



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 08:44 AM UTC

PDB ID : 7ZDP / pdb_00007zdp
EMDB ID : EMD-14664
Title : Complex I from Ovis aries at pH9, Open state
Authors : Sazanov, L.; Petrova, O.
Deposited on : 2022-03-29
Resolution : 3.88 Å (reported)
Based on initial model : 6ZKE

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:

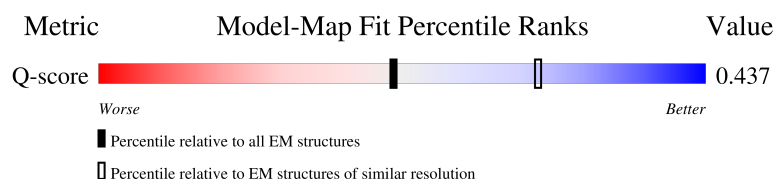
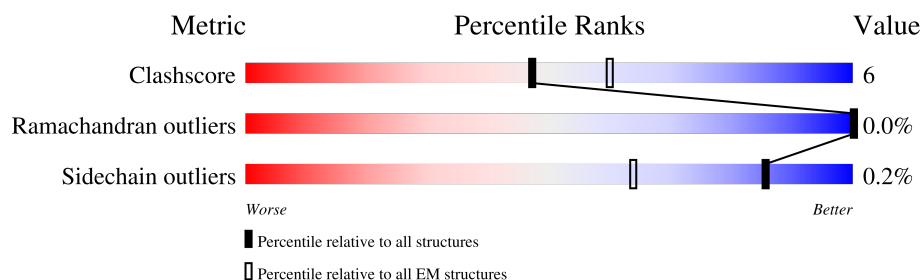
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.88 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	8773 (3.38 - 4.38)

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

Mol	Chain	Length	Quality of chain
1	4	463	5% 75% 16% 9%
2	A	115	20% 83% 11% ..
3	H	318	14% 79% 19% ..
4	J	175	22% 79% 18% .

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Mol	Chain	Length	Quality of chain
5	K	98	9% 74% 26%
6	L	606	84% 16%
7	M	459	81% 19%
8	N	347	79% 21%
9	V	140	41% 88% 12%
10	W	139	5% 89% 11%
11	X	157	8% 48% 7% 45%
11	j	157	26% 40% 11% 48%
12	Y	171	12% 87% 13%
13	Z	171	6% 90% 10%
14	k	320	17% 86% 14%
15	l	105	13% 87% 13%
16	m	80	24% 88% 12%
17	n	79	28% 87% 13%
18	o	120	8% 88% 12%
19	p	128	9% 86% 14%
20	q	144	15% 76% 19%
21	r	128	10% 64% 13% 23%
22	s	122	12% 83% 17%
23	t	177	13% 89% 11%
24	u	65	6% 85% 15%
25	v	155	8% 83% 17%
26	w	101	15% 71% 29%
27	x	49	14% 96%
28	y	50	20% 76% 22%

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Mol	Chain	Length	Quality of chain
29	z	70	
30	1	430	
31	2	213	
32	3	688	
33	5	208	
34	6	156	
35	9	176	
36	a	44	
37	b	95	
38	c	126	
39	d	380	
40	e	86	
41	f	113	
42	g	114	
43	h	114	
44	i	145	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	SF4	3	801	-	-	X	-

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 65835 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 Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4	421	Total	C	N	O	S	0	0
			3390	2165	581	619	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	110	Total	C	N	O	S	0	0
			880	593	128	153	6		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	314	Total	C	N	O	S	0	0
			2498	1685	380	414	19		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	169	Total	C	N	O	S	0	0
			1294	870	185	226	13		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	98	Total	C	N	O	S	0	0
			749	490	112	132	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	606	Total	C	N	O	S	0	0
			4806	3187	746	829	44		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	459	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 9 is a protein called Complex I-B14.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- Molecule 10 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 11 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
11	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 13 is a protein called Complex I-PDSW.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	k	320	Total	C	N	O	P	S	0	0
			2596	1659	432	494	1	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 16 is a protein called Complex I-B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 17 is a protein called Complex I-B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 19 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 21 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 22 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 23 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 26 is a protein called Complex I-ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 27 is a protein called Complex I-KFYI.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	x	49	Total	C	N	O	0	0
			412	271	70	71		

- Molecule 28 is a protein called Complex I-MNLL.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	y	50	Total	C	N	O	0	0
			436	287	77	72		

- Molecule 29 is a protein called Complex I-MWFE.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	z	70	Total	C	N	O	S	0	0
			576	369	106	96	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	213	Total	C	N	O	S	0	0
			1655	1058	278	309	10		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 33 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 34 is a protein called Complex I-20kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 35 is a protein called Complex I-23kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 36 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	297	Total	C	N	O	S	0	0
			2372	1516	432	419	5		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 41 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 42 is a protein called Complex I-B14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

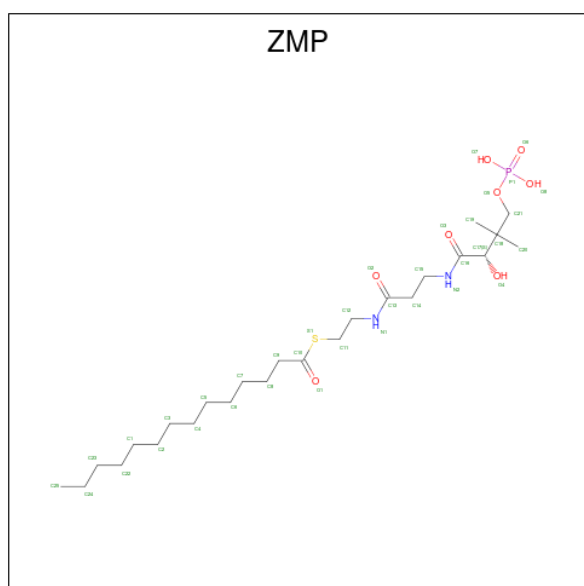
- Molecule 43 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

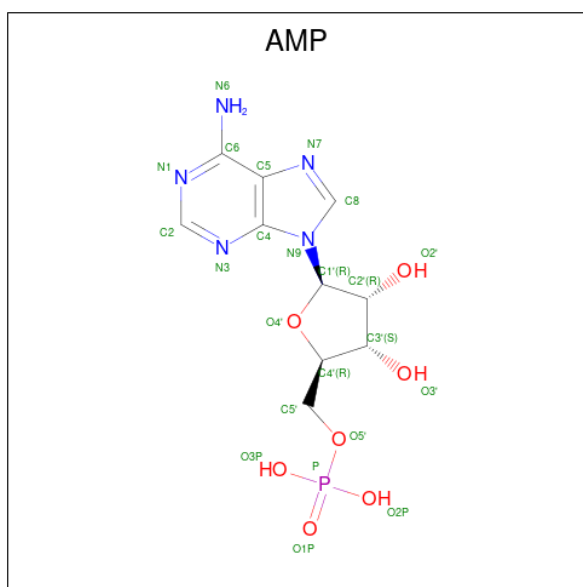
Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 45 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



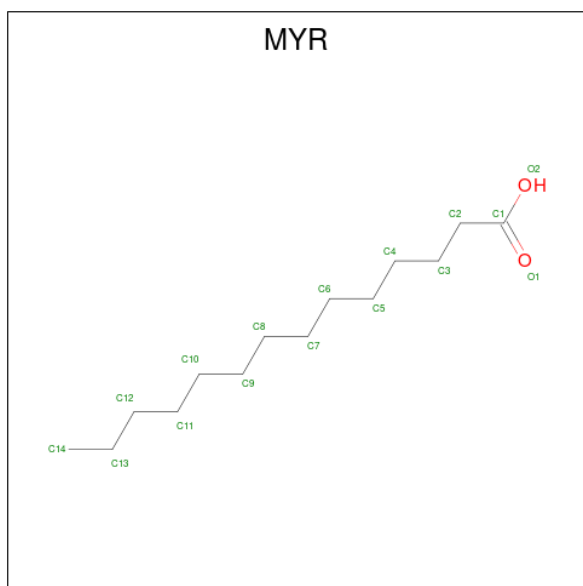
Mol	Chain	Residues	Atoms						AltConf
45	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
45	j	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 46 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



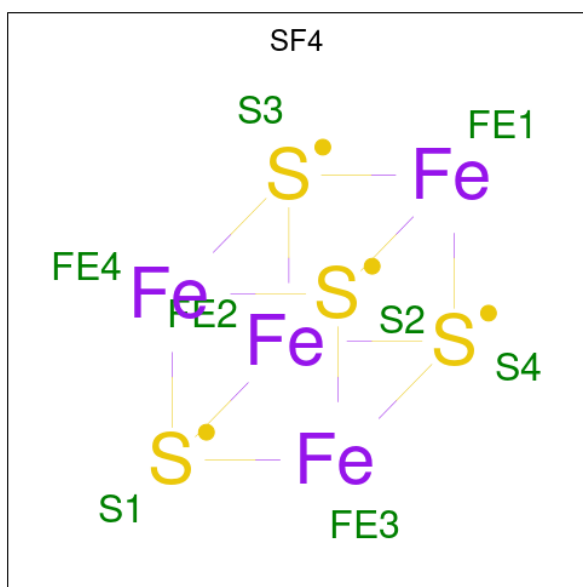
Mol	Chain	Residues	Atoms					AltConf
46	k	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 47 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



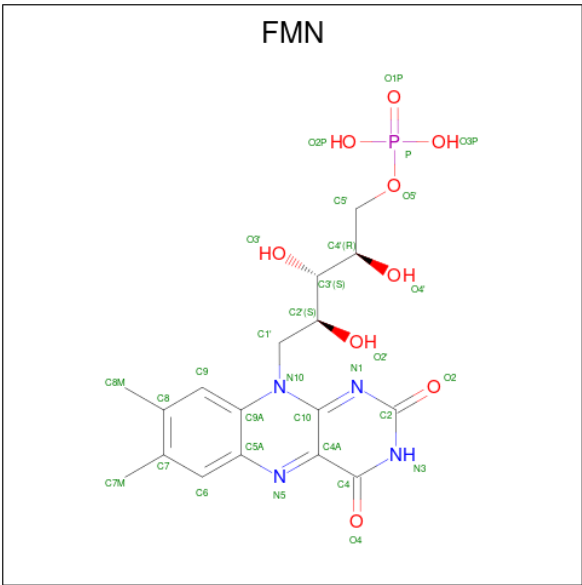
Mol	Chain	Residues	Atoms			AltConf
47	s	1	Total	C	O	0
			15	14	1	

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



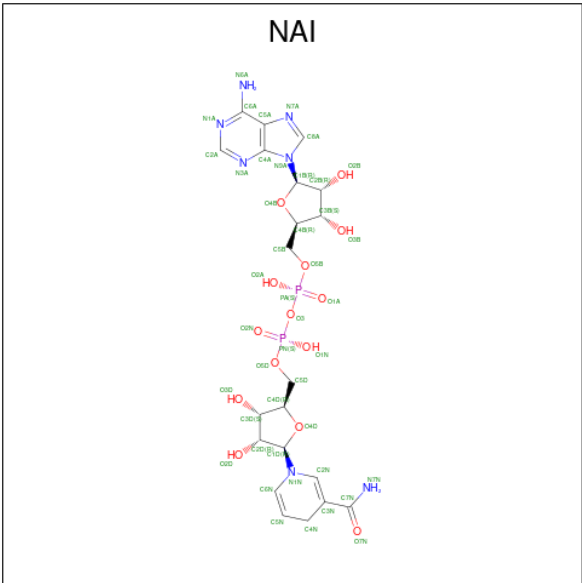
Mol	Chain	Residues	Atoms			AltConf
48	1	1	Total	Fe	S	0
			8	4	4	
48	3	1	Total	Fe	S	0
			8	4	4	
48	3	1	Total	Fe	S	0
			8	4	4	
48	6	1	Total	Fe	S	0
			8	4	4	
48	9	1	Total	Fe	S	0
			8	4	4	
48	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



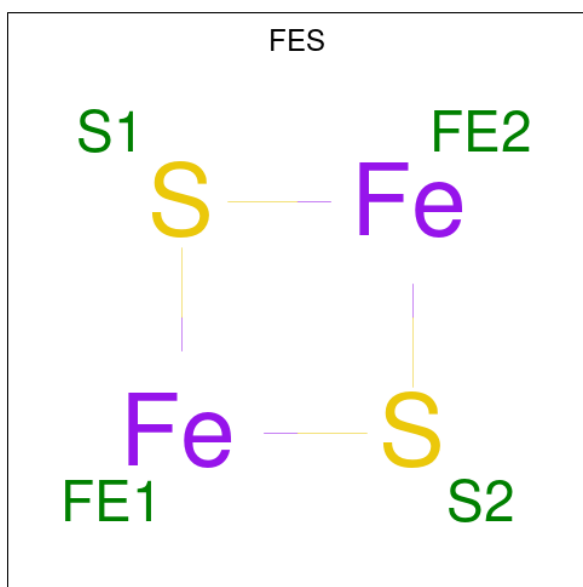
Mol	Chain	Residues	Atoms					AltConf
49	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
50	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
51	2	1	Total	Fe	S	0
			4	2	2	
51	3	1	Total	Fe	S	0
			4	2	2	

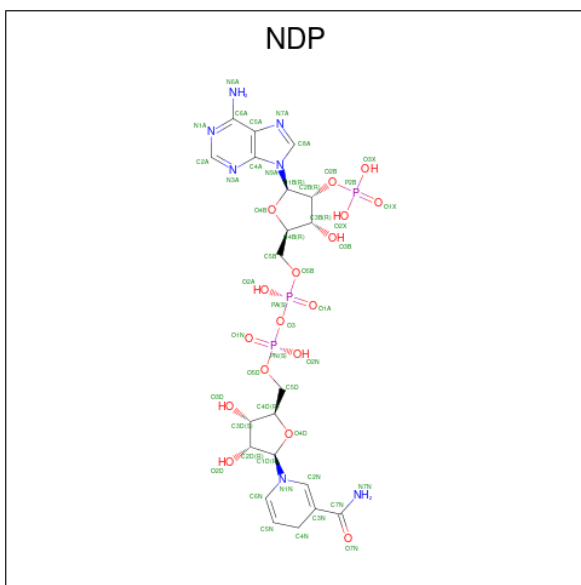
- Molecule 52 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
52	3	1	Total	K	0
			1	1	

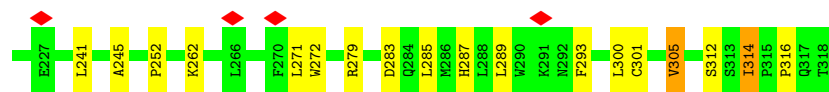
- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	b	1	Total	Zn	0
			1	1	

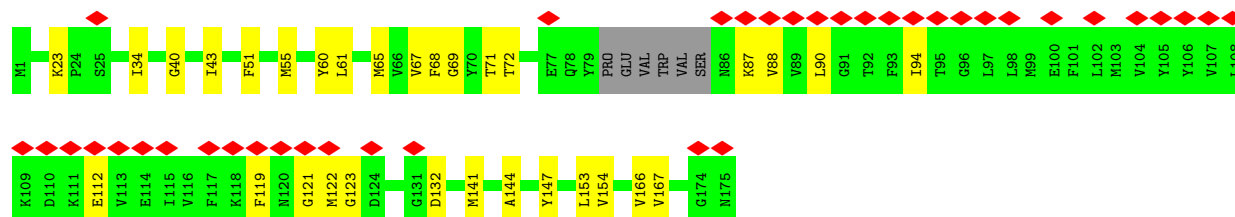
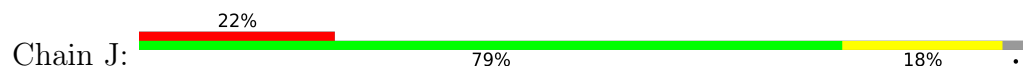
- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



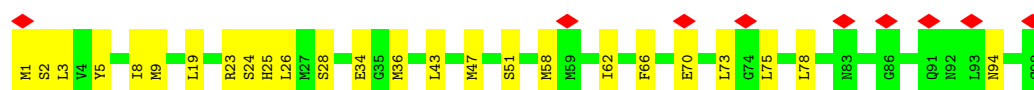
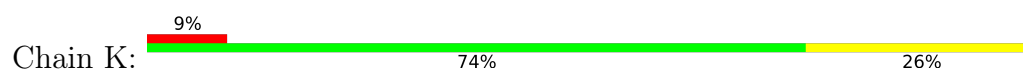
Mol	Chain	Residues	Atoms					AltConf
54	d	1	Total	C	N	O	P	0
			48	21	7	17	3	



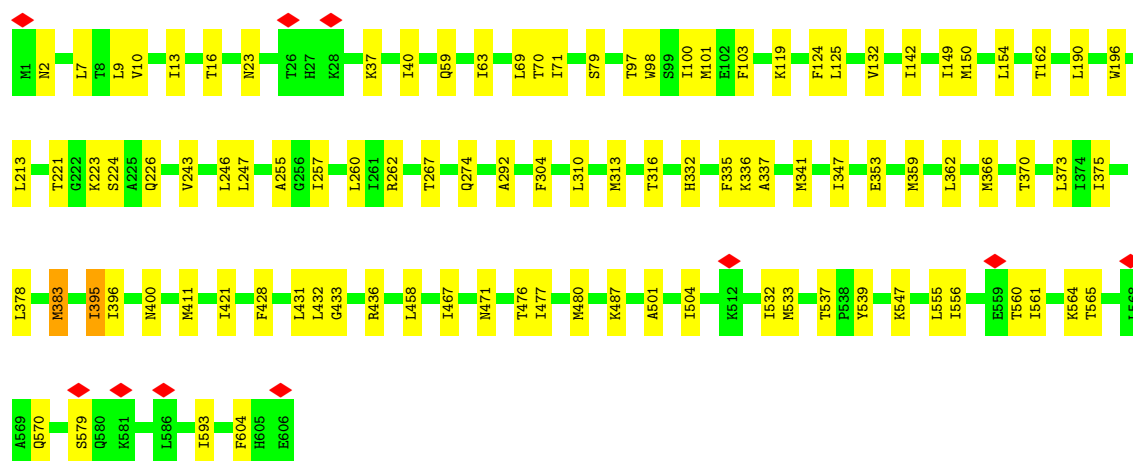
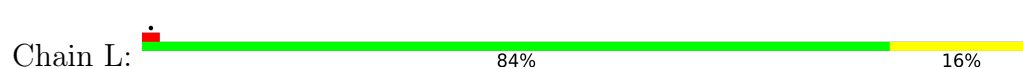
• Molecule 4: NADH-ubiquinone oxidoreductase chain 6



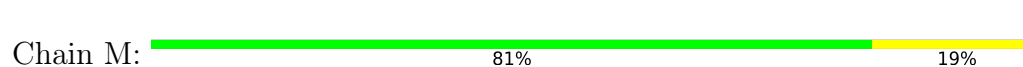
• Molecule 5: NADH-ubiquinone oxidoreductase chain 4L

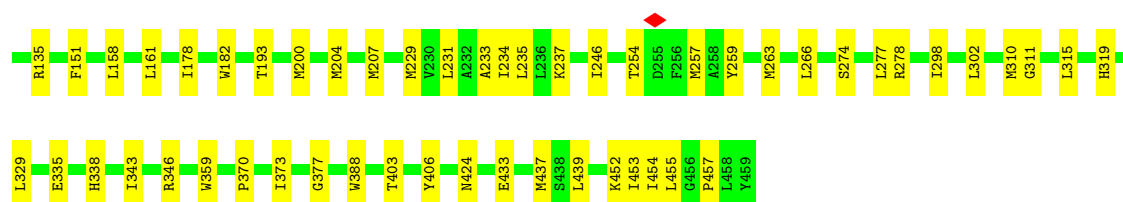


• Molecule 6: NADH-ubiquinone oxidoreductase chain 5

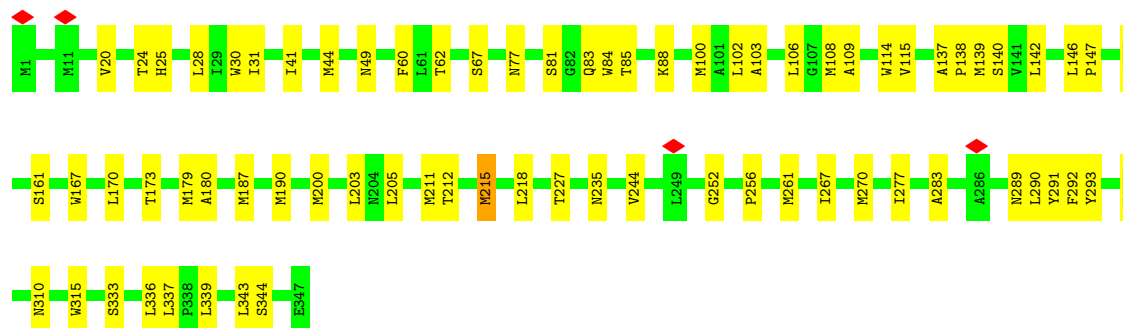
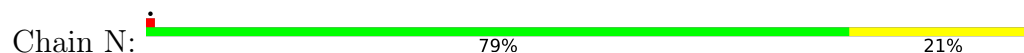


• Molecule 7: NADH-ubiquinone oxidoreductase chain 4

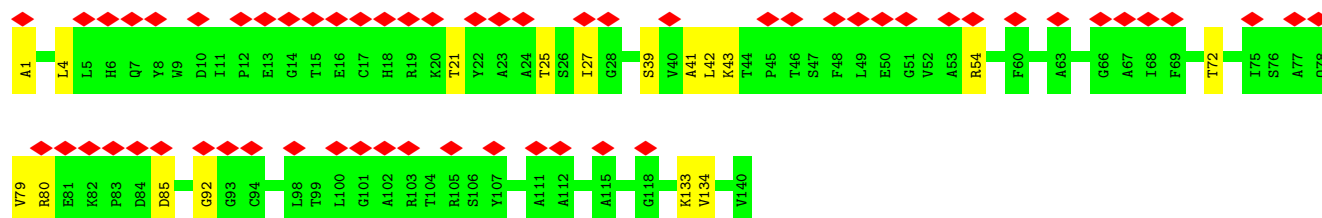
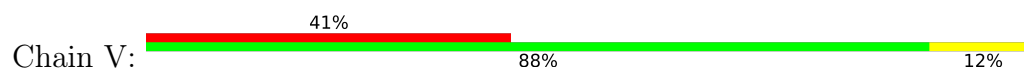




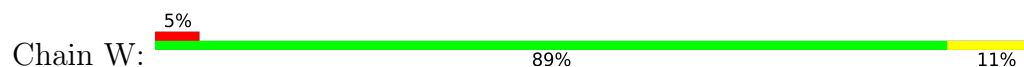
• Molecule 8: NADH-ubiquinone oxidoreductase chain 2



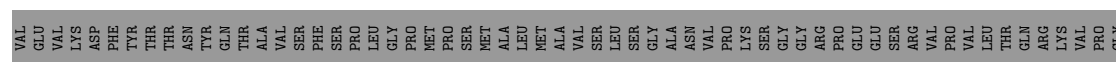
• Molecule 9: Complex I-B14.7



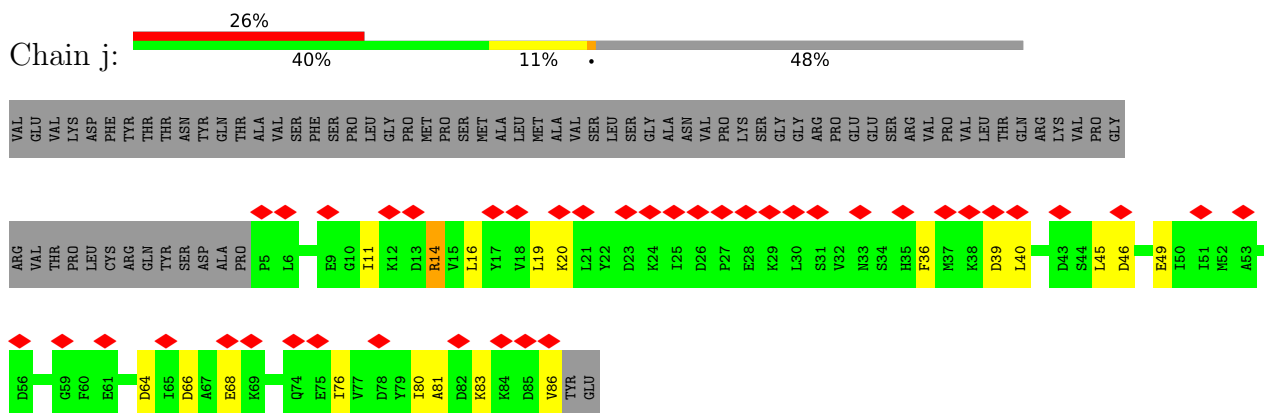
• Molecule 10: Complex I-SGDH



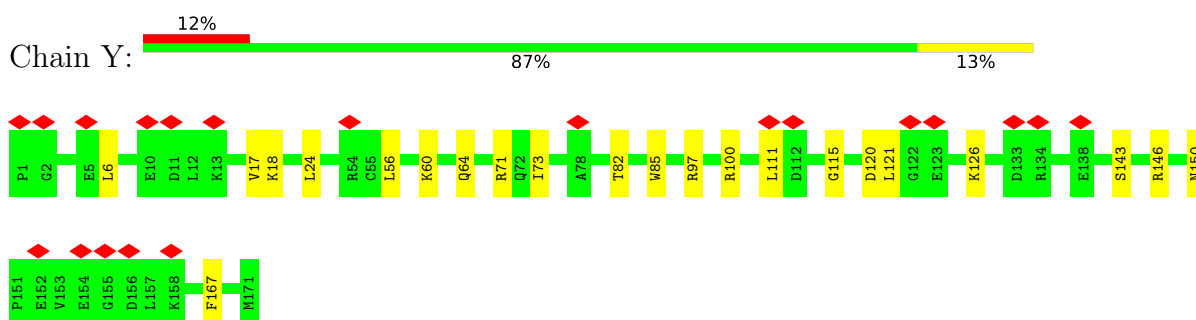
• Molecule 11: Acyl carrier protein



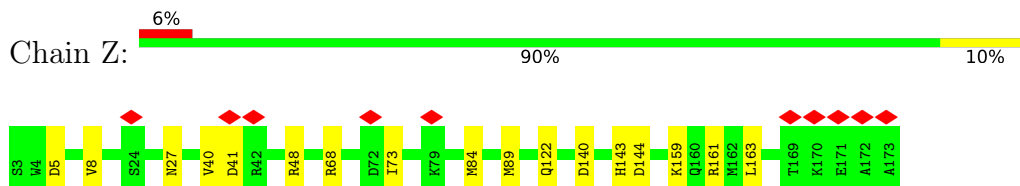
- Molecule 11: Acyl carrier protein



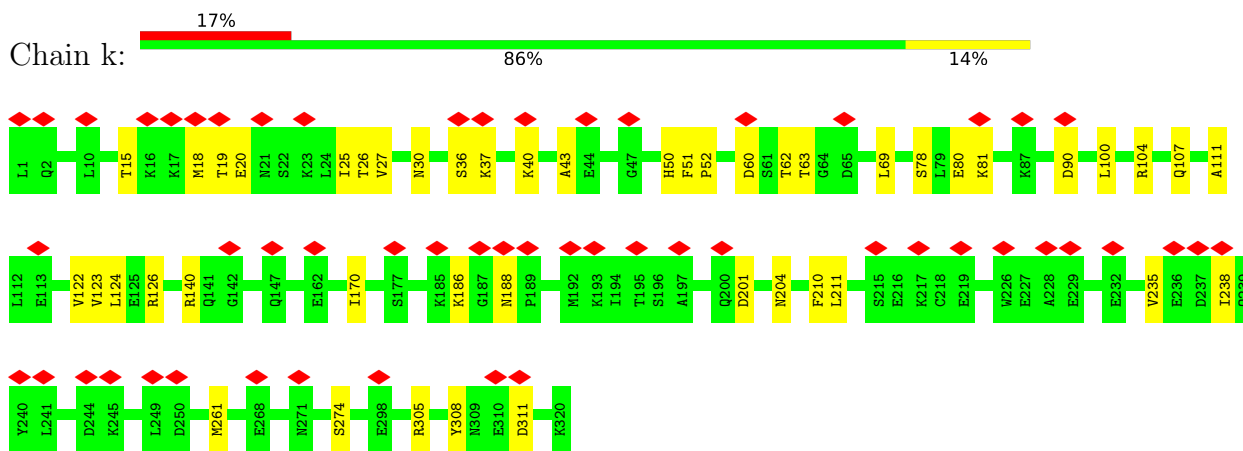
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



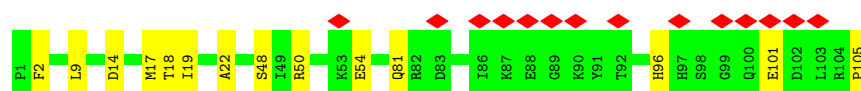
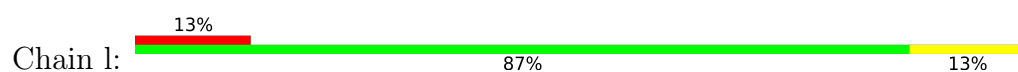
- Molecule 13: Complex I-PDSW



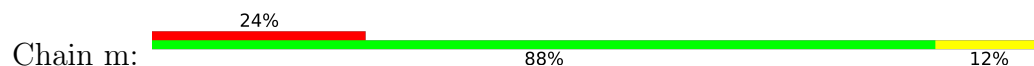
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



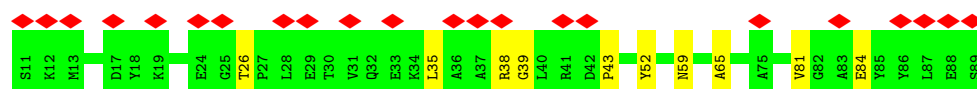
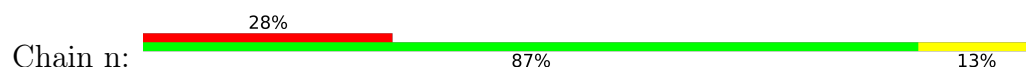
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



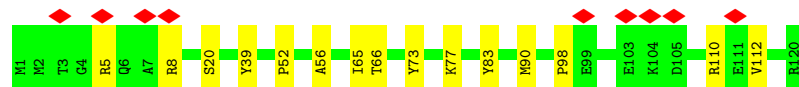
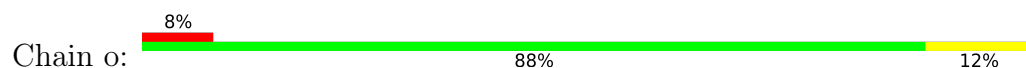
- Molecule 16: Complex I-B9



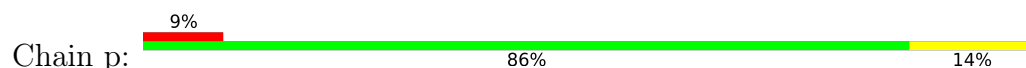
- Molecule 17: Complex I-B12



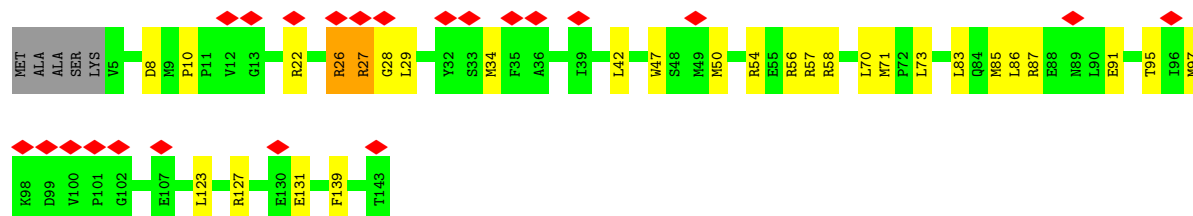
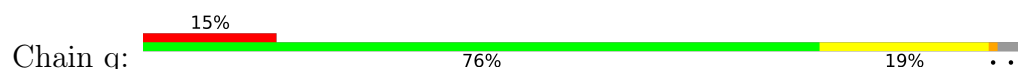
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 subunit C2



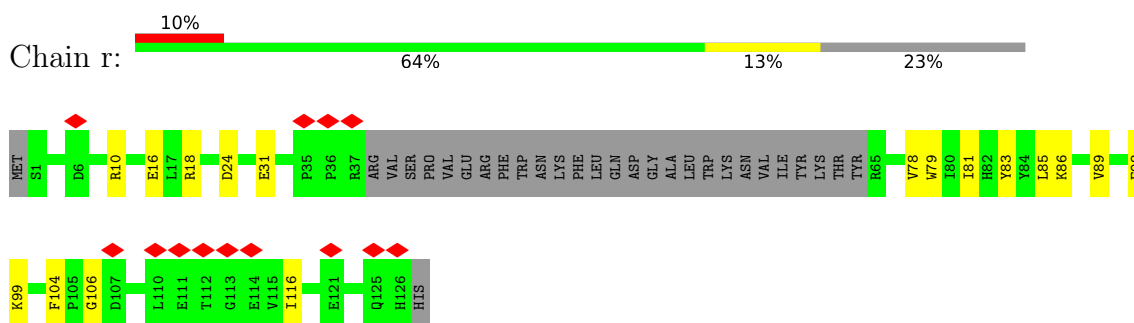
- Molecule 19: NADH:ubiquinone oxidoreductase subunit B4



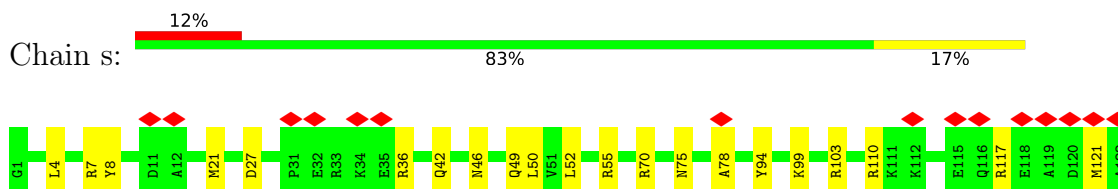
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



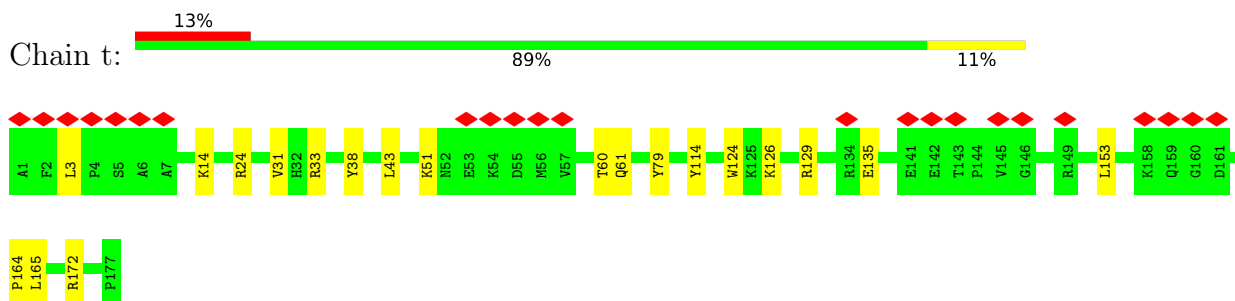
- Molecule 21: Mitochondrial complex I, B17 subunit



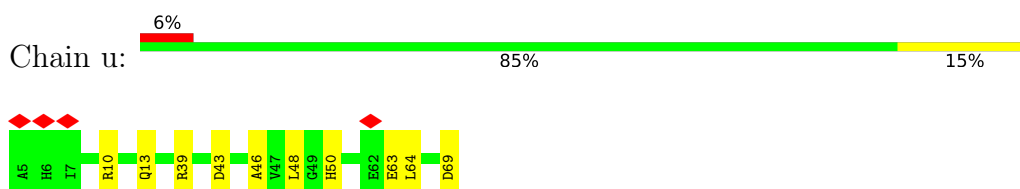
- Molecule 22: Complex I-B18



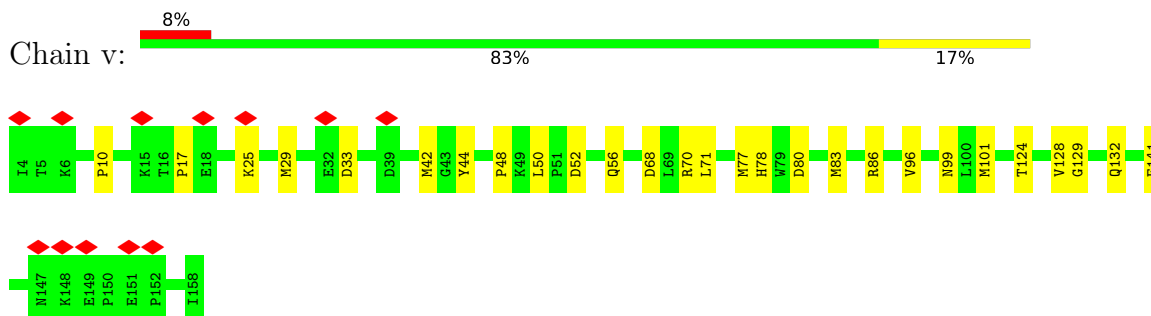
- Molecule 23: Complex I-B22



- Molecule 24: Complex I-AGGG

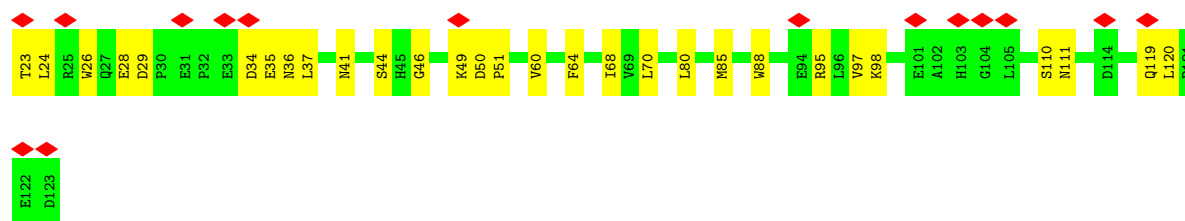


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

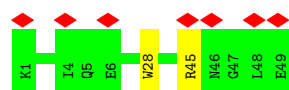


- Molecule 26: Complex I-ESSS

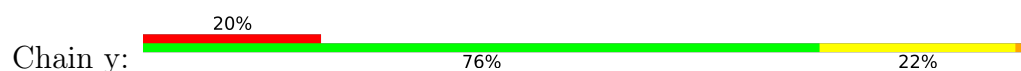




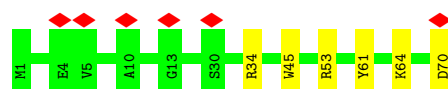
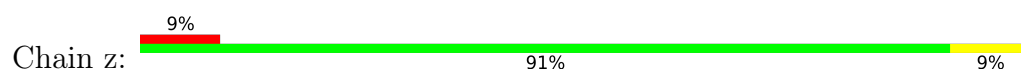
- Molecule 27: Complex I-KFYI



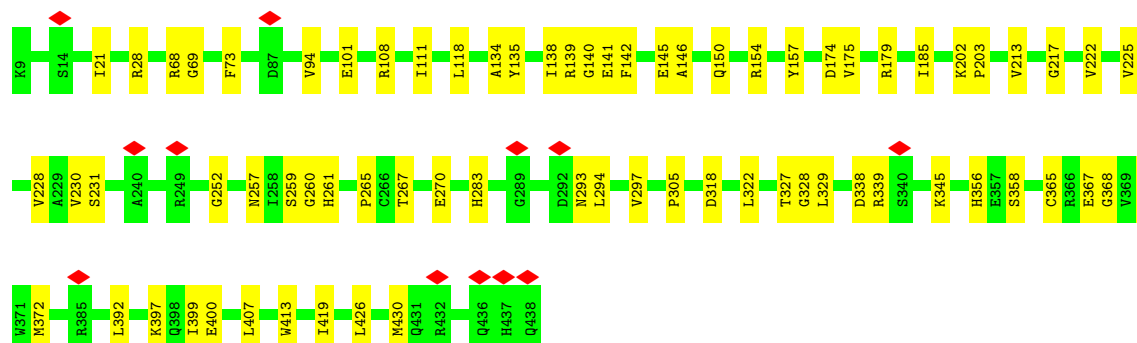
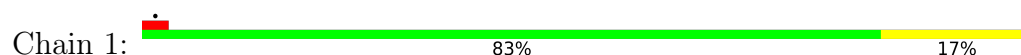
- Molecule 28: Complex I-MNLL



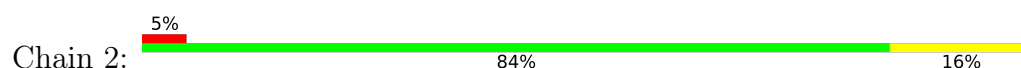
- Molecule 29: Complex I-MWFE



- Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



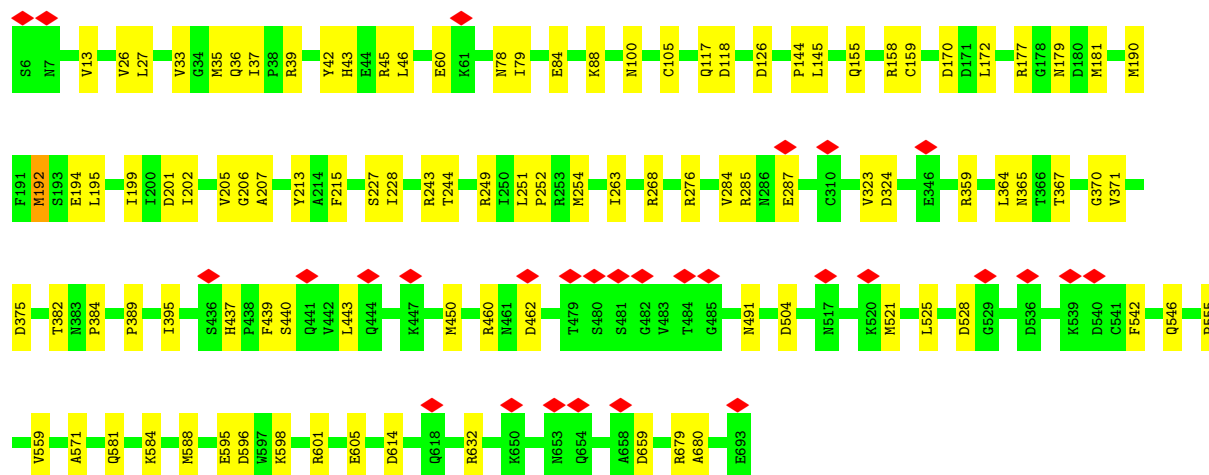
- Molecule 31: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





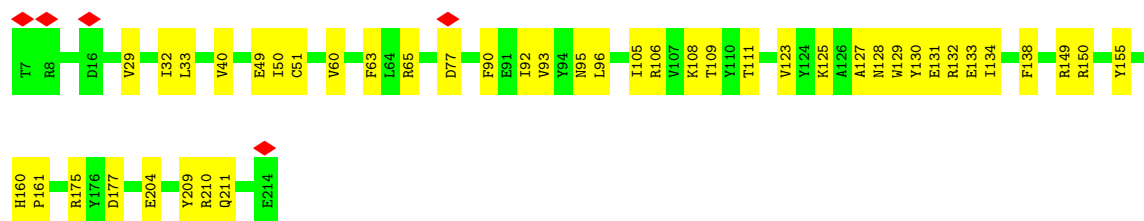
- Molecule 32: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 3: 85% 15%



- Molecule 33: Complex I-30kD

Chain 5: 79% 21%



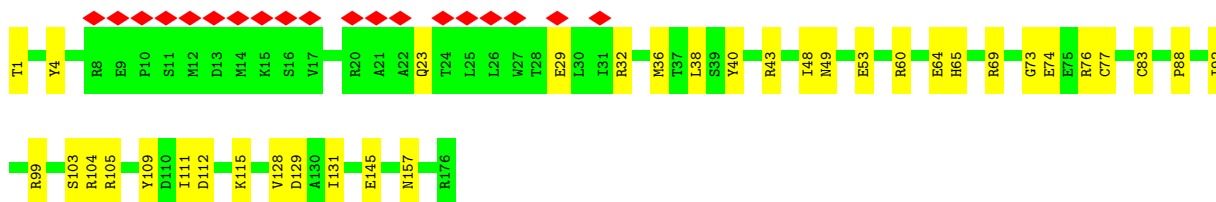
- Molecule 34: Complex I-20kD

Chain 6: 83% 17%



- Molecule 35: Complex I-23kD

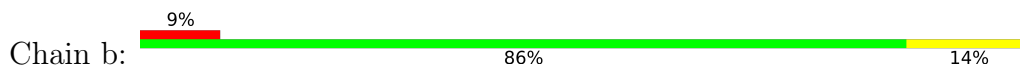
Chain 9: 11% 80% 20%



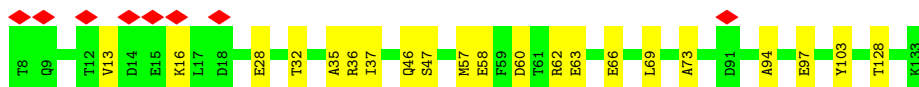
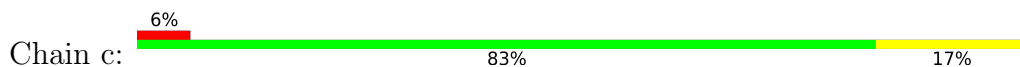
• Molecule 36: Complex I-9kD



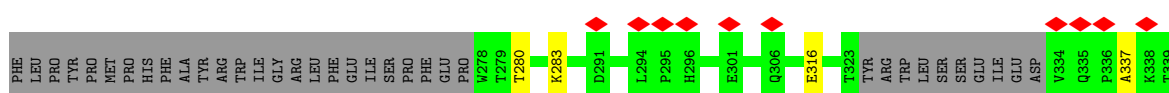
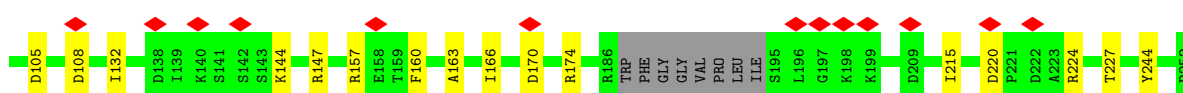
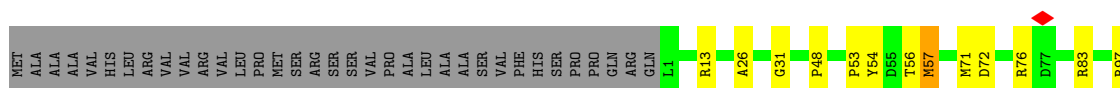
• Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



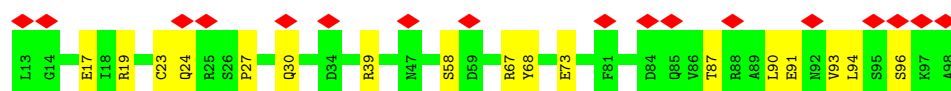
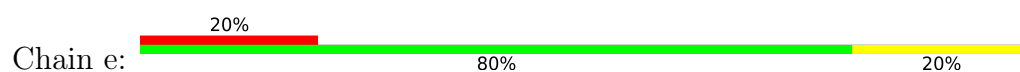
• Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



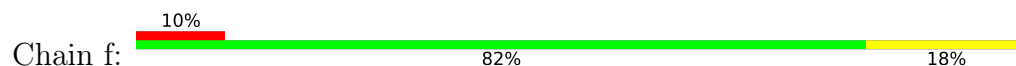
• Molecule 39: NADH:ubiquinone oxidoreductase subunit A9



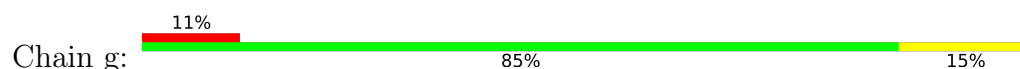
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



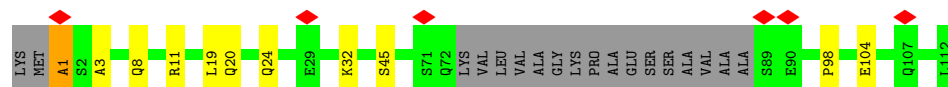
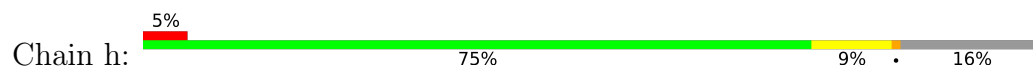
- Molecule 41: Complex I subunit B13



- Molecule 42: Complex I-B14



- Molecule 43: Mitochondrial complex I, B14.5a subunit



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35957	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.554	Depositor
Minimum map value	-0.011	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	164.7, 195.20001, 290.36002	wwPDB
Map dimensions	238, 160, 135	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZMP, FMN, SEP, AMP, AYA, SF4, FES, NDP, 2MR, MYR, NAI, FME, ZN, K

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	4	0.13	0/3463	0.35	0/4687
2	A	0.20	0/902	0.52	0/1234
3	H	0.22	0/2572	0.52	1/3517 (0.0%)
4	J	0.18	0/1324	0.47	0/1790
5	K	0.24	0/749	0.52	0/1014
6	L	0.18	0/4924	0.44	1/6698 (0.0%)
7	M	0.19	0/3731	0.45	0/5085
8	N	0.21	0/2787	0.52	1/3795 (0.0%)
9	V	0.16	0/1041	0.36	0/1412
10	W	0.14	0/1188	0.34	0/1607
11	X	0.20	0/713	0.50	0/963
11	j	0.20	0/670	0.54	0/902
12	Y	0.14	0/1440	0.39	0/1942
13	Z	0.13	0/1475	0.33	0/1989
14	k	0.12	0/2646	0.31	0/3579
15	l	0.15	0/896	0.41	0/1200
16	m	0.16	0/647	0.43	0/890
17	n	0.13	0/653	0.35	0/882
18	o	0.18	0/1035	0.45	1/1398 (0.1%)
19	p	0.21	0/1085	0.51	2/1467 (0.1%)
20	q	0.25	0/1171	0.56	1/1579 (0.1%)
21	r	0.15	0/874	0.41	1/1188 (0.1%)
22	s	0.14	0/1072	0.39	0/1436
23	t	0.15	0/1573	0.42	3/2130 (0.1%)
24	u	0.12	0/590	0.31	0/810
25	v	0.21	0/1361	0.51	2/1861 (0.1%)
26	w	0.18	0/872	0.45	0/1185
27	x	0.16	0/425	0.39	0/576
28	y	0.19	0/449	0.45	0/605
29	z	0.18	0/591	0.50	0/795
30	1	0.15	0/3386	0.37	0/4575
31	2	0.16	0/1695	0.45	0/2306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	3	0.14	0/5362	0.37	1/7266 (0.0%)
33	5	0.15	0/1776	0.36	0/2417
34	6	0.14	0/1278	0.37	0/1728
35	9	0.14	0/1445	0.34	0/1956
36	a	0.13	0/383	0.35	0/518
37	b	0.17	0/749	0.39	2/1009 (0.2%)
38	c	0.13	0/1047	0.35	0/1415
39	d	0.13	0/2424	0.30	0/3276
40	e	0.15	0/702	0.41	0/945
41	f	0.15	0/937	0.32	0/1271
42	g	0.18	0/993	0.39	0/1336
43	h	0.18	0/779	0.47	1/1053 (0.1%)
44	i	0.13	0/1250	0.36	0/1698
All	All	0.17	0/67125	0.42	17/90985 (0.0%)

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	4	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	v	17	PRO	CA-N-CD	-11.80	95.48	112.00
19	p	3	PRO	CA-N-CD	-11.01	96.59	112.00
18	o	98	PRO	CA-N-CD	-8.66	99.87	112.00
43	h	98	PRO	CA-N-CD	-7.82	101.05	112.00
3	H	90	PRO	CA-N-CD	-7.32	101.75	112.00
37	b	6	PRO	CA-N-CD	-7.21	101.91	112.00
25	v	17	PRO	N-CD-CG	-6.13	94.00	103.20
8	N	215	MET	CB-CG-SD	5.93	130.49	112.70
21	r	16	GLU	CA-CB-CG	5.81	125.72	114.10
20	q	28	GLY	N-CA-C	5.81	121.60	111.14
19	p	3	PRO	N-CD-CG	-5.67	94.70	103.20
32	3	192	MET	CB-CG-SD	5.54	129.33	112.70
23	t	61	GLN	CA-CB-CG	5.45	124.99	114.10
6	L	383	MET	CB-CG-SD	5.26	128.48	112.70
23	t	60	THR	CA-C-N	-5.13	112.53	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	t	60	THR	C-N-CA	-5.13	112.53	122.06
37	b	6	PRO	N-CD-CG	-5.08	95.58	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	4	275	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4	3390	0	3333	53	0
2	A	880	0	920	15	0
3	H	2498	0	2609	49	0
4	J	1294	0	1317	27	0
5	K	749	0	793	23	0
6	L	4806	0	4945	73	0
7	M	3647	0	3849	61	0
8	N	2723	0	2930	51	0
9	V	1028	0	1036	11	0
10	W	1155	0	1177	12	0
11	X	701	0	692	8	0
11	j	660	0	662	13	0
12	Y	1403	0	1392	17	0
13	Z	1441	0	1419	17	0
14	k	2596	0	2559	29	0
15	l	874	0	869	12	0
16	m	626	0	635	7	0
17	n	634	0	616	7	0
18	o	1004	0	995	10	0
19	p	1059	0	1062	15	0
20	q	1142	0	1136	31	0
21	r	846	0	864	15	0
22	s	1047	0	1015	18	0
23	t	1520	0	1477	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	u	563	0	509	8	0
25	v	1307	0	1207	26	0
26	w	846	0	792	21	0
27	x	412	0	411	2	0
28	y	436	0	437	8	0
29	z	576	0	570	5	0
30	1	3312	0	3266	47	0
31	2	1655	0	1668	22	0
32	3	5275	0	5300	71	0
33	5	1726	0	1676	28	0
34	6	1247	0	1256	20	0
35	9	1414	0	1369	34	0
36	a	371	0	344	9	0
37	b	737	0	710	9	0
38	c	1024	0	1023	17	0
39	d	2372	0	2407	20	0
40	e	691	0	706	9	0
41	f	917	0	958	14	0
42	g	969	0	980	12	0
43	h	769	0	780	8	0
44	i	1209	0	1182	7	0
45	X	31	0	34	1	0
45	j	34	0	40	0	0
46	k	23	0	12	1	0
47	s	15	0	27	0	0
48	1	8	0	0	0	0
48	3	16	0	0	2	0
48	6	8	0	0	0	0
48	9	16	0	0	0	0
49	1	31	0	19	0	0
50	1	44	0	27	4	0
51	2	4	0	0	0	0
51	3	4	0	0	0	0
52	3	1	0	0	0	0
53	b	1	0	0	0	0
54	d	48	0	26	2	0
All	All	65835	0	66038	794	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 6.

All (794) 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)
20:q:27:ARG:HG2	35:9:32:ARG:NH1	1.59	1.16
20:q:27:ARG:CG	35:9:32:ARG:HH12	1.68	1.06
20:q:27:ARG:HG2	35:9:32:ARG:HH12	1.14	0.96
20:q:27:ARG:HG2	35:9:32:ARG:CZ	2.03	0.88
20:q:27:ARG:CD	35:9:32:ARG:HH12	1.97	0.76
2:A:44:MET:HG3	3:H:126:LYS:HB2	1.70	0.73
1:4:164:MET:H	1:4:164:MET:HE3	1.54	0.72
33:5:125:LYS:O	33:5:128:ASN:HB3	1.88	0.72
7:M:263:MET:HA	7:M:266:LEU:HB2	1.72	0.72
33:5:90:PHE:HB2	33:5:111:THR:O	1.90	0.72
8:N:146:LEU:HD23	8:N:147:PRO:HD3	1.72	0.71
4:J:122:MET:HE3	4:J:123:GLY:H	1.56	0.71
3:H:289:LEU:HA	3:H:293:PHE:HB2	1.73	0.70
8:N:252:GLY:HA3	8:N:290:LEU:HD13	1.75	0.69
7:M:61:LEU:HB2	7:M:457:PRO:HG3	1.75	0.68
6:L:100:ILE:HG13	6:L:246:LEU:HB2	1.77	0.67
26:w:41:ASN:HD21	26:w:51:PRO:HG3	1.59	0.66
7:M:158:LEU:HD13	8:N:283:ALA:HB1	1.78	0.66
20:q:27:ARG:HG2	35:9:32:ARG:NH2	2.09	0.66
30:1:21:ILE:HG21	30:1:230:VAL:HG12	1.79	0.65
32:3:521:MET:HG3	32:3:542:PHE:HB3	1.79	0.64
34:6:38:ASN:ND2	34:6:167:ILE:O	2.30	0.64
34:6:85:VAL:HG12	34:6:112:TYR:HB2	1.80	0.64
6:L:124:PHE:HB2	6:L:150:MET:HG2	1.81	0.63
20:q:27:ARG:CG	35:9:32:ARG:NH1	2.36	0.63
33:5:129:TRP:O	33:5:132:ARG:HB3	1.98	0.63
39:d:54:TYR:O	39:d:57:MET:HB2	1.98	0.63
8:N:30:TRP:NE1	8:N:67:SER:OG	2.31	0.62
14:k:27:VAL:HG12	14:k:170:ILE:HB	1.80	0.62
32:3:450:MET:SD	32:3:491:ASN:ND2	2.71	0.62
4:J:23:LYS:HD2	5:K:28:SER:HB3	1.82	0.62
30:1:69:GLY:O	50:1:503:NAI:N7N	2.33	0.62
3:H:179:TRP:HE1	20:q:42:LEU:HG	1.65	0.61
7:M:278:ARG:NH1	25:v:83:MET:SD	2.73	0.61
6:L:103:PHE:HB2	6:L:341:MET:HE3	1.81	0.61
6:L:436:ARG:HH12	23:t:31:VAL:HG12	1.65	0.61
38:c:16:LYS:NZ	38:c:97:GLU:OE2	2.34	0.61
1:4:184:VAL:O	35:9:60:ARG:NH1	2.32	0.61
5:K:1:FME:SD	5:K:1:FME:N	2.74	0.61
1:4:328:ALA:HB3	32:3:126:ASP:HB2	1.83	0.60
22:s:117:ARG:O	22:s:121:MET:HB2	2.01	0.60
6:L:570:GLN:OE1	8:N:167:TRP:NE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:212:ASN:O	34:6:81:ARG:NH2	2.36	0.59
32:3:117:GLN:NE2	48:3:801:SF4:S3	2.76	0.59
43:h:1:AYA:OT	43:h:20:GLN:NE2	2.35	0.59
11:X:19:LEU:HB3	11:X:30:LEU:HD21	1.84	0.59
28:y:53:GLU:HG2	28:y:54:VAL:HG22	1.84	0.59
32:3:324:ASP:N	32:3:324:ASP:OD1	2.36	0.59
7:M:60:SER:HB2	7:M:457:PRO:HA	1.84	0.59
30:1:257:ASN:ND2	30:1:267:THR:OG1	2.35	0.59
7:M:73:LEU:HD13	7:M:103:GLN:HB2	1.84	0.58
15:l:14:ASP:OD1	15:l:14:ASP:N	2.36	0.58
32:3:382:THR:HG23	32:3:384:PRO:HD3	1.85	0.58
7:M:204:MET:HE1	7:M:302:LEU:HD11	1.85	0.58
14:k:311:ASP:N	14:k:311:ASP:OD1	2.37	0.58
6:L:604:PHE:O	8:N:150:ASN:ND2	2.37	0.58
30:1:101:GLU:HB2	50:1:503:NAI:H42N	1.86	0.57
1:4:354:GLU:OE2	1:4:357:GLN:NE2	2.37	0.57
1:4:231:ASN:HB3	35:9:29:GLU:HG3	1.85	0.57
2:A:63:LEU:HB2	4:J:67:VAL:HG21	1.86	0.57
14:k:52:PRO:O	14:k:107:GLN:NE2	2.37	0.57
30:1:150:GLN:HB3	36:a:54:LEU:HD13	1.85	0.57
30:1:261:HIS:ND1	30:1:338:ASP:OD1	2.36	0.57
32:3:36:GLN:NE2	38:c:47:SER:O	2.38	0.57
41:f:5:LYS:NZ	41:f:75:GLN:OE1	2.37	0.57
3:H:111:LEU:HD22	4:J:61:LEU:HD23	1.87	0.57
4:J:71:THR:HG21	5:K:75:LEU:HD22	1.87	0.57
12:Y:150:ASN:OD1	15:l:50:ARG:NH1	2.38	0.57
35:9:64:GLU:OE2	35:9:157:ASN:ND2	2.38	0.57
39:d:174:ARG:NH2	39:d:316:GLU:OE2	2.38	0.57
7:M:453:ILE:HG13	7:M:454:ILE:HG23	1.87	0.56
32:3:284:VAL:HG12	32:3:559:VAL:HG22	1.86	0.56
4:J:121:GLY:HA2	5:K:3:LEU:HD22	1.87	0.56
30:1:157:TYR:OH	30:1:174:ASP:OD1	2.19	0.56
31:2:79:ARG:NH2	32:3:170:ASP:OD1	2.38	0.56
39:d:160:PHE:HB3	39:d:163:ALA:HB2	1.87	0.56
12:Y:6:LEU:HD21	20:q:86:LEU:HB3	1.88	0.56
42:g:97:LYS:HB3	42:g:101:HIS:HB2	1.87	0.56
1:4:109:VAL:HG11	1:4:152:MET:HG2	1.87	0.56
41:f:22:ARG:NH2	41:f:84:GLU:OE2	2.38	0.56
35:9:43:ARG:NH1	43:h:24:GLN:OE1	2.39	0.56
20:q:29:LEU:HD13	20:q:34:MET:HE3	1.88	0.56
7:M:338:HIS:NE2	26:w:34:ASP:OD2	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:e:27:PRO:O	40:e:30:GLN:HB3	2.06	0.56
6:L:396:ILE:O	6:L:400:ASN:ND2	2.40	0.55
1:4:391:ILE:O	1:4:430:ARG:NH1	2.39	0.55
3:H:87:ILE:HG22	3:H:95:LEU:HD23	1.87	0.55
34:6:117:GLY:O	34:6:121:ASN:ND2	2.40	0.55
35:9:92:ILE:HG12	35:9:111:ILE:HG12	1.88	0.55
12:Y:71:ARG:NH2	29:z:70:ASP:OD2	2.40	0.55
34:6:34:ASP:O	34:6:38:ASN:HB2	2.06	0.55
4:J:153:LEU:HD21	5:K:62:ILE:HG13	1.89	0.55
6:L:221:THR:HG23	6:L:226:GLN:HB2	1.88	0.55
1:4:269:LEU:HB2	1:4:368:GLU:HB2	1.89	0.55
3:H:102:VAL:HG11	3:H:154:LEU:HD21	1.88	0.55
6:L:292:ALA:HB2	6:L:304:PHE:HB3	1.89	0.55
7:M:25:ILE:HG23	26:w:60:VAL:HG11	1.89	0.55
32:3:201:ASP:OD2	32:3:268:ARG:NH2	2.35	0.55
32:3:27:LEU:HD13	32:3:37:ILE:HB	1.88	0.55
21:r:10:ARG:NH2	23:t:164:PRO:O	2.37	0.55
8:N:310:ASN:HB2	14:k:274:SER:HB3	1.89	0.55
12:Y:126:LYS:NZ	16:m:69:PRO:O	2.40	0.55
32:3:158:ARG:HB3	32:3:202:ILE:HD12	1.87	0.55
7:M:120:ILE:HD11	8:N:337:LEU:HD21	1.89	0.55
26:w:26:TRP:NE1	26:w:28:GLU:OE1	2.37	0.54
7:M:54:LEU:HD23	10:W:93:ILE:HG23	1.90	0.54
21:r:106:GLY:H	21:r:116:ILE:HB	1.73	0.54
37:b:27:ARG:NH1	38:c:69:LEU:O	2.34	0.54
7:M:207:MET:HG2	7:M:298:ILE:HG13	1.89	0.54
7:M:388:TRP:O	19:p:108:ARG:NH1	2.41	0.54
10:W:87:TYR:HE1	13:Z:89:MET:HG2	1.72	0.54
35:9:77:CYS:O	35:9:105:ARG:NH1	2.40	0.54
1:4:110:SER:OG	1:4:149:ASN:ND2	2.41	0.54
7:M:116:ILE:HG21	12:Y:167:PHE:HB3	1.88	0.54
21:r:85:LEU:HA	21:r:89:VAL:HB	1.90	0.54
5:K:19:LEU:HD13	5:K:36:MET:HE3	1.89	0.54
26:w:64:PHE:HA	26:w:68:ILE:HB	1.90	0.54
30:1:372:MET:HE3	30:1:399:ILE:HD12	1.89	0.54
1:4:117:ALA:HB2	1:4:367:ILE:HG12	1.89	0.54
8:N:218:LEU:HD13	8:N:244:VAL:HG12	1.90	0.54
14:k:62:THR:HG23	14:k:63:THR:HG23	1.90	0.54
42:g:91:GLU:OE1	42:g:97:LYS:NZ	2.40	0.54
6:L:2:ASN:N	6:L:2:ASN:OD1	2.41	0.53
6:L:467:ILE:O	6:L:471:ASN:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:n:35:LEU:O	17:n:39:GLY:N	2.41	0.53
43:h:11:ARG:HG2	43:h:19:LEU:HD12	1.90	0.53
14:k:235:VAL:HA	14:k:238:ILE:HG12	1.90	0.53
22:s:110:ARG:NH2	24:u:69:ASP:OD2	2.41	0.53
33:5:96:LEU:HB2	33:5:105:ILE:HG22	1.90	0.53
33:5:127:ALA:HA	33:5:130:TYR:HB2	1.90	0.53
35:9:105:ARG:NH2	37:b:86:TYR:O	2.40	0.53
26:w:23:THR:OG1	26:w:24:LEU:N	2.41	0.53
30:1:260:GLY:O	31:2:111:ARG:NH1	2.42	0.53
35:9:48:ILE:HG22	44:i:58:ARG:HG2	1.90	0.53
7:M:47:ASP:OD1	7:M:47:ASP:N	2.41	0.53
9:V:39:SER:OG	9:V:54:ARG:NH2	2.42	0.53
32:3:194:GLU:HG2	32:3:195:LEU:HG	1.90	0.53
1:4:162:GLY:HA3	3:H:279:ARG:HG3	1.91	0.53
6:L:411:MET:SD	6:L:411:MET:N	2.81	0.53
7:M:1:FME:O1	7:M:3:LYS:NZ	2.38	0.53
7:M:254:THR:HA	7:M:257:MET:HB3	1.91	0.53
31:2:39:PRO:HA	36:a:65:GLN:HB3	1.91	0.53
32:3:375:ASP:OD1	32:3:375:ASP:N	2.39	0.53
32:3:601:ARG:NH2	32:3:614:ASP:OD2	2.42	0.53
39:d:157:ARG:NH2	39:d:227:THR:OG1	2.41	0.53
1:4:300:ARG:HH21	1:4:422:ASP:HB2	1.74	0.53
6:L:162:THR:OG1	25:v:86:ARG:NH2	2.42	0.53
22:s:50:LEU:HB2	22:s:55:ARG:HE	1.74	0.53
32:3:206:GLY:N	48:3:801:SF4:S2	2.78	0.53
3:H:153:VAL:HG11	3:H:241:LEU:HD21	1.91	0.53
25:v:50:LEU:HB2	25:v:78:HIS:HD2	1.74	0.53
32:3:118:ASP:OD2	38:c:46:GLN:NE2	2.42	0.53
44:i:73:THR:HG21	44:i:81:MET:HE1	1.90	0.53
6:L:337:ALA:O	6:L:341:MET:HB2	2.08	0.52
8:N:190:MET:HE1	8:N:205:LEU:HD13	1.91	0.52
14:k:25:ILE:O	14:k:123:VAL:HA	2.09	0.52
30:1:265:PRO:O	31:2:190:ARG:NH2	2.42	0.52
34:6:24:SER:N	34:6:27:GLU:OE2	2.41	0.52
6:L:243:VAL:HG13	6:L:247:LEU:HD13	1.90	0.52
32:3:126:ASP:OD1	32:3:126:ASP:N	2.39	0.52
40:e:19:ARG:NH2	40:e:73:GLU:OE2	2.38	0.52
7:M:5:ILE:HG23	7:M:104:LEU:HD11	1.91	0.52
10:W:125:TYR:HB2	15:l:48:SER:HB3	1.91	0.52
32:3:632:ARG:HH21	40:e:58:SER:HB3	1.73	0.52
7:M:343:ILE:O	7:M:346:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:65:ILE:H	11:X:65:ILE:HD12	1.74	0.52
14:k:111:ALA:HB1	14:k:122:VAL:HG11	1.89	0.52
30:1:367:GLU:OE1	32:3:100:ASN:ND2	2.43	0.52
36:a:71:GLU:OE1	36:a:75:HIS:NE2	2.43	0.52
15:l:96:HIS:HA	15:l:101:GLU:HB3	1.92	0.52
19:p:47:GLN:HG3	23:t:165:LEU:HD13	1.92	0.52
22:s:55:ARG:HH11	25:v:141:GLU:HG2	1.74	0.52
28:y:17:PRO:O	28:y:20:PHE:HB3	2.10	0.52
34:6:62:MET:HE2	34:6:156:LEU:HD23	1.90	0.52
2:A:49:LEU:HB2	3:H:126:LYS:HD3	1.92	0.52
6:L:476:THR:OG1	6:L:477:ILE:N	2.43	0.52
11:X:2:ASP:N	11:X:2:ASP:OD1	2.41	0.52
39:d:132:ILE:HD13	39:d:166:ILE:HB	1.91	0.52
6:L:10:VAL:HG11	21:r:78:VAL:HA	1.92	0.52
7:M:84:LEU:HD22	7:M:87:GLU:HG3	1.91	0.52
8:N:200:MET:HE1	8:N:343:LEU:HD13	1.92	0.52
30:1:108:ARG:NH2	31:2:162:GLU:OE2	2.41	0.52
1:4:430:ARG:NH2	33:5:133:GLU:OE1	2.43	0.52
6:L:142:ILE:HG12	7:M:370:PRO:HB2	1.92	0.52
35:9:74:GLU:HG3	37:b:44:ILE:HD12	1.92	0.52
8:N:108:MET:HE3	8:N:187:MET:HB3	1.91	0.51
31:2:100:ILE:HG12	31:2:156:ILE:HG12	1.92	0.51
32:3:42:TYR:O	32:3:158:ARG:NH2	2.39	0.51
32:3:105:CYS:SG	32:3:117:GLN:NE2	2.82	0.51
32:3:323:VAL:HG11	32:3:525:LEU:HD13	1.91	0.51
33:5:65:ARG:NH1	33:5:123:VAL:O	2.43	0.51
7:M:119:TYR:CZ	7:M:161:LEU:HB2	2.44	0.51
32:3:45:ARG:NH2	32:3:254:MET:SD	2.83	0.51
32:3:528:ASP:OD2	32:3:679:ARG:NH2	2.43	0.51
32:3:601:ARG:NH1	32:3:605:GLU:OE1	2.42	0.51
38:c:37:ILE:HG12	38:c:57:MET:HG2	1.92	0.51
41:f:67:LEU:O	41:f:71:LEU:HB2	2.11	0.51
44:i:34:ARG:NH2	44:i:58:ARG:O	2.42	0.51
6:L:373:LEU:HD13	6:L:431:LEU:HD21	1.92	0.51
18:o:5:ARG:O	18:o:8:ARG:NH1	2.42	0.51
21:r:31:GLU:HG2	23:t:114:TYR:HA	1.91	0.51
32:3:252:PRO:HG3	32:3:263:ILE:HG12	1.91	0.51
7:M:26:ASN:OD1	28:y:13:HIS:NE2	2.40	0.51
22:s:103:ARG:HB2	24:u:64:LEU:HD22	1.92	0.51
42:g:63:ARG:NH1	11:j:46:ASP:OD1	2.44	0.51
6:L:556:ILE:O	6:L:560:THR:OG1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:v:29:MET:HE3	25:v:48:PRO:HG2	1.92	0.51
32:3:324:ASP:HB3	32:3:571:ALA:HB1	1.92	0.51
4:J:40:GLY:HA2	4:J:43:ILE:HD12	1.93	0.51
5:K:24:SER:OG	5:K:25:HIS:N	2.40	0.51
6:L:501:ALA:HA	6:L:504:ILE:HG12	1.93	0.51
7:M:42:LEU:HB3	26:w:80:LEU:HD21	1.92	0.51
12:Y:82:THR:HA	12:Y:85:TRP:CD1	2.46	0.51
18:o:20:SER:OG	27:x:45:ARG:NH1	2.43	0.51
25:v:56:GLN:HA	25:v:70:ARG:HH21	1.75	0.51
28:y:30:ASN:HA	28:y:33:LYS:HE2	1.92	0.51
30:1:111:ILE:HD12	30:1:138:ILE:HD11	1.92	0.51
6:L:316:THR:HB	6:L:395:ILE:HD12	1.93	0.51
6:L:487:LYS:NZ	24:u:46:ALA:O	2.43	0.51
12:Y:6:LEU:O	20:q:87:ARG:NH1	2.43	0.51
30:1:142:PHE:HB3	30:1:145:GLU:HB2	1.92	0.51
31:2:16:ASN:OD1	31:2:16:ASN:N	2.44	0.51
32:3:26:VAL:HG13	32:3:79:ILE:HD13	1.92	0.51
34:6:114:VAL:HG22	34:6:144:ILE:HB	1.92	0.51
43:h:3:ALA:O	43:h:8:GLN:NE2	2.42	0.51
8:N:261:MET:HE1	8:N:336:LEU:HB3	1.93	0.51
37:b:9:GLU:OE2	37:b:33:LYS:NZ	2.40	0.51
6:L:97:THR:HG22	6:L:101:MET:HE2	1.93	0.50
17:n:38:ARG:NH2	23:t:38:TYR:OH	2.39	0.50
33:5:175:ARG:HD2	39:d:13:ARG:HH11	1.76	0.50
35:9:76:ARG:NH1	35:9:128:VAL:O	2.43	0.50
1:4:204:PRO:HD2	1:4:207:LEU:HD22	1.93	0.50
12:Y:17:VAL:HG21	20:q:73:LEU:HD21	1.92	0.50
14:k:186:LYS:HD3	14:k:188:ASN:HB2	1.92	0.50
22:s:27:ASP:OD1	22:s:27:ASP:N	2.40	0.50
26:w:95:ARG:O	26:w:98:LYS:HB3	2.12	0.50
6:L:433:GLY:O	17:n:59:ASN:ND2	2.44	0.50
6:L:533:MET:SD	6:L:537:THR:OG1	2.70	0.50
11:X:23:ASP:HB2	17:n:43:PRO:HA	1.94	0.50
13:Z:48:ARG:HD3	21:r:83:TYR:HE1	1.76	0.50
35:9:43:ARG:HG2	43:h:11:ARG:HD2	1.93	0.50
13:Z:161:ARG:NH2	26:w:110:SER:O	2.44	0.50
16:m:78:GLU:OE1	16:m:82:ARG:NH2	2.45	0.50
19:p:74:ASN:HD22	25:v:10:PRO:HB2	1.76	0.50
31:2:74:GLN:O	36:a:74:ARG:NH2	2.44	0.50
32:3:525:LEU:HD23	32:3:546:GLN:HB3	1.94	0.50
6:L:190:LEU:HB2	6:L:196:TRP:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:132:ASP:OD1	4:J:132:ASP:N	2.45	0.50
6:L:71:ILE:HD13	7:M:455:LEU:HD13	1.92	0.50
7:M:233:ALA:HA	7:M:237:LYS:HZ3	1.76	0.50
1:4:335:ARG:NH2	35:9:129:ASP:OD1	2.45	0.50
3:H:24:GLU:OE2	3:H:195:ARG:NH2	2.45	0.50
11:j:81:ALA:HB1	11:j:86:VAL:HG11	1.94	0.50
1:4:238:ARG:NH1	3:H:279:ARG:O	2.44	0.50
3:H:212:ASN:HD22	3:H:223:PHE:HD2	1.58	0.50
7:M:124:ALA:HB1	8:N:256:PRO:HG3	1.94	0.50
26:w:41:ASN:HB3	26:w:44:SER:HB2	1.94	0.50
34:6:86:MET:HB2	34:6:107:MET:HE1	1.94	0.49
6:L:539:TYR:OH	19:p:9:ARG:NH1	2.45	0.49
32:3:276:ARG:NH1	32:3:680:ALA:O	2.46	0.49
1:4:77:ASP:OD2	33:5:149:ARG:NH2	2.45	0.49
1:4:346:ILE:HG12	32:3:117:GLN:HG2	1.94	0.49
3:H:283:ASP:OD1	3:H:283:ASP:N	2.45	0.49
19:p:35:ARG:NH2	25:v:33:ASP:OD2	2.44	0.49
21:r:24:ASP:OD2	23:t:124:TRP:NE1	2.39	0.49
32:3:588:MET:HG3	38:c:63:GLU:HG3	1.94	0.49
34:6:168:LYS:NZ	44:i:76:ASP:OD1	2.40	0.49
35:9:1:THR:N	43:h:104:GLU:O	2.37	0.49
6:L:362:LEU:HD23	6:L:366:MET:HG3	1.93	0.49
7:M:106:LEU:HD13	7:M:234:ILE:HG21	1.95	0.49
1:4:393:ALA:HB3	1:4:396:PHE:HB2	1.92	0.49
4:J:60:TYR:OH	5:K:34:GLU:O	2.31	0.49
19:p:1:SER:OG	19:p:2:PHE:N	2.44	0.49
25:v:96:VAL:HB	25:v:101:MET:HE2	1.94	0.49
33:5:32:ILE:HG23	33:5:33:LEU:HG	1.94	0.49
34:6:71:ARG:NH2	35:9:49:ASN:OD1	2.45	0.49
39:d:144:LYS:HD2	39:d:147:ARG:HH21	1.77	0.49
3:H:37:PRO:HA	34:6:71:ARG:HA	1.95	0.49
4:J:167:VAL:HG11	5:K:73:LEU:HD12	1.95	0.49
30:1:134:ALA:HB3	30:1:175:VAL:HG12	1.94	0.49
35:9:83:CYS:SG	35:9:109:TYR:OH	2.69	0.49
35:9:99:ARG:HE	35:9:103:SER:HB2	1.77	0.49
7:M:122:PHE:O	7:M:125:THR:OG1	2.31	0.49
14:k:26:THR:HG22	14:k:124:LEU:HB2	1.94	0.49
35:9:65:HIS:HB3	35:9:131:ILE:HD11	1.94	0.49
16:m:12:TRP:HA	16:m:19:VAL:HG11	1.95	0.49
1:4:94:LYS:NZ	35:9:88:PRO:O	2.40	0.48
8:N:235:ASN:HB3	8:N:315:TRP:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:175:VAL:O	36:a:62:ARG:NH1	2.42	0.48
11:j:66:ASP:OD1	11:j:66:ASP:N	2.40	0.48
10:W:140:THR:O	10:W:143:ASN:ND2	2.46	0.48
19:p:21:GLU:OE2	23:t:14:LYS:NZ	2.41	0.48
30:1:270:GLU:OE1	30:1:283:HIS:NE2	2.43	0.48
14:k:104:ARG:HH21	46:k:501:AMP:H8	1.61	0.48
18:o:66:THR:OG1	27:x:28:TRP:NE1	2.46	0.48
31:2:163:ASP:OD2	31:2:190:ARG:NH1	2.46	0.48
39:d:76:ARG:NH2	39:d:108:ASP:OD2	2.45	0.48
3:H:90:PRO:HG3	3:H:162:LEU:HG	1.96	0.48
7:M:346:ARG:NE	25:v:68:ASP:OD2	2.46	0.48
30:1:259:SER:HA	30:1:265:PRO:HB3	1.95	0.48
1:4:322:GLU:HG3	1:4:324:LYS:H	1.79	0.48
3:H:108:MET:HA	3:H:111:LEU:HG	1.95	0.48
3:H:124:ASN:N	3:H:124:ASN:OD1	2.41	0.48
6:L:547:LYS:NZ	25:v:44:TYR:OH	2.43	0.48
33:5:93:VAL:HG22	33:5:108:LYS:HG2	1.95	0.48
39:d:280:THR:HG23	39:d:283:LYS:H	1.78	0.48
6:L:59:GLN:NE2	21:r:98:GLU:OE2	2.47	0.48
6:L:593:ILE:HD12	9:V:41:ALA:HB2	1.96	0.48
8:N:170:LEU:HD11	8:N:291:TYR:HD2	1.78	0.48
8:N:267:ILE:HA	8:N:270:MET:HG2	1.96	0.48
12:Y:143:SER:OG	12:Y:146:ARG:NH1	2.46	0.48
14:k:30:ASN:O	14:k:126:ARG:NH2	2.44	0.48
18:o:110:ARG:NH2	26:w:119:GLN:OE1	2.47	0.48
3:H:216:ALA:HB3	3:H:219:PRO:HD2	1.95	0.48
4:J:88:VAL:HG12	5:K:23:ARG:HH22	1.78	0.48
30:1:28:ARG:NH1	36:a:35:ASN:O	2.45	0.48
30:1:426:LEU:O	30:1:430:MET:HG2	2.14	0.48
1:4:233:ARG:NH2	35:9:23:GLN:O	2.46	0.48
11:X:51:ILE:HG21	11:X:67:ALA:HB1	1.95	0.48
29:z:64:LYS:HA	29:z:64:LYS:HD3	1.71	0.48
30:1:370:ASP:OD2	32:3:179:ASN:ND2	2.46	0.48
11:j:80:ILE:HA	11:j:83:LYS:HG2	1.95	0.48
16:m:80:LEU:O	20:q:58:ARG:NH1	2.46	0.48
31:2:16:ASN:OD1	31:2:19:THR:OG1	2.31	0.48
32:3:155:GLN:HG2	32:3:181:MET:HE3	1.96	0.48
32:3:215:PHE:HB3	35:9:104:ARG:HG3	1.96	0.48
34:6:179:ARG:NH1	54:d:401:NDP:O2X	2.43	0.48
1:4:106:LEU:HD13	1:4:391:ILE:HG21	1.96	0.48
1:4:226:GLU:OE2	20:q:22:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:402:LEU:HA	1:4:405:MET:HB2	1.94	0.48
2:A:87:MET:HG3	4:J:147:TYR:HB3	1.95	0.48
5:K:66:PHE:CE2	8:N:31:ILE:HG12	2.49	0.48
14:k:60:ASP:HB3	14:k:69:LEU:HD13	1.96	0.48
23:t:153:LEU:HD21	23:t:165:LEU:HD12	1.95	0.48
41:f:13:LEU:HD11	41:f:77:GLU:HB3	1.95	0.48
7:M:178:ILE:O	7:M:182:TRP:N	2.47	0.47
13:Z:163:LEU:HD13	26:w:120:LEU:HD22	1.96	0.47
35:9:112:ASP:HB3	35:9:115:LYS:HB2	1.96	0.47
5:K:5:TYR:O	5:K:9:MET:HG2	2.14	0.47
8:N:109:ALA:HB3	8:N:161:SER:HA	1.96	0.47
14:k:210:PHE:HD2	14:k:211:LEU:HD22	1.79	0.47
24:u:10:ARG:HB3	24:u:13:GLN:HG3	1.97	0.47
31:2:165:THR:H	31:2:168:ASP:HB2	1.79	0.47
4:J:141:MET:HA	4:J:144:ALA:HB3	1.95	0.47
13:Z:68:ARG:NH1	28:y:43:LEU:O	2.47	0.47
13:Z:161:ARG:NH2	26:w:111:ASN:OD1	2.42	0.47
22:s:7:ARG:NH2	22:s:8:TYR:OH	2.47	0.47
32:3:144:PRO:HD3	32:3:190:MET:HE3	1.96	0.47
5:K:2:SER:HB3	5:K:5:TYR:HD2	1.78	0.47
6:L:555:LEU:HD13	19:p:75:VAL:HG11	1.97	0.47
33:5:211:GLN:OE1	41:f:112:LYS:NZ	2.46	0.47
35:9:69:ARG:NH1	35:9:73:GLY:O	2.47	0.47
38:c:60:ASP:N	38:c:60:ASP:OD1	2.46	0.47
38:c:128:THR:O	38:c:128:THR:OG1	2.32	0.47
2:A:42:ASP:OD1	2:A:42:ASP:N	2.46	0.47
3:H:180:PRO:HB2	3:H:300:LEU:HD11	1.96	0.47
7:M:231:LEU:HD23	7:M:235:LEU:HD12	1.96	0.47
13:Z:41:ASP:OD1	21:r:86:LYS:NZ	2.48	0.47
14:k:15:THR:HA	14:k:18:MET:HB2	1.97	0.47
32:3:60:GLU:HG2	32:3:78:ASN:HB3	1.96	0.47
33:5:29:VAL:HG11	33:5:50:ILE:HD13	1.97	0.47
39:d:105:ASP:OD1	39:d:105:ASP:N	2.45	0.47
44:i:1:MET:SD	44:i:1:MET:N	2.80	0.47
1:4:46:ASN:OD1	1:4:46:ASN:N	2.48	0.47
8:N:173:THR:O	8:N:227:THR:OG1	2.33	0.47
12:Y:111:LEU:HA	12:Y:115:GLY:HA2	1.97	0.47
19:p:39:ARG:NH2	23:t:3:LEU:O	2.46	0.47
20:q:85:MET:HB3	20:q:123:LEU:HD22	1.97	0.47
20:q:139:PHE:HB2	29:z:45:TRP:CD1	2.50	0.47
32:3:243:ARG:HD2	32:3:244:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:2:LEU:HD23	28:y:26:LEU:HD22	1.97	0.47
16:m:83:LEU:HD12	20:q:58:ARG:HH12	1.78	0.47
30:1:228:VAL:O	30:1:231:SER:OG	2.30	0.47
6:L:132:VAL:O	6:L:262:ARG:NH2	2.48	0.47
8:N:137:ALA:O	8:N:140:SER:OG	2.29	0.47
19:p:50:TYR:O	19:p:55:ARG:NH2	2.48	0.47
19:p:51:ASN:HD22	23:t:165:LEU:HD22	1.80	0.47
32:3:13:VAL:HG21	32:3:33:VAL:HG21	1.97	0.47
42:g:83:ILE:HG22	42:g:87:MET:HE3	1.95	0.47
6:L:13:ILE:HA	6:L:16:THR:HG22	1.96	0.46
9:V:21:THR:O	9:V:25:THR:OG1	2.30	0.46
19:p:47:GLN:O	19:p:51:ASN:ND2	2.48	0.46
21:r:99:LYS:NZ	22:s:49:GLN:OE1	2.44	0.46
22:s:99:LYS:NZ	24:u:63:GLU:OE1	2.41	0.46
31:2:84:ALA:HA	31:2:90:TYR:HD2	1.79	0.46
32:3:659:ASP:N	32:3:659:ASP:OD1	2.48	0.46
40:e:23:CYS:SG	40:e:24:GLN:N	2.87	0.46
6:L:432:LEU:HD21	17:n:65:ALA:HB2	1.96	0.46
7:M:403:THR:HA	7:M:406:TYR:CE2	2.50	0.46
8:N:77:ASN:O	8:N:81:SER:HB3	2.15	0.46
13:Z:140:ASP:O	13:Z:161:ARG:NH1	2.49	0.46
42:g:32:ARG:NH1	11:j:68:GLU:OE1	2.48	0.46
8:N:28:LEU:HD12	8:N:31:ILE:HD12	1.97	0.46
33:5:40:VAL:HG22	33:5:50:ILE:HG23	1.97	0.46
1:4:49:LEU:HD22	2:A:43:PRO:HB2	1.98	0.46
8:N:62:THR:HG21	8:N:114:TRP:CD1	2.50	0.46
13:Z:40:VAL:HG13	21:r:79:TRP:HD1	1.79	0.46
14:k:51:PHE:HB2	14:k:124:LEU:HD23	1.97	0.46
14:k:78:SER:OG	14:k:80:GLU:OE1	2.33	0.46
33:5:175:ARG:NH2	33:5:177:ASP:OD1	2.49	0.46
43:h:45:SER:O	43:h:45:SER:OG	2.32	0.46
7:M:10:MET:HG3	28:y:15:LEU:HG	1.98	0.46
13:Z:122:GLN:OE1	22:s:46:ASN:ND2	2.49	0.46
31:2:61:LEU:HD12	31:2:90:TYR:HB3	1.96	0.46
41:f:25:ILE:HD12	41:f:25:ILE:HA	1.83	0.46
41:f:57:ILE:HD11	41:f:70:GLN:HG3	1.97	0.46
2:A:10:ASN:OD1	3:H:83:LEU:HB3	2.15	0.46
3:H:152:SER:OG	3:H:301:CYS:SG	2.74	0.46
5:K:1:FME:HB3	5:K:2:SER:H	1.55	0.46
13:Z:5:ASP:HB3	13:Z:8:VAL:HG22	1.97	0.46
16:m:27:LEU:O	16:m:31:LEU:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:292:ASP:OD1	1:4:292:ASP:N	2.41	0.46
6:L:9:LEU:HB3	21:r:81:ILE:HD13	1.97	0.46
6:L:23:ASN:OD1	6:L:119:LYS:NZ	2.48	0.46
8:N:83:GLN:OE1	8:N:85:THR:N	2.35	0.46
8:N:100:MET:HE2	8:N:100:MET:HB3	1.88	0.46
25:v:71:LEU:HD21	25:v:77:MET:HB3	1.97	0.46
42:g:42:VAL:HG11	42:g:59:ARG:HG3	1.97	0.46
44:i:32:ASP:OD2	44:i:34:ARG:NH1	2.49	0.46
6:L:63:ILE:O	6:L:79:SER:HA	2.16	0.46
7:M:82:HIS:NE2	7:M:335:GLU:OE2	2.48	0.46
14:k:90:ASP:OD1	14:k:90:ASP:N	2.49	0.46
15:l:105:PRO:HG2	29:z:53:ARG:HB3	1.97	0.46
25:v:99:ASN:OD1	25:v:99:ASN:N	2.49	0.46
3:H:272:TRP:CZ2	35:9:38:LEU:HB2	2.51	0.46
3:H:314:ILE:O	20:q:57:ARG:NH1	2.49	0.46
6:L:224:SER:HB3	6:L:310:LEU:HD12	1.96	0.46
15:l:50:ARG:O	15:l:54:GLU:HB2	2.16	0.46
17:n:81:VAL:HA	17:n:84:GLU:HG2	1.98	0.46
31:2:50:VAL:O	31:2:53:LEU:HB3	2.16	0.46
40:e:17:GLU:HG2	40:e:67:ARG:HB3	1.98	0.46
1:4:371:LYS:HG2	1:4:422:ASP:HB3	1.98	0.46
4:J:90:LEU:O	4:J:94:ILE:HG12	2.15	0.46
8:N:203:LEU:HD13	8:N:343:LEU:HB3	1.97	0.46
32:3:213:TYR:OH	32:3:249:ARG:NH1	2.49	0.46
32:3:439:PHE:O	32:3:443:LEU:HD12	2.15	0.46
38:c:36:ARG:NH1	38:c:58:GLU:OE2	2.49	0.46
39:d:220:ASP:O	39:d:224:ARG:NH2	2.49	0.46
32:3:227:SER:OG	32:3:228:ILE:N	2.49	0.45
39:d:48:PRO:HA	39:d:71:MET:O	2.15	0.45
11:j:16:LEU:HD23	11:j:19:LEU:HD23	1.97	0.45
6:L:480:MET:SD	24:u:50:HIS:ND1	2.90	0.45
32:3:359:ARG:NH2	32:3:504:ASP:OD2	2.49	0.45
1:4:243:GLY:O	1:4:296:ARG:NH2	2.49	0.45
7:M:9:MET:HE3	7:M:104:LEU:HD21	1.99	0.45
31:2:24:THR:OG1	31:2:27:ASN:OD1	2.35	0.45
37:b:57:ILE:HG22	37:b:73:ILE:HB	1.98	0.45
6:L:223:LYS:HG2	6:L:255:ALA:HB3	1.98	0.45
9:V:80:ARG:NH1	9:V:85:ASP:OD2	2.47	0.45
26:w:49:LYS:HA	26:w:49:LYS:HD3	1.81	0.45
38:c:28:GLU:O	38:c:32:THR:OG1	2.32	0.45
40:e:68:TYR:OH	40:e:96:SER:OG	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:206:GLY:N	20:q:8:ASP:OD1	2.49	0.45
7:M:200:MET:O	7:M:204:MET:HG2	2.17	0.45
13:Z:159:LYS:NZ	18:o:112:VAL:O	2.49	0.45
14:k:37:LYS:O	14:k:40:LYS:HB2	2.16	0.45
20:q:22:ARG:HH21	20:q:26:ARG:HH22	1.64	0.45
32:3:371:VAL:HG11	32:3:395:ILE:HG12	1.97	0.45
2:A:75:LEU:HD13	3:H:305:VAL:HG21	1.99	0.45
3:H:198:PHE:HB3	3:H:285:LEU:HD13	1.99	0.45
6:L:13:ILE:HG13	21:r:81:ILE:HD11	1.98	0.45
6:L:213:LEU:HD23	6:L:213:LEU:HA	1.87	0.45
7:M:38:SER:HB2	7:M:70:MET:HE3	1.99	0.45
8:N:83:GLN:OE1	8:N:84:TRP:N	2.50	0.45
14:k:140:ARG:NH1	14:k:201:ASP:OD1	2.50	0.45
11:j:11:ILE:HA	11:j:14:ARG:HE	1.82	0.45
3:H:22:LEU:HB2	3:H:48:PRO:HG3	1.99	0.45
6:L:370:THR:HG23	6:L:431:LEU:HD22	1.99	0.45
6:L:421:ILE:HG12	6:L:501:ALA:HB2	1.98	0.45
7:M:433:GLU:O	7:M:437:MET:HG3	2.17	0.45
8:N:293:TYR:O	8:N:297:THR:HG23	2.17	0.45
1:4:216:LYS:NZ	1:4:217:ASN:OD1	2.44	0.45
6:L:436:ARG:HG3	23:t:33:ARG:HD3	1.99	0.45
12:Y:97:ARG:HA	12:Y:100:ARG:HD3	1.97	0.45
22:s:21:MET:HE1	25:v:129:GLY:HA2	1.99	0.45
33:5:77:ASP:HB2	33:5:95:ASN:HD22	1.81	0.45
36:a:50:THR:O	36:a:54:LEU:HB2	2.17	0.45
1:4:360:PRO:HD2	33:5:209:TYR:CD2	2.52	0.44
7:M:329:LEU:HD13	7:M:359:TRP:CD2	2.51	0.44
30:1:345:LYS:NZ	31:2:109:MET:SD	2.83	0.44
38:c:13:VAL:O	42:g:14:THR:OG1	2.34	0.44
8:N:88:LYS:HB3	8:N:147:PRO:HB2	2.00	0.44
11:X:43:ASP:OD2	23:t:51:LYS:NZ	2.40	0.44
23:t:135:GLU:HB2	23:t:164:PRO:HA	1.99	0.44
32:3:244:THR:HB	38:c:73:ALA:HB2	1.99	0.44
1:4:283:PHE:HB3	1:4:310:ILE:HD11	1.99	0.44
22:s:36:ARG:NH2	25:v:132:GLN:OE1	2.37	0.44
32:3:39:ARG:HD3	32:3:42:TYR:HB3	1.99	0.44
33:5:131:GLU:O	33:5:134:ILE:HB	2.17	0.44
1:4:87:THR:HG21	1:4:106:LEU:HD21	1.98	0.44
3:H:22:LEU:HD13	3:H:47:GLN:HB3	1.99	0.44
3:H:92:PRO:HG3	3:H:252:PRO:HB3	1.98	0.44
3:H:183:MET:O	3:H:187:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:115:VAL:HG12	8:N:180:ALA:HB1	1.99	0.44
12:Y:73:ILE:HD13	12:Y:73:ILE:HA	1.88	0.44
23:t:24:ARG:HD3	23:t:24:ARG:HA	1.82	0.44
7:M:66:LEU:O	7:M:70:MET:HG2	2.18	0.44
30:1:94:VAL:HB	30:1:222:VAL:HG22	2.00	0.44
31:2:129:GLY:HA2	31:2:140:ILE:HG22	1.98	0.44
32:3:199:ILE:HA	32:3:202:ILE:HG12	2.00	0.44
30:1:400:GLU:OE2	30:1:413:TRP:NE1	2.49	0.44
32:3:546:GLN:HE22	32:3:596:ASP:HA	1.81	0.44
1:4:261:ARG:NH1	1:4:268:ASP:OD1	2.51	0.44
1:4:429:ASP:OD1	1:4:429:ASP:N	2.50	0.44
3:H:22:LEU:HG	3:H:26:LYS:NZ	2.33	0.44
30:1:213:VAL:HG13	30:1:217:GLY:HA2	1.99	0.44
41:f:67:LEU:HD23	41:f:67:LEU:HA	1.85	0.44
13:Z:27:ASN:OD1	13:Z:27:ASN:N	2.46	0.44
21:r:18:ARG:NH1	23:t:172:ARG:O	2.50	0.44
24:u:39:ARG:NH1	24:u:43:ASP:OD2	2.51	0.44
30:1:185:ILE:HD13	30:1:407:LEU:HD13	2.00	0.44
30:1:356:HIS:O	32:3:177:ARG:NH2	2.51	0.44
1:4:175:GLU:OE2	1:4:188:ARG:NH2	2.51	0.44
2:A:54:LYS:HB2	2:A:54:LYS:HE3	1.80	0.44
2:A:104:TYR:HE2	4:J:166:VAL:HG22	1.83	0.44
3:H:18:ALA:O	3:H:21:THR:OG1	2.30	0.44
14:k:140:ARG:HH12	14:k:204:ASN:HB2	1.83	0.44
32:3:145:LEU:HD12	32:3:192:MET:HE1	2.00	0.44
11:j:39:ASP:OD1	11:j:39:ASP:N	2.50	0.44
28:y:28:ARG:O	28:y:31:ASP:HB3	2.17	0.43
30:1:305:PRO:HG3	30:1:413:TRP:HB3	2.00	0.43
32:3:159:CYS:HB3	32:3:172:LEU:HD13	1.99	0.43
33:5:77:ASP:HB2	33:5:95:ASN:HB2	1.99	0.43
36:a:49:TYR:HD1	36:a:52:LEU:HD12	1.83	0.43
1:4:183:ARG:NH1	1:4:210:ASP:OD2	2.49	0.43
3:H:316:PRO:HG3	20:q:56:ARG:HB3	2.00	0.43
7:M:373:ILE:HD12	7:M:454:ILE:HD11	2.01	0.43
14:k:81:LYS:HD2	14:k:81:LYS:HA	1.77	0.43
20:q:47:TRP:HA	20:q:50:MET:HE2	2.00	0.43
26:w:35:GLU:HG2	26:w:49:LYS:HZ1	1.82	0.43
33:5:204:GLU:OE2	33:5:210:ARG:NE	2.51	0.43
39:d:72:ASP:O	39:d:83:ARG:NH2	2.50	0.43
6:L:428:PHE:HA	6:L:432:LEU:HD12	1.99	0.43
19:p:66:ARG:HG3	25:v:10:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:s:52:LEU:HD11	25:v:141:GLU:HB3	2.00	0.43
30:1:322:LEU:HD13	30:1:329:LEU:HA	1.99	0.43
33:5:49:GLU:HG2	33:5:106:ARG:HB3	2.00	0.43
2:A:90:MET:HG3	4:J:154:VAL:HG11	1.99	0.43
32:3:285:ARG:NH2	32:3:555:PRO:O	2.42	0.43
34:6:81:ARG:H	34:6:81:ARG:HG2	1.61	0.43
3:H:24:GLU:HG3	3:H:271:LEU:HD22	2.00	0.43
7:M:75:LEU:HD11	7:M:439:LEU:HB3	2.00	0.43
7:M:91:ARG:HD3	7:M:135:ARG:HH21	1.82	0.43
11:X:25:ILE:HD11	11:X:40:LEU:HD21	2.00	0.43
26:w:29:ASP:N	26:w:29:ASP:OD1	2.51	0.43
30:1:293:ASN:O	30:1:339:ARG:N	2.51	0.43
1:4:69:SER:O	1:4:69:SER:OG	2.35	0.43
2:A:49:LEU:HD12	2:A:50:PRO:HD2	2.00	0.43
6:L:336:LYS:HA	6:L:336:LYS:HD3	1.72	0.43
8:N:211:MET:HG2	8:N:333:SER:HB2	2.00	0.43
30:1:118:LEU:HD13	30:1:225:VAL:HG13	2.00	0.43
37:b:55:ARG:NH1	37:b:76:ASP:OD1	2.51	0.43
1:4:287:ILE:HD11	35:9:4:TYR:HE1	1.83	0.43
2:A:115:GLU:HB3	3:H:287:HIS:HB2	1.99	0.43
6:L:579:SER:O	9:V:43:LYS:NZ	2.51	0.43
9:V:4:LEU:HD23	9:V:4:LEU:HA	1.91	0.43
12:Y:120:ASP:OD1	12:Y:121:LEU:N	2.49	0.43
20:q:127:ARG:NH1	20:q:131:GLU:OE1	2.52	0.43
32:3:43:HIS:HB3	32:3:46:LEU:HB2	2.01	0.43
42:g:69:ASN:HD21	42:g:81:LEU:HD22	1.83	0.43
1:4:88:GLU:H	1:4:88:GLU:HG2	1.65	0.43
3:H:81:LEU:HD13	3:H:112:ALA:HA	2.00	0.43
5:K:70:GLU:HG2	8:N:60:PHE:HE1	1.84	0.43
7:M:329:LEU:HA	7:M:437:MET:HE1	2.01	0.43
18:o:52:PRO:HG2	18:o:56:ALA:HB2	2.00	0.43
31:2:78:MET:HE3	31:2:82:GLU:HG3	2.00	0.43
5:K:26:LEU:HB2	5:K:78:LEU:HD12	2.00	0.43
6:L:97:THR:HG21	6:L:125:LEU:HD22	2.01	0.43
15:l:81:GLN:HG2	20:q:97:MET:HB3	2.00	0.43
20:q:27:ARG:HD3	35:9:32:ARG:HH12	1.82	0.43
20:q:91:GLU:O	20:q:95:THR:HG22	2.18	0.43
30:1:139:ARG:NE	30:1:141:GLU:OE1	2.43	0.43
32:3:84:GLU:HG2	32:3:88:LYS:HE2	2.00	0.43
32:3:181:MET:HE2	32:3:181:MET:HB3	1.75	0.43
33:5:150:ARG:HD2	33:5:155:TYR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:i:73:THR:O	44:i:73:THR:OG1	2.37	0.43
11:j:76:ILE:O	11:j:80:ILE:HG22	2.18	0.43
5:k:73:LEU:HD11	8:n:41:ILE:HG21	2.00	0.43
8:n:106:LEU:HD11	8:n:138:PRO:HB2	2.01	0.43
12:y:18:LYS:HE2	12:y:18:LYS:HB2	1.82	0.43
13:z:73:ILE:HD11	13:z:84:MET:HG3	2.00	0.43
30:1:318:ASP:OD1	30:1:318:ASP:N	2.48	0.43
42:g:56:LYS:HD3	42:g:56:LYS:HA	1.77	0.43
3:h:99:ASN:OD1	3:h:161:THR:OG1	2.36	0.42
4:j:69:GLY:HA2	4:j:72:THR:HG22	2.01	0.42
6:l:260:LEU:HD23	6:l:260:LEU:HA	1.88	0.42
11:x:37:MET:SD	11:x:37:MET:N	2.92	0.42
25:v:25:LYS:HE3	25:v:25:LYS:HB3	1.93	0.42
32:3:437:HIS:O	32:3:440:SER:OG	2.37	0.42
35:9:36:MET:HE3	35:9:40:TYR:HB2	2.00	0.42
3:h:186:PHE:HA	3:h:189:THR:HG22	2.01	0.42
4:j:51:PHE:HE1	4:j:55:MET:HE2	1.85	0.42
7:m:315:LEU:O	7:m:319:HIS:HB3	2.19	0.42
8:n:139:MET:HE2	8:n:139:MET:HA	2.00	0.42
29:z:34:ARG:NH1	29:z:61:TYR:O	2.49	0.42
50:1:503:NAI:H6N	50:1:503:NAI:H2D	1.78	0.42
31:2:166:PRO:HA	31:2:169:ILE:HG22	2.01	0.42
32:3:365:ASN:N	32:3:491:ASN:OD1	2.53	0.42
34:6:48:MET:HG2	34:6:80:PRO:HB3	2.01	0.42
38:c:94:ALA:HA	38:c:97:GLU:HG3	2.01	0.42
4:j:34:ILE:HG23	4:j:61:LEU:HD11	2.01	0.42
4:j:87:LYS:HD3	4:j:88:VAL:HG23	2.01	0.42
6:l:149:ILE:HD13	6:l:149:ILE:HA	1.90	0.42
6:l:564:LYS:HD2	6:l:564:LYS:HA	1.70	0.42
8:n:44:MET:HE2	8:n:44:MET:HB3	1.95	0.42
30:1:68:ARG:HH22	30:1:252:GLY:HA3	1.84	0.42
4:j:65:MET:HA	4:j:68:PHE:HB2	2.01	0.42
6:l:359:MET:O	6:l:436:ARG:NE	2.43	0.42
6:l:375:ILE:HD12	6:l:458:LEU:HD11	2.00	0.42
7:m:64:PRO:HB3	7:m:454:ILE:HG22	2.01	0.42
14:k:261:MET:HE3	14:k:261:MET:HB3	1.80	0.42
15:l:19:ILE:HG13	15:l:22:ALA:HB2	2.00	0.42
18:o:39:TYR:HD1	18:o:65:ILE:HD11	1.84	0.42
32:3:364:LEU:HD12	32:3:491:ASN:HB3	2.01	0.42
32:3:367:THR:HB	32:3:370:GLY:H	1.84	0.42
39:d:170:ASP:N	39:d:170:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:j:45:LEU:O	11:j:49:GLU:HG2	2.19	0.42
2:A:78:ALA:HA	4:J:144:ALA:HB1	2.02	0.42
5:K:5:TYR:HE1	5:K:47:MET:HG2	1.84	0.42
8:N:179:MET:HE2	8:N:212:THR:HG23	2.00	0.42
31:2:158:ASP:OD1	31:2:158:ASP:N	2.51	0.42
32:3:581:GLN:HE21	32:3:581:GLN:HB2	1.69	0.42
4:J:23:LYS:HE2	4:J:23:LYS:HB2	1.84	0.42
5:K:94:ASN:OD1	5:K:94:ASN:N	2.53	0.42
7:M:151:PHE:CZ	8:N:291:TYR:HB2	2.55	0.42
9:V:133:LYS:HA	9:V:133:LYS:HD2	1.81	0.42
10:W:136:SER:O	10:W:138:LYS:NZ	2.51	0.42
13:Z:143:HIS:ND1	13:Z:144:ASP:OD1	2.53	0.42
32:3:194:GLU:HG3	32:3:389:PRO:HB3	2.01	0.42
32:3:287:GLU:H	32:3:287:GLU:HG3	1.62	0.42
37:b:57:ILE:HD12	37:b:57:ILE:HA	1.90	0.42
39:d:97:ARG:NH2	54:d:401:NDP:O3X	2.45	0.42
3:H:79:LEU:O	3:H:83:LEU:HB2	2.19	0.42
3:H:213:VAL:O	34:6:81:ARG:NE	2.49	0.42
4:J:112:GLU:HA	4:J:119:PHE:O	2.20	0.42
7:M:452:LYS:HA	7:M:455:LEU:HD12	2.02	0.42
8:N:289:ASN:HA	8:N:292:PHE:CE2	2.54	0.42
12:Y:24:LEU:HB3	20:q:70:LEU:HD11	2.01	0.42
37:b:60:ASP:OD1	37:b:60:ASP:N	2.51	0.42
39:d:97:ARG:HA	39:d:97:ARG:HD3	1.86	0.42
41:f:6:LYS:H	41:f:6:LYS:HG2	1.64	0.42
7:M:259:TYR:HB3	19:p:101:TYR:HE1	1.84	0.42
14:k:51:PHE:HB3	14:k:107:GLN:HE21	1.84	0.42
39:d:244:TYR:HB2	39:d:337:ALA:HB2	2.01	0.42
21:r:104:PHE:HE2	22:s:70:ARG:HD3	1.84	0.42
26:w:70:LEU:HD23	26:w:70:LEU:HA	1.86	0.42
33:5:134:ILE:O	33:5:138:PHE:N	2.53	0.42
35:9:49:ASN:O	35:9:53:GLU:N	2.47	0.42
5:K:8:ILE:HG21	5:K:43:LEU:HB2	2.01	0.42
6:L:532:ILE:HD11	25:v:101:MET:HB3	2.02	0.42
7:M:193:THR:HG23	7:M:257:MET:HE1	2.02	0.42
9:V:42:LEU:HD23	9:V:42:LEU:HA	1.84	0.42
14:k:100:LEU:HD23	14:k:100:LEU:HA	1.83	0.42
30:1:327:THR:OG1	30:1:328:GLY:N	2.53	0.42
33:5:92:ILE:HB	33:5:109:THR:HG23	2.02	0.42
1:4:149:ASN:HD22	1:4:370:PRO:HB2	1.84	0.41
3:H:181:LEU:HG	3:H:300:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:561:ILE:O	6:L:565:THR:OG1	2.38	0.41
7:M:311:GLY:HA2	7:M:377:GLY:HA2	2.02	0.41
14:k:19:THR:OG1	14:k:20:GLU:N	2.53	0.41
26:w:37:LEU:HD23	26:w:46:GLY:HA2	2.02	0.41
31:2:105:THR:HG22	31:2:107:PRO:HD2	2.02	0.41
3:H:156:MET:HE2	3:H:156:MET:HB2	2.00	0.41
6:L:7:LEU:HD23	6:L:7:LEU:HA	1.86	0.41
6:L:257:ILE:HD13	6:L:257:ILE:HA	1.96	0.41
30:1:358:SER:OG	30:1:365:CYS:SG	2.78	0.41
37:b:22:ASP:OD2	37:b:24:ARG:NH2	2.53	0.41
1:4:165:THR:HB	1:4:228:MET:HE1	2.02	0.41
1:4:208:MET:HE1	20:q:10:PRO:HD3	2.03	0.41
6:L:353:GLU:OE2	23:t:79:TYR:OH	2.38	0.41
8:N:20:VAL:HG11	8:N:137:ALA:HB1	2.03	0.41
8:N:277:ILE:HB	9:V:134:VAL:HG23	2.02	0.41
10:W:38:ILE:HD13	10:W:38:ILE:HA	1.89	0.41
14:k:43:ALA:HB2	14:k:50:HIS:HB3	2.02	0.41
25:v:42:MET:HE2	25:v:42:MET:HB2	1.94	0.41
25:v:77:MET:H	25:v:77:MET:HG2	1.66	0.41
25:v:80:ASP:HB3	25:v:83:MET:HE2	2.02	0.41
30:1:94:VAL:HG22	30:1:135:TYR:HB2	2.01	0.41
30:1:368:GLY:HA3	30:1:399:ILE:HD11	2.02	0.41
43:h:32:LYS:HA	43:h:32:LYS:HD3	1.80	0.41
11:j:16:LEU:O	11:j:20:LYS:HG3	2.20	0.41
3:H:22:LEU:HG	3:H:26:LYS:HZ1	1.83	0.41
3:H:312:SER:HB3	20:q:54:ARG:HH21	1.86	0.41
7:M:231:LEU:HD23	7:M:231:LEU:HA	1.90	0.41
10:W:40:ILE:HD13	10:W:40:ILE:HA	1.92	0.41
15:l:14:ASP:O	15:l:18:THR:OG1	2.38	0.41
17:n:26:THR:HG22	17:n:52:TYR:HB2	2.02	0.41
19:p:5:TYR:HD2	19:p:13:LEU:HD12	1.85	0.41
26:w:85:MET:O	26:w:88:TRP:HB3	2.20	0.41
40:e:91:GLU:HA	40:e:94:LEU:HG	2.02	0.41
41:f:45:LYS:HB3	41:f:45:LYS:HE2	1.82	0.41
42:g:29:ARG:NE	11:j:64:ASP:OD2	2.38	0.41
5:K:58:MET:HE2	15:l:17:MET:HE1	2.03	0.41
6:L:267:THR:O	6:L:274:GLN:NE2	2.54	0.41
6:L:378:LEU:HD13	6:L:383:MET:HG2	2.01	0.41
8:N:215:MET:HA	8:N:215:MET:HE2	2.03	0.41
8:N:336:LEU:HD12	8:N:339:LEU:HD12	2.02	0.41
14:k:19:THR:OG1	14:k:20:GLU:OE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:k:305:ARG:HB3	14:k:308:TYR:HD2	1.85	0.41
22:s:75:ASN:HB3	22:s:78:ALA:HB2	2.03	0.41
30:1:138:ILE:HG21	30:1:146:ALA:HB2	2.02	0.41
30:1:140:GLY:O	30:1:179:ARG:NH2	2.44	0.41
32:3:35:MET:HE3	32:3:35:MET:HB2	1.87	0.41
32:3:595:GLU:HB3	32:3:598:LYS:HG3	2.01	0.41
1:4:3:GLN:OE1	1:4:5:GLN:NE2	2.52	0.41
6:L:37:LYS:HD3	6:L:98:TRP:HE1	1.86	0.41
6:L:40:ILE:HG13	6:L:101:MET:HE3	2.02	0.41
6:L:69:LEU:HD12	6:L:69:LEU:HA	1.94	0.41
24:u:48:LEU:HD23	24:u:48:LEU:HA	1.89	0.41
33:5:49:GLU:OE2	33:5:106:ARG:NH1	2.47	0.41
38:c:62:ARG:NH1	42:g:126:ASP:OD1	2.54	0.41
7:M:424:ASN:OD1	7:M:424:ASN:N	2.52	0.41
8:N:41:ILE:HD13	8:N:41:ILE:HA	1.97	0.41
30:1:294:LEU:HD11	30:1:297:VAL:HG23	2.03	0.41
33:5:60:VAL:O	33:5:63:PHE:HB3	2.21	0.41
41:f:61:GLU:HA	41:f:62:PRO:HD3	1.94	0.41
3:H:197:PRO:HG2	3:H:198:PHE:CE1	2.55	0.41
6:L:332:HIS:HA	6:L:335:PHE:CE2	2.54	0.41
7:M:246:ILE:HD13	7:M:246:ILE:HA	1.90	0.41
10:W:62:GLU:OE1	10:W:64:TRP:NE1	2.47	0.41
10:W:75:ILE:HD13	10:W:75:ILE:HA	1.92	0.41
10:W:110:VAL:HG11	18:o:90:MET:HG3	2.03	0.41
16:m:52:TYR:CD2	20:q:71:MET:HE2	2.56	0.41
25:v:52:ASP:OD1	25:v:78:HIS:NE2	2.54	0.41
39:d:26:ALA:HA	39:d:31:GLY:HA3	2.03	0.41
1:4:96:TYR:HE2	1:4:378:LEU:HD21	1.85	0.41
1:4:112:MET:HE3	1:4:112:MET:HB3	1.89	0.41
1:4:145:THR:HA	1:4:148:LEU:HB2	2.03	0.41
1:4:180:PHE:O	1:4:184:VAL:HG12	2.21	0.41
3:H:150:LEU:HD12	3:H:150:LEU:HA	1.89	0.41
6:L:154:LEU:HD23	6:L:154:LEU:HA	1.95	0.41
7:M:274:SER:O	7:M:277:LEU:HB2	2.21	0.41
8:N:25:HIS:NE2	15:l:17:MET:HG2	2.36	0.41
8:N:49:ASN:OD1	8:N:49:ASN:N	2.54	0.41
8:N:103:ALA:HA	8:N:108:MET:HG3	2.03	0.41
12:Y:60:LYS:O	12:Y:64:GLN:NE2	2.54	0.41
13:Z:163:LEU:HD12	13:Z:163:LEU:HA	1.92	0.41
22:s:94:TYR:CZ	25:v:128:VAL:HG11	2.56	0.41
30:1:73:PHE:HB2	50:1:503:NAI:H51A	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:154:ARG:HA	36:a:58:LEU:HD21	2.01	0.41
30:1:397:LYS:HA	30:1:397:LYS:HD3	1.88	0.41
39:d:53:PRO:O	39:d:56:THR:OG1	2.36	0.41
41:f:54:LYS:HA	41:f:57:ILE:HG22	2.01	0.41
11:j:36:PHE:HA	11:j:40:LEU:HD12	2.03	0.41
6:L:100:ILE:HD13	6:L:100:ILE:HA	1.85	0.41
8:N:344:SER:HB3	18:o:83:TYR:HE1	1.86	0.41
9:V:72:THR:HB	9:V:92:GLY:HA2	2.01	0.41
18:o:73:TYR:CE2	18:o:77:LYS:HD2	2.56	0.41
1:4:148:LEU:HD22	1:4:177:MET:SD	2.61	0.40
1:4:241:ASP:OD1	1:4:241:ASP:N	2.55	0.40
10:W:81:ASP:OD1	10:W:81:ASP:N	2.53	0.40
38:c:35:ALA:O	38:c:103:TYR:HA	2.20	0.40
39:d:215:ILE:HD13	39:d:215:ILE:HA	1.93	0.40
3:H:24:GLU:HA	3:H:271:LEU:HD13	2.03	0.40
3:H:40:VAL:HG13	34:6:39:TRP:HE1	1.85	0.40
3:H:245:ALA:HB2	3:H:262:LYS:HE3	2.02	0.40
7:M:22:MET:O	7:M:26:ASN:ND2	2.53	0.40
8:N:102:LEU:HD13	8:N:142:LEU:HG	2.03	0.40
9:V:27:ILE:HD13	9:V:27:ILE:HA	1.90	0.40
22:s:4:LEU:HD21	25:v:124:THR:HA	2.04	0.40
31:2:159:ASN:HB3	31:2:184:PRO:HB3	2.04	0.40
32:3:249:ARG:HE	32:3:251:LEU:HD11	1.87	0.40
32:3:584:LYS:HE3	38:c:36:ARG:HD2	2.02	0.40
40:e:90:LEU:HA	40:e:93:VAL:HG12	2.04	0.40
1:4:175:GLU:HG2	34:6:66:ARG:HD2	2.03	0.40
2:A:104:TYR:CE2	4:J:166:VAL:HG22	2.56	0.40
6:L:313:MET:HA	6:L:316:THR:HG22	2.04	0.40
7:M:76:MET:HG2	7:M:229:MET:HE3	2.03	0.40
8:N:24:THR:HG22	15:l:2:PHE:HZ	1.85	0.40
10:W:19:LYS:HA	10:W:19:LYS:HD3	1.83	0.40
12:Y:56:LEU:HD21	20:q:83:LEU:HD12	2.03	0.40
13:Z:8:VAL:HG12	26:w:97:VAL:HG13	2.04	0.40
22:s:42:GLN:O	22:s:46:ASN:HB2	2.22	0.40
30:1:202:LYS:HA	30:1:203:PRO:HD3	1.93	0.40
30:1:392:LEU:HD23	30:1:419:ILE:HD11	2.02	0.40
34:6:91:THR:HA	34:6:119:CYS:HB3	2.04	0.40
41:f:39:LYS:HA	41:f:44:ARG:HD2	2.04	0.40
4:J:88:VAL:HG12	5:K:23:ARG:NH2	2.37	0.40
5:K:51:SER:O	5:K:51:SER:OG	2.38	0.40
23:t:126:LYS:HA	23:t:129:ARG:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:v:68:ASP:OD1	25:v:68:ASP:N	2.47	0.40
32:3:205:VAL:HG23	32:3:207:ALA:H	1.86	0.40
33:5:51:CYS:HB3	41:f:111:TRP:CE2	2.56	0.40
33:5:160:HIS:HA	33:5:161:PRO:HD3	1.89	0.40
34:6:175:ILE:HD13	34:6:175:ILE:HA	1.92	0.40
6:L:71:ILE:HD11	7:M:310:MET:SD	2.62	0.40
6:L:347:ILE:HD13	6:L:347:ILE:HA	1.91	0.40
45:X:101:ZMP:H5A	23:t:43:LEU:HD11	2.03	0.40
26:w:50:ASP:HA	26:w:51:PRO:HD3	1.95	0.40
32:3:192:MET:HA	32:3:192:MET:HE3	2.03	0.40
32:3:460:ARG:NH2	32:3:462:ASP:OD2	2.54	0.40
38:c:66:GLU:H	38:c:66:GLU:HG3	1.73	0.40
40:e:39:ARG:NH1	40:e:87:THR:OG1	2.55	0.40
42:g:75:PRO:O	42:g:79:ASP:HB2	2.22	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	4	414/463 (89%)	398 (96%)	16 (4%)	0	100	100
2	A	106/115 (92%)	98 (92%)	8 (8%)	0	100	100
3	H	310/318 (98%)	301 (97%)	9 (3%)	0	100	100
4	J	165/175 (94%)	157 (95%)	8 (5%)	0	100	100
5	K	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
6	L	604/606 (100%)	576 (95%)	28 (5%)	0	100	100
7	M	457/459 (100%)	446 (98%)	11 (2%)	0	100	100
8	N	345/347 (99%)	335 (97%)	10 (3%)	0	100	100
9	V	138/140 (99%)	137 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	W	137/139 (99%)	137 (100%)	0	0	100	100
11	X	85/157 (54%)	79 (93%)	6 (7%)	0	100	100
11	j	80/157 (51%)	79 (99%)	1 (1%)	0	100	100
12	Y	169/171 (99%)	164 (97%)	5 (3%)	0	100	100
13	Z	169/171 (99%)	167 (99%)	2 (1%)	0	100	100
14	k	317/320 (99%)	308 (97%)	9 (3%)	0	100	100
15	l	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
16	m	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
17	n	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
18	o	118/120 (98%)	116 (98%)	2 (2%)	0	100	100
19	p	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
20	q	137/144 (95%)	134 (98%)	2 (2%)	1 (1%)	18	52
21	r	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
22	s	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
23	t	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
24	u	63/65 (97%)	62 (98%)	1 (2%)	0	100	100
25	v	153/155 (99%)	147 (96%)	6 (4%)	0	100	100
26	w	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
27	x	47/49 (96%)	47 (100%)	0	0	100	100
28	y	48/50 (96%)	48 (100%)	0	0	100	100
29	z	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
30	1	428/430 (100%)	419 (98%)	9 (2%)	0	100	100
31	2	211/213 (99%)	194 (92%)	17 (8%)	0	100	100
32	3	686/688 (100%)	661 (96%)	25 (4%)	0	100	100
33	5	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
34	6	154/156 (99%)	150 (97%)	4 (3%)	0	100	100
35	9	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
36	a	42/44 (96%)	42 (100%)	0	0	100	100
37	b	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
38	c	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
39	d	289/380 (76%)	285 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	e	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	f	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
42	g	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
43	h	92/114 (81%)	91 (99%)	1 (1%)	0	100	100
44	i	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
All	All	8048/8497 (95%)	7793 (97%)	254 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	q	26	ARG

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	4	363/391 (93%)	362 (100%)	1 (0%)	86	85
2	A	99/103 (96%)	98 (99%)	1 (1%)	68	75
3	H	274/278 (99%)	272 (99%)	2 (1%)	76	78
4	J	138/144 (96%)	138 (100%)	0	100	100
5	K	86/86 (100%)	86 (100%)	0	100	100
6	L	538/538 (100%)	536 (100%)	2 (0%)	84	83
7	M	411/411 (100%)	411 (100%)	0	100	100
8	N	315/315 (100%)	315 (100%)	0	100	100
9	V	101/101 (100%)	100 (99%)	1 (1%)	68	75
10	W	122/122 (100%)	122 (100%)	0	100	100
11	X	80/141 (57%)	80 (100%)	0	100	100
11	j	76/141 (54%)	75 (99%)	1 (1%)	61	71
12	Y	154/154 (100%)	154 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	Z	155/155 (100%)	155 (100%)	0	100	100
14	k	283/283 (100%)	283 (100%)	0	100	100
15	l	94/94 (100%)	93 (99%)	1 (1%)	65	73
16	m	69/69 (100%)	69 (100%)	0	100	100
17	n	61/61 (100%)	61 (100%)	0	100	100
18	o	107/107 (100%)	107 (100%)	0	100	100
19	p	114/114 (100%)	114 (100%)	0	100	100
20	q	119/122 (98%)	118 (99%)	1 (1%)	73	77
21	r	95/122 (78%)	95 (100%)	0	100	100
22	s	110/110 (100%)	110 (100%)	0	100	100
23	t	159/159 (100%)	159 (100%)	0	100	100
24	u	59/59 (100%)	59 (100%)	0	100	100
25	v	140/140 (100%)	140 (100%)	0	100	100
26	w	92/92 (100%)	91 (99%)	1 (1%)	65	73
27	x	44/44 (100%)	44 (100%)	0	100	100
28	y	46/46 (100%)	45 (98%)	1 (2%)	45	64
29	z	59/59 (100%)	59 (100%)	0	100	100
30	1	344/344 (100%)	344 (100%)	0	100	100
31	2	183/183 (100%)	181 (99%)	2 (1%)	65	73
32	3	578/578 (100%)	578 (100%)	0	100	100
33	5	189/189 (100%)	189 (100%)	0	100	100
34	6	132/132 (100%)	132 (100%)	0	100	100
35	9	151/151 (100%)	150 (99%)	1 (1%)	76	78
36	a	43/43 (100%)	43 (100%)	0	100	100
37	b	79/79 (100%)	79 (100%)	0	100	100
38	c	113/113 (100%)	113 (100%)	0	100	100
39	d	255/326 (78%)	254 (100%)	1 (0%)	84	83
40	e	76/76 (100%)	76 (100%)	0	100	100
41	f	101/101 (100%)	101 (100%)	0	100	100
42	g	107/107 (100%)	107 (100%)	0	100	100
43	h	84/96 (88%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	i	131/131 (100%)	130 (99%)	1 (1%)	73	77
All	All	7129/7410 (96%)	7112 (100%)	17 (0%)	85	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4	178	PHE
2	A	10	ASN
3	H	305	VAL
3	H	314	ILE
6	L	70	THR
6	L	395	ILE
9	V	79	VAL
15	l	9	LEU
20	q	27	ARG
26	w	36	ASN
28	y	43	LEU
31	2	47	VAL
31	2	89	MET
35	9	145	GLU
39	d	57	MET
44	i	32	ASP
11	j	14	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	4	54	GLN
1	4	79	HIS
1	4	149	ASN
1	4	237	ASN
5	K	97	GLN
6	L	109	HIS
6	L	113	ASN
6	L	165	ASN
6	L	192	ASN
6	L	296	ASN
6	L	471	ASN
6	L	479	GLN
6	L	506	ASN
6	L	603	ASN

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Mol	Chain	Res	Type
7	M	220	HIS
7	M	374	ASN
7	M	422	HIS
8	N	112	HIS
8	N	144	GLN
8	N	289	ASN
10	W	124	GLN
10	W	143	ASN
11	X	47	GLN
12	Y	34	GLN
12	Y	39	ASN
12	Y	142	HIS
13	Z	54	GLN
13	Z	58	ASN
13	Z	133	GLN
14	k	97	GLN
14	k	114	HIS
14	k	180	GLN
14	k	184	GLN
14	k	287	HIS
19	p	51	ASN
22	s	54	GLN
23	t	12	GLN
23	t	50	HIS
24	u	42	HIS
25	v	104	HIS
26	w	41	ASN
29	z	27	HIS
30	1	257	ASN
30	1	264	ASN
31	2	55	GLN
31	2	155	GLN
32	3	117	GLN
34	6	94	ASN
35	9	170	GLN
36	a	65	GLN
39	d	87	HIS
39	d	103	ASN
39	d	184	ASN
39	d	243	GLN
40	e	47	ASN
42	g	107	HIS

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Mol	Chain	Res	Type
42	g	125	HIS
44	i	113	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	AYA	V	1	9	6,7,8	1.22	1 (16%)	6,8,10	1.52	2 (33%)
5	FME	K	1	5	8,9,10	0.98	0	8,9,11	0.82	0
14	SEP	k	36	14	8,9,10	1.60	1 (12%)	7,12,14	1.37	1 (14%)
1	2MR	4	85	1	10,12,13	2.53	2 (20%)	5,13,15	0.99	0
6	FME	L	1	6	8,9,10	0.98	0	8,9,11	0.84	0
43	AYA	h	1	43	6,7,8	1.26	1 (16%)	6,8,10	1.25	1 (16%)
7	FME	M	1	7	8,9,10	1.00	0	8,9,11	0.92	0

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
9	AYA	V	1	9	-	2/5/6/8	-
5	FME	K	1	5	-	3/7/9/11	-
14	SEP	k	36	14	-	4/6/8/10	-
1	2MR	4	85	1	-	2/10/13/15	-
6	FME	L	1	6	-	1/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	AYA	h	1	43	-	0/5/6/8	-
7	FME	M	1	7	-	3/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	85	2MR	CZ-NH2	5.45	1.44	1.33
1	4	85	2MR	CZ-NE	5.25	1.45	1.34
14	k	36	SEP	P-O1P	3.54	1.61	1.50
43	h	1	AYA	CA-N	-2.34	1.44	1.46
9	V	1	AYA	CA-N	-2.08	1.44	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	k	36	SEP	OG-CB-CA	3.02	111.08	108.14
43	h	1	AYA	CB-CA-N	2.80	112.84	109.68
9	V	1	AYA	CB-CA-N	2.71	112.74	109.68
9	V	1	AYA	CA-N-CT	2.10	124.21	121.50

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	FME	O-C-CA-CB
7	M	1	FME	O-C-CA-CB
14	k	36	SEP	CB-OG-P-O1P
14	k	36	SEP	CB-OG-P-O2P
14	k	36	SEP	CB-OG-P-O3P
6	L	1	FME	CA-CB-CG-SD
9	V	1	AYA	OT-CT-N-CA
9	V	1	AYA	CM-CT-N-CA
5	K	1	FME	N-CA-CB-CG
1	4	85	2MR	C-CA-CB-CG
14	k	36	SEP	CA-CB-OG-P
1	4	85	2MR	CA-CB-CG-CD
7	M	1	FME	C-CA-CB-CG
5	K	1	FME	CB-CA-N-CN
7	M	1	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	FME	2	0
43	h	1	AYA	1	0
7	M	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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
46	AMP	k	501	-	25,25,25	1.42	4 (16%)	37,38,38	2.06	7 (18%)
48	SF4	9	202	35	0,12,12	-	-	-		
48	SF4	1	501	30	0,12,12	-	-	-		
51	FES	2	300	31	0,4,4	-	-	-		
50	NAI	1	503	-	47,48,48	0.42	1 (2%)	64,73,73	1.78	4 (6%)
45	ZMP	j	101	11	28,33,36	0.69	1 (3%)	32,40,45	1.00	1 (3%)
47	MYR	s	201	22	13,14,15	0.17	0	12,13,15	0.13	0
48	SF4	3	802	32	0,12,12	-	-	-		
45	ZMP	X	101	11	25,30,36	0.70	1 (4%)	29,37,45	0.98	1 (3%)
49	FMN	1	502	-	33,33,33	1.04	2 (6%)	48,50,50	1.25	8 (16%)
48	SF4	9	201	35	0,12,12	-	-	-		
51	FES	3	803	32	0,4,4	-	-	-		
48	SF4	3	801	32	0,12,12	-	-	-		
48	SF4	6	300	34	0,12,12	-	-	-		
54	NDP	d	401	-	51,52,52	0.32	0	71,80,80	0.34	0

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
46	AMP	k	501	-	-	9/10/26/26	0/3/3/3
48	SF4	9	202	35	-	-	0/6/5/5
48	SF4	1	501	30	-	-	0/6/5/5
51	FES	2	300	31	-	-	0/1/1/1
50	NAI	1	503	-	-	9/29/72/72	0/5/5/5
45	ZMP	j	101	11	-	4/38/40/43	-
47	MYR	s	201	22	-	1/12/12/13	-
48	SF4	3	802	32	-	-	0/6/5/5
45	ZMP	X	101	11	-	15/35/37/43	-
49	FMN	1	502	-	-	7/18/18/18	0/3/3/3
48	SF4	9	201	35	-	-	0/6/5/5
51	FES	3	803	32	-	-	0/1/1/1
48	SF4	3	801	32	-	-	0/6/5/5
48	SF4	6	300	34	-	-	0/6/5/5
54	NDP	d	401	-	-	9/34/77/77	0/5/5/5

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	k	501	AMP	C5-C4	4.91	1.47	1.39
49	1	502	FMN	C4A-N5	3.26	1.37	1.30
46	k	501	AMP	C5-C6	2.66	1.48	1.41
45	j	101	ZMP	C9-C10	2.54	1.53	1.50
46	k	501	AMP	C5-N7	-2.47	1.34	1.39
49	1	502	FMN	C10-N1	2.43	1.38	1.33
50	1	503	NAI	PA-O5B	2.20	1.68	1.59
45	X	101	ZMP	C9-C10	2.17	1.53	1.50
46	k	501	AMP	C8-N7	2.08	1.35	1.31

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	503	NAI	O5B-PA-O1A	-9.54	71.11	108.94
50	1	503	NAI	O2A-PA-O1A	-8.22	74.23	112.44
46	k	501	AMP	C5-C4-N3	-7.04	117.03	126.72
50	1	503	NAI	O3-PA-O1A	-5.78	93.31	110.70
46	k	501	AMP	N3-C4-N9	5.77	136.98	127.17
46	k	501	AMP	C2-N3-C4	4.14	121.95	111.83
49	1	502	FMN	C4-N3-C2	-3.32	119.75	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	k	501	AMP	N3-C2-N1	-3.27	123.62	128.58
46	k	501	AMP	C4-C5-N7	-3.05	107.10	110.58
49	1	502	FMN	C4A-C10-N10	2.75	120.41	116.48
45	X	101	ZMP	O1-C10-C9	-2.72	120.84	123.98
45	j	101	ZMP	O1-C10-C9	-2.62	120.96	123.98
49	1	502	FMN	C4A-C4-N3	2.62	119.91	113.25
49	1	502	FMN	O4-C4-C4A	-2.51	119.90	126.53
50	1	503	NAI	O2A-PA-O5B	2.47	118.75	107.57
46	k	501	AMP	C1'-N9-C8	-2.44	121.69	127.09
49	1	502	FMN	C10-C4A-N5	-2.31	120.09	124.81
46	k	501	AMP	C5-N7-C8	2.29	107.05	103.45
49	1	502	FMN	C4A-C10-N1	-2.15	119.33	124.59
49	1	502	FMN	C5A-C9A-N10	2.11	119.88	117.97
49	1	502	FMN	C9A-C5A-N5	-2.04	120.29	122.45

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	X	101	ZMP	C17-C18-C21-O5
45	X	101	ZMP	O4-C17-C18-C21
45	X	101	ZMP	C16-C17-C18-C21
45	X	101	ZMP	O3-C16-C17-O4
45	X	101	ZMP	C17-C16-N2-C15
45	X	101	ZMP	C12-C11-S1-C10
45	j	101	ZMP	S1-C11-C12-N1
46	k	501	AMP	C5'-O5'-P-O1P
46	k	501	AMP	C5'-O5'-P-O2P
46	k	501	AMP	C5'-O5'-P-O3P
47	s	201	MYR	C1-C2-C3-C4
49	1	502	FMN	N10-C1'-C2'-O2'
49	1	502	FMN	N10-C1'-C2'-C3'
49	1	502	FMN	C5'-O5'-P-O2P
49	1	502	FMN	C5'-O5'-P-O3P
50	1	503	NAI	C5B-O5B-PA-O1A
50	1	503	NAI	PN-O3-PA-O5B
50	1	503	NAI	C5D-O5D-PN-O3
50	1	503	NAI	C2D-C1D-N1N-C6N
54	d	401	NDP	C2N-C3N-C7N-N7N
45	X	101	ZMP	O3-C16-N2-C15
50	1	503	NAI	C2D-C1D-N1N-C2N
46	k	501	AMP	C3'-C4'-C5'-O5'

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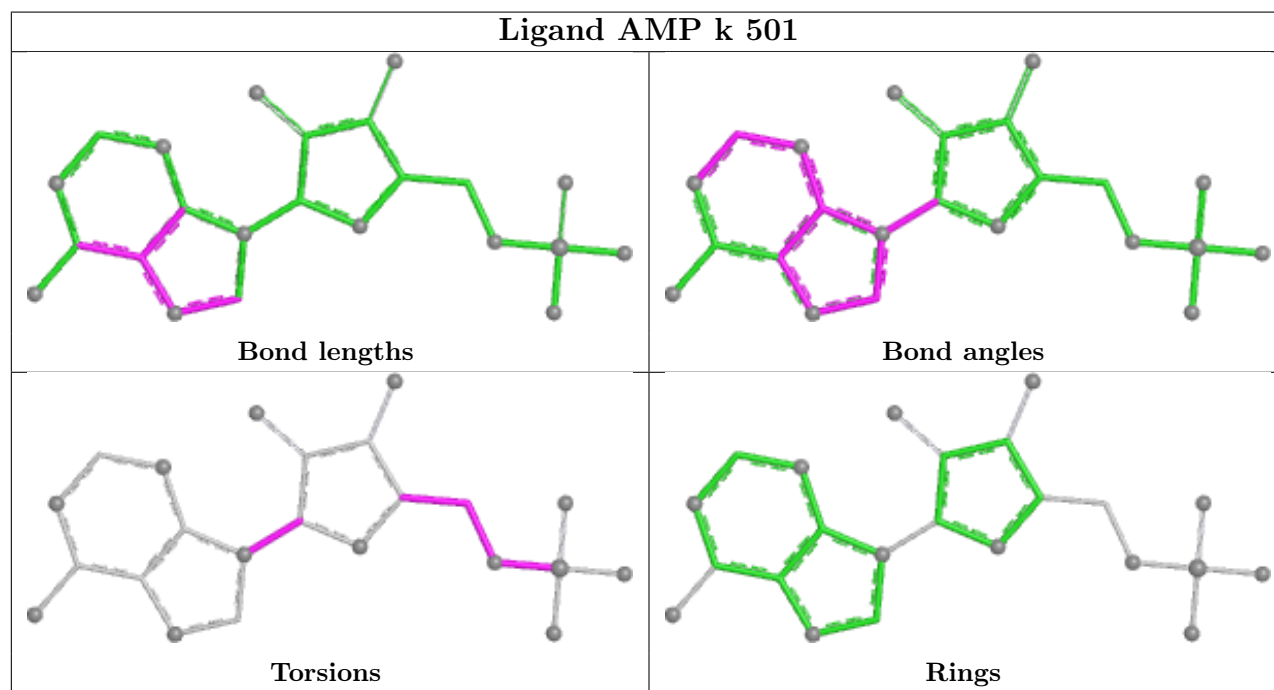
Mol	Chain	Res	Type	Atoms
49	1	502	FMN	C5'-O5'-P-O1P
46	k	501	AMP	O4'-C4'-C5'-O5'
45	X	101	ZMP	O1-C10-S1-C11
45	j	101	ZMP	O1-C10-S1-C11
45	X	101	ZMP	C9-C10-S1-C11
45	j	101	ZMP	C9-C10-S1-C11
45	X	101	ZMP	C16-C17-C18-C20
54	d	401	NDP	PN-O3-PA-O1A
45	X	101	ZMP	C19-C18-C21-O5
45	X	101	ZMP	C20-C18-C21-O5
54	d	401	NDP	C2N-C3N-C7N-O7N
46	k	501	AMP	C2'-C1'-N9-C4
50	1	503	NAI	O4D-C1D-N1N-C6N
50	1	503	NAI	C4D-C5D-O5D-PN
46	k	501	AMP	C2'-C1'-N9-C8
50	1	503	NAI	O4D-C1D-N1N-C2N
50	1	503	NAI	C2N-C3N-C7N-N7N
54	d	401	NDP	O4D-C1D-N1N-C6N
54	d	401	NDP	C2D-C1D-N1N-C6N
49	1	502	FMN	O2'-C2'-C3'-C4'
45	X	101	ZMP	C16-C17-C18-C19
49	1	502	FMN	O2'-C2'-C3'-O3'
54	d	401	NDP	C3B-C2B-O2B-P2B
45	X	101	ZMP	O4-C17-C18-C19
54	d	401	NDP	PN-O3-PA-O2A
46	k	501	AMP	O4'-C1'-N9-C8
54	d	401	NDP	C1B-C2B-O2B-P2B
54	d	401	NDP	O4B-C4B-C5B-O5B
45	X	101	ZMP	N2-C16-C17-O4
45	j	101	ZMP	N2-C16-C17-O4
46	k	501	AMP	C4'-C5'-O5'-P

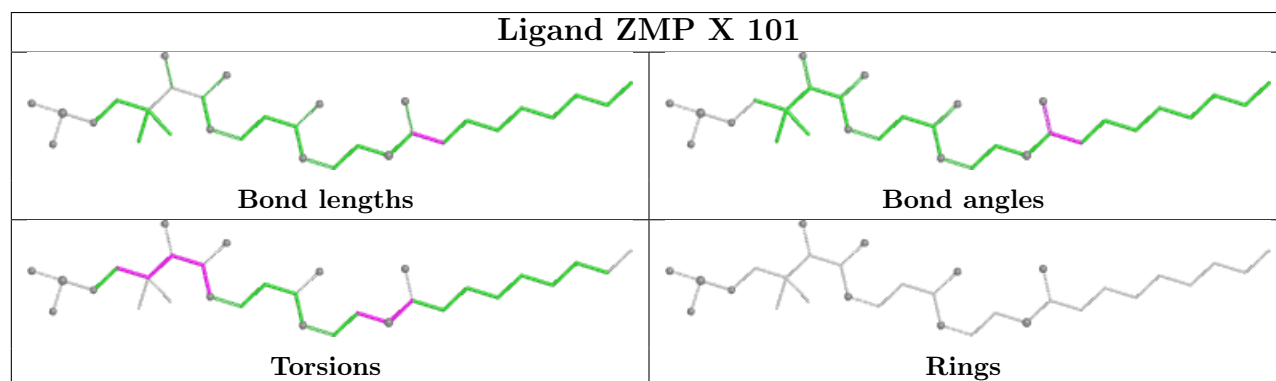
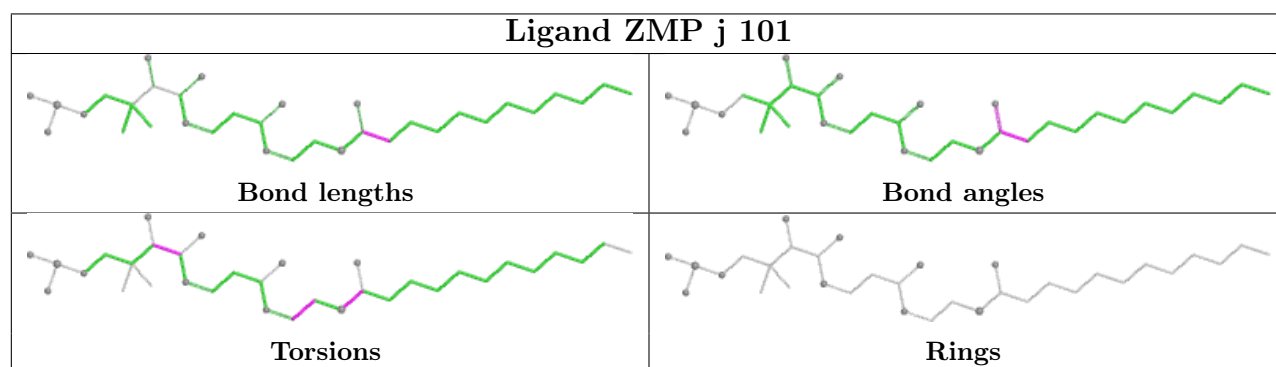
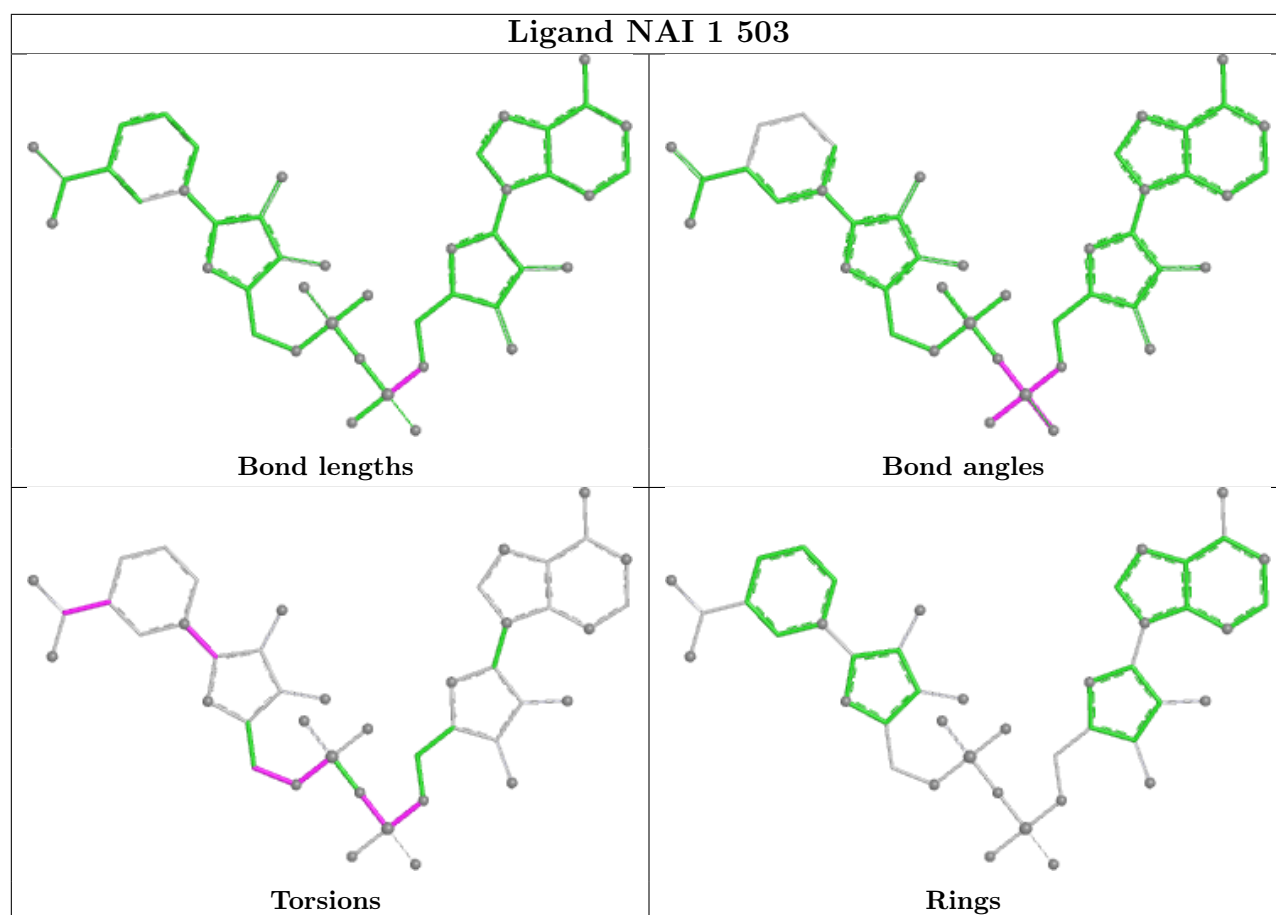
There are no ring outliers.

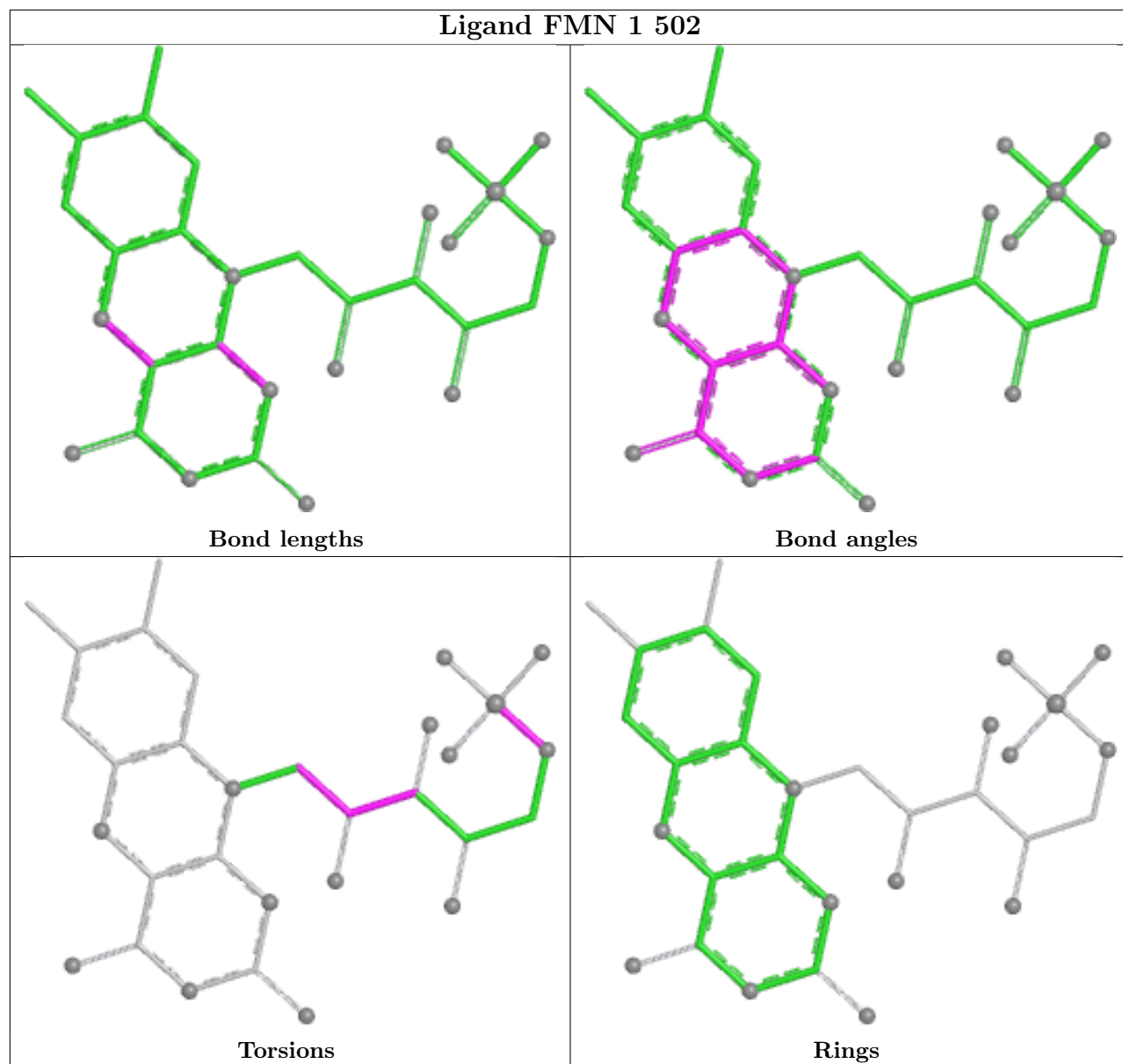
5 monomers are involved in 10 short contacts:

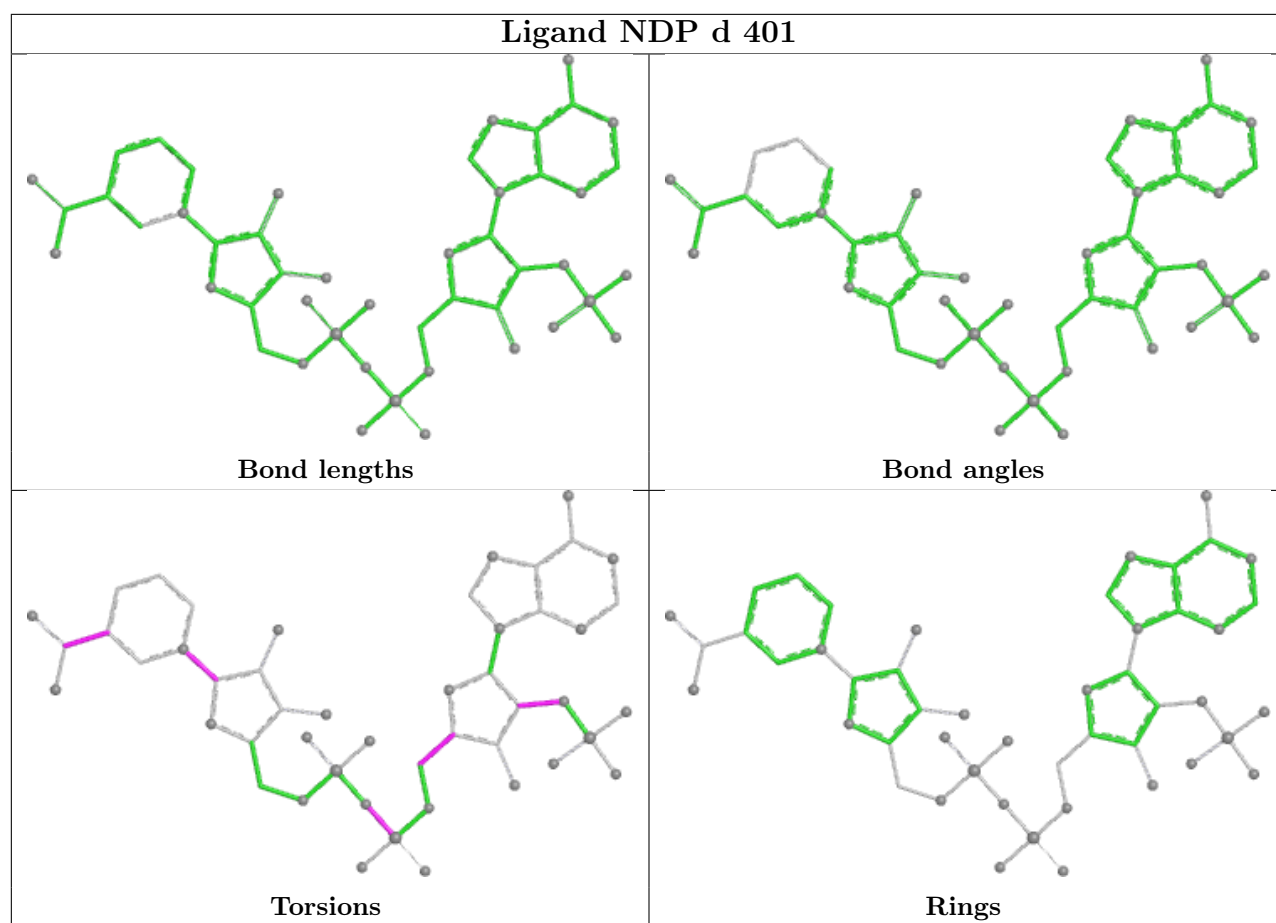
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	k	501	AMP	1	0
50	1	503	NAI	4	0
45	X	101	ZMP	1	0
48	3	801	SF4	2	0
54	d	401	NDP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

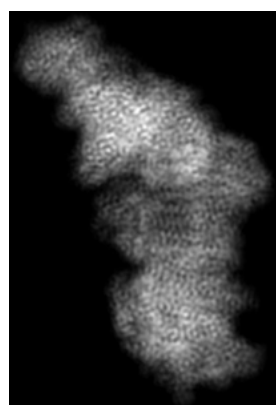
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14664. These allow visual inspection of the internal detail of the map and identification of artifacts.

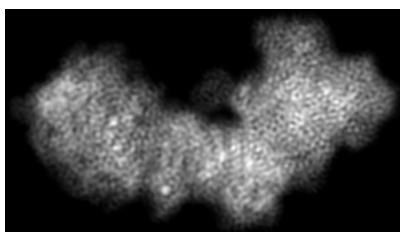
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

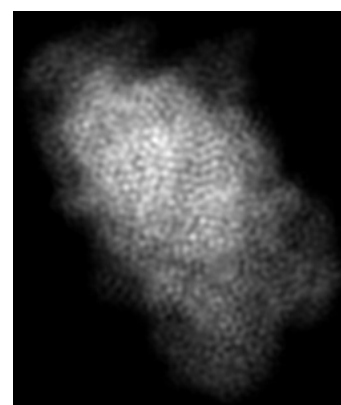
6.1.1 Primary map



X



Y



Z

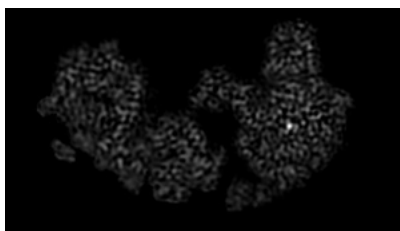
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 67



Y Index: 80

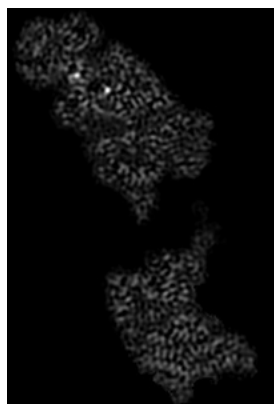


Z Index: 119

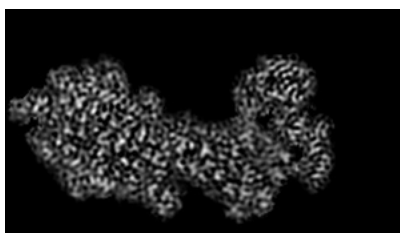
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

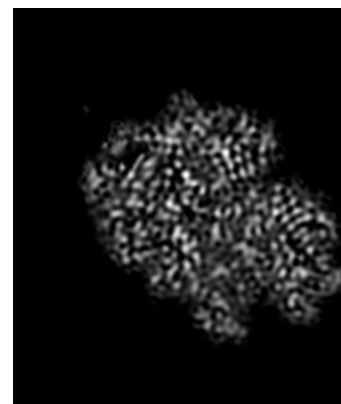
6.3.1 Primary map



X Index: 79



Y Index: 103

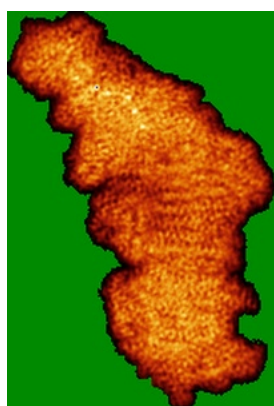


Z Index: 172

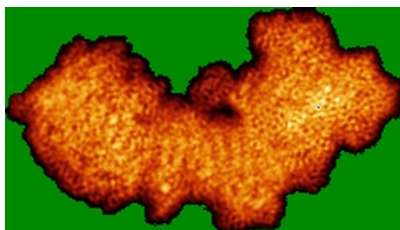
The images above show the largest variance slices of the map in three orthogonal directions.

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

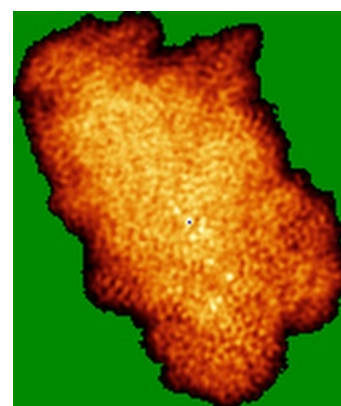
6.4.1 Primary map



X



Y

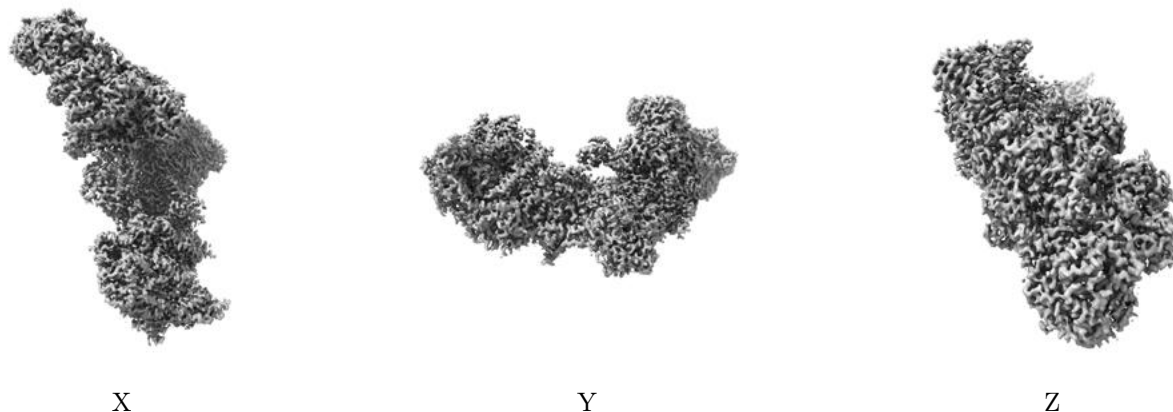


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

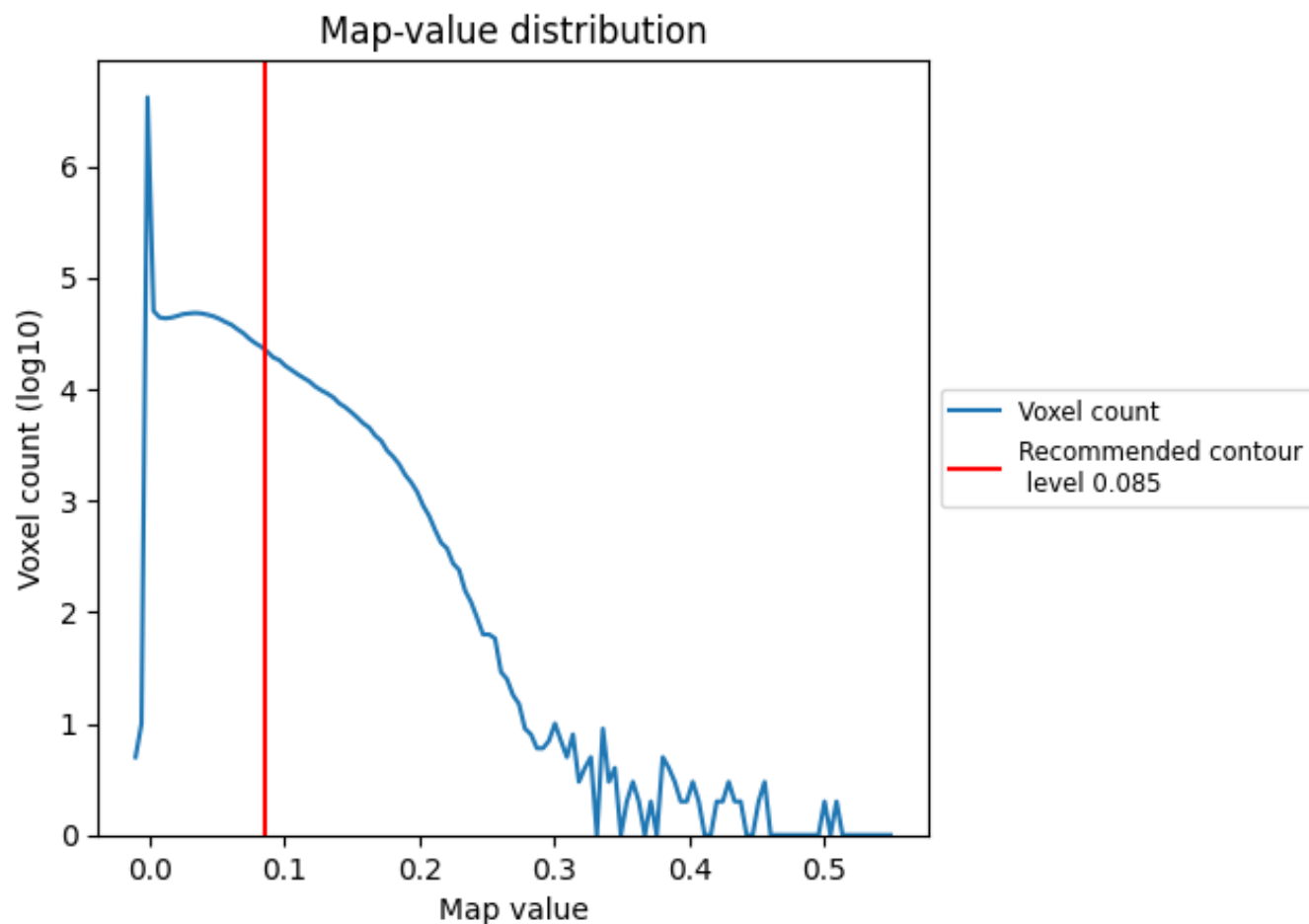
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

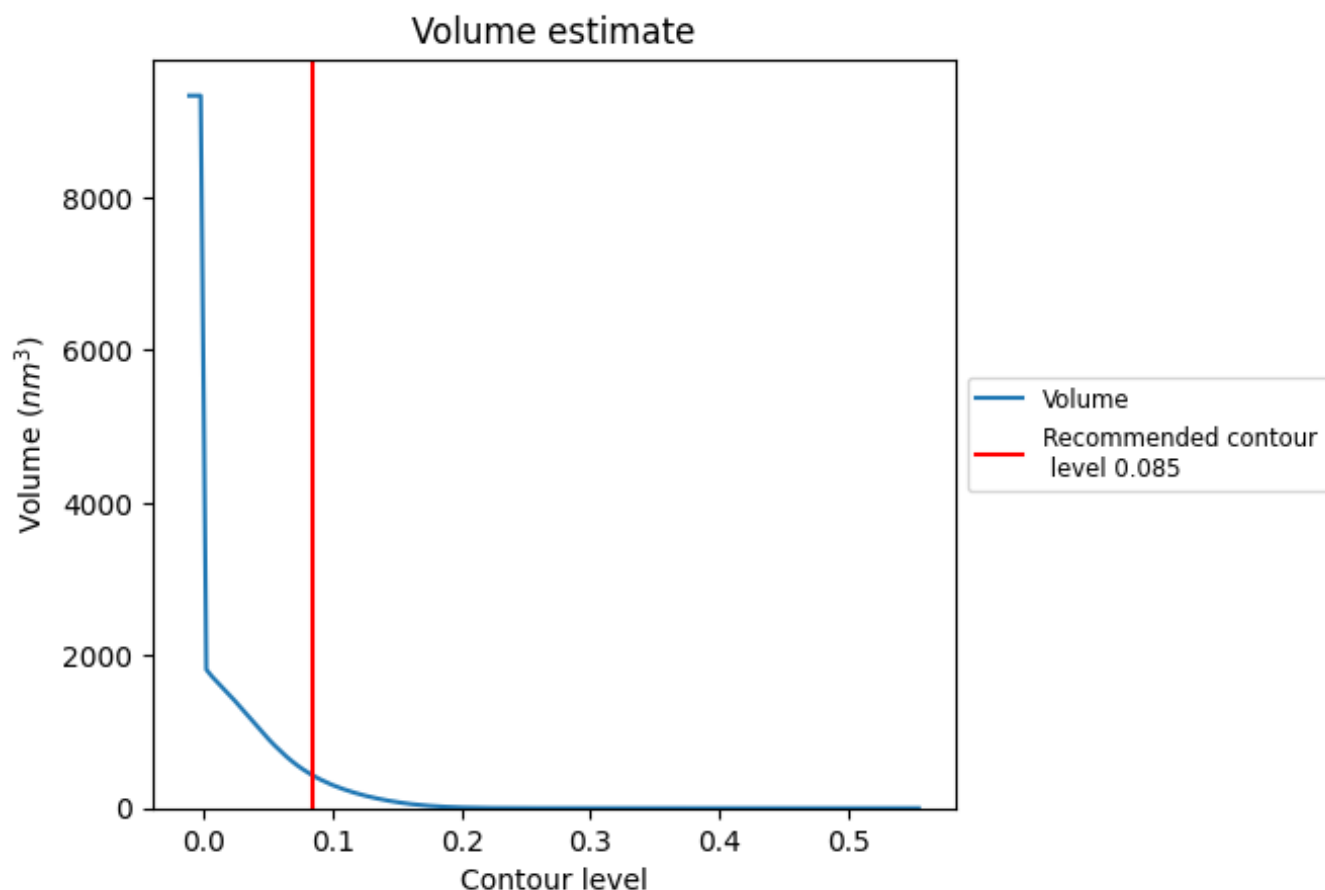
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 430 nm³; this corresponds to an approximate mass of 389 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.

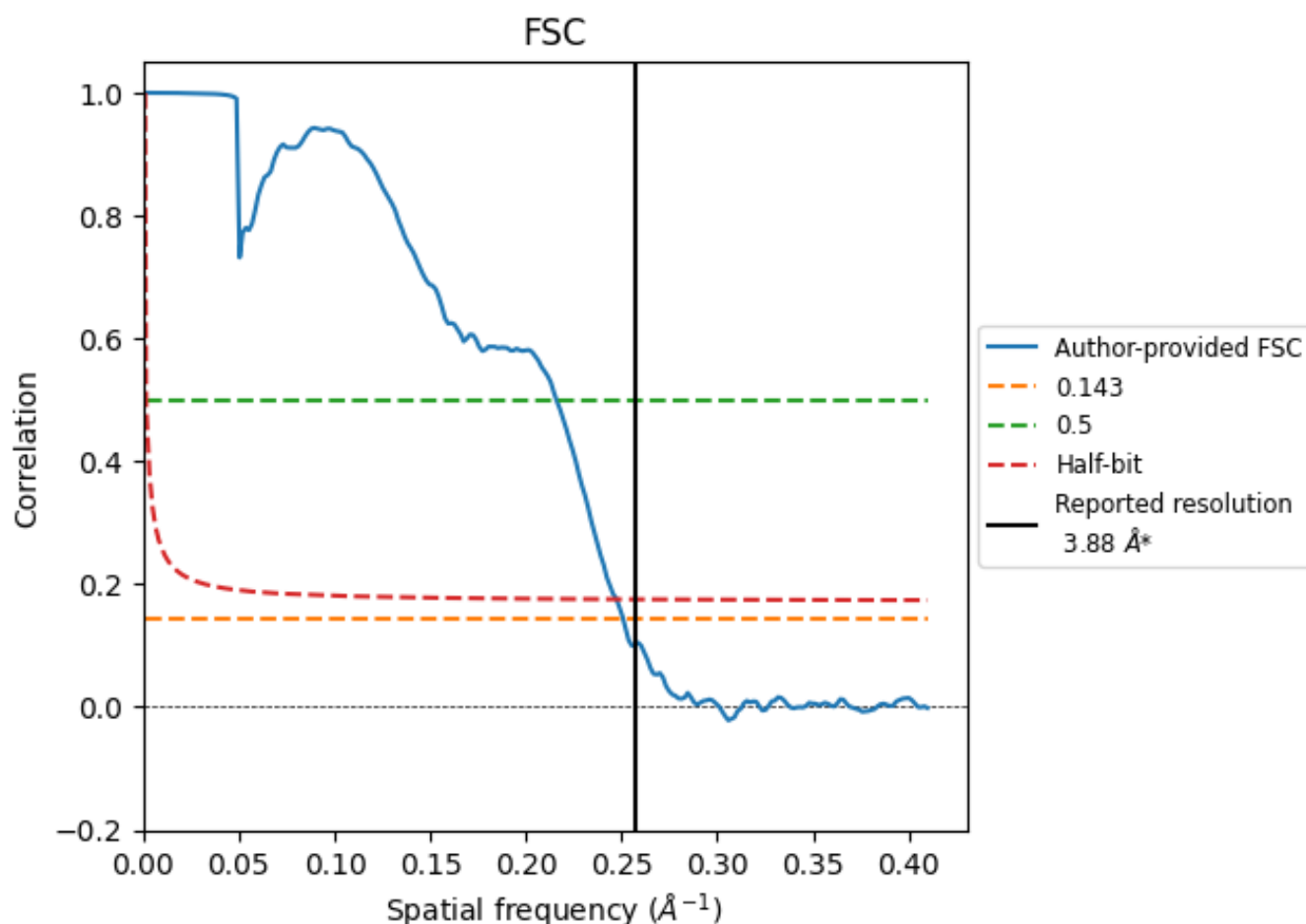
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.258 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

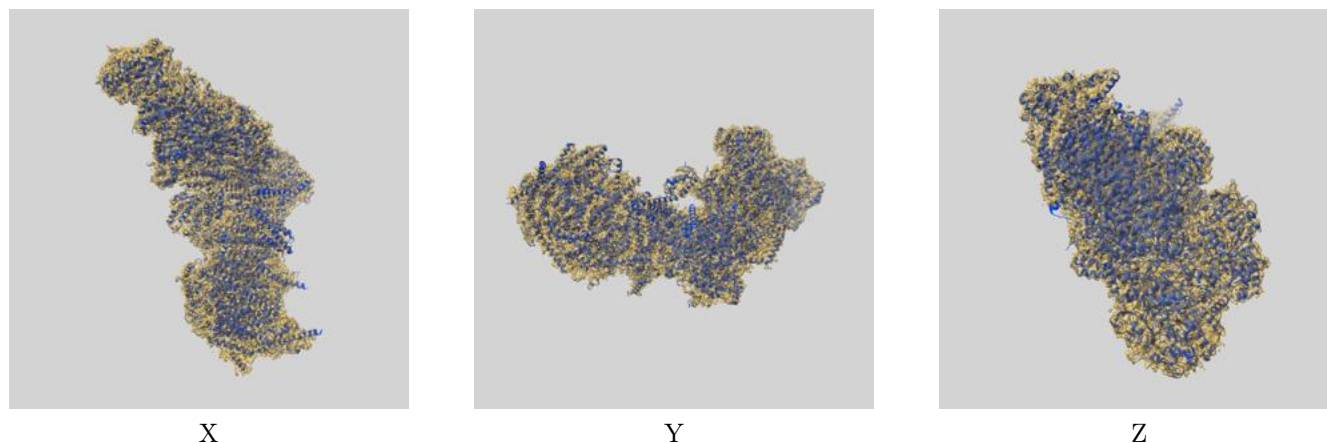
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.88	-	-
Author-provided FSC curve	3.99	4.63	4.04
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

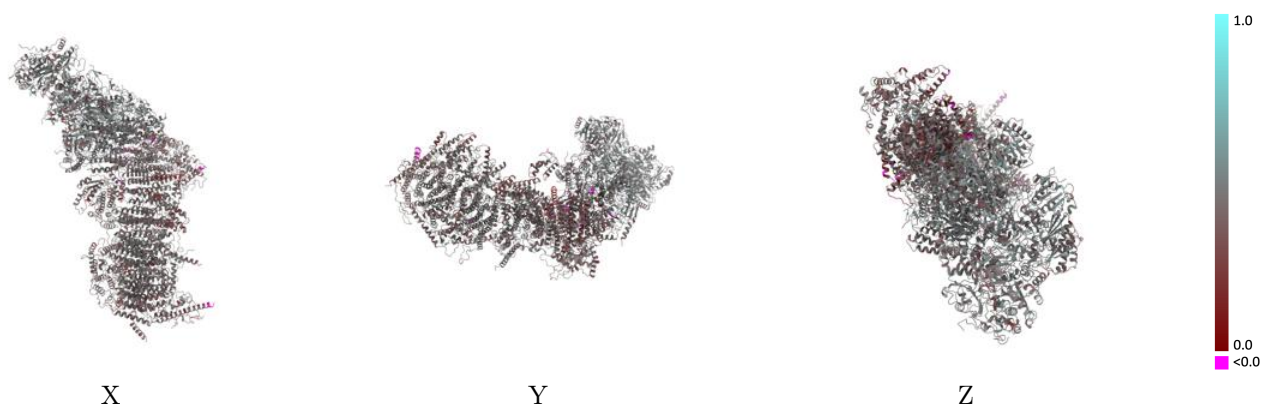
This section contains information regarding the fit between EMDB map EMD-14664 and PDB model 7ZDP. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



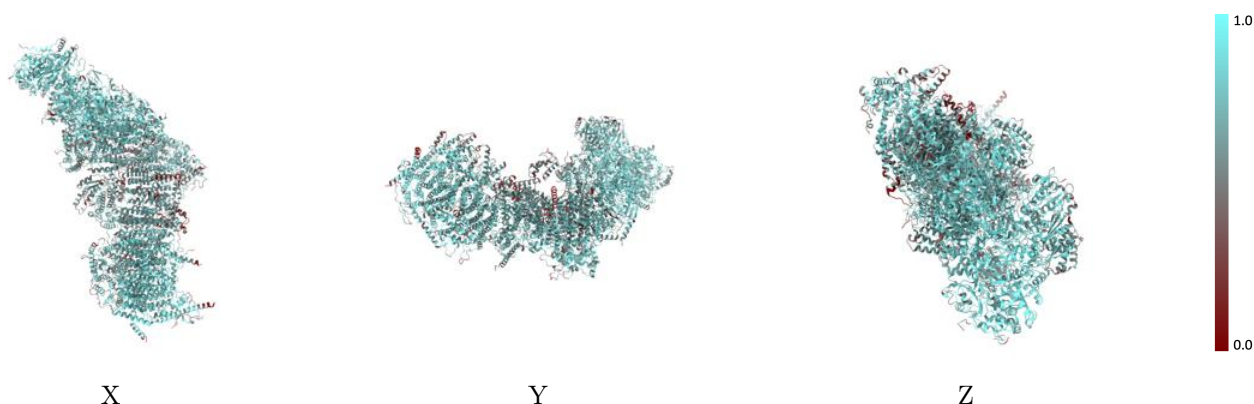
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



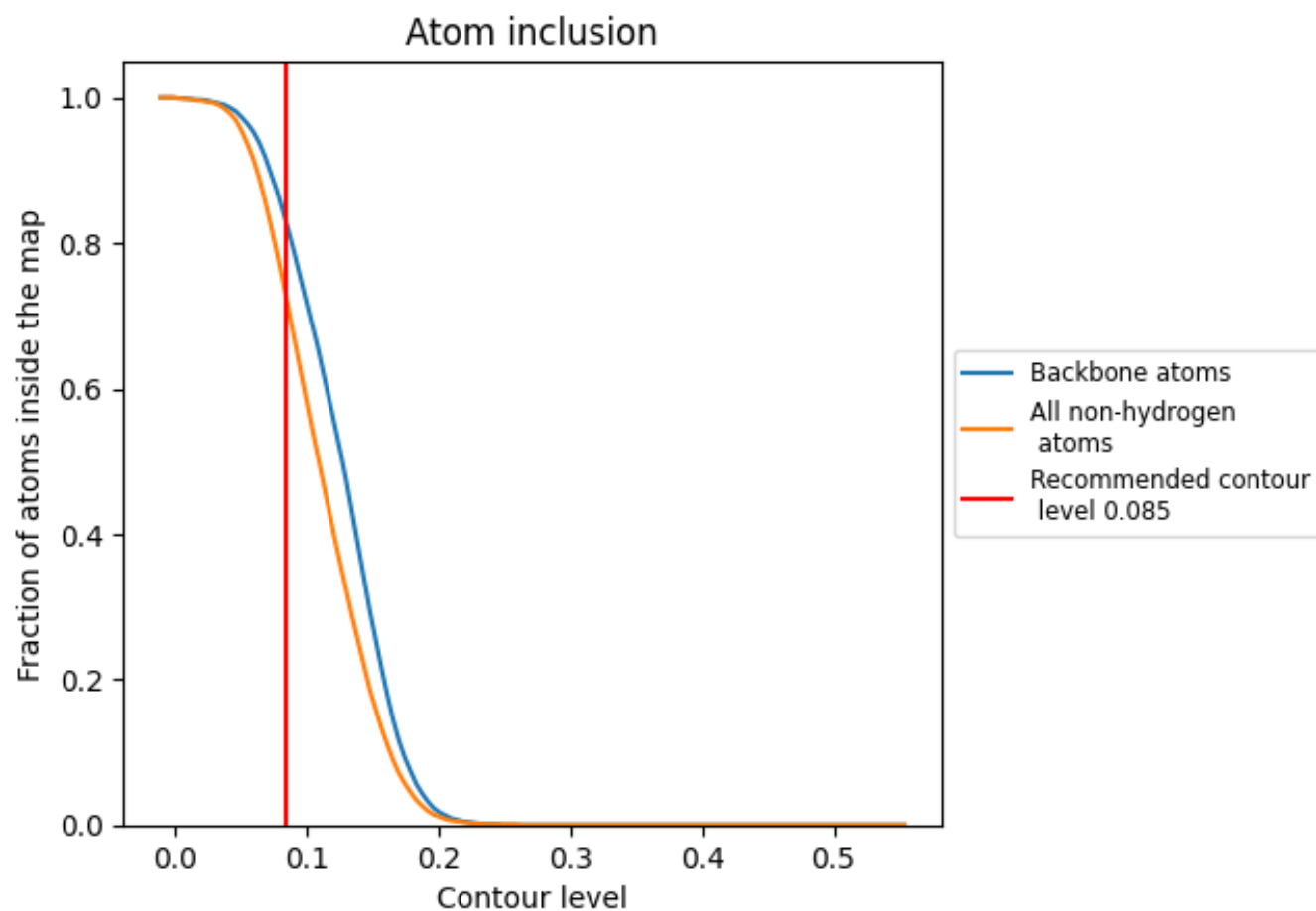
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7240	 0.4370
1	 0.8020	 0.4610
2	 0.7610	 0.4610
3	 0.7710	 0.4740
4	 0.7750	 0.4790
5	 0.7940	 0.4880
6	 0.8320	 0.4750
9	 0.7780	 0.4480
A	 0.5640	 0.3410
H	 0.6670	 0.3620
J	 0.6060	 0.3540
K	 0.6920	 0.4060
L	 0.7950	 0.4290
M	 0.8040	 0.4490
N	 0.7570	 0.4370
V	 0.4590	 0.3740
W	 0.7470	 0.4440
X	 0.6280	 0.4060
Y	 0.6700	 0.4180
Z	 0.7330	 0.4230
a	 0.8070	 0.4520
b	 0.7350	 0.4930
c	 0.7520	 0.4820
d	 0.7160	 0.4660
e	 0.6320	 0.4560
f	 0.6670	 0.4460
g	 0.6810	 0.4600
h	 0.7000	 0.4740
i	 0.7660	 0.4850
j	 0.4310	 0.3750
k	 0.6280	 0.4130
l	 0.6670	 0.4050
m	 0.5830	 0.3900
n	 0.6050	 0.3860
o	 0.7110	 0.4360



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Chain	Atom inclusion	Q-score
p	 0.7120	 0.4350
q	 0.6730	 0.3950
r	 0.6800	 0.4240
s	 0.7040	 0.3760
t	 0.6950	 0.4230
u	 0.7700	 0.4160
v	 0.7680	 0.4470
w	 0.6780	 0.4390
x	 0.6450	 0.4310
y	 0.6050	 0.4170
z	 0.7540	 0.3990