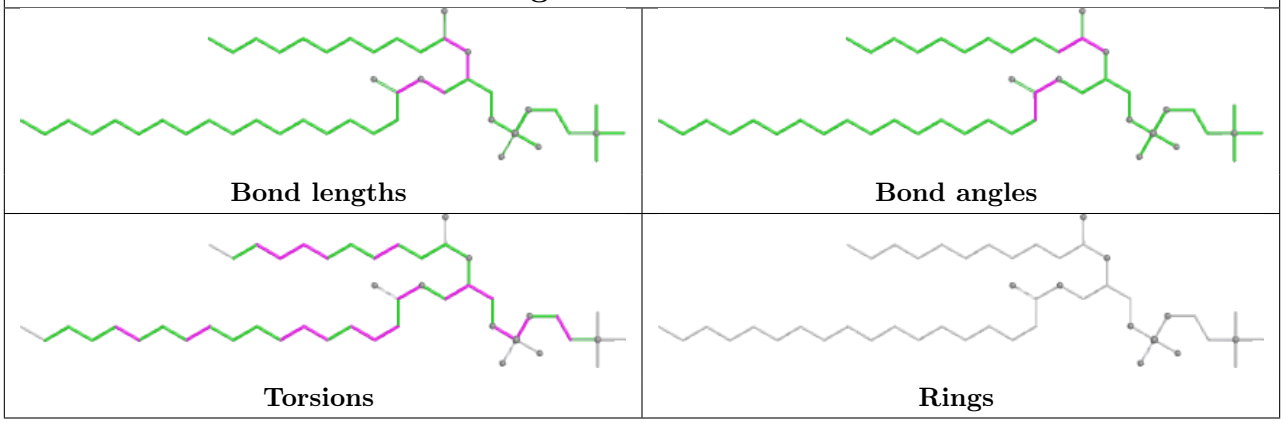


Bond angles

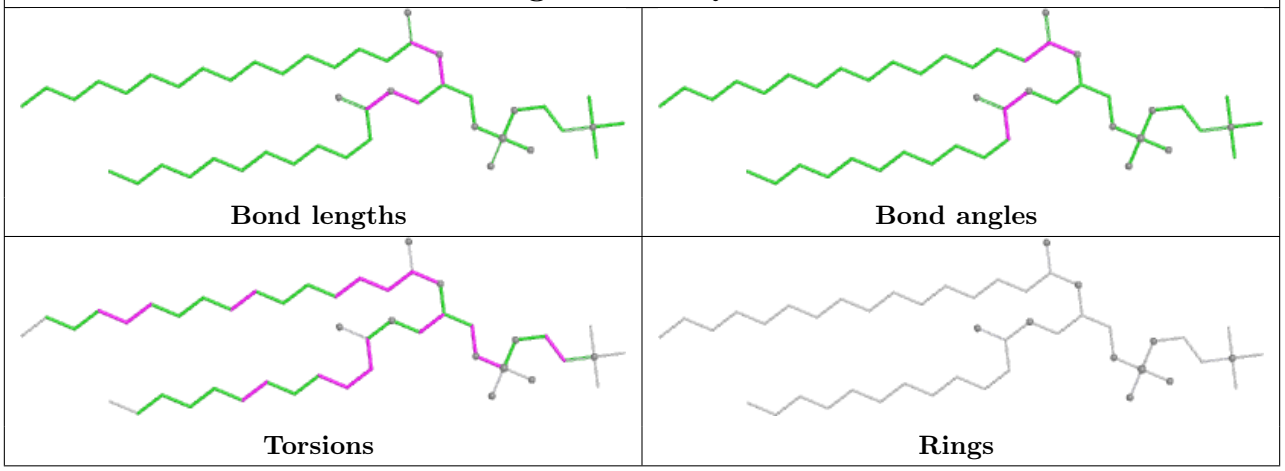
Torsions

Rings

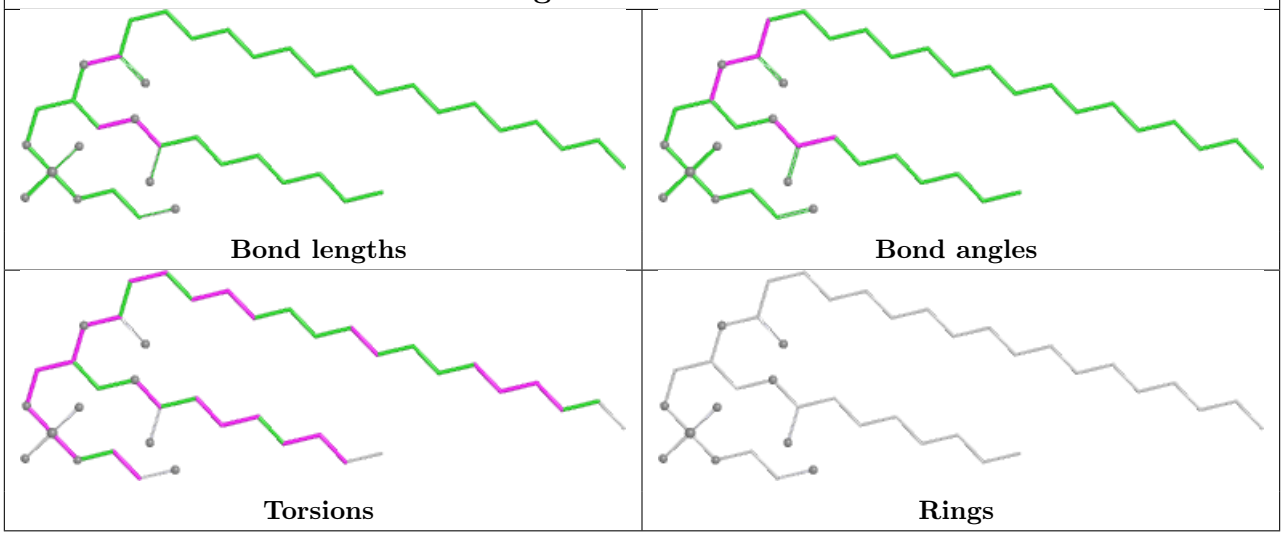
Ligand PC1 L 200



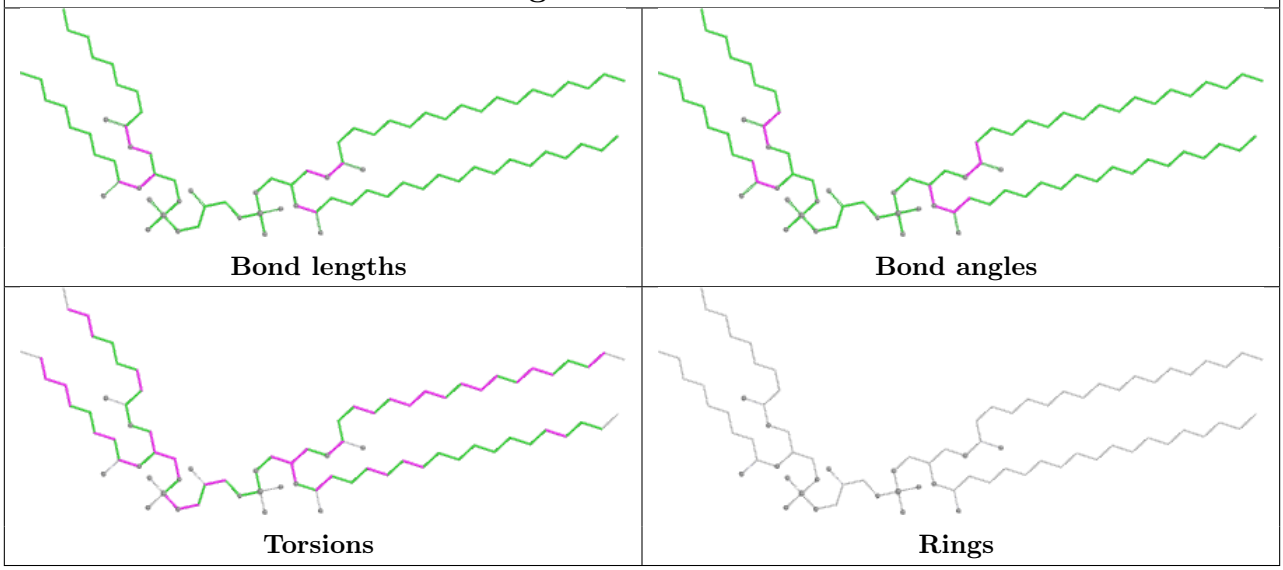
Ligand PC1 Q 201



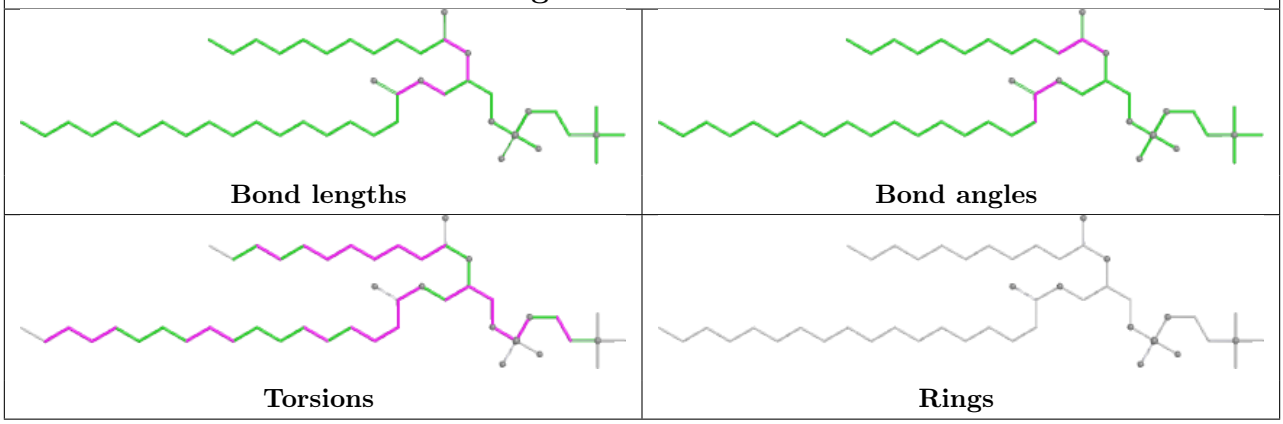
Ligand 3PE 4 502



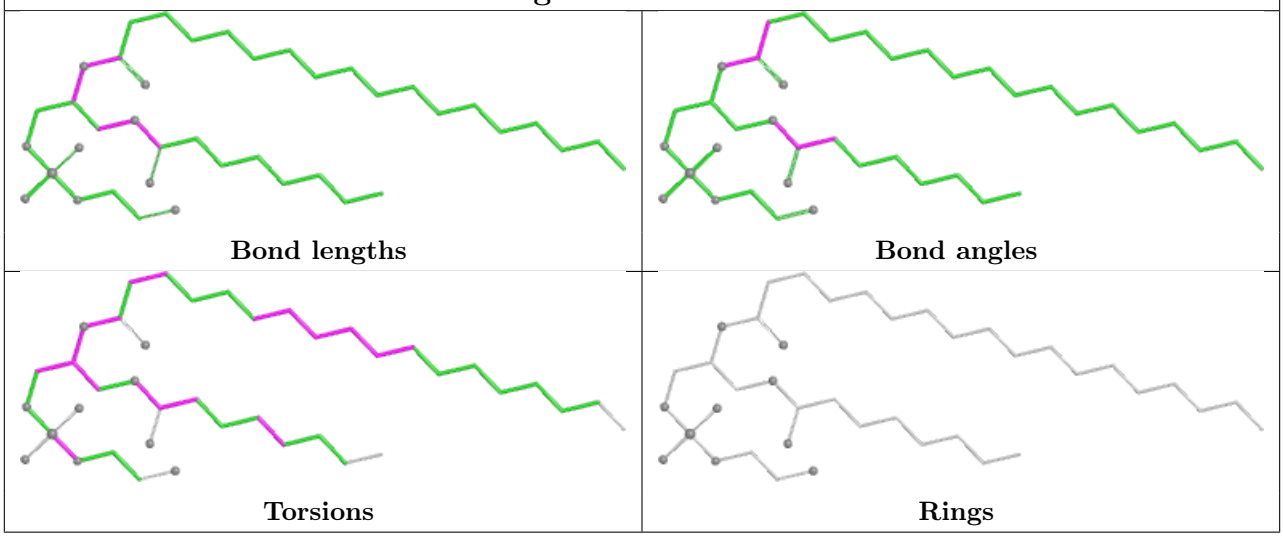
Ligand CDL 4 501



Ligand PC1 S 401



Ligand 3PE 2 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

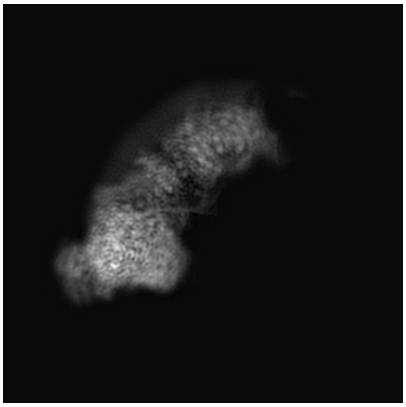
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30676. These allow visual inspection of the internal detail of the map and identification of artifacts.

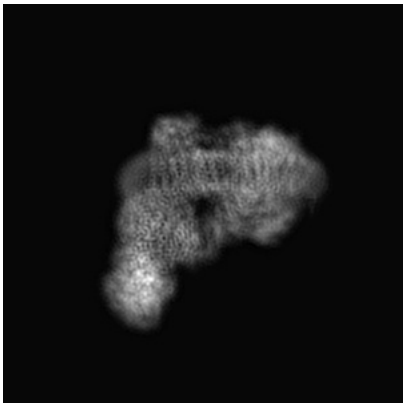
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

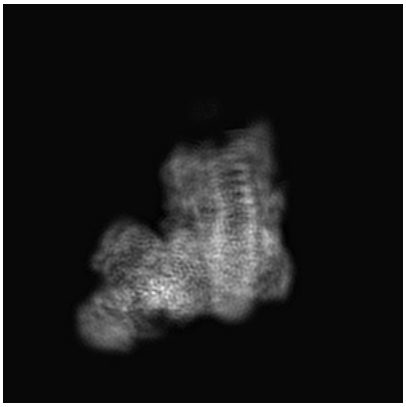
6.1.1 Primary map



X



Y

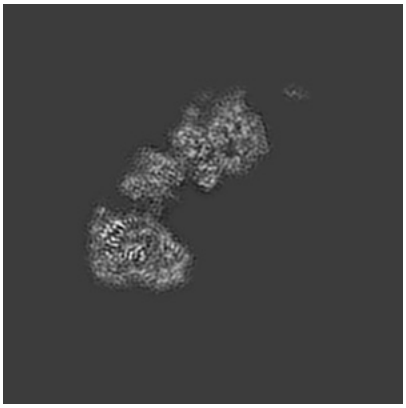


Z

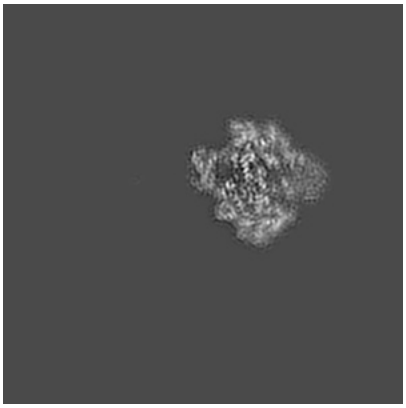
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 140



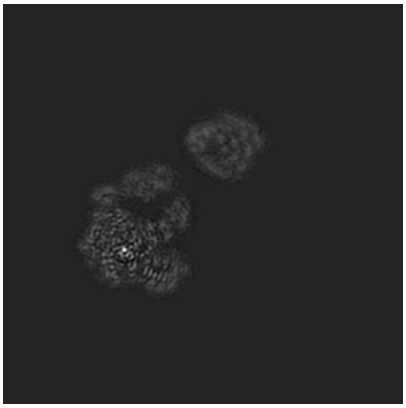
Y Index: 140

Z Index: 140

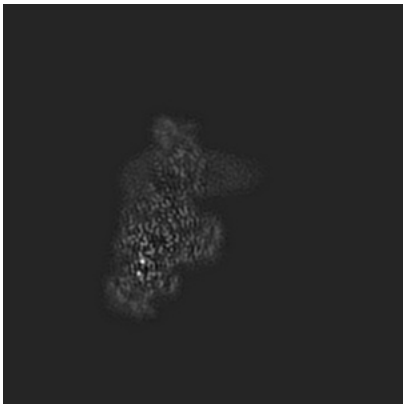
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

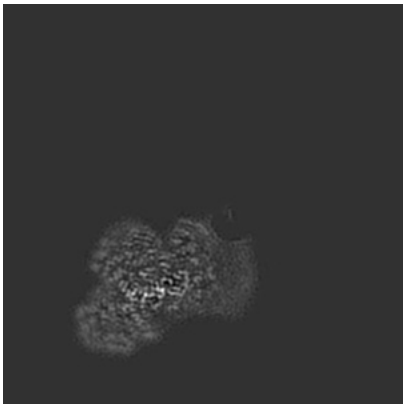
6.3.1 Primary map



X Index: 124



Y Index: 76

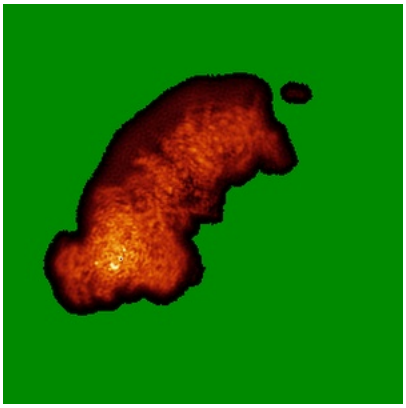


Z Index: 96

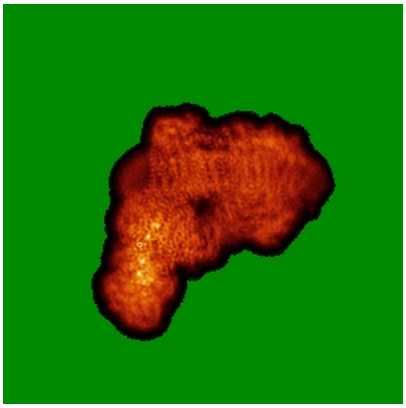
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

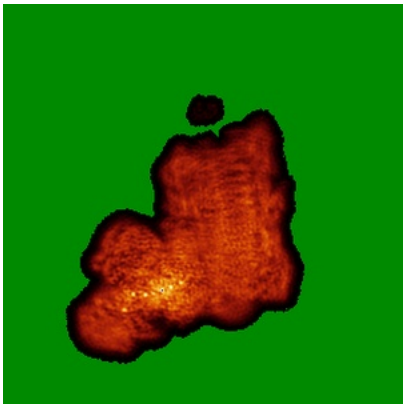
6.4.1 Primary map



X



Y

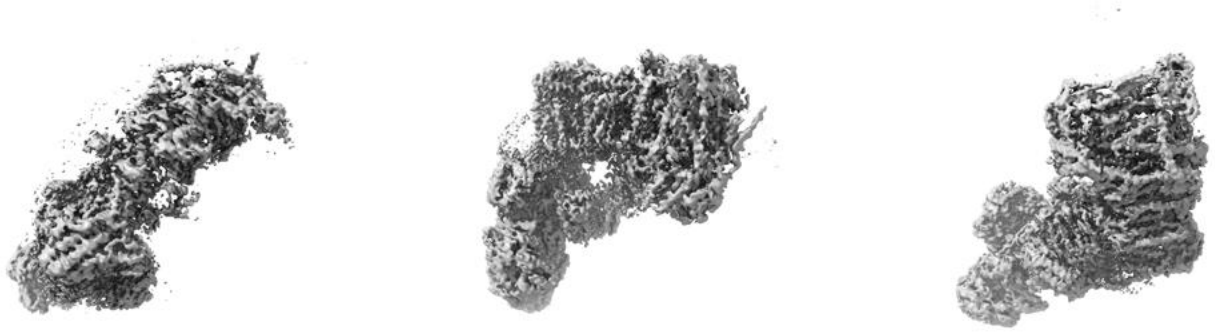


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.111. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

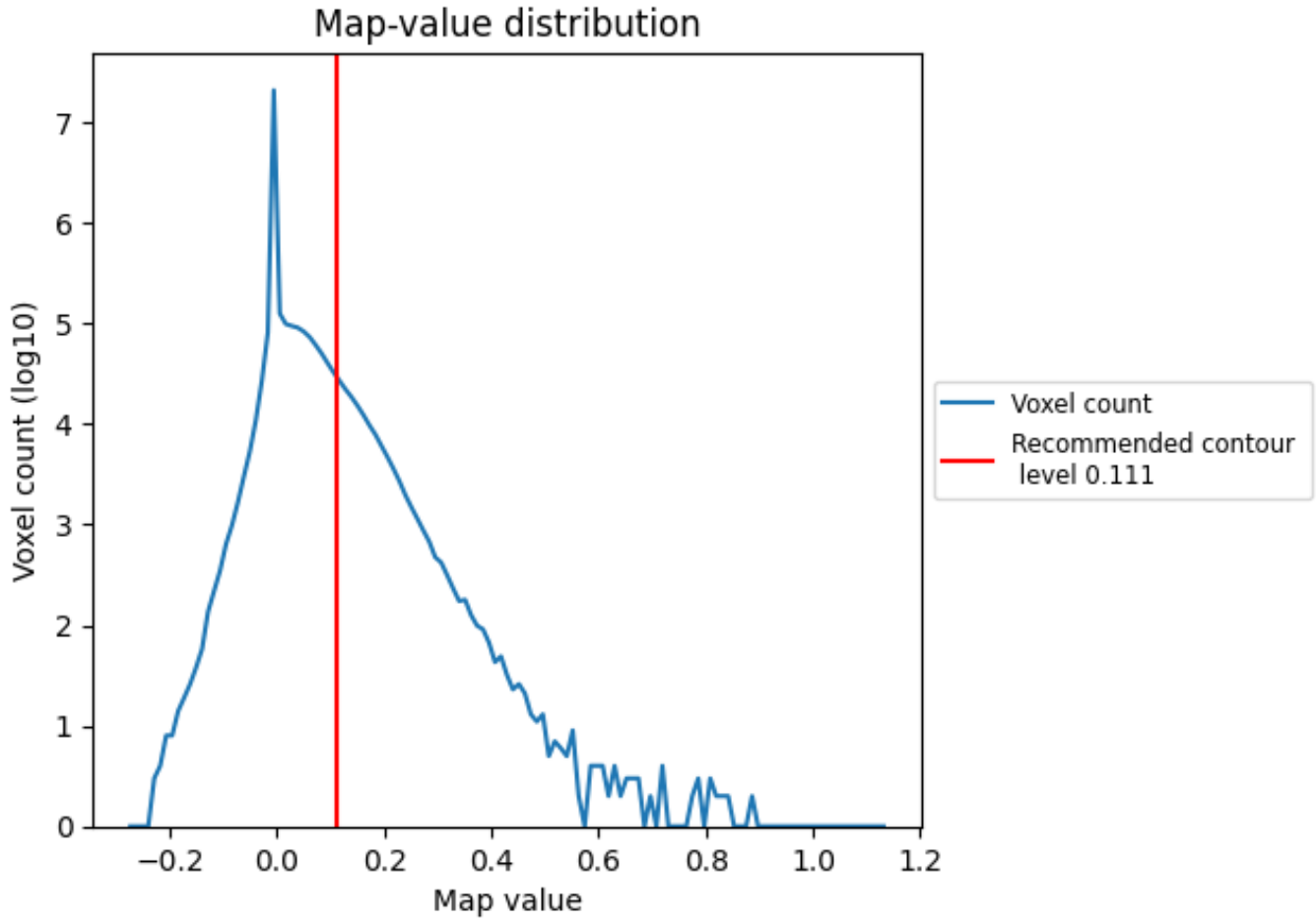
6.6 Mask visualisation (i)

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

7 Map analysis

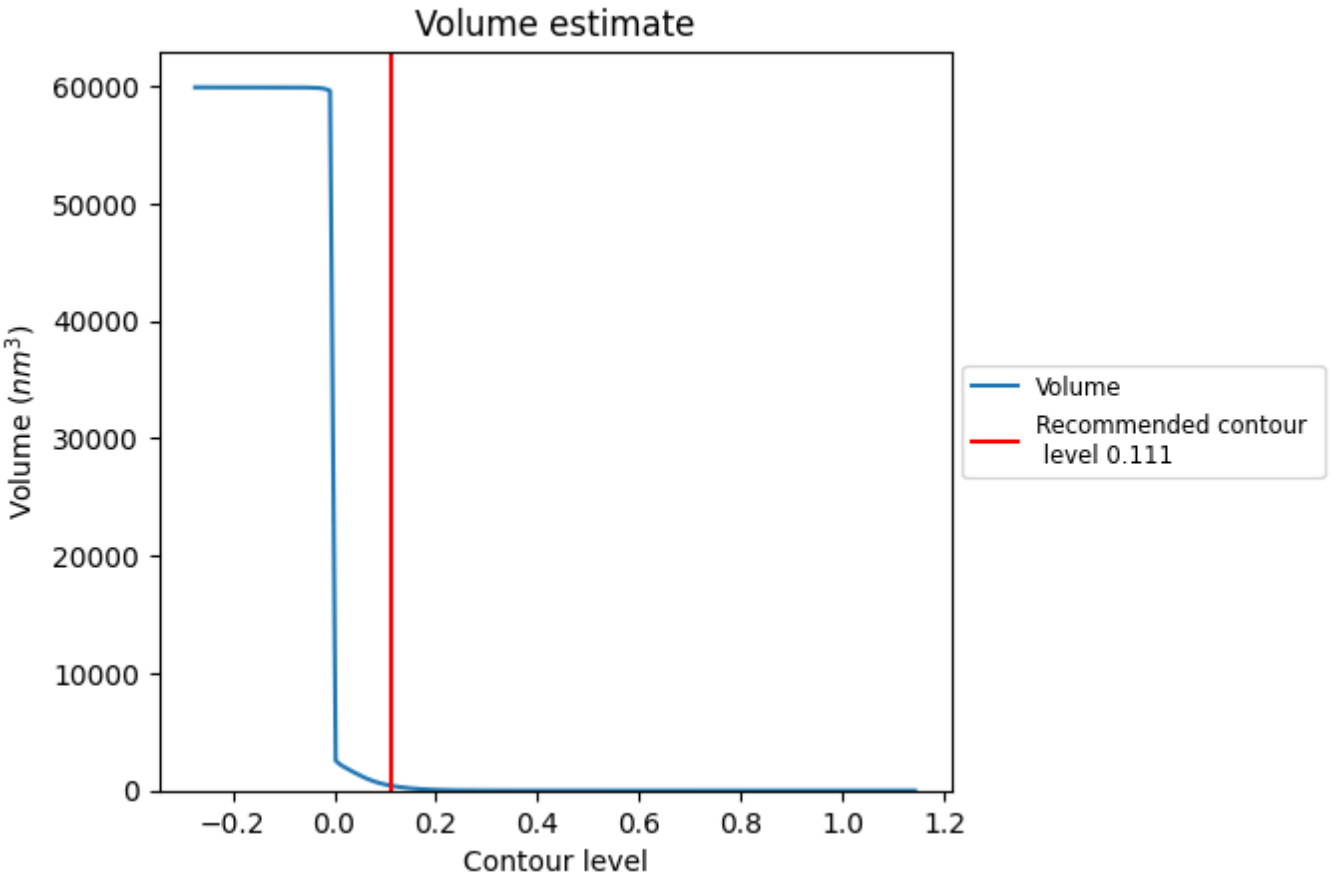
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

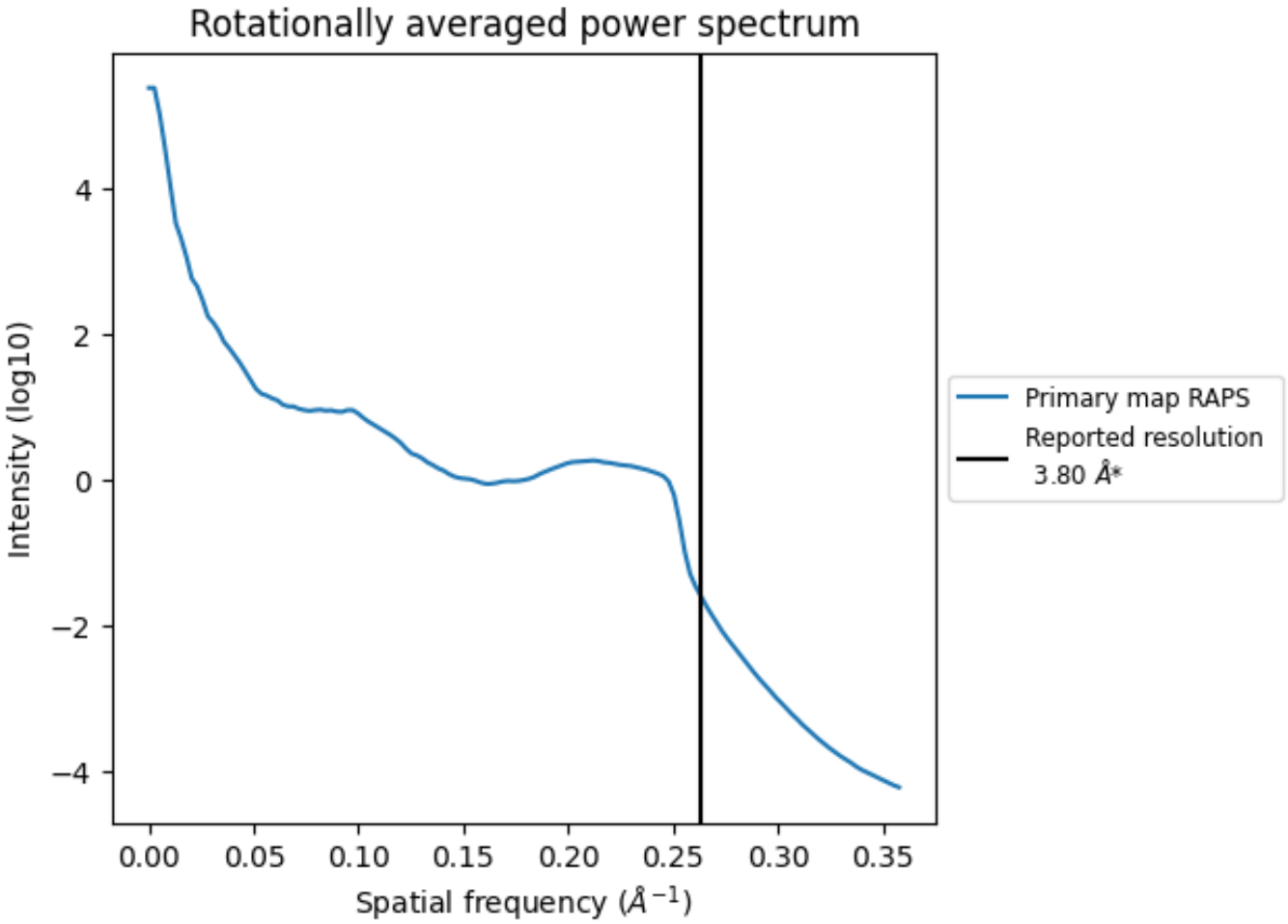
7.2 Volume estimate



The volume at the recommended contour level is 422 nm^3; this corresponds to an approximate mass of 381 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

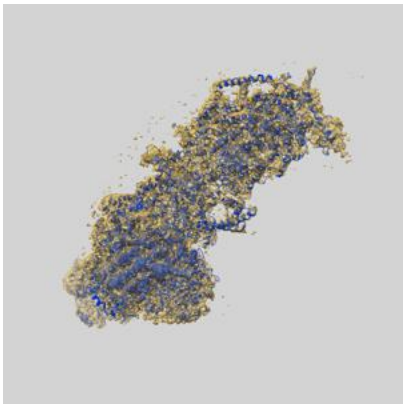
8 Fourier-Shell correlation

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

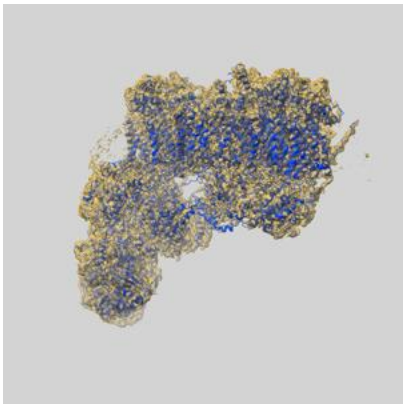
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30676 and PDB model 7DGZ. Per-residue inclusion information can be found in section 3 on page 18.

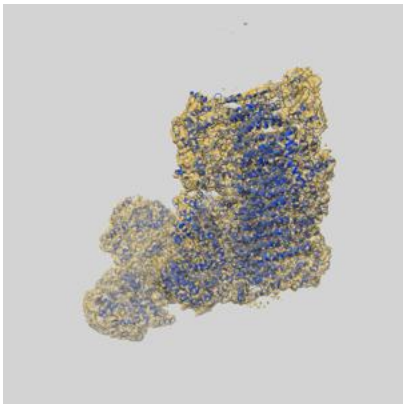
9.1 Map-model overlay



X



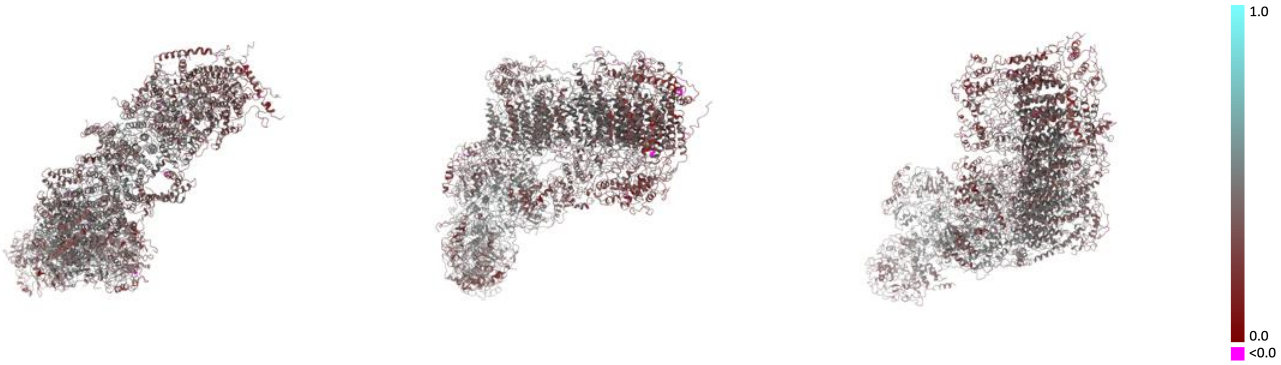
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.111 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.

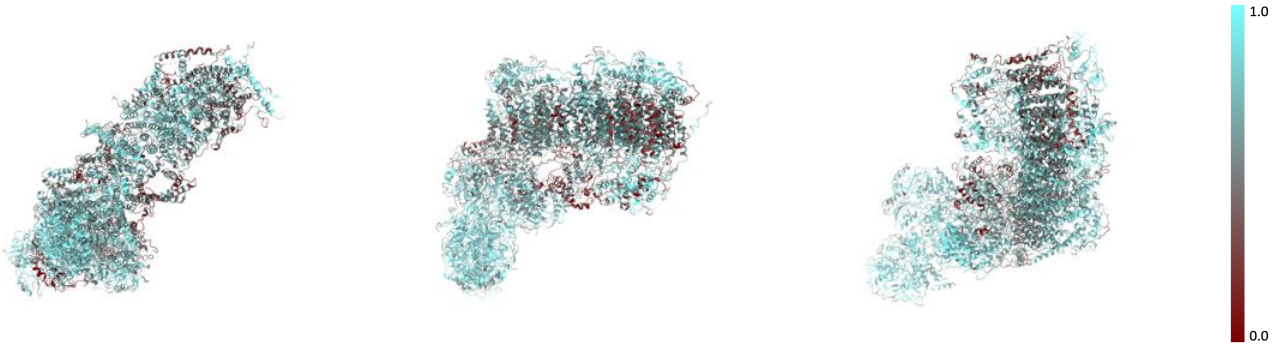
9.2 Q-score mapped to coordinate model



X Y Z

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.

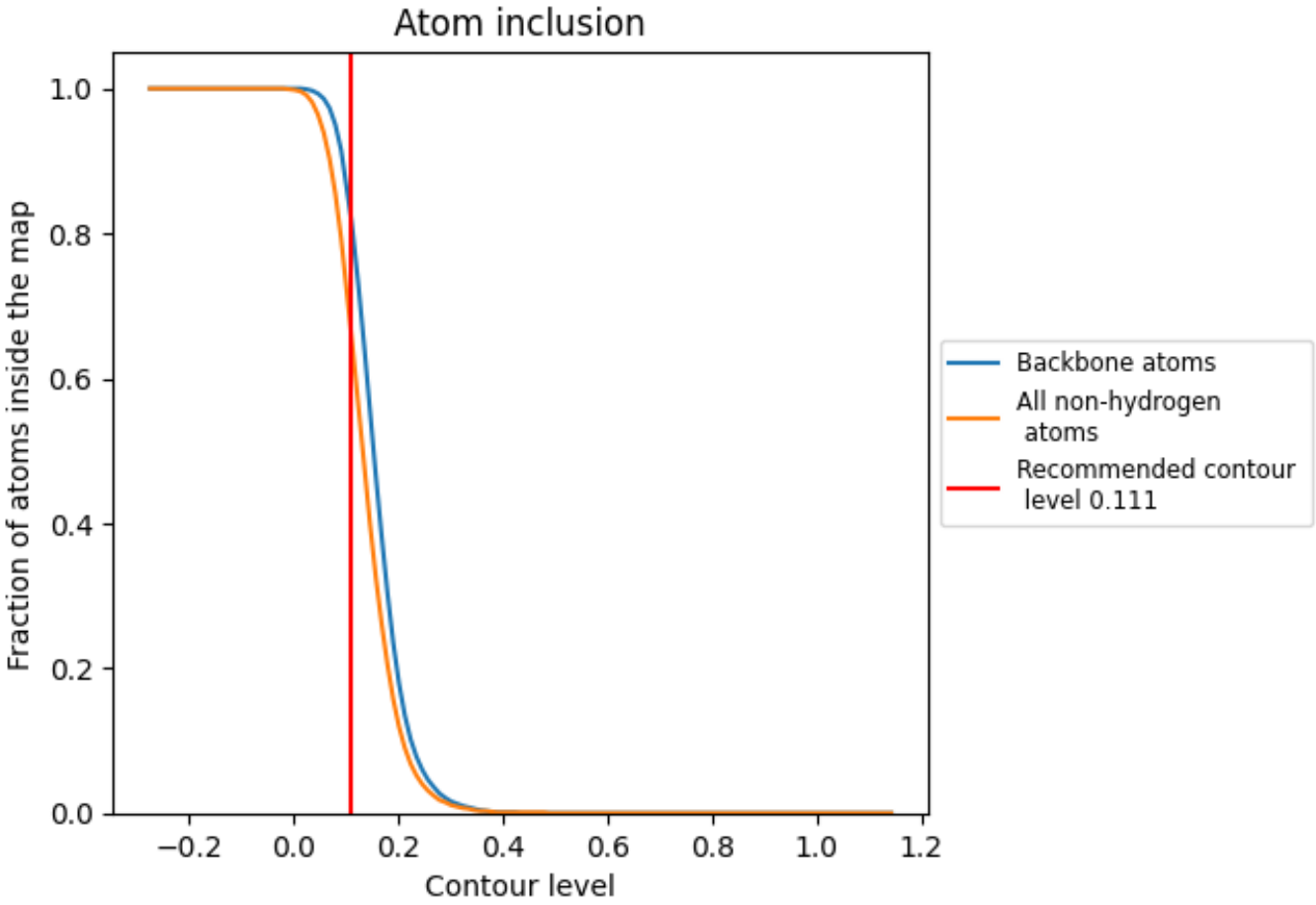
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.111).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.111) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6580	0.3970
1	0.6540	0.4450
2	0.7030	0.4400
3	0.4720	0.3970
4	0.6490	0.4310
5	0.6520	0.4170
6	0.5000	0.3600
7	0.5220	0.3890
8	0.8220	0.3680
9	0.7550	0.3410
A	0.8070	0.4290
B	0.7360	0.4640
C	0.8110	0.4650
D	0.7850	0.4690
E	0.8440	0.4640
F	0.5470	0.2900
G	0.7300	0.4560
H	0.7210	0.4280
I	0.5480	0.4010
J	0.6890	0.4240
K	0.7460	0.3520
L	0.5670	0.3910
M	0.3970	0.2920
N	0.7400	0.3910
O	0.6880	0.4050
P	0.5360	0.3740
Q	0.7160	0.3820
R	0.6200	0.3730
S	0.4020	0.3490
T	0.4500	0.3680
U	0.3600	0.3690
V	0.6960	0.3990
W	0.5870	0.2980
X	0.5380	0.3400
Y	0.5730	0.3310

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Chain	Atom inclusion	Q-score
Z	0.5330	0.3110
a	0.6220	0.3860
b	0.7390	0.4150
c	0.6590	0.3290
d	0.7850	0.2910
e	0.5590	0.3690
f	0.6880	0.3400
g	0.6150	0.3390
h	0.6310	0.3680
i	0.6590	0.3650
j	0.6680	0.4040