



Full wwPDB EM Validation Report ⓘ

Mar 30, 2026 – 02:14 AM UTC

PDB ID : 7ZEB / pdb_00007zeb
EMDB ID : EMD-14688
Title : Complex I from Ovis aries at pH9, Closed state
Authors : Sazanov, L.; Petrova, O.
Deposited on : 2022-03-30
Resolution : 3.80 Å(reported)
Based on initial model : 6ZKC

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

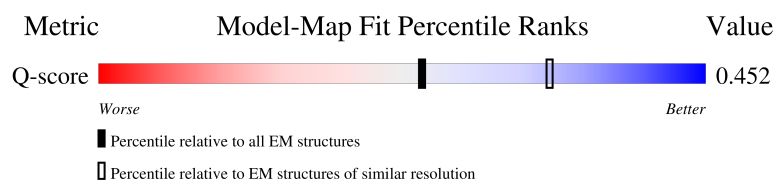
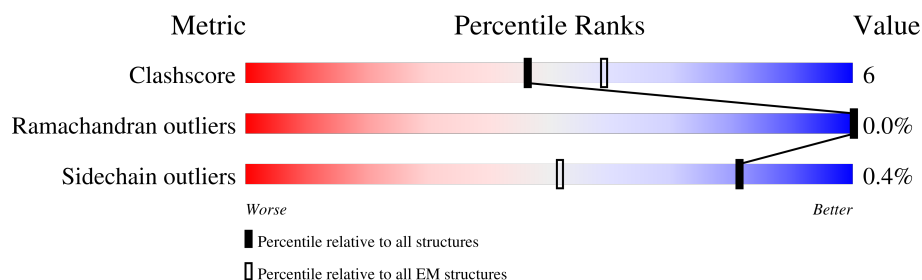
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



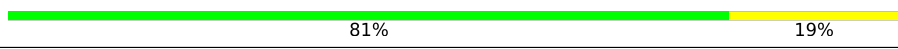
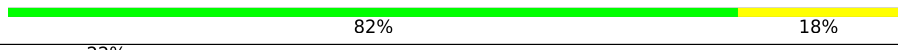
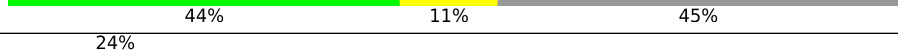
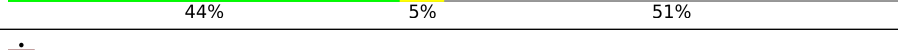
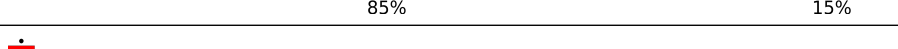
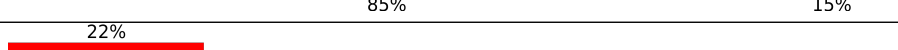
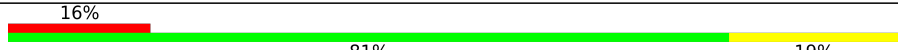
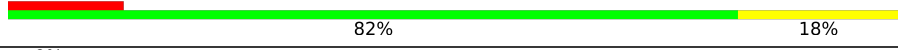
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	430	
2	A	115	
3	H	318	
4	J	175	

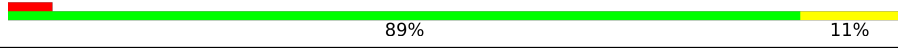
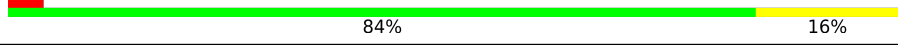
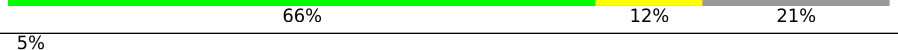
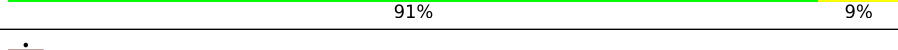
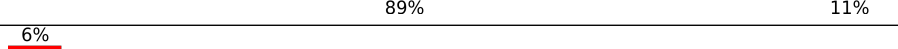
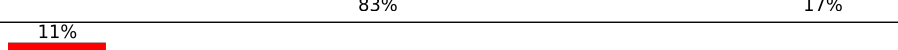
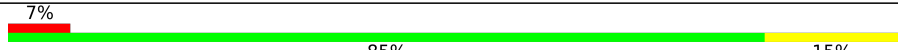
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Mol	Chain	Length	Quality of chain
5	K	98	
6	L	606	
7	M	459	
8	N	347	
9	V	140	
10	W	139	
11	X	157	
11	j	157	
12	Y	171	
13	Z	171	
14	k	320	
15	l	105	
16	m	80	
17	n	79	
18	o	120	
19	p	128	
20	q	139	
21	r	126	
22	s	122	
23	t	177	
24	u	65	
25	v	155	
26	w	101	
27	x	49	
28	y	50	

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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	150	
35	9	217	
36	a	44	
37	b	95	
38	c	126	
39	d	340	
40	e	86	
41	f	113	
42	g	114	
43	h	112	
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
49	SF4	3	801	-	-	X	-

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 66396 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4	423	Total	C	N	O	S	0	0
			3404	2172	586	621	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	115	Total	C	N	O	S	0	0
			922	621	133	161	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	318	Total	C	N	O	S	0	0
			2528	1704	384	421	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	175	Total	C	N	O	S	0	0
			1344	904	192	235	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
			4807	3188	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	77	Total	C	N	O	S	0	0
			619	399	92	123	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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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 NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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 NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	6	150	Total	C	N	O	S	0	0
			1198	765	216	203	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	171	Total	C	N	O	S	0	0
			1376	867	238	260	11		

- 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	331	Total	C	N	O	S	0	0
			2662	1715	474	468	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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-

unit 5.

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		

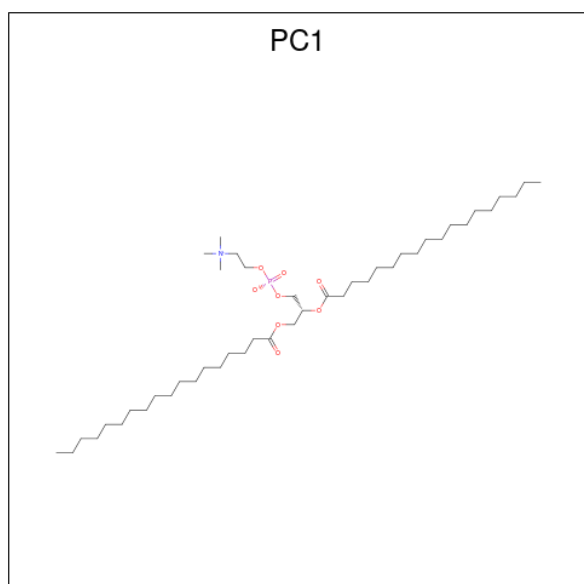
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 7.

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 sub-unit 12.

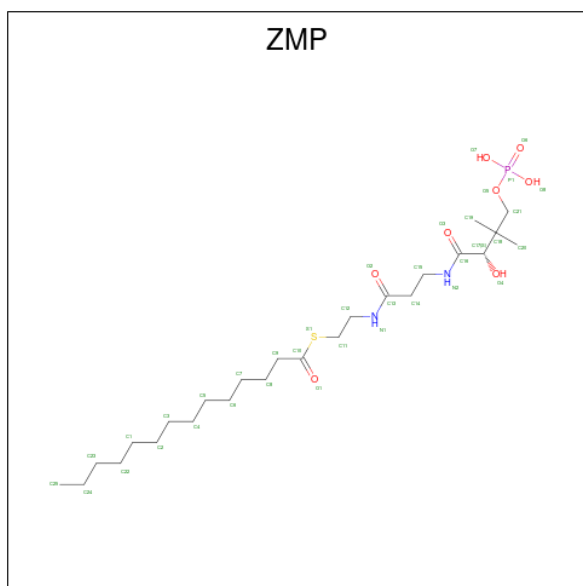
Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



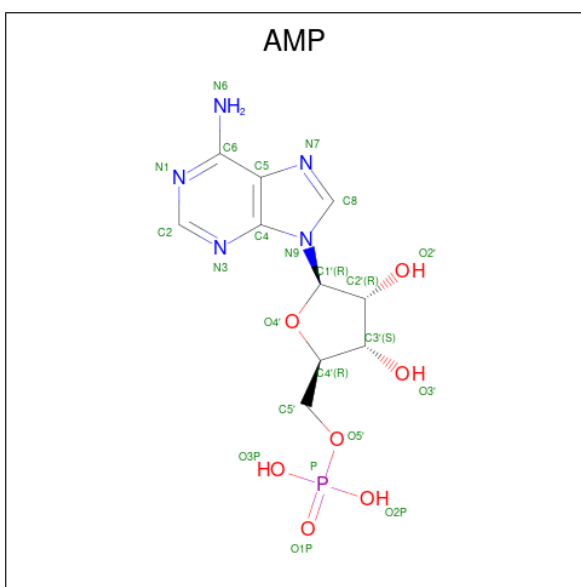
Mol	Chain	Residues	Atoms					AltConf
45	H	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	L	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	M	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	w	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	d	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 46 is S-[2-(N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl)amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



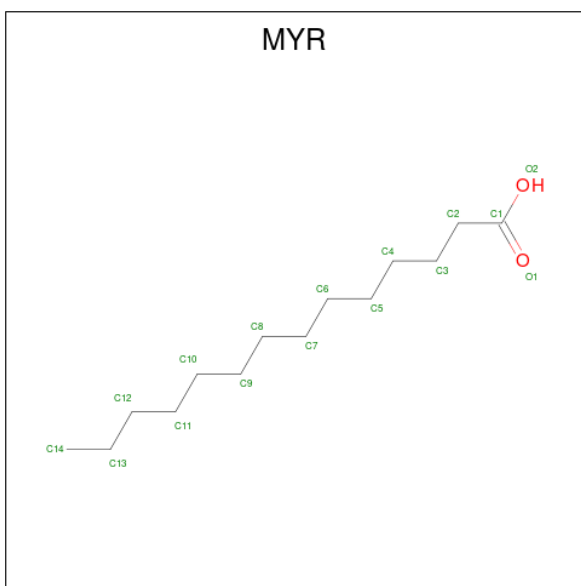
Mol	Chain	Residues	Atoms						AltConf
46	X	1	Total 31	C 20	N 2	O 7	P 1	S 1	0
46	j	1	Total 34	C 23	N 2	O 7	P 1	S 1	0

- Molecule 47 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



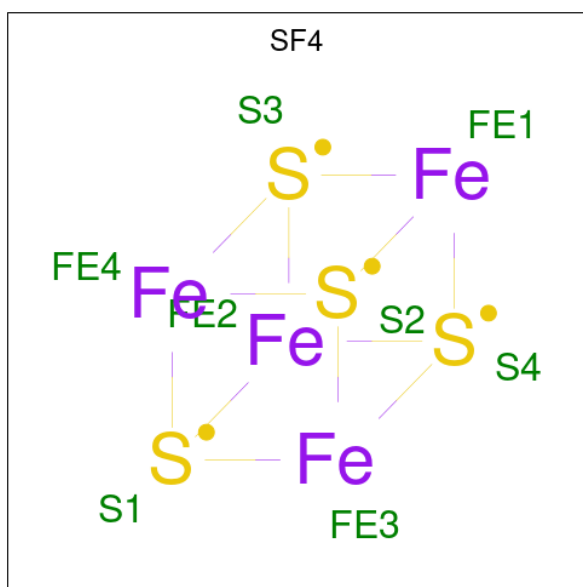
Mol	Chain	Residues	Atoms					AltConf
47	k	1	Total	C	N	O	P	0
			23	10	5	7	1	

- Molecule 48 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



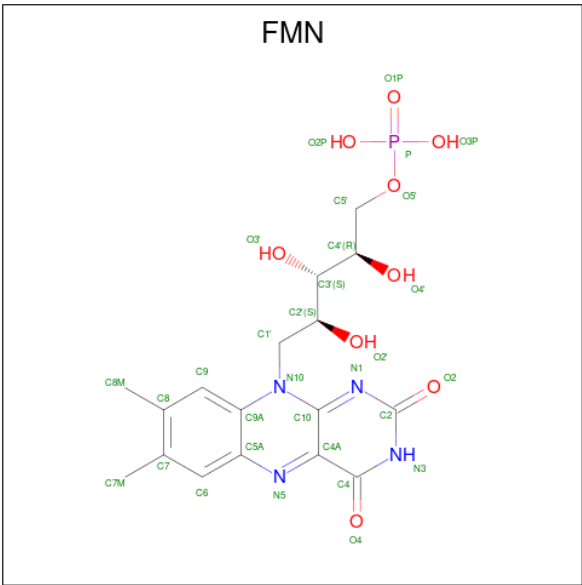
Mol	Chain	Residues	Atoms			AltConf
48	s	1	Total	C	O	0
			15	14	1	

- Molecule 49 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



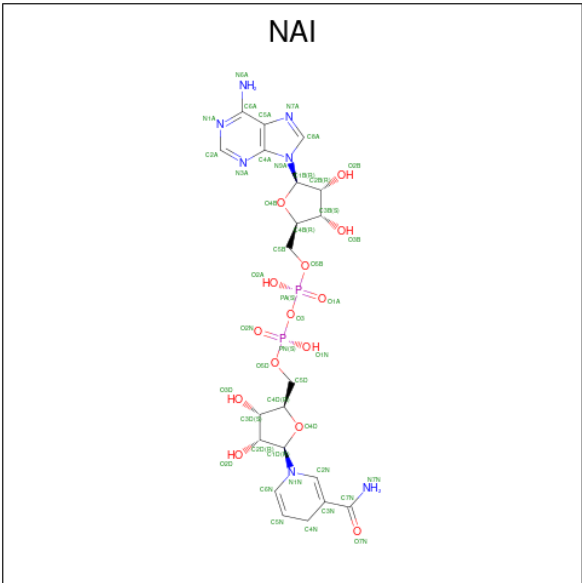
Mol	Chain	Residues	Atoms			AltConf
49	1	1	Total	Fe	S	0
			8	4	4	
49	3	1	Total	Fe	S	0
			8	4	4	
49	3	1	Total	Fe	S	0
			8	4	4	
49	6	1	Total	Fe	S	0
			8	4	4	
49	9	1	Total	Fe	S	0
			8	4	4	
49	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



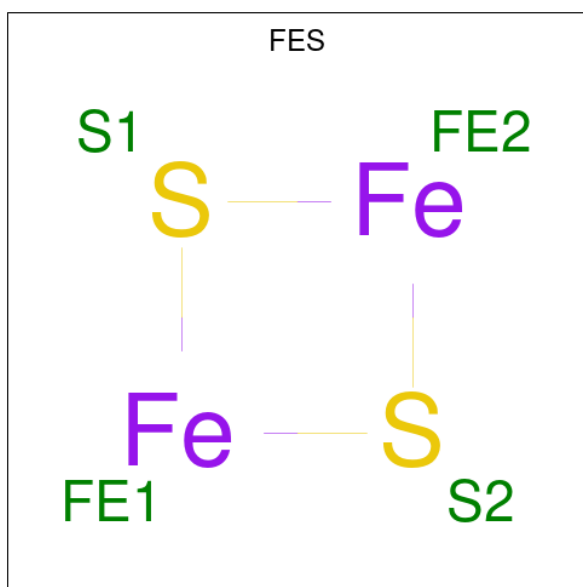
Mol	Chain	Residues	Atoms					AltConf
50	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
51	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

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



Mol	Chain	Residues	Atoms			AltConf
52	2	1	Total	Fe	S	0
			4	2	2	
52	3	1	Total	Fe	S	0
			4	2	2	

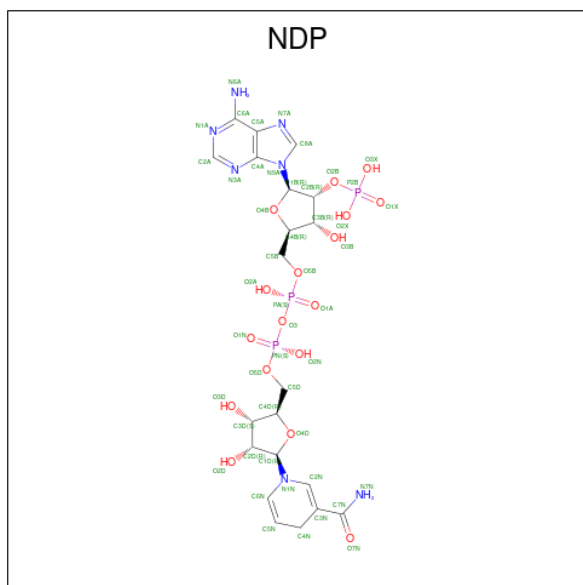
- Molecule 53 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
53	3	1	Total	K	0
			1	1	

- Molecule 54 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

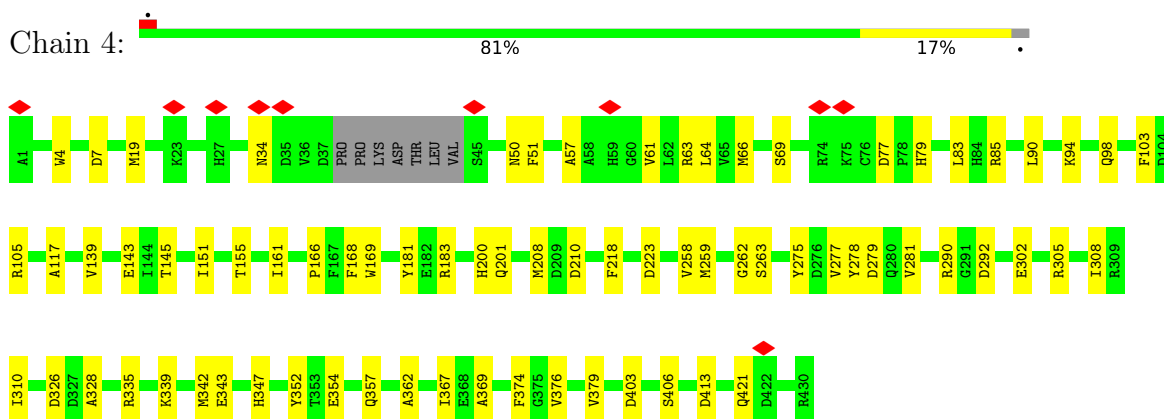


Mol	Chain	Residues	Atoms					AltConf
55	d	1	Total	C	N	O	P	0
			48	21	7	17	3	

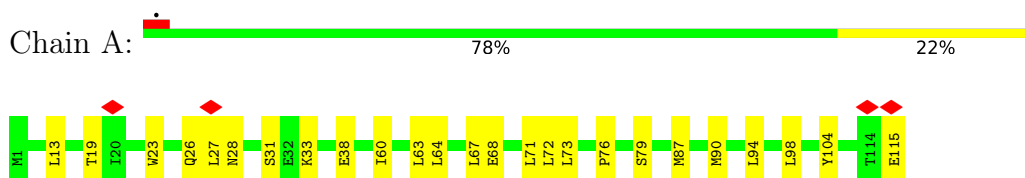
3 Residue-property plots

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

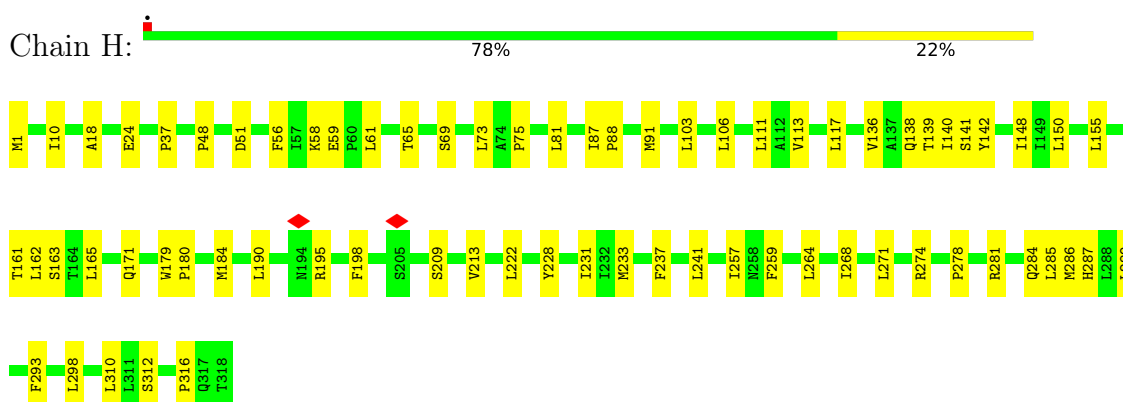
- Molecule 1: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



- Molecule 2: NADH-ubiquinone oxidoreductase chain 3

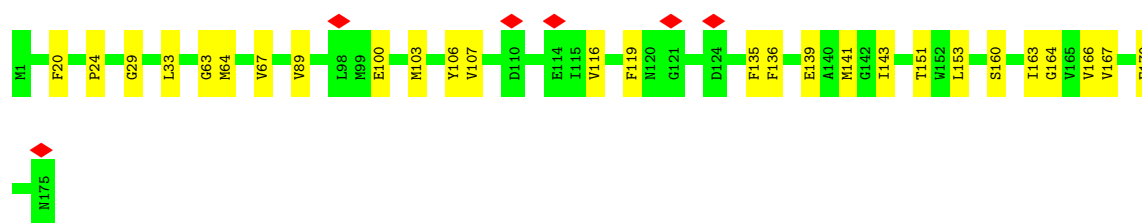


- Molecule 3: NADH-ubiquinone oxidoreductase chain 1



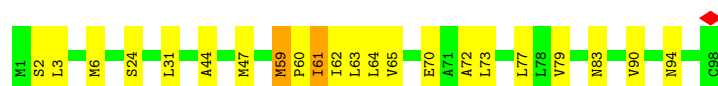
- Molecule 4: NADH-ubiquinone oxidoreductase chain 6

Chain J:  85% 15%



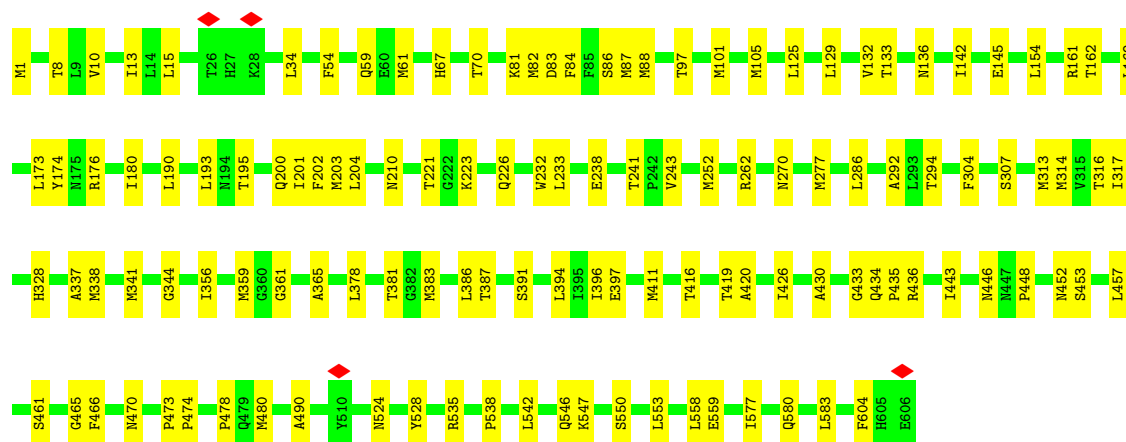
- Molecule 5: NADH-ubiquinone oxidoreductase chain 4L

Chain K:  78% 20%



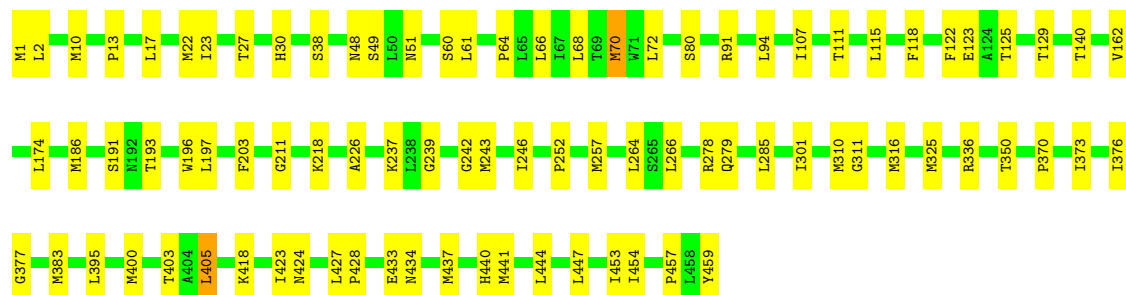
- Molecule 6: NADH-ubiquinone oxidoreductase chain 5

Chain L:  80% 20%

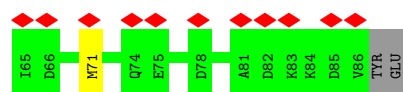


- Molecule 7: NADH-ubiquinone oxidoreductase chain 4

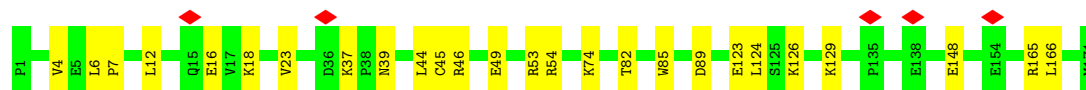
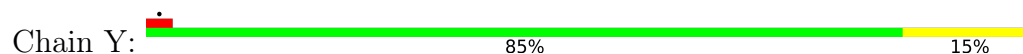
Chain M:  81% 19%



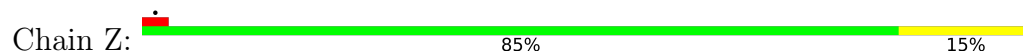
- Molecule 8: NADH-ubiquinone oxidoreductase chain 2



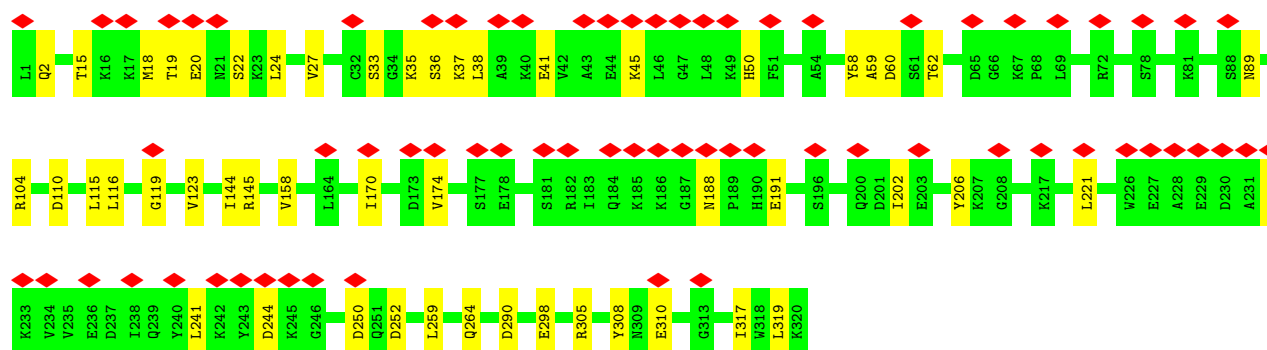
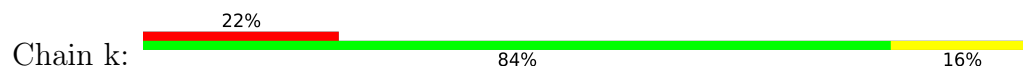
- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



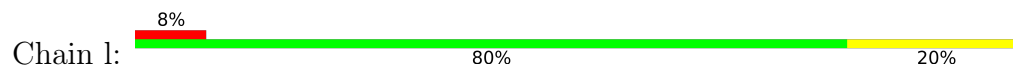
- Molecule 13: Complex I-PDSW



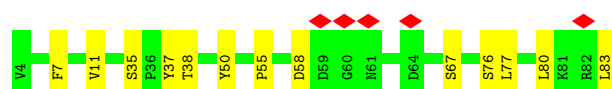
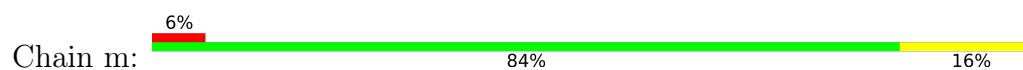
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



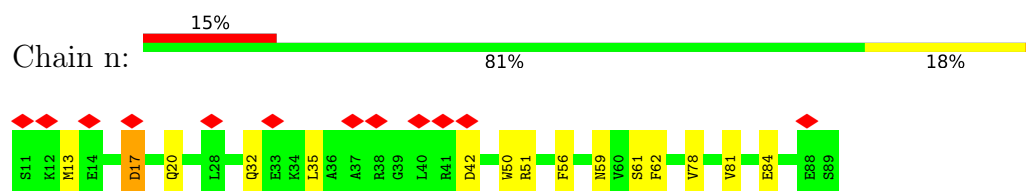
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



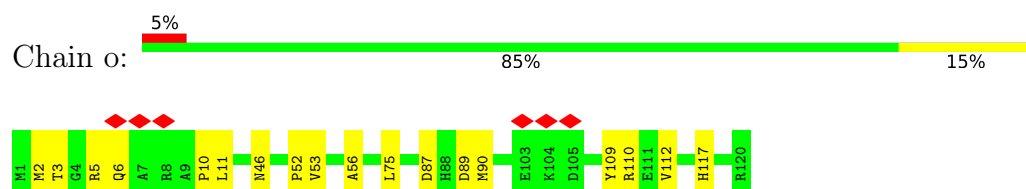
- Molecule 16: Complex I-B9



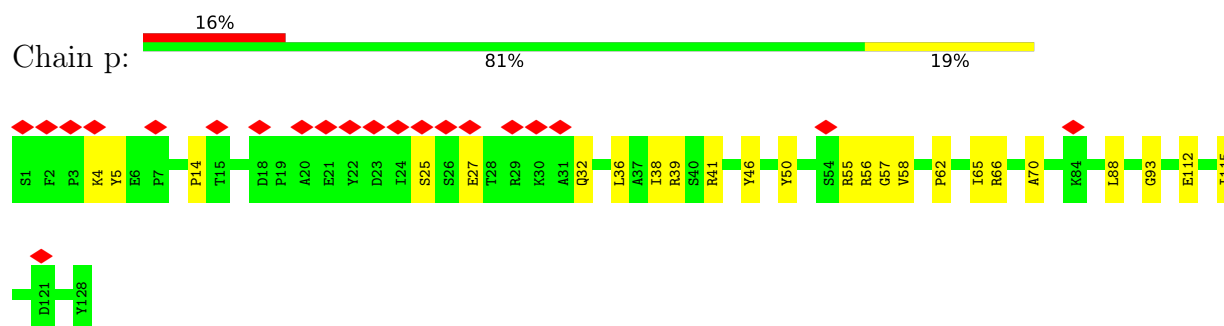
- Molecule 17: Complex I-B12



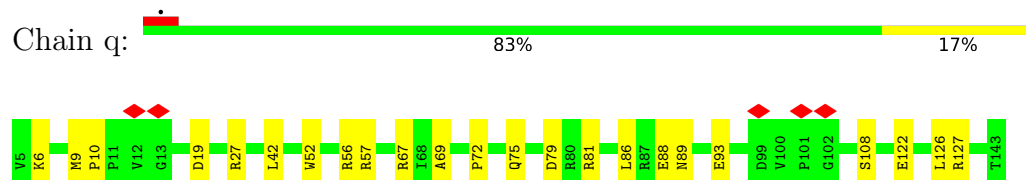
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 subunit C2



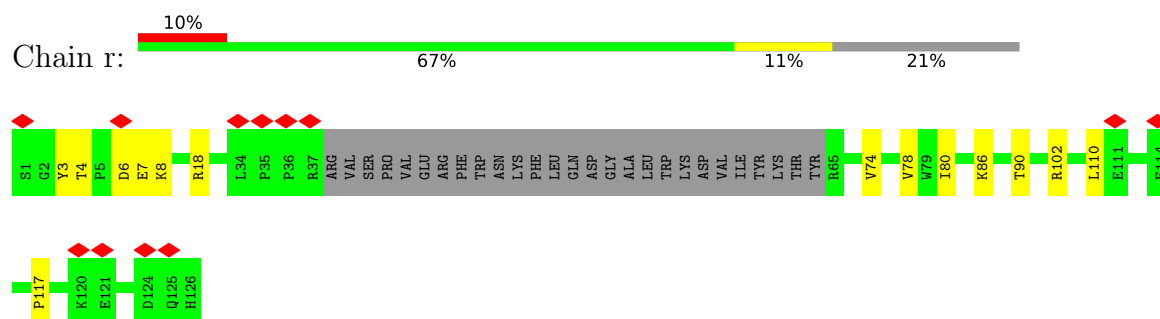
- Molecule 19: NADH:ubiquinone oxidoreductase subunit B4



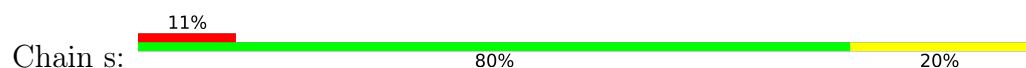
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

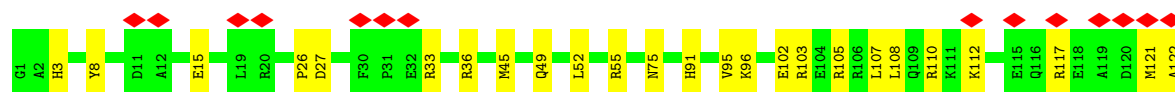


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

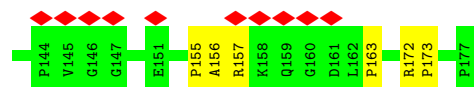
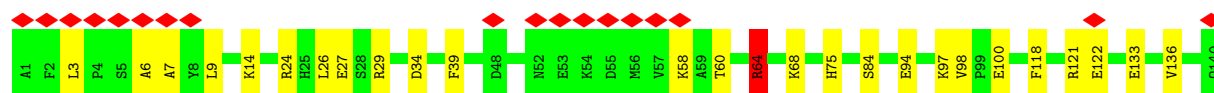
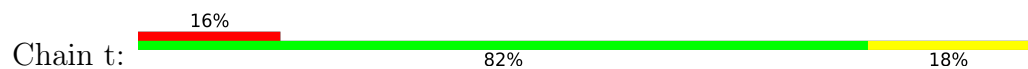


- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

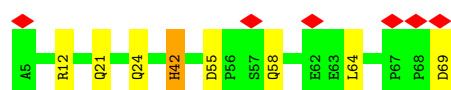
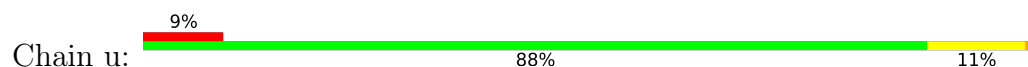




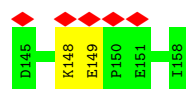
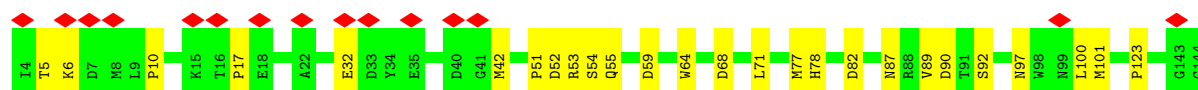
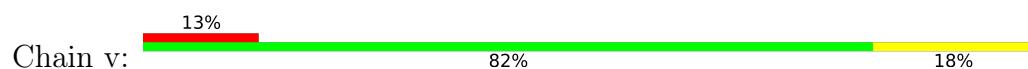
- Molecule 23: Complex I-B22



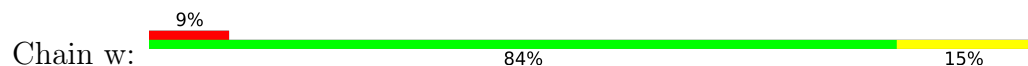
- Molecule 24: Complex I-AGGG



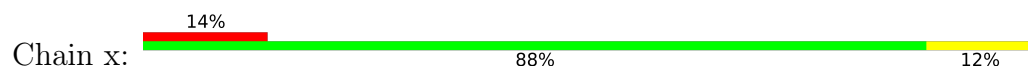
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



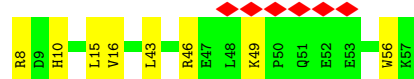
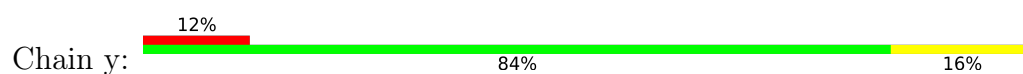
- Molecule 26: Complex I-ESSS



- Molecule 27: Complex I-KFYI



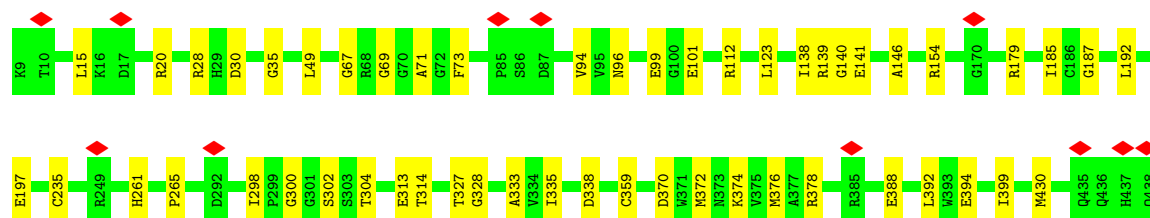
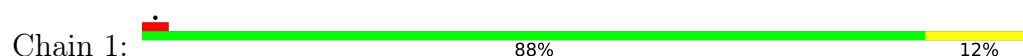
- Molecule 28: Complex I-MNLL



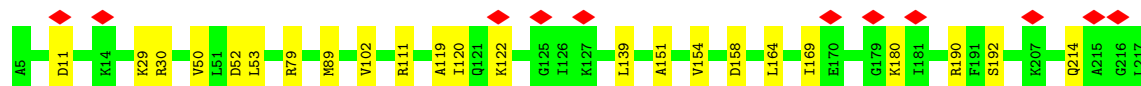
• Molecule 29: Complex I-MWFE



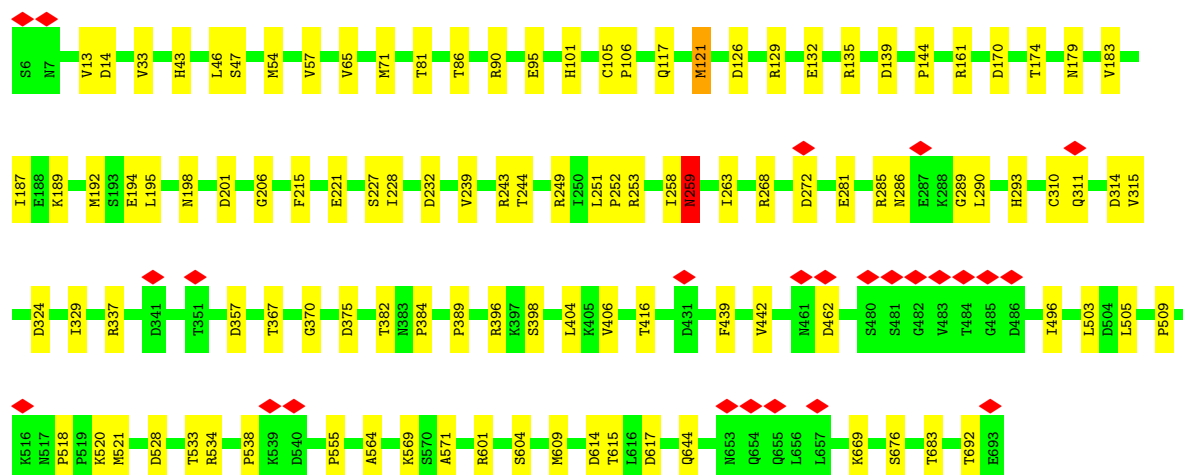
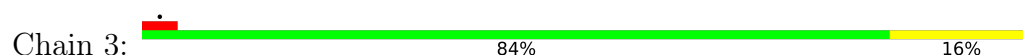
• Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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



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



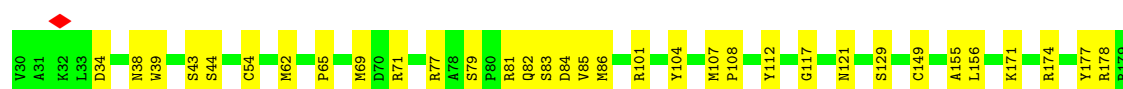
- Molecule 33: Complex I-30kD

Chain 5:  86% 14%



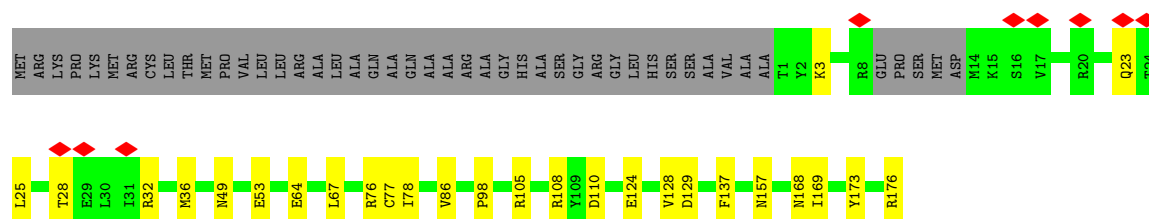
- Molecule 34: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 6:  78% 22%

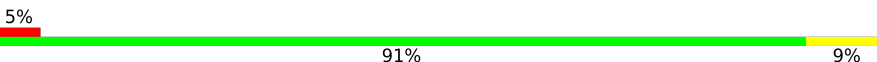


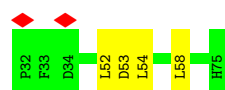
- Molecule 35: Complex I-23kD

Chain 9:  66% 12% 21%



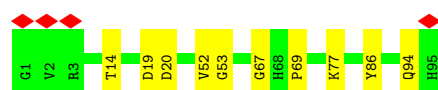
- Molecule 36: Complex I-9kD

Chain a:  5% 91% 9%



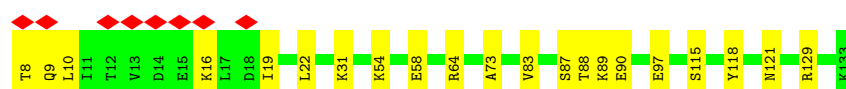
- Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain b:  89% 11%

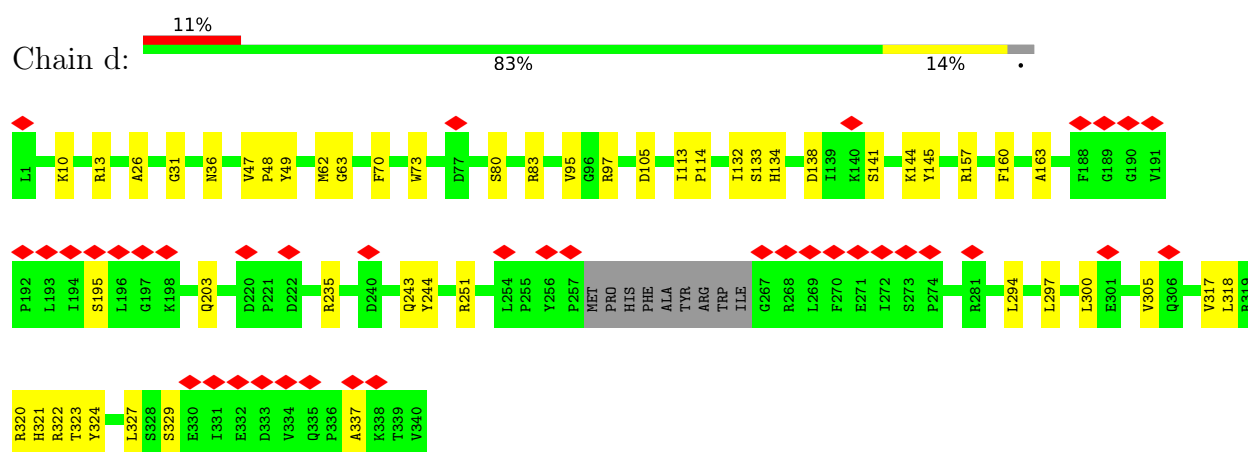


- Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

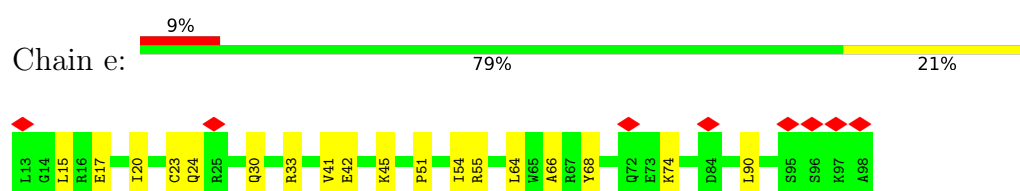
Chain c:  6% 83% 17%



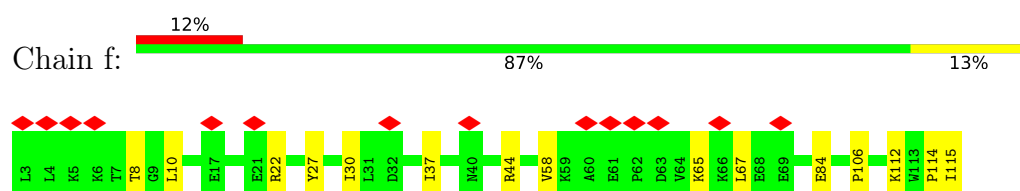
- Molecule 39: NADH:ubiquinone oxidoreductase subunit A9



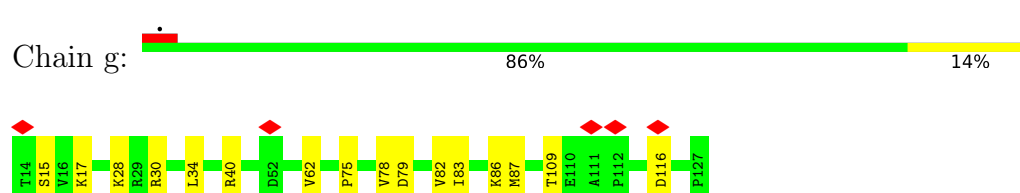
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



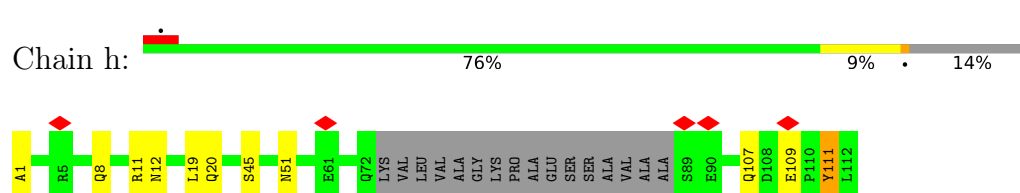
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



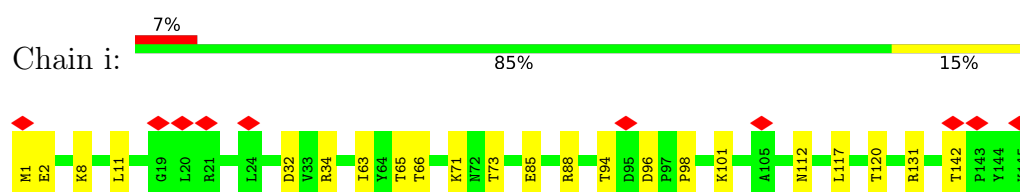
- Molecule 42: Complex I-B14



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



- 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	41421	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	0.532	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.077	Depositor
Map size (Å)	165.92, 196.42, 287.92	wwPDB
Map dimensions	236, 161, 136	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: AYA, FME, ZMP, ZN, FMN, PC1, FES, NAI, SF4, NDP, AMP, 2MR, K, MYR, SEP

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	0.16	0/3479	0.39	0/4711
2	A	0.20	0/947	0.45	0/1296
3	H	0.19	0/2603	0.49	0/3561
4	J	0.20	0/1378	0.52	0/1868
5	K	0.22	0/749	0.50	1/1014 (0.1%)
6	L	0.19	0/4925	0.45	1/6700 (0.0%)
7	M	0.19	0/3731	0.48	0/5085
8	N	0.21	0/2787	0.47	0/3795
9	V	0.19	0/1041	0.46	0/1412
10	W	0.14	0/1188	0.34	0/1607
11	X	0.15	0/713	0.37	0/963
11	j	0.20	0/627	0.51	0/842
12	Y	0.15	0/1440	0.34	0/1942
13	Z	0.15	0/1475	0.35	0/1989
14	k	0.16	0/2646	0.39	0/3579
15	l	0.15	0/896	0.43	0/1200
16	m	0.16	0/647	0.45	0/890
17	n	0.17	0/653	0.43	0/882
18	o	0.20	0/1035	0.47	1/1398 (0.1%)
19	p	0.19	0/1085	0.43	0/1467
20	q	0.19	0/1171	0.46	0/1579
21	r	0.19	0/874	0.47	1/1188 (0.1%)
22	s	0.15	0/1072	0.42	0/1436
23	t	0.16	0/1573	0.43	1/2130 (0.0%)
24	u	0.11	0/590	0.33	0/810
25	v	0.17	0/1361	0.47	1/1861 (0.1%)
26	w	0.17	0/872	0.46	0/1185
27	x	0.16	0/425	0.43	0/576
28	y	0.19	0/449	0.49	0/605
29	z	0.22	0/591	0.51	0/795
30	1	0.16	0/3386	0.37	0/4575
31	2	0.17	0/1695	0.41	0/2306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	3	0.14	0/5362	0.38	0/7266
33	5	0.14	0/1776	0.38	0/2417
34	6	0.17	0/1228	0.39	0/1661
35	9	0.16	0/1405	0.36	0/1900
36	a	0.10	0/383	0.27	0/518
37	b	0.14	0/749	0.33	0/1009
38	c	0.12	0/1047	0.31	0/1415
39	d	0.15	0/2731	0.35	0/3701
40	e	0.16	0/702	0.42	0/945
41	f	0.19	0/937	0.42	0/1271
42	g	0.17	0/993	0.34	0/1336
43	h	0.15	0/779	0.40	0/1053
44	i	0.14	0/1250	0.34	0/1698
All	All	0.17	0/67446	0.42	6/91437 (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
7	M	0	1
32	3	0	1
All	All	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	v	17	PRO	CA-N-CD	-7.49	101.51	112.00
18	o	10	PRO	CA-N-CD	-6.54	102.84	112.00
23	t	64	ARG	CA-CB-CG	-6.22	101.65	114.10
5	K	59	MET	CB-CG-SD	5.47	129.10	112.70
6	L	101	MET	CB-CG-SD	5.36	128.78	112.70
21	r	117	PRO	CA-N-CD	-5.10	104.86	112.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	3	259	ASN	Peptide
1	4	275	TYR	Peptide
7	M	123	GLU	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	3404	0	3339	51	0
2	A	922	0	953	22	0
3	H	2528	0	2641	51	0
4	J	1344	0	1364	23	0
5	K	749	0	793	20	0
6	L	4807	0	4949	87	0
7	M	3647	0	3849	60	0
8	N	2723	0	2930	45	0
9	V	1028	0	1036	8	0
10	W	1155	0	1177	17	0
11	X	701	0	692	13	0
11	j	619	0	620	6	0
12	Y	1403	0	1392	21	0
13	Z	1441	0	1419	22	0
14	k	2596	0	2559	31	0
15	l	874	0	869	16	0
16	m	626	0	635	11	0
17	n	634	0	616	11	0
18	o	1004	0	995	11	0
19	p	1059	0	1062	16	0
20	q	1142	0	1137	22	0
21	r	846	0	864	13	0
22	s	1047	0	1013	18	0
23	t	1520	0	1477	26	0
24	u	563	0	509	7	0
25	v	1307	0	1207	22	0
26	w	846	0	792	14	0
27	x	412	0	411	3	0
28	y	436	0	437	7	0
29	z	576	0	570	11	0
30	1	3312	0	3266	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	2	1655	0	1668	16	0
32	3	5275	0	5300	73	0
33	5	1726	0	1676	21	0
34	6	1198	0	1211	22	0
35	9	1376	0	1339	25	0
36	a	371	0	344	4	0
37	b	737	0	710	8	0
38	c	1024	0	1023	14	0
39	d	2662	0	2682	31	0
40	e	691	0	706	13	0
41	f	917	0	958	10	0
42	g	969	0	980	13	0
43	h	769	0	780	8	0
44	i	1209	0	1182	13	0
45	H	54	0	88	2	0
45	L	54	0	88	3	0
45	M	54	0	88	4	0
45	d	46	0	69	1	0
45	w	54	0	88	2	0
46	X	31	0	34	1	0
46	j	34	0	40	4	0
47	k	23	0	12	1	0
48	s	15	0	27	0	0
49	1	8	0	0	0	0
49	3	16	0	0	2	0
49	6	8	0	0	1	0
49	9	16	0	0	0	0
50	1	31	0	19	0	0
51	1	44	0	27	3	0
52	2	4	0	0	0	0
52	3	4	0	0	0	0
53	3	1	0	0	0	0
54	b	1	0	0	0	0
55	d	48	0	26	1	0
All	All	66396	0	66738	805	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 (805) 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:9:MET:HE3	20:q:10:PRO:HD2	1.66	0.78
40:e:30:GLN:HA	40:e:33:ARG:HE	1.56	0.71
6:L:203:MET:HB2	13:Z:113:GLN:HG3	1.73	0.70
7:M:118:PHE:O	7:M:122:PHE:HB3	1.93	0.69
10:W:43:ILE:HD11	10:W:70:PRO:HB2	1.75	0.69
30:1:300:GLY:HA2	30:1:333:ALA:H	1.58	0.69
3:H:195:ARG:HE	3:H:274:ARG:HD2	1.59	0.68
19:p:70:ALA:HB2	25:v:10:PRO:HG2	1.78	0.66
14:k:202:ILE:O	14:k:206:TYR:HB2	1.96	0.65
6:L:378:LEU:HB3	6:L:383:MET:HG2	1.78	0.65
3:H:24:GLU:HG3	3:H:271:LEU:HD21	1.79	0.64
22:s:36:ARG:HH12	22:s:96:LYS:HG3	1.62	0.64
40:e:23:CYS:SG	40:e:24:GLN:N	2.70	0.64
14:k:104:ARG:NH2	47:k:501:AMP:N7	2.46	0.63
25:v:52:ASP:HA	25:v:78:HIS:HE2	1.63	0.63
8:N:77:ASN:O	8:N:81:SER:HB3	1.99	0.63
23:t:60:THR:HG23	23:t:64:ARG:HH21	1.62	0.63
7:M:38:SER:OG	7:M:70:MET:SD	2.55	0.63
19:p:46:TYR:O	19:p:50:TYR:HB3	1.99	0.63
33:5:32:ILE:HG22	33:5:33:LEU:HG	1.81	0.62
23:t:155:PRO:HD2	23:t:157:ARG:HH21	1.64	0.62
32:3:201:ASP:OD2	32:3:268:ARG:NH2	2.30	0.62
18:o:46:ASN:HB3	18:o:53:VAL:HA	1.82	0.62
19:p:38:ILE:HA	19:p:41:ARG:HE	1.65	0.62
18:o:52:PRO:HG2	18:o:56:ALA:HB2	1.82	0.62
7:M:10:MET:HE3	28:y:15:LEU:HG	1.81	0.61
31:2:30:ARG:HH21	36:a:53:ASP:HB2	1.65	0.61
4:J:136:PHE:HB2	4:J:141:MET:HE1	1.82	0.61
12:Y:23:VAL:HG21	29:z:65:GLY:HA2	1.82	0.60
11:j:37:MET:HE2	11:j:71:MET:HE1	1.82	0.60
1:4:328:ALA:HB3	32:3:126:ASP:HB2	1.82	0.60
1:4:223:ASP:OD1	1:4:305:ARG:NH2	2.35	0.60
45:L:701:PC1:H3B1	21:r:80:ILE:HD12	1.82	0.60
44:i:32:ASP:OD2	44:i:34:ARG:NH1	2.35	0.60
39:d:324:TYR:HA	39:d:327:LEU:HB2	1.84	0.60
3:H:284:GLN:HA	3:H:287:HIS:HB2	1.84	0.59
4:J:64:MET:HA	4:J:67:VAL:HB	1.83	0.59
40:e:20:ILE:HD11	40:e:90:LEU:HD21	1.84	0.59
2:A:90:MET:HE1	4:J:151:THR:HA	1.85	0.59
13:Z:27:ASN:HB2	13:Z:29:ILE:HD12	1.83	0.59
16:m:77:LEU:HD11	16:m:80:LEU:HD23	1.84	0.59
32:3:314:ASP:HB3	32:3:520:LYS:HG2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:281:VAL:HG11	1:4:310:ILE:HG23	1.85	0.59
12:Y:123:GLU:HA	12:Y:126:LYS:HE3	1.83	0.59
15:l:5:VAL:HG12	18:o:11:LEU:HD21	1.84	0.59
39:d:36:ASN:HB2	39:d:62:MET:HE2	1.83	0.59
1:4:77:ASP:OD2	33:5:149:ARG:NH2	2.35	0.59
6:L:84:PHE:O	6:L:88:MET:HB3	2.02	0.59
7:M:453:ILE:HG13	7:M:454:ILE:HG23	1.83	0.59
32:3:117:GLN:NE2	49:3:801:SF4:S3	2.76	0.59
30:1:265:PRO:O	31:2:190:ARG:NH2	2.36	0.58
26:w:40:LYS:H	26:w:40:LYS:HD2	1.68	0.58
39:d:322:ARG:NH1	39:d:329:SER:OG	2.36	0.58
1:4:335:ARG:NH2	35:9:129:ASP:OD1	2.37	0.58
3:H:24:GLU:OE2	3:H:195:ARG:NH2	2.36	0.58
35:9:49:ASN:HB3	35:9:53:GLU:HG3	1.85	0.58
6:L:86:SER:HG	6:L:262:ARG:HH22	1.51	0.58
1:4:258:VAL:O	1:4:262:GLY:N	2.37	0.57
15:l:14:ASP:OD1	15:l:14:ASP:N	2.36	0.57
22:s:103:ARG:NH1	24:u:64:LEU:O	2.36	0.57
31:2:53:LEU:HD12	36:a:52:LEU:HD13	1.85	0.57
6:L:132:VAL:HG23	6:L:133:THR:HG23	1.87	0.57
14:k:89:ASN:O	26:w:23:THR:N	2.38	0.57
17:n:32:GLN:HG2	17:n:42:ASP:HB3	1.87	0.57
34:6:117:GLY:O	34:6:121:ASN:ND2	2.37	0.57
3:H:161:THR:HG22	3:H:163:SER:H	1.69	0.57
32:3:382:THR:HG23	32:3:384:PRO:HD3	1.85	0.57
4:J:153:LEU:HD21	5:K:62:ILE:HG13	1.86	0.57
8:N:179:MET:HE1	8:N:215:MET:HB3	1.85	0.57
42:g:78:VAL:HG23	46:j:101:ZMP:HN1	1.70	0.57
45:M:501:PC1:H252	8:N:277:ILE:HG22	1.86	0.57
7:M:310:MET:HE2	7:M:459:TYR:HA	1.86	0.57
5:K:44:ALA:HB1	5:K:59:MET:HE1	1.86	0.56
7:M:418:LYS:HB3	25:v:68:ASP:HB2	1.87	0.56
9:V:11:ILE:HB	9:V:20:LYS:HD3	1.87	0.56
30:1:69:GLY:O	51:1:503:NAI:N7N	2.35	0.56
38:c:16:LYS:NZ	38:c:97:GLU:O	2.38	0.56
4:J:167:VAL:HG13	8:N:42:PRO:HG3	1.88	0.56
6:L:180:ILE:HD11	7:M:400:MET:HB3	1.87	0.56
8:N:30:TRP:NE1	8:N:67:SER:OG	2.34	0.56
8:N:316:GLN:NE2	14:k:60:ASP:OD1	2.39	0.56
20:q:89:ASN:ND2	20:q:122:GLU:O	2.37	0.56
6:L:162:THR:OG1	25:v:87:ASN:OD1	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:9:3:LYS:NZ	43:h:109:GLU:OE1	2.39	0.56
18:o:5:ARG:NH1	18:o:89:ASP:OD1	2.39	0.56
6:L:294:THR:O	6:L:524:ASN:ND2	2.38	0.56
11:X:63:PRO:HG2	11:X:66:ASP:HB2	1.87	0.56
1:4:90:LEU:HD11	34:6:129:SER:HB2	1.88	0.56
32:3:252:PRO:HG3	32:3:263:ILE:HG12	1.87	0.56
6:L:396:ILE:HG21	6:L:490:ALA:HB2	1.88	0.55
32:3:221:GLU:OE2	32:3:243:ARG:NH1	2.38	0.55
7:M:203:PHE:HB3	7:M:239:GLY:HA2	1.88	0.55
13:Z:161:ARG:NH2	26:w:111:ASN:OD1	2.39	0.55
30:1:313:GLU:HG3	30:1:314:THR:HG23	1.89	0.55
30:1:376:MET:HE1	30:1:392:LEU:HD21	1.88	0.55
11:j:49:GLU:HA	11:j:52:MET:HE2	1.89	0.55
8:N:337:LEU:O	8:N:340:THR:OG1	2.20	0.55
14:k:38:LEU:O	14:k:41:GLU:HB3	2.06	0.55
8:N:232:HIS:HB3	8:N:311:MET:HE1	1.89	0.55
16:m:50:TYR:O	20:q:67:ARG:NH1	2.40	0.55
6:L:190:LEU:HD23	7:M:383:MET:HG2	1.87	0.55
30:1:185:ILE:HG12	30:1:359:CYS:HB3	1.88	0.55
33:5:49:GLU:OE2	33:5:106:ARG:NH1	2.40	0.55
6:L:277:MET:HE3	6:L:317:ILE:HG23	1.89	0.55
6:L:378:LEU:HD13	6:L:383:MET:HE3	1.88	0.55
15:l:96:HIS:HA	15:l:101:GLU:HB3	1.89	0.55
44:i:71:LYS:HE2	44:i:73:THR:HG22	1.89	0.55
7:M:30:HIS:HB3	28:y:16:VAL:HG21	1.89	0.55
44:i:94:THR:HG23	44:i:96:ASP:H	1.72	0.55
32:3:601:ARG:NH2	32:3:614:ASP:OD1	2.39	0.55
7:M:60:SER:HB2	7:M:457:PRO:HA	1.88	0.55
6:L:223:LYS:HD2	6:L:252:MET:HE3	1.88	0.54
6:L:314:MET:HA	6:L:317:ILE:HG22	1.88	0.54
14:k:310:GLU:HG2	14:k:317:ILE:HD12	1.89	0.54
19:p:55:ARG:NH1	19:p:57:GLY:O	2.40	0.54
32:3:398:SER:HB3	32:3:404:LEU:HD13	1.89	0.54
33:5:129:TRP:O	33:5:132:ARG:HB3	2.08	0.54
39:d:294:LEU:HD13	39:d:297:LEU:HD12	1.88	0.54
6:L:446:ASN:ND2	24:u:21:GLN:OE1	2.41	0.54
7:M:336:ARG:NH2	7:M:428:PRO:O	2.40	0.54
33:5:33:LEU:HD13	33:5:60:VAL:HG22	1.88	0.54
7:M:91:ARG:NH2	14:k:290:ASP:OD2	2.40	0.54
37:b:14:THR:O	44:i:131:ARG:NH1	2.40	0.54
4:J:164:GLY:HA2	8:N:38:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:25:LEU:HD12	22:s:75:ASN:HB2	1.89	0.54
32:3:105:CYS:SG	32:3:117:GLN:NE2	2.80	0.54
8:N:277:ILE:HD11	9:V:134:VAL:HG12	1.89	0.54
15:l:19:ILE:HG23	15:l:22:ALA:HB2	1.90	0.54
18:o:110:ARG:NH1	26:w:119:GLN:OE1	2.41	0.54
30:1:141:GLU:HG3	31:2:89:MET:HE1	1.90	0.54
32:3:329:ILE:HD13	32:3:505:LEU:HD22	1.89	0.54
1:4:117:ALA:HB2	1:4:367:ILE:HG12	1.90	0.54
7:M:162:VAL:HG22	8:N:267:ILE:HG21	1.90	0.54
15:l:37:LYS:NZ	15:l:41:GLU:OE1	2.41	0.54
23:t:24:ARG:NH1	23:t:27:GLU:OE1	2.41	0.54
25:v:148:LYS:NZ	25:v:149:GLU:O	2.40	0.54
1:4:279:ASP:OD1	1:4:279:ASP:N	2.36	0.54
12:Y:148:GLU:O	15:l:50:ARG:NH2	2.39	0.54
19:p:39:ARG:NH2	23:t:3:LEU:O	2.41	0.54
32:3:135:ARG:NH1	32:3:179:ASN:OD1	2.41	0.54
13:Z:143:HIS:ND1	13:Z:144:ASP:OD1	2.40	0.54
42:g:62:VAL:HG22	46:j:101:ZMP:H3A	1.91	0.53
2:A:31:SER:HB2	39:d:320:ARG:HB3	1.89	0.53
6:L:435:PRO:HG2	17:n:51:ARG:HB3	1.90	0.53
10:W:88:GLU:OE1	28:y:56:TRP:NE1	2.33	0.53
31:2:119:ALA:HA	31:2:122:LYS:HG2	1.90	0.53
37:b:52:VAL:O	37:b:94:GLN:NE2	2.40	0.53
45:L:701:PC1:H3G2	21:r:80:ILE:HG13	1.89	0.53
6:L:221:THR:HG23	6:L:226:GLN:HB2	1.89	0.53
28:y:8:ARG:HG3	28:y:10:HIS:H	1.72	0.53
32:3:324:ASP:HB3	32:3:571:ALA:HB1	1.90	0.53
35:9:76:ARG:NH1	35:9:128:VAL:O	2.41	0.53
3:H:310:LEU:HD12	16:m:35:SER:HB3	1.89	0.53
5:K:24:SER:HA	5:K:90:VAL:HG22	1.91	0.53
38:c:118:TYR:O	38:c:121:ASN:ND2	2.42	0.53
7:M:1:FME:HE3	7:M:111:THR:HG21	1.91	0.53
3:H:37:PRO:HA	34:6:71:ARG:HA	1.91	0.53
14:k:15:THR:HA	14:k:18:MET:HE2	1.90	0.53
30:1:101:GLU:OE2	30:1:302:SER:N	2.42	0.53
32:3:396:ARG:NH1	32:3:416:THR:O	2.42	0.53
12:Y:7:PRO:HD3	12:Y:53:ARG:HG2	1.91	0.52
33:5:47:GLU:OE1	33:5:106:ARG:NH2	2.41	0.52
6:L:542:LEU:HB3	7:M:278:ARG:HH11	1.74	0.52
32:3:174:THR:HG22	32:3:183:VAL:HG22	1.92	0.52
32:3:310:CYS:SG	32:3:311:GLN:N	2.82	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:289:LEU:HA	3:H:293:PHE:HB2	1.90	0.52
3:H:312:SER:HB3	16:m:37:TYR:HB3	1.91	0.52
7:M:68:LEU:O	7:M:72:LEU:HB2	2.09	0.52
8:N:81:SER:OG	8:N:83:GLN:NE2	2.42	0.52
8:N:289:ASN:HD22	8:N:292:PHE:HE2	1.58	0.52
2:A:33:LYS:NZ	3:H:59:GLU:OE2	2.38	0.52
14:k:27:VAL:HG22	14:k:170:ILE:HB	1.92	0.52
30:1:71:ALA:HB2	51:1:503:NAI:H4D	1.90	0.52
1:4:354:GLU:OE2	1:4:357:GLN:NE2	2.42	0.52
7:M:203:PHE:HB2	7:M:243:MET:HE3	1.92	0.52
33:5:14:ARG:NH1	33:5:16:ASP:OD1	2.43	0.52
15:l:82:ARG:NH2	20:q:126:LEU:O	2.42	0.52
25:v:71:LEU:HD21	25:v:77:MET:HG2	1.91	0.52
11:X:22:TYR:HB3	11:X:25:ILE:HG12	1.92	0.52
19:p:36:LEU:HD22	23:t:7:ALA:HB2	1.90	0.52
2:A:71:LEU:HB3	2:A:94:LEU:HD11	1.90	0.52
4:J:119:PHE:CG	5:K:6:MET:HB2	2.44	0.52
7:M:61:LEU:HB2	7:M:457:PRO:HG3	1.90	0.52
16:m:58:ASP:OD1	16:m:58:ASP:N	2.42	0.52
21:r:4:THR:HB	21:r:7:GLU:HG2	1.91	0.52
33:5:193:GLU:OE2	38:c:64:ARG:NH1	2.43	0.52
35:9:105:ARG:NH2	37:b:86:TYR:O	2.41	0.52
1:4:343:GLU:O	1:4:347:HIS:ND1	2.36	0.51
1:4:413:ASP:OD2	3:H:281:ARG:NH1	2.43	0.51
3:H:138:GLN:NE2	3:H:198:PHE:O	2.43	0.51
3:H:141:SER:HB3	3:H:286:MET:HG3	1.91	0.51
4:J:160:SER:HB2	8:N:35:MET:HE2	1.90	0.51
27:x:34:GLN:NE2	27:x:38:ASP:OD1	2.43	0.51
30:1:99:GLU:O	30:1:139:ARG:NH1	2.43	0.51
38:c:8:THR:OG1	38:c:9:GLN:N	2.42	0.51
39:d:138:ASP:HB2	39:d:141:SER:HB2	1.92	0.51
3:H:58:LYS:NZ	34:6:84:ASP:OD1	2.43	0.51
4:J:100:GLU:HA	4:J:103:MET:HE3	1.91	0.51
10:W:62:GLU:HB2	10:W:65:GLU:HG3	1.91	0.51
15:l:103:LEU:HD13	20:q:81:ARG:HD2	1.92	0.51
24:u:55:ASP:O	24:u:58:GLN:NE2	2.43	0.51
31:2:79:ARG:NH2	32:3:170:ASP:OD1	2.42	0.51
32:3:215:PHE:HB2	35:9:98:PRO:HD3	1.92	0.51
6:L:546:GLN:HA	6:L:550:SER:HB3	1.93	0.51
19:p:32:GLN:HB3	23:t:7:ALA:HB1	1.90	0.51
32:3:615:THR:OG1	32:3:617:ASP:OD1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:97:THR:HG21	6:L:125:LEU:HD13	1.92	0.51
6:L:341:MET:HE1	6:L:453:SER:HB3	1.92	0.51
30:1:112:ARG:NH2	31:2:192:SER:OG	2.43	0.51
31:2:164:LEU:HD23	31:2:169:ILE:HB	1.93	0.51
33:5:37:VAL:HA	33:5:52:ILE:HG22	1.93	0.51
1:4:183:ARG:NH1	1:4:210:ASP:OD2	2.43	0.51
6:L:558:LEU:HD13	7:M:211:GLY:HA2	1.93	0.51
7:M:243:MET:HB3	7:M:301:ILE:HG21	1.92	0.51
8:N:266:ILE:HG22	8:N:270:MET:HE2	1.93	0.51
30:1:101:GLU:HB2	51:1:503:NAI:H42N	1.92	0.51
30:1:235:CYS:O	31:2:214:GLN:NE2	2.43	0.51
30:1:298:ILE:HB	30:1:335:ILE:HB	1.92	0.51
39:d:251:ARG:HH22	39:d:323:THR:HG23	1.76	0.51
8:N:265:MET:HE1	12:Y:166:LEU:HD21	1.91	0.51
33:5:127:ALA:HA	33:5:130:TYR:HB2	1.92	0.51
6:L:359:MET:O	6:L:436:ARG:NH2	2.44	0.51
12:Y:39:ASN:HB3	20:q:72:PRO:HG2	1.93	0.51
12:Y:129:LYS:NZ	16:m:67:SER:OG	2.44	0.51
17:n:61:SER:OG	17:n:62:PHE:N	2.44	0.51
38:c:54:LYS:HD2	38:c:87:SER:HA	1.93	0.51
19:p:62:PRO:O	19:p:66:ARG:HB2	2.10	0.50
25:v:51:PRO:HB2	25:v:53:ARG:HE	1.76	0.50
39:d:160:PHE:HB3	39:d:163:ALA:HB2	1.93	0.50
39:d:244:TYR:HB2	39:d:337:ALA:HB2	1.93	0.50
2:A:67:LEU:HD12	5:K:65:VAL:HG22	1.92	0.50
11:X:69:LYS:HB3	21:r:3:TYR:HE1	1.77	0.50
22:s:52:LEU:HA	22:s:55:ARG:HG3	1.92	0.50
23:t:64:ARG:HG3	23:t:64:ARG:HH11	1.75	0.50
32:3:194:GLU:HG2	32:3:195:LEU:HG	1.93	0.50
32:3:518:PRO:HB2	32:3:538:PRO:HD3	1.93	0.50
6:L:54:PHE:HB3	6:L:87:MET:HE1	1.93	0.50
32:3:272:ASP:OD2	32:3:683:THR:OG1	2.25	0.50
1:4:342:MET:HE2	32:3:101:HIS:HD2	1.76	0.50
5:K:70:GLU:O	5:K:73:LEU:HB3	2.12	0.50
6:L:174:TYR:HD2	6:L:232:TRP:HB3	1.76	0.50
30:1:372:MET:HE3	30:1:399:ILE:HD12	1.94	0.50
31:2:120:ILE:HG21	31:2:139:LEU:HD13	1.94	0.50
32:3:244:THR:HB	38:c:73:ALA:HB2	1.93	0.50
40:e:15:LEU:HD11	40:e:66:ALA:HB1	1.94	0.50
5:K:79:VAL:O	5:K:83:ASN:N	2.45	0.50
6:L:193:LEU:HD23	6:L:201:ILE:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:43:ILE:HG13	10:W:47:ILE:HB	1.92	0.50
19:p:5:TYR:HE2	19:p:14:PRO:HD3	1.77	0.50
3:H:165:LEU:HD21	3:H:241:LEU:HA	1.92	0.50
16:m:35:SER:HG	16:m:38:THR:HG1	1.58	0.50
5:K:2:SER:OG	5:K:3:LEU:N	2.41	0.50
5:K:47:MET:HE1	15:l:66:LEU:HD21	1.94	0.50
6:L:292:ALA:HB2	6:L:304:PHE:HB3	1.92	0.50
12:Y:74:LYS:NZ	29:z:69:ILE:O	2.45	0.50
25:v:97:ASN:HB2	25:v:100:LEU:HB2	1.92	0.50
6:L:478:PRO:HB2	6:L:480:MET:HE3	1.94	0.50
38:c:58:GLU:HG2	38:c:83:VAL:HG22	1.92	0.50
41:f:22:ARG:NH2	41:f:84:GLU:OE2	2.45	0.50
45:H:401:PC1:H271	35:9:25:LEU:HB3	1.94	0.50
6:L:1:FME:O1	6:L:59:GLN:NE2	2.44	0.50
32:3:195:LEU:HB3	32:3:198:ASN:HD22	1.77	0.50
42:g:116:ASP:N	42:g:116:ASP:OD1	2.44	0.50
6:L:448:PRO:O	6:L:452:ASN:ND2	2.42	0.49
25:v:32:GLU:N	25:v:32:GLU:OE1	2.44	0.49
33:5:96:LEU:HB2	33:5:105:ILE:HG22	1.93	0.49
39:d:317:VAL:HG12	39:d:318:LEU:HG	1.94	0.49
41:f:58:VAL:HA	41:f:67:LEU:HD11	1.94	0.49
42:g:83:ILE:O	42:g:87:MET:HG2	2.12	0.49
4:J:67:VAL:HG11	5:K:31:LEU:HD21	1.93	0.49
22:s:26:PRO:O	22:s:33:ARG:NH1	2.46	0.49
25:v:54:SER:OG	25:v:55:GLN:N	2.45	0.49
1:4:139:VAL:HG21	1:4:277:VAL:HG12	1.94	0.49
3:H:65:THR:HA	39:d:324:TYR:HB3	1.93	0.49
4:J:163:ILE:HG21	8:N:12:THR:HG21	1.93	0.49
7:M:122:PHE:O	7:M:125:THR:OG1	2.29	0.49
20:q:88:GLU:OE1	20:q:127:ARG:NH2	2.45	0.49
32:3:281:GLU:OE1	32:3:293:HIS:ND1	2.45	0.49
44:i:65:THR:OG1	44:i:66:THR:N	2.45	0.49
1:4:218:PHE:HD2	1:4:308:ILE:HD11	1.77	0.49
3:H:180:PRO:HB3	45:H:401:PC1:H281	1.94	0.49
32:3:194:GLU:HG3	32:3:389:PRO:HB3	1.95	0.49
12:Y:6:LEU:HD21	20:q:86:LEU:HB3	1.93	0.49
21:r:6:ASP:OD2	23:t:157:ARG:NH2	2.46	0.49
22:s:91:HIS:O	22:s:95:VAL:HG23	2.13	0.49
32:3:564:ALA:HB3	32:3:569:LYS:HD3	1.93	0.49
14:k:58:TYR:OH	14:k:110:ASP:OD2	2.31	0.49
32:3:126:ASP:OD1	32:3:126:ASP:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:h:8:GLN:O	43:h:12:ASN:ND2	2.44	0.49
1:4:352:TYR:HD1	35:9:86:VAL:HG21	1.78	0.49
3:H:162:LEU:HD21	3:H:237:PHE:HE1	1.77	0.49
32:3:337:ARG:HG2	32:3:609:MET:HB3	1.94	0.49
6:L:538:PRO:HB2	25:v:89:VAL:HG22	1.95	0.49
14:k:24:LEU:HG	14:k:115:LEU:HD22	1.95	0.49
32:3:503:LEU:HD21	32:3:509:PRO:HB3	1.95	0.49
2:A:60:ILE:HG23	5:K:72:ALA:HB1	1.94	0.49
8:N:234:TRP:NE1	8:N:305:PHE:O	2.40	0.49
4:J:163:ILE:HG22	8:N:38:LEU:HD22	1.95	0.49
34:6:39:TRP:O	34:6:43:SER:OG	2.26	0.49
42:g:40:ARG:NH1	11:j:56:ASP:OD1	2.32	0.49
22:s:110:ARG:NH2	24:u:69:ASP:OD2	2.42	0.48
7:M:242:GLY:O	7:M:246:ILE:HB	2.12	0.48
14:k:19:THR:OG1	14:k:20:GLU:N	2.46	0.48
14:k:50:HIS:HB2	14:k:123:VAL:HB	1.95	0.48
15:l:69:GLN:HA	15:l:72:MET:HG3	1.94	0.48
30:1:30:ASP:HB3	30:1:35:GLY:HA3	1.94	0.48
32:3:95:GLU:OE1	32:3:129:ARG:NH2	2.46	0.48
32:3:285:ARG:NH2	32:3:555:PRO:O	2.44	0.48
3:H:198:PHE:HD1	3:H:285:LEU:HD11	1.78	0.48
6:L:535:ARG:HH12	25:v:92:SER:H	1.61	0.48
30:1:394:GLU:OE1	32:3:129:ARG:NH1	2.46	0.48
33:5:60:VAL:O	33:5:63:PHE:HB3	2.13	0.48
41:f:8:THR:HG23	41:f:10:LEU:H	1.78	0.48
6:L:394:LEU:HA	6:L:397:GLU:HG2	1.94	0.48
30:1:154:ARG:HA	36:a:58:LEU:HD21	1.95	0.48
39:d:203:GLN:OE1	39:d:235:ARG:NH1	2.46	0.48
41:f:112:LYS:NZ	41:f:115:ILE:O	2.46	0.48
1:4:302:GLU:HG2	35:9:3:LYS:HD2	1.95	0.48
29:z:3:PHE:O	29:z:6:LEU:HB2	2.13	0.48
32:3:375:ASP:OD1	32:3:375:ASP:N	2.45	0.48
3:H:180:PRO:O	3:H:184:MET:HG2	2.13	0.48
39:d:251:ARG:NH2	39:d:321:HIS:O	2.46	0.48
1:4:326:ASP:OD2	43:h:45:SER:OG	2.28	0.48
32:3:206:GLY:N	49:3:801:SF4:S2	2.77	0.48
35:9:108:ARG:NH1	35:9:110:ASP:OD2	2.47	0.48
40:e:17:GLU:HB3	40:e:51:PRO:HG2	1.95	0.48
40:e:30:GLN:OE1	40:e:33:ARG:NH2	2.46	0.48
1:4:151:ILE:O	1:4:155:THR:OG1	2.21	0.48
2:A:63:LEU:HD22	5:K:72:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:b:19:ASP:OD1	37:b:20:ASP:N	2.46	0.48
6:L:8:THR:HB	6:L:82:MET:HE1	1.96	0.48
37:b:53:GLY:HA2	37:b:94:GLN:HE22	1.78	0.48
1:4:292:ASP:OD1	1:4:292:ASP:N	2.46	0.47
6:L:337:ALA:O	6:L:341:MET:HG2	2.14	0.47
8:N:342:ILE:HD11	18:o:75:LEU:HB3	1.96	0.47
13:Z:117:GLY:O	13:Z:120:HIS:ND1	2.39	0.47
23:t:156:ALA:HB2	23:t:163:PRO:HA	1.96	0.47
30:1:67:GLY:N	30:1:73:PHE:O	2.44	0.47
35:9:64:GLU:OE2	35:9:157:ASN:ND2	2.47	0.47
2:A:73:LEU:HD21	3:H:103:LEU:HD11	1.96	0.47
6:L:81:LYS:NZ	6:L:83:ASP:OD2	2.41	0.47
7:M:278:ARG:NE	25:v:82:ASP:OD1	2.47	0.47
7:M:447:LEU:HD11	45:w:801:PC1:H3F1	1.96	0.47
27:x:28:TRP:O	27:x:32:ILE:HG12	2.14	0.47
44:i:117:LEU:O	44:i:120:THR:OG1	2.32	0.47
1:4:166:PRO:HA	1:4:169:TRP:HB2	1.96	0.47
1:4:201:GLN:HE21	35:9:176:ARG:HG2	1.79	0.47
2:A:63:LEU:HD12	4:J:63:GLY:HA2	1.95	0.47
7:M:191:SER:HB3	45:M:501:PC1:H31	1.96	0.47
7:M:424:ASN:O	19:p:56:ARG:NH1	2.47	0.47
8:N:139:MET:HE2	8:N:139:MET:HA	1.96	0.47
13:Z:96:LYS:NZ	26:w:84:ARG:O	2.44	0.47
46:j:101:ZMP:O2	46:j:101:ZMP:N2	2.45	0.47
3:H:87:ILE:HG13	3:H:88:PRO:HD3	1.96	0.47
7:M:48:ASN:ND2	10:W:86:ASN:OD1	2.47	0.47
45:M:501:PC1:H381	45:M:501:PC1:H281	1.96	0.47
23:t:64:ARG:HG3	23:t:64:ARG:NH1	2.28	0.47
5:K:60:PRO:O	5:K:63:LEU:HB3	2.14	0.47
7:M:66:LEU:HD22	7:M:107:ILE:HG13	1.95	0.47
8:N:20:VAL:HG11	8:N:137:ALA:HB1	1.96	0.47
10:W:133:ILE:HD11	15:l:40:ILE:HB	1.96	0.47
30:1:378:ARG:NH2	30:1:388:GLU:OE1	2.46	0.47
30:1:430:MET:HE2	30:1:430:MET:HB3	1.84	0.47
6:L:210:ASN:OD1	6:L:270:ASN:ND2	2.47	0.47
6:L:433:GLY:O	17:n:59:ASN:ND2	2.47	0.47
14:k:35:LYS:HA	14:k:38:LEU:HB3	1.97	0.47
14:k:250:ASP:OD1	14:k:250:ASP:N	2.39	0.47
16:m:80:LEU:HA	16:m:83:LEU:HG	1.97	0.47
22:s:117:ARG:NH1	22:s:121:MET:SD	2.86	0.47
23:t:100:GLU:HB2	23:t:121:ARG:HH12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:9:23:GLN:HG3	35:9:28:THR:HB	1.97	0.47
40:e:54:ILE:O	40:e:55:ARG:NH1	2.41	0.47
3:H:264:LEU:HD11	29:z:9:ILE:HG12	1.96	0.47
10:W:114:MET:HE2	10:W:120:GLY:HA3	1.96	0.47
32:3:315:VAL:HG12	32:3:521:MET:HB3	1.97	0.47
1:4:369:ALA:HB2	1:4:374:PHE:HB2	1.97	0.47
12:Y:82:THR:HA	12:Y:85:TRP:CD1	2.49	0.47
15:l:13:LEU:O	15:l:16:TRP:NE1	2.45	0.47
27:x:7:PRO:HG2	27:x:10:GLY:HA3	1.96	0.47
30:1:261:HIS:ND1	30:1:338:ASP:OD1	2.48	0.47
42:g:34:LEU:HD21	42:g:86:LYS:HG3	1.97	0.47
11:X:2:ASP:N	11:X:2:ASP:OD1	2.47	0.47
34:6:155:ALA:HB2	35:9:137:PHE:HD2	1.80	0.47
35:9:168:ASN:OD1	44:i:88:ARG:NH1	2.48	0.47
1:4:143:GLU:OE2	1:4:278:TYR:OH	2.30	0.46
2:A:72:LEU:HD13	2:A:94:LEU:HD22	1.96	0.46
8:N:170:LEU:O	8:N:295:ARG:NH1	2.46	0.46
4:J:107:VAL:HG21	5:K:3:LEU:HD13	1.97	0.46
6:L:387:THR:OG1	6:L:461:SER:O	2.29	0.46
6:L:466:PHE:O	6:L:470:ASN:ND2	2.48	0.46
14:k:45:LYS:NZ	14:k:232:GLU:OE2	2.48	0.46
7:M:237:LYS:HD2	7:M:316:MET:HG2	1.97	0.46
34:6:79:SER:O	34:6:83:SER:OG	2.34	0.46
1:4:50:ASN:HD21	2:A:38:GLU:HG3	1.79	0.46
12:Y:124:LEU:HD13	20:q:69:ALA:HB2	1.97	0.46
32:3:139:ASP:O	37:b:77:LYS:NZ	2.39	0.46
32:3:144:PRO:HD2	32:3:192:MET:HE1	1.95	0.46
32:3:249:ARG:HE	32:3:251:LEU:HD21	1.80	0.46
23:t:3:LEU:HD12	23:t:6:ALA:HB3	1.98	0.46
32:3:357:ASP:N	32:3:357:ASP:OD1	2.49	0.46
34:6:177:TYR:HD2	34:6:178:ARG:HH21	1.62	0.46
1:4:200:HIS:NE2	35:9:124:GLU:OE1	2.49	0.46
30:1:197:GLU:OE1	38:c:129:ARG:NH2	2.47	0.46
30:1:327:THR:OG1	30:1:328:GLY:N	2.46	0.46
32:3:533:THR:OG1	32:3:534:ARG:N	2.48	0.46
1:4:339:LYS:HB3	37:b:69:PRO:HA	1.97	0.46
6:L:142:ILE:HG12	7:M:370:PRO:HB2	1.98	0.46
29:z:2:TRP:O	29:z:5:VAL:HG12	2.15	0.46
31:2:111:ARG:HD3	31:2:151:ALA:HB3	1.98	0.46
3:H:209:SER:HB3	3:H:213:VAL:HA	1.97	0.46
6:L:604:PHE:O	8:N:150:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:374:LYS:HB3	32:3:132:GLU:HG2	1.97	0.46
39:d:133:SER:OG	39:d:134:HIS:N	2.49	0.46
1:4:69:SER:OG	2:A:115:GLU:OE2	2.33	0.46
6:L:10:VAL:HG21	21:r:78:VAL:HG22	1.98	0.46
32:3:669:LYS:HE3	32:3:692:THR:HG22	1.98	0.46
1:4:145:THR:OG1	1:4:181:TYR:OH	2.30	0.45
6:L:577:ILE:O	6:L:580:GLN:NE2	2.40	0.45
8:N:24:THR:HG22	15:l:2:PHE:HZ	1.81	0.45
12:Y:89:ASP:OD1	29:z:34:ARG:NH1	2.44	0.45
13:Z:141:ARG:NH2	26:w:109:GLU:OE1	2.49	0.45
13:Z:163:LEU:HD21	26:w:121:PRO:HD2	1.97	0.45
31:2:50:VAL:O	31:2:53:LEU:HB3	2.15	0.45
32:3:285:ARG:NH1	32:3:289:GLY:O	2.43	0.45
32:3:367:THR:OG1	32:3:370:GLY:N	2.49	0.45
1:4:51:PHE:HB2	1:4:66:MET:HE2	1.97	0.45
2:A:19:THR:HG23	2:A:23:TRP:HD1	1.79	0.45
3:H:257:ILE:HG13	29:z:17:PHE:HE2	1.81	0.45
4:J:170:GLU:HG2	8:N:1:MET:HE3	1.97	0.45
6:L:154:LEU:HD13	6:L:243:VAL:HG22	1.98	0.45
6:L:161:ARG:NE	6:L:238:GLU:OE1	2.37	0.45
38:c:88:THR:OG1	38:c:89:LYS:N	2.49	0.45
2:A:104:TYR:CZ	4:J:166:VAL:HG23	2.52	0.45
3:H:228:TYR:HA	3:H:231:ILE:HG22	1.98	0.45
17:n:13:MET:SD	17:n:13:MET:N	2.86	0.45
25:v:59:ASP:O	25:v:64:TRP:NE1	2.41	0.45
1:4:7:ASP:OD1	1:4:7:ASP:N	2.47	0.45
10:W:18:ASP:OD1	10:W:18:ASP:N	2.48	0.45
32:3:14:ASP:OD2	32:3:81:THR:OG1	2.29	0.45
32:3:258:ILE:HG22	32:3:259:ASN:HB3	1.99	0.45
3:H:148:ILE:HD13	3:H:148:ILE:HA	1.84	0.45
6:L:61:MET:HE3	6:L:61:MET:HB3	1.83	0.45
20:q:19:ASP:OD1	20:q:19:ASP:N	2.49	0.45
23:t:94:GLU:HA	23:t:97:LYS:HG2	1.97	0.45
32:3:404:LEU:HD23	32:3:406:VAL:HG22	1.99	0.45
33:5:38:GLN:HG2	41:f:106:PRO:HD3	1.99	0.45
34:6:171:LYS:HE2	34:6:174:ARG:HD3	1.97	0.45
8:N:62:THR:HG21	8:N:114:TRP:CD1	2.52	0.45
8:N:66:ALA:HB2	8:N:104:MET:HB3	1.99	0.45
8:N:193:VAL:HG11	8:N:266:ILE:HD12	1.99	0.45
8:N:241:THR:HA	8:N:244:VAL:HG12	1.97	0.45
39:d:26:ALA:HB3	39:d:47:VAL:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:325:MET:HE1	7:M:441:MET:HE3	1.99	0.45
11:X:47:GLN:NE2	11:X:71:MET:SD	2.89	0.45
23:t:26:LEU:HD11	23:t:39:PHE:HB3	1.98	0.45
23:t:155:PRO:HG2	23:t:157:ARG:HE	1.81	0.45
32:3:47:SER:O	32:3:161:ARG:NH1	2.42	0.45
39:d:132:ILE:HD13	39:d:132:ILE:HA	1.85	0.45
1:4:406:SER:O	1:4:406:SER:OG	2.31	0.45
3:H:316:PRO:HG3	20:q:56:ARG:HB3	1.99	0.45
30:1:140:GLY:O	30:1:179:ARG:NH2	2.44	0.45
32:3:57:VAL:HA	32:3:86:THR:HG23	1.99	0.45
42:g:75:PRO:O	42:g:79:ASP:HB2	2.16	0.45
12:Y:12:LEU:O	15:l:104:ARG:NH2	2.50	0.45
35:9:49:ASN:O	35:9:53:GLU:N	2.49	0.45
11:j:54:MET:HE2	11:j:54:MET:HB2	1.84	0.45
2:A:98:LEU:HD22	3:H:298:LEU:HD21	1.99	0.45
7:M:434:ASN:HD22	7:M:434:ASN:HA	1.60	0.45
38:c:31:LYS:HE2	38:c:31:LYS:HB2	1.77	0.45
2:A:26:GLN:NE2	2:A:27:LEU:O	2.51	0.44
7:M:373:ILE:HA	7:M:376:ILE:HD12	1.99	0.44
8:N:181:TYR:HA	8:N:184:ILE:HD12	1.98	0.44
14:k:59:ALA:HA	14:k:62:THR:HG22	1.99	0.44
32:3:106:PRO:HB2	35:9:78:ILE:HD11	1.99	0.44
39:d:80:SER:HA	39:d:83:ARG:HE	1.82	0.44
11:X:6:LEU:HD13	11:X:14:ARG:HH12	1.82	0.44
21:r:86:LYS:O	21:r:90:THR:OG1	2.35	0.44
30:1:304:THR:OG1	30:1:327:THR:OG1	2.33	0.44
44:i:101:LYS:HE3	44:i:101:LYS:HB3	1.80	0.44
4:J:103:MET:HA	4:J:106:TYR:HB2	1.98	0.44
6:L:535:ARG:HH22	25:v:92:SER:HG	1.63	0.44
10:W:13:PRO:HD3	23:t:98:VAL:HG21	1.99	0.44
20:q:27:ARG:HG2	35:9:32:ARG:HD3	1.98	0.44
1:4:63:ARG:HB3	1:4:79:HIS:HB2	1.99	0.44
1:4:362:ALA:HB2	1:4:379:VAL:HG13	1.99	0.44
3:H:179:TRP:HE1	20:q:42:LEU:HG	1.83	0.44
6:L:136:ASN:OD1	6:L:136:ASN:N	2.51	0.44
7:M:80:SER:HB2	7:M:226:ALA:HB2	1.99	0.44
12:Y:37:LYS:HE3	12:Y:37:LYS:HB3	1.77	0.44
32:3:439:PHE:HA	32:3:442:VAL:HB	2.00	0.44
42:g:30:ARG:HB3	42:g:82:VAL:HG11	2.00	0.44
3:H:1:MET:HE1	29:z:29:PHE:HD2	1.83	0.44
8:N:274:ASP:HB2	9:V:139:LYS:HZ1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:l:78:ILE:HD12	20:q:93:GLU:HG3	1.99	0.44
22:s:102:GLU:OE2	22:s:105:ARG:NH2	2.50	0.44
39:d:113:ILE:HG23	39:d:114:PRO:HD3	2.00	0.44
39:d:157:ARG:HA	39:d:157:ARG:HD3	1.82	0.44
17:n:84:GLU:OE1	24:u:42:HIS:NE2	2.49	0.44
20:q:6:LYS:HD2	20:q:6:LYS:HA	1.89	0.44
3:H:56:PHE:HD2	45:d:401:PC1:H3G2	1.81	0.44
6:L:328:HIS:ND1	6:L:391:SER:OG	2.46	0.44
6:L:387:THR:HG23	6:L:465:GLY:HA3	1.98	0.44
7:M:279:GLN:HB2	7:M:285:LEU:HD12	1.99	0.44
8:N:165:GLY:HA2	8:N:181:TYR:HD1	1.83	0.44
10:W:87:TYR:HE1	13:Z:89:MET:HG3	1.82	0.44
12:Y:44:LEU:HB2	16:m:55:PRO:HG2	1.99	0.44
12:Y:49:GLU:OE2	12:Y:54:ARG:NH2	2.48	0.44
17:n:17:ASP:OD2	17:n:20:GLN:N	2.51	0.44
32:3:13:VAL:HB	32:3:33:VAL:HG21	2.00	0.44
38:c:19:ILE:HG22	38:c:22:LEU:HB2	2.00	0.44
42:g:28:LYS:NZ	46:j:101:ZMP:O3	2.51	0.44
43:h:45:SER:O	43:h:51:ASN:ND2	2.50	0.44
3:H:233:MET:HE3	3:H:233:MET:HB3	1.73	0.44
6:L:195:THR:HG21	6:L:200:GLN:HB3	1.99	0.44
9:V:65:ILE:HD11	9:V:100:LEU:HB2	2.00	0.44
33:5:184:VAL:HG21	42:g:109:THR:HG21	1.98	0.44
34:6:54:CYS:HB2	49:6:300:SF4:S1	2.58	0.44
40:e:24:GLN:O	40:e:33:ARG:NH1	2.51	0.44
4:J:139:GLU:O	4:J:143:ILE:HG12	2.18	0.44
8:N:178:ILE:HG23	8:N:292:PHE:HE1	1.83	0.44
11:X:37:MET:SD	11:X:37:MET:N	2.90	0.44
29:z:57:VAL:HB	29:z:59:ARG:HG3	1.99	0.44
35:9:77:CYS:O	35:9:105:ARG:NH1	2.51	0.44
2:A:79:SER:HA	2:A:87:MET:HE2	2.00	0.43
8:N:221:ALA:HB1	8:N:323:MET:HE2	1.99	0.43
12:Y:165:ARG:NH2	18:o:87:ASP:OD1	2.49	0.43
21:r:74:VAL:O	21:r:78:VAL:HG23	2.18	0.43
32:3:43:HIS:HB3	32:3:46:LEU:HB2	2.00	0.43
32:3:604:SER:OG	32:3:609:MET:O	2.29	0.43
1:4:94:LYS:HB3	1:4:98:GLN:HB2	1.99	0.43
6:L:286:LEU:HD13	6:L:411:MET:HB3	2.00	0.43
6:L:356:ILE:HD11	6:L:430:ALA:HB2	2.00	0.43
6:L:559:GLU:OE2	7:M:218:LYS:NZ	2.39	0.43
8:N:243:LEU:HA	8:N:246:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:t:118:PHE:O	23:t:122:GLU:HG2	2.19	0.43
36:a:54:LEU:HD23	36:a:54:LEU:HA	1.90	0.43
39:d:105:ASP:OD1	39:d:105:ASP:N	2.44	0.43
4:J:163:ILE:HA	4:J:166:VAL:HG12	2.00	0.43
6:L:67:HIS:CE1	6:L:70:THR:HG23	2.53	0.43
6:L:173:LEU:HD12	7:M:405:LEU:HD11	2.00	0.43
6:L:547:LYS:HB3	6:L:547:LYS:HE2	1.76	0.43
8:N:102:LEU:HD13	8:N:142:LEU:HG	2.00	0.43
8:N:312:LYS:HA	8:N:315:TRP:CD2	2.53	0.43
9:V:85:ASP:O	9:V:88:ASN:ND2	2.51	0.43
10:W:63:HIS:NE2	10:W:76:ALA:O	2.45	0.43
23:t:58:LYS:HD2	23:t:58:LYS:HA	1.74	0.43
25:v:5:THR:OG1	25:v:6:LYS:N	2.46	0.43
33:5:211:GLN:NE2	41:f:114:PRO:O	2.52	0.43
39:d:300:LEU:HD22	39:d:305:VAL:HG11	2.00	0.43
40:e:64:LEU:HD11	40:e:90:LEU:HG	2.01	0.43
1:4:19:MET:HE2	8:N:295:ARG:HD3	2.00	0.43
2:A:76:PRO:O	2:A:79:SER:HB2	2.18	0.43
6:L:553:LEU:HD11	19:p:93:GLY:HA2	1.99	0.43
26:w:39:GLU:OE1	26:w:39:GLU:N	2.51	0.43
30:1:94:VAL:HG11	30:1:192:LEU:HD21	2.01	0.43
33:5:135:TRP:HE1	42:g:87:MET:HE2	1.83	0.43
1:4:51:PHE:HZ	1:4:57:ALA:HB3	1.82	0.43
3:H:61:LEU:HD21	34:6:81:ARG:HH11	1.84	0.43
3:H:136:VAL:O	3:H:140:ILE:HG12	2.18	0.43
6:L:202:PHE:O	13:Z:121:ARG:NH1	2.51	0.43
7:M:373:ILE:HD11	7:M:444:LEU:HD12	2.00	0.43
10:W:12:LYS:HB2	10:W:12:LYS:HE3	1.76	0.43
14:k:33:SER:HA	14:k:174:VAL:HG21	2.01	0.43
39:d:97:ARG:NH2	55:d:402:NDP:O1A	2.52	0.43
3:H:75:PRO:HB2	3:H:222:LEU:HD12	2.01	0.43
7:M:427:LEU:HD22	26:w:38:TYR:HD2	1.83	0.43
11:X:50:ILE:O	11:X:54:MET:HG2	2.19	0.43
14:k:252:ASP:OD1	14:k:252:ASP:N	2.44	0.43
32:3:215:PHE:HD2	35:9:98:PRO:HB3	1.82	0.43
34:6:77:ARG:NH2	34:6:82:GLN:OE1	2.43	0.43
38:c:10:LEU:HD12	42:g:15:SER:HB3	2.00	0.43
3:H:18:ALA:HB1	3:H:48:PRO:HB3	2.00	0.43
5:K:61:ILE:O	5:K:64:LEU:HB3	2.18	0.43
6:L:129:LEU:HA	6:L:132:VAL:HG22	2.00	0.43
7:M:325:MET:HB2	7:M:440:HIS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:61:GLU:HB3	23:t:84:SER:HB2	2.00	0.43
19:p:4:LYS:HA	19:p:4:LYS:HD2	1.91	0.43
1:4:290:ARG:NH1	1:4:292:ASP:OD2	2.49	0.43
6:L:15:LEU:HD23	6:L:15:LEU:HA	1.86	0.43
6:L:381:THR:HG22	6:L:420:ALA:HA	2.00	0.43
7:M:51:ASN:ND2	10:W:90:THR:OG1	2.45	0.43
8:N:88:LYS:HE3	8:N:88:LYS:HB2	1.87	0.43
13:Z:41:ASP:OD2	21:r:86:LYS:NZ	2.51	0.43
6:L:241:THR:HG21	6:L:344:GLY:HA3	2.01	0.43
31:2:158:ASP:OD1	31:2:158:ASP:N	2.48	0.43
33:5:136:ASP:OD2	33:5:151:ILE:N	2.49	0.43
39:d:49:TYR:HE2	39:d:70:PHE:HB3	1.83	0.43
39:d:95:VAL:HG11	39:d:113:ILE:HD13	2.01	0.43
1:4:208:MET:HE1	20:q:10:PRO:HD3	2.01	0.43
7:M:64:PRO:HB3	7:M:454:ILE:HG22	1.99	0.43
7:M:423:ILE:HG12	19:p:58:VAL:HG22	2.01	0.43
14:k:319:LEU:HD23	14:k:319:LEU:HA	1.86	0.43
26:w:64:PHE:HA	26:w:68:ILE:HB	2.00	0.43
32:3:329:ILE:HD12	32:3:329:ILE:HA	1.86	0.43
1:4:105:ARG:NH2	34:6:149:CYS:SG	2.90	0.42
3:H:81:LEU:HD11	3:H:111:LEU:HG	2.00	0.42
3:H:106:LEU:HD21	3:H:150:LEU:HD23	2.00	0.42
4:J:20:PHE:HB2	4:J:29:GLY:HA2	2.01	0.42
6:L:193:LEU:HG	6:L:204:LEU:HD12	2.01	0.42
6:L:203:MET:HE3	13:Z:128:LEU:HD22	2.01	0.42
6:L:535:ARG:HH12	25:v:92:SER:N	2.16	0.42
7:M:196:TRP:HE3	7:M:197:LEU:HD23	1.84	0.42
11:X:24:LYS:HE3	11:X:42:LEU:HD23	2.01	0.42
14:k:116:LEU:HD11	14:k:259:LEU:HD23	2.01	0.42
22:s:27:ASP:OD1	22:s:27:ASP:N	2.37	0.42
38:c:115:SER:O	38:c:115:SER:OG	2.30	0.42
1:4:61:VAL:HG21	1:4:83:LEU:HB2	1.99	0.42
2:A:67:LEU:HD12	5:K:65:VAL:HA	2.01	0.42
6:L:84:PHE:O	6:L:88:MET:CB	2.66	0.42
10:W:39:GLY:O	10:W:43:ILE:HG22	2.18	0.42
30:1:49:LEU:HD11	30:1:123:LEU:HD21	2.01	0.42
33:5:131:GLU:O	33:5:134:ILE:HB	2.19	0.42
34:6:34:ASP:OD1	34:6:38:ASN:ND2	2.52	0.42
38:c:90:GLU:OE2	38:c:90:GLU:N	2.51	0.42
41:f:65:LYS:HD2	41:f:65:LYS:HA	1.89	0.42
1:4:339:LYS:NZ	37:b:67:GLY:O	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:434:GLN:O	6:L:436:ARG:NE	2.51	0.42
14:k:298:GLU:H	14:k:298:GLU:HG3	1.66	0.42
22:s:8:TYR:OH	25:v:123:PRO:O	2.31	0.42
40:e:42:GLU:HA	40:e:45:LYS:HB2	2.01	0.42
1:4:4:TRP:CD2	7:M:140:THR:HG22	2.55	0.42
3:H:91:MET:HG2	3:H:259:PHE:CZ	2.53	0.42
4:J:24:PRO:HB3	4:J:89:VAL:HG11	2.00	0.42
5:K:94:ASN:HB3	6:L:583:LEU:HD23	2.00	0.42
9:V:89:TYR:HB3	9:V:121:ALA:HB1	2.01	0.42
19:p:56:ARG:HA	19:p:56:ARG:HD3	1.86	0.42
19:p:112:GLU:HA	19:p:115:ILE:HG22	2.02	0.42
32:3:239:VAL:HG23	32:3:253:ARG:HG3	2.00	0.42
33:5:116:PRO:HG2	42:g:17:LYS:HE3	2.01	0.42
39:d:134:HIS:HD2	39:d:145:TYR:HE1	1.68	0.42
39:d:195:SER:O	39:d:195:SER:OG	2.34	0.42
41:f:27:TYR:HA	41:f:30:ILE:HG22	2.00	0.42
44:i:8:LYS:HD2	44:i:11:LEU:HD21	2.01	0.42
6:L:10:VAL:HA	6:L:13:ILE:HG22	2.01	0.42
6:L:365:ALA:HB1	6:L:443:ILE:HD13	2.00	0.42
11:X:38:LYS:HE2	11:X:38:LYS:HB2	1.78	0.42
22:s:108:LEU:O	22:s:112:LYS:HG2	2.20	0.42
23:t:29:ARG:HH11	23:t:75:HIS:HD2	1.67	0.42
29:z:70:ASP:OD1	29:z:70:ASP:N	2.40	0.42
4:J:135:PHE:HD2	20:q:67:ARG:HD2	1.84	0.42
6:L:169:LEU:HD11	7:M:405:LEU:HD13	2.00	0.42
46:X:101:ZMP:H15	46:X:101:ZMP:H17	1.58	0.42
13:Z:108:ARG:NH1	26:w:101:GLU:OE2	2.52	0.42
14:k:305:ARG:HB3	14:k:308:TYR:HD2	1.84	0.42
21:r:3:TYR:HB3	21:r:8:LYS:HB2	2.01	0.42
26:w:36:ASN:O	26:w:40:LYS:NZ	2.40	0.42
30:1:15:LEU:O	30:1:20:ARG:NH1	2.52	0.42
30:1:28:ARG:HA	30:1:28:ARG:HD3	1.87	0.42
32:3:121:MET:HE2	32:3:121:MET:HB3	1.91	0.42
3:H:51:ASP:OD1	34:6:44:SER:OG	2.33	0.42
3:H:139:THR:HA	3:H:142:TYR:CD2	2.55	0.42
3:H:268:ILE:HD13	3:H:268:ILE:HA	1.90	0.42
6:L:313:MET:HA	6:L:316:THR:HG22	2.02	0.42
7:M:115:LEU:HD12	7:M:174:LEU:HD22	2.02	0.42
14:k:144:ILE:HG22	14:k:145:ARG:H	1.85	0.42
3:H:171:GLN:HG3	20:q:52:TRP:HB2	2.02	0.42
7:M:424:ASN:OD1	7:M:424:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:5:15:ASN:OD1	33:5:15:ASN:N	2.48	0.42
1:4:161:ILE:HG22	3:H:278:PRO:HB3	2.02	0.42
1:4:168:PHE:HD1	34:6:65:PRO:HD3	1.85	0.42
6:L:361:GLY:HA2	17:n:59:ASN:HD21	1.84	0.42
7:M:266:LEU:HB3	7:M:395:LEU:HD13	2.02	0.42
9:V:94:CYS:HA	9:V:114:CYS:HA	2.02	0.42
14:k:244:ASP:OD1	14:k:244:ASP:N	2.52	0.42
15:l:19:ILE:HG13	15:l:21:SER:H	1.83	0.42
28:y:46:ARG:HH12	28:y:49:LYS:HG3	1.84	0.42
31:2:29:LYS:HB3	31:2:29:LYS:HE2	1.70	0.42
34:6:86:MET:HE1	34:6:104:TYR:HB2	2.01	0.42
44:i:85:GLU:HB2	44:i:98:PRO:HB3	2.02	0.42
8:N:238:PRO:O	8:N:241:THR:OG1	2.29	0.42
13:Z:48:ARG:HA	13:Z:48:ARG:HD2	1.85	0.42
21:r:18:ARG:NH1	23:t:172:ARG:O	2.40	0.42
21:r:102:ARG:H	21:r:102:ARG:HG2	1.59	0.42
22:s:3:HIS:HB2	22:s:15:GLU:HG2	2.01	0.42
29:z:51:ASP:HA	29:z:54:VAL:HG12	2.02	0.42
30:1:96:ASN:ND2	30:1:187:GLY:O	2.42	0.42
41:f:37:ILE:HB	41:f:44:ARG:HG3	2.02	0.42
4:J:33:LEU:HD22	4:J:64:MET:SD	2.60	0.41
5:K:59:MET:HE3	5:K:60:PRO:HD3	2.02	0.41
6:L:473:PRO:HA	6:L:474:PRO:HD3	1.95	0.41
7:M:13:PRO:O	7:M:17:LEU:N	2.50	0.41
10:W:103:LEU:HD23	10:W:103:LEU:HA	1.88	0.41
22:s:103:ARG:HB2	24:u:64:LEU:HD22	2.02	0.41
32:3:227:SER:OG	32:3:228:ILE:N	2.52	0.41
32:3:644:GLN:HG3	40:e:41:VAL:HG22	2.01	0.41
33:5:211:GLN:NE2	41:f:115:ILE:O	2.52	0.41
43:h:11:ARG:HB3	43:h:19:LEU:HD12	2.02	0.41
6:L:145:GLU:OE2	6:L:176:ARG:NH1	2.53	0.41
6:L:223:LYS:HA	6:L:223:LYS:HD3	1.79	0.41
14:k:221:LEU:HD11	14:k:241:LEU:HD11	2.02	0.41
23:t:68:LYS:HA	23:t:68:LYS:HD3	1.84	0.41
30:1:370:ASP:OD2	32:3:179:ASN:ND2	2.39	0.41
32:3:54:MET:HE3	32:3:90:ARG:HG2	2.02	0.41
32:3:232:ASP:OD1	32:3:232:ASP:N	2.53	0.41
32:3:243:ARG:HD2	32:3:244:THR:HG23	2.01	0.41
39:d:13:ARG:NH2	39:d:63:GLY:O	2.53	0.41
1:4:403:ASP:OD1	1:4:403:ASP:N	2.54	0.41
13:Z:70:VAL:HG21	28:y:43:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:528:ASP:OD2	32:3:676:SER:OG	2.36	0.41
34:6:79:SER:HB2	34:6:82:GLN:HG2	2.02	0.41
7:M:23:ILE:O	7:M:27:THR:OG1	2.30	0.41
12:Y:16:GLU:HB2	12:Y:18:LYS:HE3	2.01	0.41
12:Y:46:ARG:NH2	20:q:79:ASP:OD2	2.50	0.41
13:Z:136:LYS:HD2	13:Z:136:LYS:HA	1.92	0.41
1:4:263:SER:O	1:4:263:SER:OG	2.35	0.41
7:M:400:MET:HA	7:M:403:THR:HG22	2.02	0.41
14:k:37:LYS:O	14:k:41:GLU:N	2.51	0.41
2:A:28:ASN:O	2:A:33:LYS:NZ	2.48	0.41
6:L:535:ARG:NH1	25:v:90:ASP:O	2.53	0.41
7:M:49:SER:OG	7:M:51:ASN:OD1	2.38	0.41
7:M:94:LEU:HD12	7:M:94:LEU:HA	1.91	0.41
8:N:170:LEU:HD11	8:N:288:LEU:HD11	2.03	0.41
8:N:246:ILE:HD12	8:N:334:THR:HG21	2.01	0.41
16:m:7:PHE:O	16:m:11:VAL:HG22	2.19	0.41
16:m:76:SER:OG	16:m:77:LEU:N	2.53	0.41
18:o:3:THR:O	18:o:6:GLN:C	2.63	0.41
20:q:57:ARG:HD2	20:q:57:ARG:HA	1.88	0.41
32:3:462:ASP:OD1	32:3:462:ASP:N	2.54	0.41
35:9:169:ILE:O	35:9:173:TYR:HB3	2.20	0.41
39:d:10:LYS:HE3	39:d:10:LYS:HB3	1.96	0.41
40:e:68:TYR:HE2	40:e:74:LYS:HB2	1.86	0.41
1:4:103:PHE:HE2	1:4:376:VAL:HG11	1.86	0.41
10:W:107:GLU:OE2	10:W:111:ARG:NE	2.54	0.41
13:Z:18:ALA:HA	21:r:110:LEU:HD21	2.02	0.41
14:k:22:SER:OG	14:k:119:GLY:O	2.30	0.41
17:n:78:VAL:HA	17:n:81:VAL:HG12	2.03	0.41
19:p:25:SER:OG	19:p:27:GLU:OE1	2.26	0.41
22:s:45:MET:HE3	22:s:55:ARG:HD3	2.03	0.41
34:6:101:ARG:HA	34:6:101:ARG:HD2	1.76	0.41
35:9:3:LYS:HD3	43:h:111:TYR:HD2	1.85	0.41
1:4:34:ASN:HB3	14:k:158:VAL:HB	2.02	0.41
1:4:259:MET:HE1	1:4:421:GLN:HG2	2.03	0.41
6:L:553:LEU:HD23	6:L:553:LEU:HA	1.90	0.41
45:M:501:PC1:H2F1	8:N:284:ILE:HG13	2.02	0.41
9:V:72:THR:O	9:V:76:SER:OG	2.31	0.41
22:s:121:MET:SD	22:s:122:ALA:N	2.94	0.41
31:2:102:VAL:HG13	31:2:154:VAL:HG12	2.03	0.41
39:d:48:PRO:HB2	39:d:73:TRP:CD1	2.56	0.41
3:H:69:SER:O	3:H:73:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:59:MET:HE2	8:N:84:TRP:HH2	1.85	0.41
6:L:34:LEU:HB2	6:L:105:MET:HE1	2.02	0.41
6:L:338:MET:HB2	6:L:457:LEU:HB3	2.01	0.41
6:L:528:TYR:CG	25:v:101:MET:HG2	2.56	0.41
7:M:264:LEU:HD23	7:M:264:LEU:HA	1.96	0.41
11:X:83:LYS:HD2	11:X:83:LYS:HA	1.72	0.41
17:n:35:LEU:HD23	17:n:42:ASP:HB2	2.03	0.41
23:t:9:LEU:HD23	23:t:14:LYS:HD3	2.02	0.41
23:t:172:ARG:HA	23:t:173:PRO:HD3	1.89	0.41
25:v:42:MET:HE2	25:v:42:MET:HB2	1.93	0.41
30:1:138:ILE:HG21	30:1:146:ALA:HB2	2.03	0.41
32:3:564:ALA:O	32:3:569:LYS:NZ	2.41	0.41
43:h:107:GLN:OE1	43:h:107:GLN:N	2.54	0.41
11:j:52:MET:HA	11:j:55:GLU:HG3	2.03	0.41
2:A:13:LEU:HD13	3:H:10:ILE:HD12	2.03	0.41
3:H:24:GLU:HA	3:H:271:LEU:HD11	2.02	0.41
6:L:88:MET:HE2	6:L:88:MET:HB2	1.80	0.41
13:Z:8:VAL:HG12	26:w:97:VAL:HG13	2.02	0.41
14:k:2:GLN:NE2	14:k:264:GLN:OE1	2.54	0.41
22:s:107:LEU:HD23	22:s:107:LEU:HA	1.90	0.41
32:3:496:ILE:HD13	32:3:496:ILE:HA	1.96	0.41
34:6:62:MET:SD	34:6:69:MET:HB3	2.61	0.41
34:6:107:MET:HA	34:6:108:PRO:HD3	1.96	0.41
40:e:55:ARG:HA	40:e:55:ARG:HD3	1.91	0.41
44:i:1:MET:HE3	44:i:2:GLU:N	2.36	0.41
5:K:77:LEU:HD23	5:K:77:LEU:HA	1.90	0.40
13:Z:67:PHE:HB3	28:y:43:LEU:HD11	2.03	0.40
26:w:80:LEU:HD22	26:w:83:TYR:HD2	1.86	0.40
35:9:36:MET:HE3	35:9:36:MET:HB2	1.86	0.40
39:d:144:LYS:HE2	39:d:144:LYS:HB3	1.95	0.40
11:j:51:ILE:HD13	11:j:51:ILE:HA	1.91	0.40
2:A:64:LEU:O	2:A:68:GLU:HG2	2.21	0.40
3:H:113:VAL:O	3:H:117:LEU:HG	2.21	0.40
6:L:426:ILE:O	6:L:430:ALA:HB3	2.21	0.40
13:Z:118:GLU:N	22:s:49:GLN:OE1	2.54	0.40
18:o:109:TYR:HA	18:o:112:VAL:HG12	2.04	0.40
34:6:85:VAL:HG12	34:6:112:TYR:HB2	2.04	0.40
3:H:155:LEU:HD23	3:H:155:LEU:HA	1.88	0.40
6:L:233:LEU:HD23	6:L:307:SER:HB3	2.04	0.40
6:L:416:THR:O	6:L:419:THR:OG1	2.33	0.40
45:L:701:PC1:H32	45:w:801:PC1:H153	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:2:LEU:HD12	7:M:2:LEU:HA	1.90	0.40
7:M:252:PRO:HG3	18:o:117:HIS:CD2	2.56	0.40
7:M:433:GLU:O	7:M:437:MET:HG2	2.21	0.40
10:W:107:GLU:HA	18:o:90:MET:HE2	2.04	0.40
14:k:188:ASN:HB3	14:k:191:GLU:HG2	2.04	0.40
17:n:50:TRP:CD2	24:u:12:ARG:HB2	2.56	0.40
20:q:75:GLN:NE2	20:q:79:ASP:OD1	2.44	0.40
31:2:180:LYS:HA	31:2:180:LYS:HD2	1.75	0.40
35:9:67:LEU:HD23	35:9:67:LEU:HA	1.97	0.40
43:h:8:GLN:NE2	43:h:20:GLN:HG3	2.36	0.40
44:i:112:ASN:OD1	44:i:112:ASN:N	2.55	0.40
3:H:190:LEU:HB3	3:H:198:PHE:CD2	2.56	0.40
7:M:311:GLY:HA2	7:M:377:GLY:HA2	2.04	0.40
12:Y:45:CYS:O	12:Y:49:GLU:HB2	2.21	0.40
13:Z:159:LYS:O	13:Z:163:LEU:HG	2.21	0.40
23:t:14:LYS:HA	23:t:14:LYS:HD2	1.77	0.40
25:v:148:LYS:HD2	25:v:148:LYS:HA	1.84	0.40
32:3:71:MET:HE2	32:3:71:MET:HB2	1.89	0.40
32:3:187:ILE:HG13	32:3:189:LYS:HB2	2.03	0.40
39:d:26:ALA:HA	39:d:31:GLY:HA3	2.03	0.40
11:X:24:LYS:HE3	11:X:24:LYS:HB3	1.84	0.40
12:Y:4:VAL:HG13	20:q:108:SER:HB2	2.04	0.40
23:t:133:GLU:HA	23:t:136:VAL:HG22	2.03	0.40
32:3:286:ASN:OD1	32:3:290:LEU:N	2.53	0.40
44:i:63:ILE:HD13	44:i:63:ILE:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	418/430 (97%)	398 (95%)	20 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
3	H	316/318 (99%)	305 (96%)	11 (4%)	0	100	100
4	J	173/175 (99%)	165 (95%)	7 (4%)	1 (1%)	21	54
5	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
6	L	604/606 (100%)	576 (95%)	28 (5%)	0	100	100
7	M	457/459 (100%)	445 (97%)	12 (3%)	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
10	W	137/139 (99%)	137 (100%)	0	0	100	100
11	X	85/157 (54%)	81 (95%)	4 (5%)	0	100	100
11	j	73/157 (46%)	73 (100%)	0	0	100	100
12	Y	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
13	Z	169/171 (99%)	167 (99%)	2 (1%)	0	100	100
14	k	317/320 (99%)	300 (95%)	17 (5%)	0	100	100
15	l	103/105 (98%)	95 (92%)	8 (8%)	0	100	100
16	m	78/80 (98%)	70 (90%)	8 (10%)	0	100	100
17	n	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
18	o	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
19	p	126/128 (98%)	121 (96%)	5 (4%)	0	100	100
20	q	137/139 (99%)	133 (97%)	4 (3%)	0	100	100
21	r	95/126 (75%)	91 (96%)	4 (4%)	0	100	100
22	s	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
23	t	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
24	u	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
25	v	153/155 (99%)	140 (92%)	13 (8%)	0	100	100
26	w	99/101 (98%)	92 (93%)	7 (7%)	0	100	100
27	x	47/49 (96%)	47 (100%)	0	0	100	100
28	y	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
29	z	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
30	1	428/430 (100%)	416 (97%)	12 (3%)	0	100	100
31	2	211/213 (99%)	195 (92%)	16 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	3	686/688 (100%)	656 (96%)	30 (4%)	0	100	100
33	5	206/208 (99%)	196 (95%)	10 (5%)	0	100	100
34	6	148/150 (99%)	145 (98%)	3 (2%)	0	100	100
35	9	167/217 (77%)	160 (96%)	7 (4%)	0	100	100
36	a	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
37	b	93/95 (98%)	90 (97%)	3 (3%)	0	100	100
38	c	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
39	d	327/340 (96%)	319 (98%)	8 (2%)	0	100	100
40	e	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
41	f	111/113 (98%)	106 (96%)	5 (4%)	0	100	100
42	g	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
43	h	92/112 (82%)	87 (95%)	5 (5%)	0	100	100
44	i	143/145 (99%)	138 (96%)	5 (4%)	0	100	100
All	All	8091/8450 (96%)	7780 (96%)	310 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	116	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4	363/370 (98%)	362 (100%)	1 (0%)	86	84
2	A	103/103 (100%)	103 (100%)	0	100	100
3	H	278/278 (100%)	278 (100%)	0	100	100
4	J	144/144 (100%)	144 (100%)	0	100	100
5	K	86/86 (100%)	85 (99%)	1 (1%)	63	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	L	538/538 (100%)	537 (100%)	1 (0%)	87	87
7	M	411/411 (100%)	403 (98%)	8 (2%)	50	66
8	N	315/315 (100%)	314 (100%)	1 (0%)	86	84
9	V	101/101 (100%)	101 (100%)	0	100	100
10	W	122/122 (100%)	122 (100%)	0	100	100
11	X	80/141 (57%)	80 (100%)	0	100	100
11	j	71/141 (50%)	71 (100%)	0	100	100
12	Y	154/154 (100%)	154 (100%)	0	100	100
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%)	94 (100%)	0	100	100
16	m	69/69 (100%)	69 (100%)	0	100	100
17	n	61/61 (100%)	59 (97%)	2 (3%)	33	56
18	o	107/107 (100%)	106 (99%)	1 (1%)	70	74
19	p	114/114 (100%)	112 (98%)	2 (2%)	51	67
20	q	119/119 (100%)	119 (100%)	0	100	100
21	r	95/120 (79%)	95 (100%)	0	100	100
22	s	110/110 (100%)	110 (100%)	0	100	100
23	t	159/159 (100%)	157 (99%)	2 (1%)	61	71
24	u	59/59 (100%)	57 (97%)	2 (3%)	32	55
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%)	46 (100%)	0	100	100
29	z	59/59 (100%)	58 (98%)	1 (2%)	53	67
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%)	575 (100%)	3 (0%)	81	81
33	5	189/189 (100%)	189 (100%)	0	100	100
34	6	127/127 (100%)	126 (99%)	1 (1%)	73	76
35	9	146/179 (82%)	146 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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	286/294 (97%)	285 (100%)	1 (0%)	86	84
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	84/94 (89%)	83 (99%)	1 (1%)	63	72
44	i	131/131 (100%)	130 (99%)	1 (1%)	73	76
All	All	7159/7373 (97%)	7127 (100%)	32 (0%)	81	83

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4	64	LEU
5	K	61	ILE
6	L	386	LEU
7	M	22	MET
7	M	70	MET
7	M	129	THR
7	M	186	MET
7	M	193	THR
7	M	257	MET
7	M	350	THR
7	M	405	LEU
8	N	14	MET
17	n	17	ASP
17	n	56	PHE
18	o	2	MET
19	p	65	ILE
19	p	88	LEU
23	t	34	ASP
23	t	64	ARG
24	u	24	GLN
24	u	42	HIS
26	w	68	ILE
29	z	57	VAL
31	2	11	ASP
31	2	52	ASP

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Mol	Chain	Res	Type
32	3	65	VAL
32	3	121	MET
32	3	259	ASN
34	6	156	LEU
39	d	243	GLN
43	h	111	TYR
44	i	142	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	4	201	GLN
1	4	409	HIS
2	A	2	ASN
2	A	85	ASN
3	H	194	ASN
3	H	235	ASN
3	H	317	GLN
5	K	7	ASN
6	L	59	GLN
6	L	113	ASN
6	L	470	ASN
6	L	524	ASN
6	L	603	ASN
7	M	48	ASN
7	M	51	ASN
7	M	184	GLN
7	M	304	GLN
8	N	49	ASN
8	N	289	ASN
10	W	95	GLN
10	W	124	GLN
11	X	33	ASN
12	Y	15	GLN
13	Z	90	GLN
14	k	2	GLN
14	k	153	ASN
14	k	190	HIS
14	k	251	GLN
14	k	288	GLN
15	l	15	HIS
22	s	42	GLN

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Mol	Chain	Res	Type
22	s	116	GLN
23	t	17	GLN
23	t	74	GLN
27	x	5	GLN
27	x	46	ASN
28	y	13	HIS
30	1	250	ASN
30	1	293	ASN
30	1	398	GLN
30	1	421	HIS
31	2	101	GLN
32	3	117	GLN
32	3	141	ASN
32	3	237	ASN
32	3	444	GLN
32	3	581	GLN
34	6	164	GLN
35	9	144	HIS
37	b	94	GLN
39	d	44	GLN
39	d	67	GLN
39	d	87	HIS
39	d	148	ASN
40	e	85	GLN
40	e	92	ASN
41	f	49	GLN
42	g	125	HIS
43	h	35	GLN
44	i	72	ASN
11	j	33	ASN

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
1	2MR	4	85	1	10,12,13	2.50	2 (20%)	5,13,15	0.95	0
7	FME	M	1	7	8,9,10	0.97	0	8,9,11	0.88	0
9	AYA	V	1	9	6,7,8	1.22	1 (16%)	6,8,10	1.64	2 (33%)
6	FME	L	1	6	8,9,10	0.98	0	8,9,11	0.87	0
14	SEP	k	36	14	8,9,10	1.59	1 (12%)	7,12,14	1.33	1 (14%)
43	AYA	h	1	43	6,7,8	1.25	1 (16%)	6,8,10	1.13	1 (16%)
5	FME	K	1	5	8,9,10	0.96	0	8,9,11	0.94	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
1	2MR	4	85	1	-	1/10/13/15	-
7	FME	M	1	7	-	2/7/9/11	-
9	AYA	V	1	9	-	3/5/6/8	-
6	FME	L	1	6	-	1/7/9/11	-
14	SEP	k	36	14	-	4/6/8/10	-
43	AYA	h	1	43	-	1/5/6/8	-
5	FME	K	1	5	-	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	5.38	1.44	1.33
1	4	85	2MR	CZ-NE	5.17	1.45	1.34
14	k	36	SEP	P-O1P	3.50	1.61	1.50
43	h	1	AYA	CA-N	-2.26	1.44	1.46
9	V	1	AYA	CA-N	-2.07	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	2.89	110.95	108.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	AYA	CB-CA-N	2.72	112.75	109.68
43	h	1	AYA	CB-CA-N	2.51	112.51	109.68
9	V	1	AYA	CA-N-CT	2.46	124.68	121.50

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	M	1	FME	1	0
6	L	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
55	NDP	d	402	-	51,52,52	0.33	0	71,80,80	0.35	0
52	FES	3	803	32	0,4,4	-	-	-		
50	FMN	1	502	-	33,33,33	1.02	2 (6%)	48,50,50	1.22	8 (16%)
45	PC1	w	801	-	53,53,53	0.28	0	59,61,61	0.27	0
46	ZMP	X	101	11	25,30,36	0.79	1 (4%)	29,37,45	0.92	2 (6%)
51	NAI	1	503	-	47,48,48	0.43	1 (2%)	64,73,73	1.78	4 (6%)
52	FES	2	300	31	0,4,4	-	-	-		
45	PC1	L	701	-	53,53,53	0.31	0	59,61,61	0.57	2 (3%)
49	SF4	1	501	30	0,12,12	-	-	-		
49	SF4	3	802	32	0,12,12	-	-	-		
45	PC1	M	501	-	53,53,53	0.30	0	59,61,61	0.32	0
46	ZMP	j	101	11	28,33,36	0.69	1 (3%)	32,40,45	1.10	2 (6%)
45	PC1	H	401	-	53,53,53	0.30	0	59,61,61	0.46	0
49	SF4	6	300	34	0,12,12	-	-	-		
45	PC1	d	401	-	45,45,53	0.32	0	51,53,61	0.31	0
49	SF4	9	201	35	0,12,12	-	-	-		
49	SF4	9	202	35	0,12,12	-	-	-		
49	SF4	3	801	32	0,12,12	-	-	-		
48	MYR	s	201	22	13,14,15	0.17	0	12,13,15	0.14	0
47	AMP	k	501	-	25,25,25	1.41	4 (16%)	37,38,38	1.87	8 (21%)

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
55	NDP	d	402	-	-	5/34/77/77	0/5/5/5
52	FES	3	803	32	-	-	0/1/1/1
50	FMN	1	502	-	-	9/18/18/18	0/3/3/3
45	PC1	w	801	-	-	5/57/57/57	-
46	ZMP	X	101	11	-	15/35/37/43	-
51	NAI	1	503	-	-	11/29/72/72	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	FES	2	300	31	-	-	0/1/1/1
45	PC1	L	701	-	-	12/57/57/57	-
49	SF4	1	501	30	-	-	0/6/5/5
49	SF4	3	802	32	-	-	0/6/5/5
45	PC1	M	501	-	-	17/57/57/57	-
46	ZMP	j	101	11	-	16/38/40/43	-
45	PC1	H	401	-	-	13/57/57/57	-
49	SF4	6	300	34	-	-	0/6/5/5
45	PC1	d	401	-	-	12/49/49/57	-
49	SF4	9	201	35	-	-	0/6/5/5
49	SF4	9	202	35	-	-	0/6/5/5
49	SF4	3	801	32	-	-	0/6/5/5
48	MYR	s	201	22	-	0/12/12/13	-
47	AMP	k	501	-	-	3/10/26/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	k	501	AMP	C5-C4	4.72	1.47	1.39
50	1	502	FMN	C4A-N5	3.32	1.37	1.30
46	X	101	ZMP	C9-C10	2.77	1.53	1.50
47	k	501	AMP	C5-C6	2.70	1.48	1.41
46	j	101	ZMP	C9-C10	2.43	1.53	1.50
50	1	502	FMN	C10-N1	2.37	1.38	1.33
47	k	501	AMP	C8-N7	2.32	1.36	1.31
47	k	501	AMP	C5-N7	-2.30	1.34	1.39
51	1	503	NAI	PA-O5B	2.22	1.68	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	1	503	NAI	O5B-PA-O1A	-9.53	71.17	108.94
51	1	503	NAI	O2A-PA-O1A	-8.19	74.36	112.44
47	k	501	AMP	C5-C4-N3	-5.83	118.69	126.72
51	1	503	NAI	O3-PA-O1A	-5.78	93.32	110.70
47	k	501	AMP	N3-C4-N9	4.65	135.08	127.17
47	k	501	AMP	C2-N3-C4	3.68	120.82	111.83
47	k	501	AMP	C4-C5-N7	-3.41	106.68	110.58
50	1	502	FMN	C4-N3-C2	-3.27	119.83	125.64
47	k	501	AMP	N3-C2-N1	-3.20	123.73	128.58
46	j	101	ZMP	O1-C10-C9	-3.10	120.40	123.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	1	502	FMN	C4A-C10-N10	2.81	120.50	116.48
47	k	501	AMP	C4-N9-C8	2.60	108.47	105.74
50	1	502	FMN	C4A-C4-N3	2.59	119.85	113.25
47	k	501	AMP	C5-N7-C8	2.56	107.47	103.45
50	1	502	FMN	O4-C4-C4A	-2.47	120.00	126.53
51	1	503	NAI	O2A-PA-O5B	2.45	118.67	107.57
46	X	101	ZMP	O1-C10-C9	-2.42	121.19	123.98
45	L	701	PC1	O21-C2-C1	2.36	116.80	108.34
50	1	502	FMN	C10-C4A-N5	-2.35	120.02	124.81
45	L	701	PC1	C2-O21-C21	2.31	123.32	117.80
46	X	101	ZMP	C15-C14-C13	-2.21	108.71	112.39
50	1	502	FMN	C5A-C9A-N10	2.10	119.87	117.97
50	1	502	FMN	C4A-C10-N1	-2.08	119.50	124.59
46	j	101	ZMP	C14-C15-N2	-2.07	107.59	112.00
50	1	502	FMN	C9A-C5A-N5	-2.04	120.28	122.45
47	k	501	AMP	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (118) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	H	401	PC1	C11-O13-P-O12
45	H	401	PC1	C11-O13-P-O14
45	H	401	PC1	C11-O13-P-O11
45	H	401	PC1	C1-O11-P-O14
45	H	401	PC1	C1-O11-P-O13
45	L	701	PC1	C1-O11-P-O12
45	L	701	PC1	C1-O11-P-O14
45	L	701	PC1	C1-O11-P-O13
45	M	501	PC1	C11-O13-P-O11
45	M	501	PC1	C1-O11-P-O12
45	M	501	PC1	C1-O11-P-O13
45	w	801	PC1	C11-O13-P-O12
45	w	801	PC1	C11-O13-P-O11
45	d	401	PC1	C1-O11-P-O12
45	d	401	PC1	C1-O11-P-O14
45	d	401	PC1	C1-O11-P-O13
46	X	101	ZMP	O4-C17-C18-C21
46	X	101	ZMP	C16-C17-C18-C21
46	X	101	ZMP	C17-C16-N2-C15
46	X	101	ZMP	O1-C10-S1-C11
46	X	101	ZMP	C9-C10-S1-C11

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Mol	Chain	Res	Type	Atoms
46	X	101	ZMP	C7-C8-C9-C10
46	j	101	ZMP	C19-C18-C21-O5
46	j	101	ZMP	C20-C18-C21-O5
46	j	101	ZMP	C17-C18-C21-O5
46	j	101	ZMP	O4-C17-C18-C21
46	j	101	ZMP	C16-C17-C18-C21
46	j	101	ZMP	O4-C17-C18-C19
46	j	101	ZMP	S1-C11-C12-N1
46	j	101	ZMP	C7-C8-C9-C10
47	k	501	AMP	O4'-C4'-C5'-O5'
50	1	502	FMN	N10-C1'-C2'-O2'
50	1	502	FMN	N10-C1'-C2'-C3'
50	1	502	FMN	C1'-C2'-C3'-C4'
50	1	502	FMN	C5'-O5'-P-O2P
50	1	502	FMN	C5'-O5'-P-O3P
51	1	503	NAI	C5D-O5D-PN-O1N
55	d	402	NDP	C2N-C3N-C7N-N7N
46	X	101	ZMP	O3-C16-N2-C15
47	k	501	AMP	C3'-C4'-C5'-O5'
45	M	501	PC1	C11-C12-N-C14
45	d	401	PC1	C11-C12-N-C14
45	H	401	PC1	C21-C22-C23-C24
51	1	503	NAI	C2D-C1D-N1N-C6N
45	M	501	PC1	C11-C12-N-C15
45	d	401	PC1	C11-C12-N-C15
51	1	503	NAI	C2D-C1D-N1N-C2N
45	M	501	PC1	C3A-C3B-C3C-C3D
45	d	401	PC1	C3B-C3C-C3D-C3E
45	L	701	PC1	C31-C32-C33-C34
45	L	701	PC1	C38-C39-C3A-C3B
45	M	501	PC1	C11-C12-N-C13
45	d	401	PC1	C11-C12-N-C13
46	j	101	ZMP	C22-C1-C2-C3
50	1	502	FMN	C5'-O5'-P-O1P
45	w	801	PC1	C3E-C3F-C3G-C3H
45	M	501	PC1	O31-C31-C32-C33
55	d	402	NDP	PN-O3-PA-O1A
45	L	701	PC1	C2-C1-O11-P
45	M	501	PC1	O11-C1-C2-C3
50	1	502	FMN	O2'-C2'-C3'-C4'
50	1	502	FMN	O2'-C2'-C3'-O3'
51	1	503	NAI	PN-O3-PA-O5B

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Mol	Chain	Res	Type	Atoms
45	L	701	PC1	O11-C1-C2-C3
45	H	401	PC1	C2B-C2C-C2D-C2E
46	X	101	ZMP	C4-C5-C6-C7
46	X	101	ZMP	C16-C17-C18-C19
46	X	101	ZMP	C16-C17-C18-C20
46	j	101	ZMP	C16-C17-C18-C19
46	j	101	ZMP	C16-C17-C18-C20
46	j	101	ZMP	C3-C4-C5-C6
51	1	503	NAI	O4D-C1D-N1N-C6N
45	H	401	PC1	O13-C11-C12-N
45	L	701	PC1	O13-C11-C12-N
46	X	101	ZMP	O3-C16-C17-O4
51	1	503	NAI	O4D-C1D-N1N-C2N
45	L	701	PC1	O11-C1-C2-O21
45	M	501	PC1	O11-C1-C2-O21
55	d	402	NDP	C2N-C3N-C7N-O7N
45	H	401	PC1	C1-O11-P-O12
45	M	501	PC1	C11-O13-P-O14
45	M	501	PC1	C1-O11-P-O14
51	1	503	NAI	C5B-O5B-PA-O1A
51	1	503	NAI	C5D-O5D-PN-O3
51	1	503	NAI	C5D-O5D-PN-O2N
45	M	501	PC1	C2-C1-O11-P
51	1	503	NAI	C4D-C5D-O5D-PN
45	M	501	PC1	C36-C37-C38-C39
45	H	401	PC1	C2C-C2D-C2E-C2F
46	X	101	ZMP	O4-C17-C18-C19
45	L	701	PC1	C24-C25-C26-C27
45	L	701	PC1	O31-C31-C32-C33
45	d	401	PC1	C2-C1-O11-P
45	M	501	PC1	O32-C31-C32-C33
47	k	501	AMP	C4'-C5'-O5'-P
46	X	101	ZMP	C5-C6-C7-C8
45	H	401	PC1	C3-C2-O21-C21
45	L	701	PC1	C1-C2-O21-C21
46	j	101	ZMP	C4-C5-C6-C7
51	1	503	NAI	C2N-C3N-C7N-N7N
55	d	402	NDP	O4D-C1D-N1N-C6N
45	M	501	PC1	C25-C26-C27-C28
50	1	502	FMN	C1'-C2'-C3'-O3'
45	d	401	PC1	O31-C31-C32-C33
46	j	101	ZMP	C2-C1-C22-C23

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Mol	Chain	Res	Type	Atoms
55	d	402	NDP	C2D-C1D-N1N-C6N
46	X	101	ZMP	O4-C17-C18-C20
46	j	101	ZMP	O3-C16-C17-O4
45	w	801	PC1	O31-C31-C32-C33
45	d	401	PC1	O21-C21-C22-C23
45	H	401	PC1	C23-C24-C25-C26
45	d	401	PC1	C22-C23-C24-C25
45	d	401	PC1	O22-C21-C22-C23
46	X	101	ZMP	N2-C16-C17-O4
46	j	101	ZMP	N2-C16-C17-O4
45	M	501	PC1	O21-C21-C22-C23
45	w	801	PC1	O32-C31-C32-C33
45	H	401	PC1	C34-C35-C36-C37

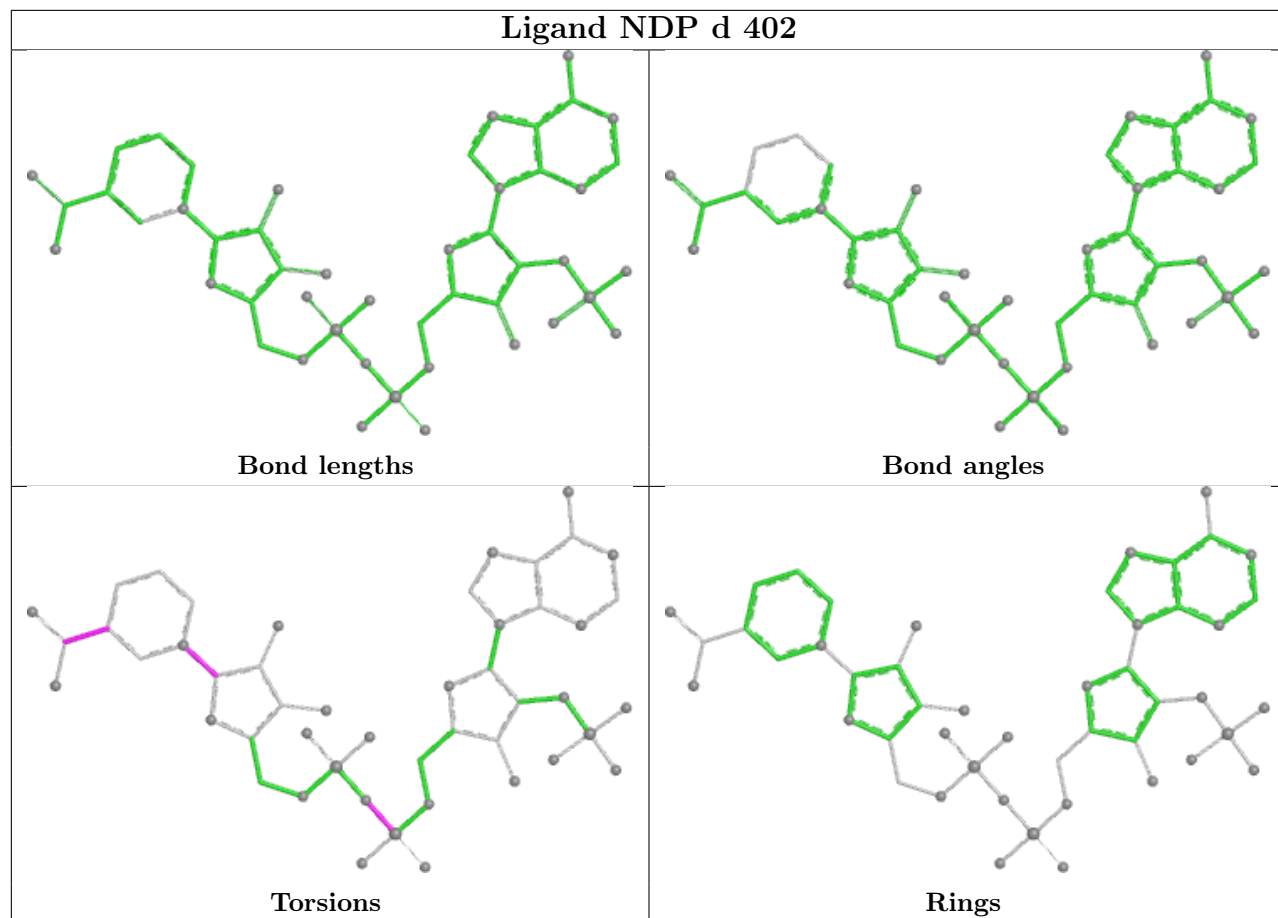
There are no ring outliers.

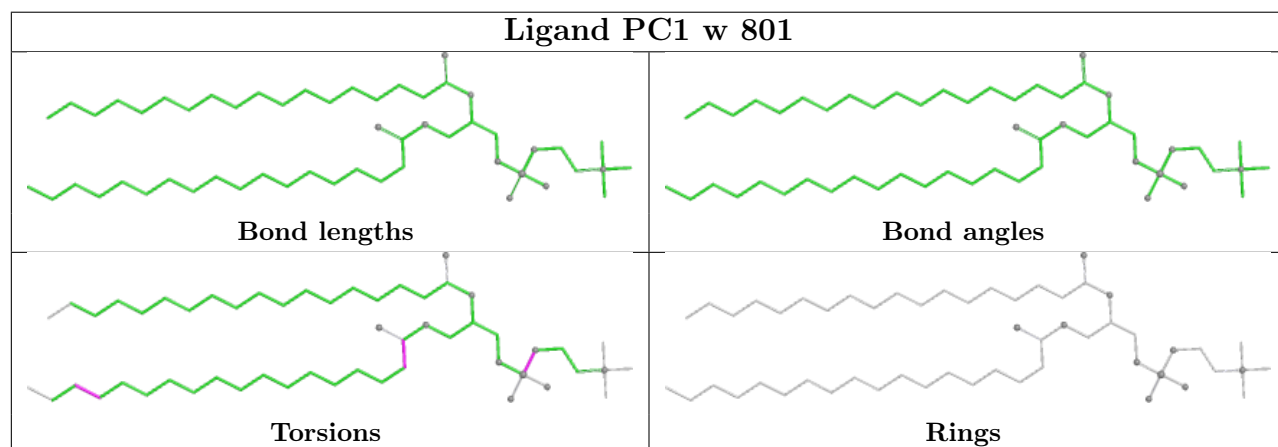
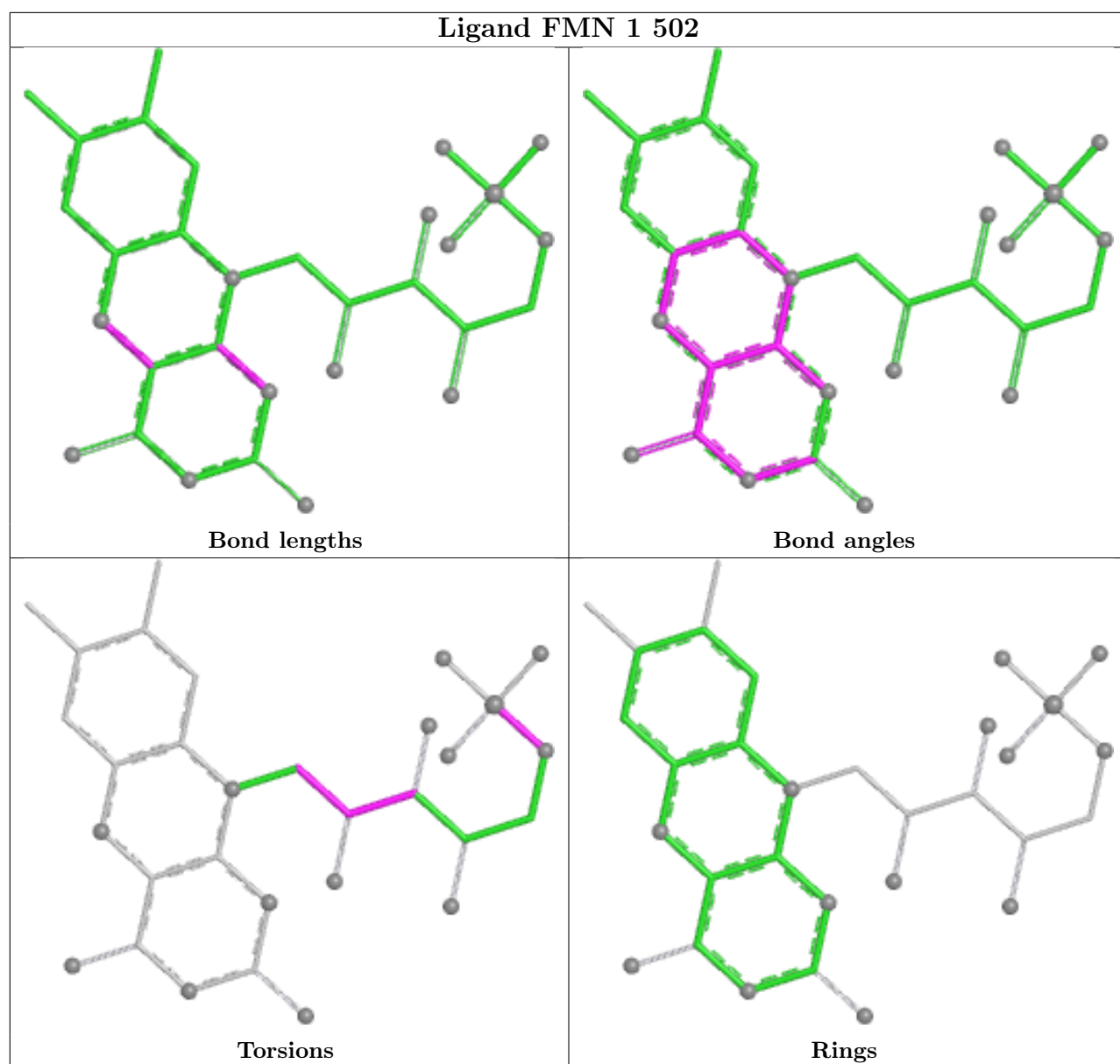
12 monomers are involved in 24 short contacts:

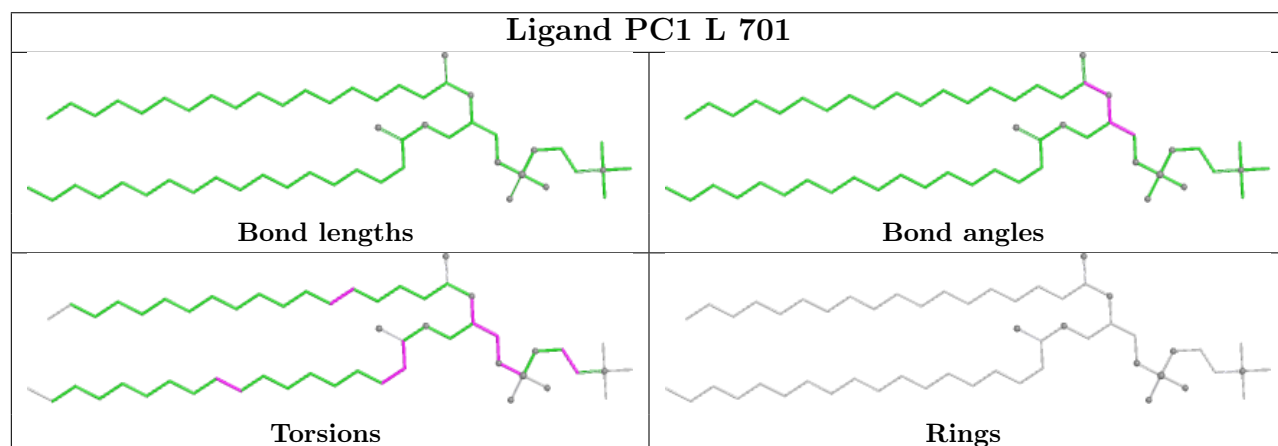
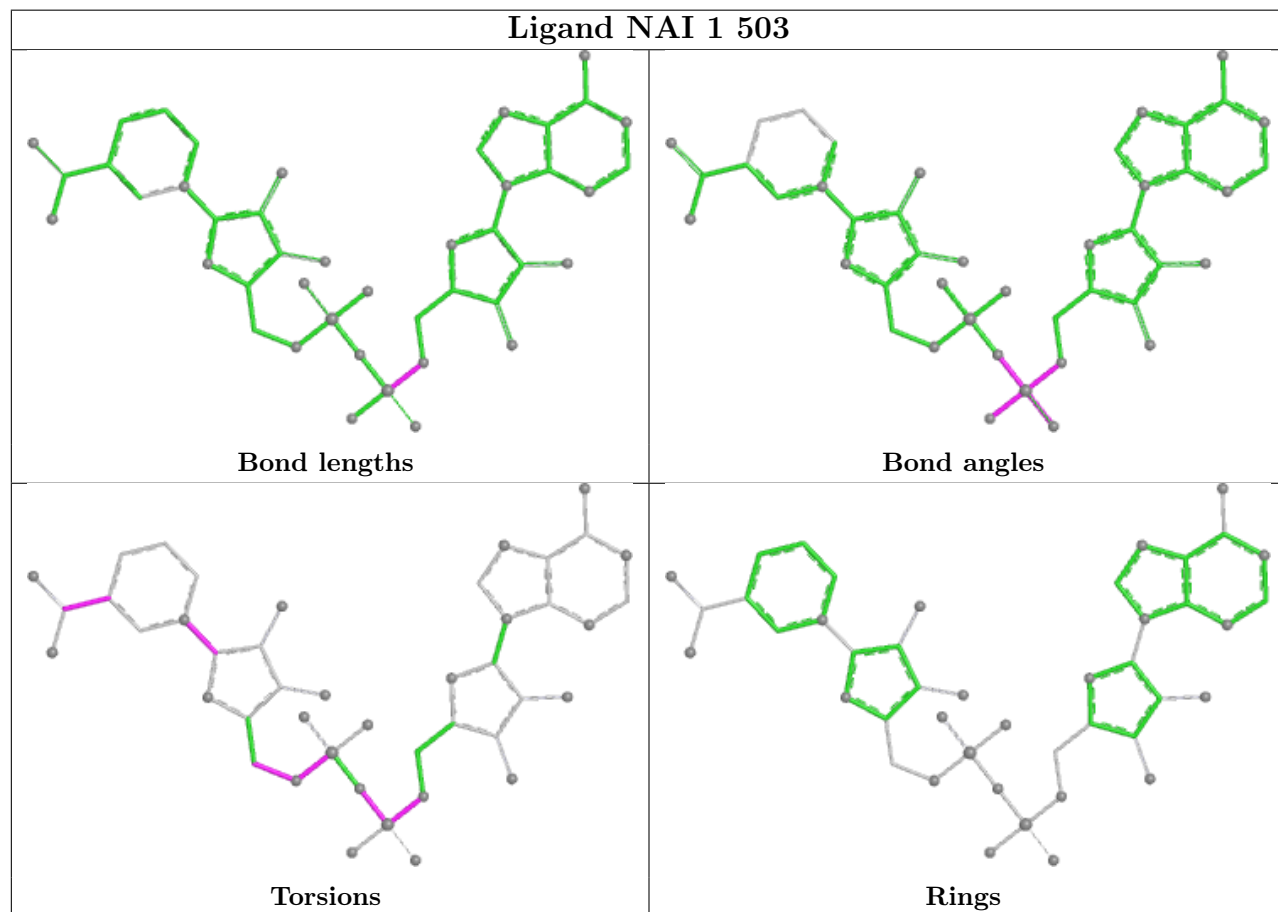
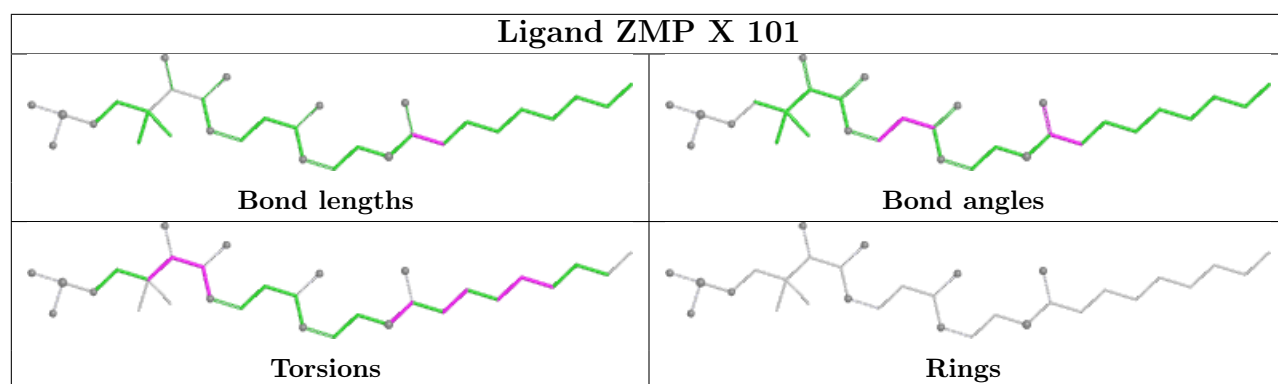
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	d	402	NDP	1	0
45	w	801	PC1	2	0
46	X	101	ZMP	1	0
51	1	503	NAI	3	0
45	L	701	PC1	3	0
45	M	501	PC1	4	0
46	j	101	ZMP	4	0
45	H	401	PC1	2	0
49	6	300	SF4	1	0
45	d	401	PC1	1	0
49	3	801	SF4	2	0
47	k	501	AMP	1	0

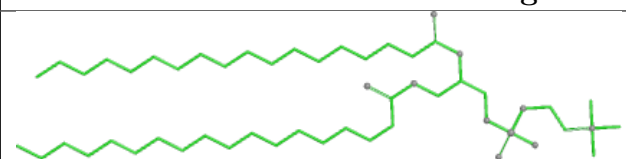
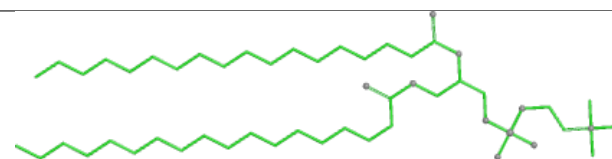
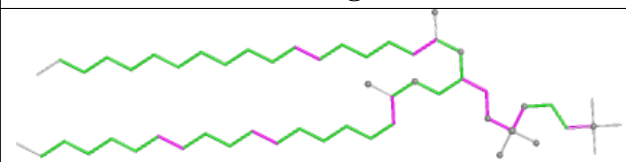
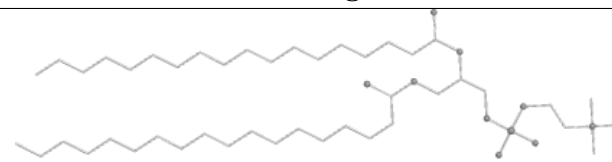
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

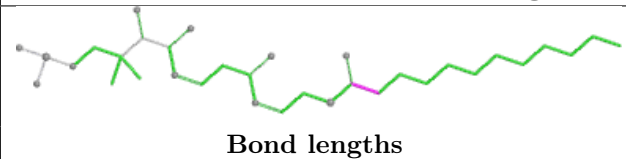
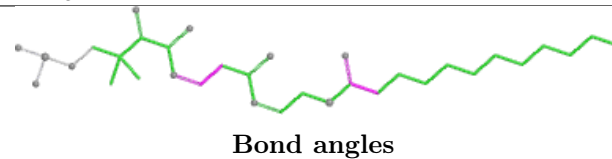
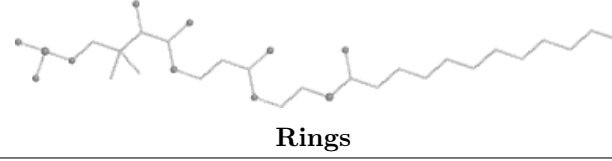
equivalents in the CSD to analyse the geometry.

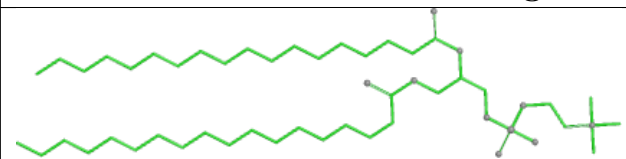
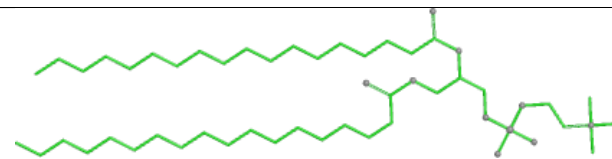
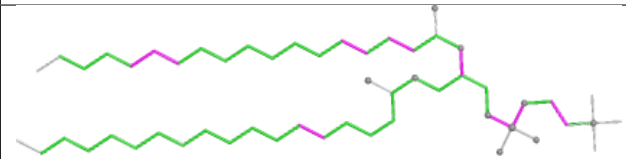
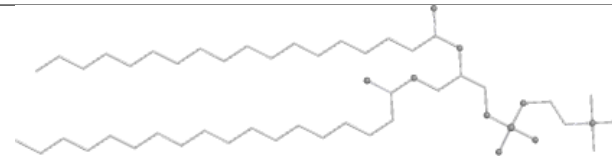


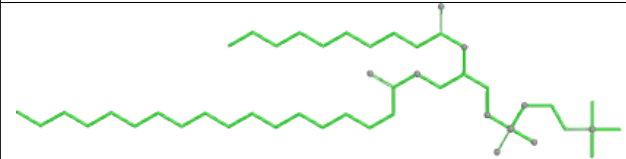
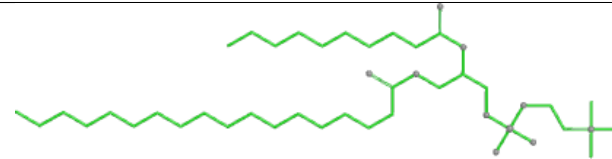
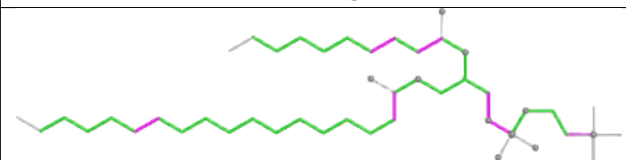
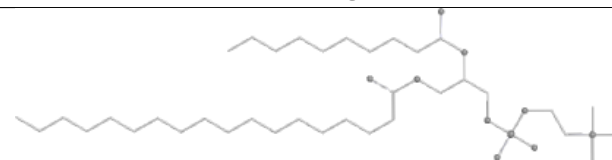


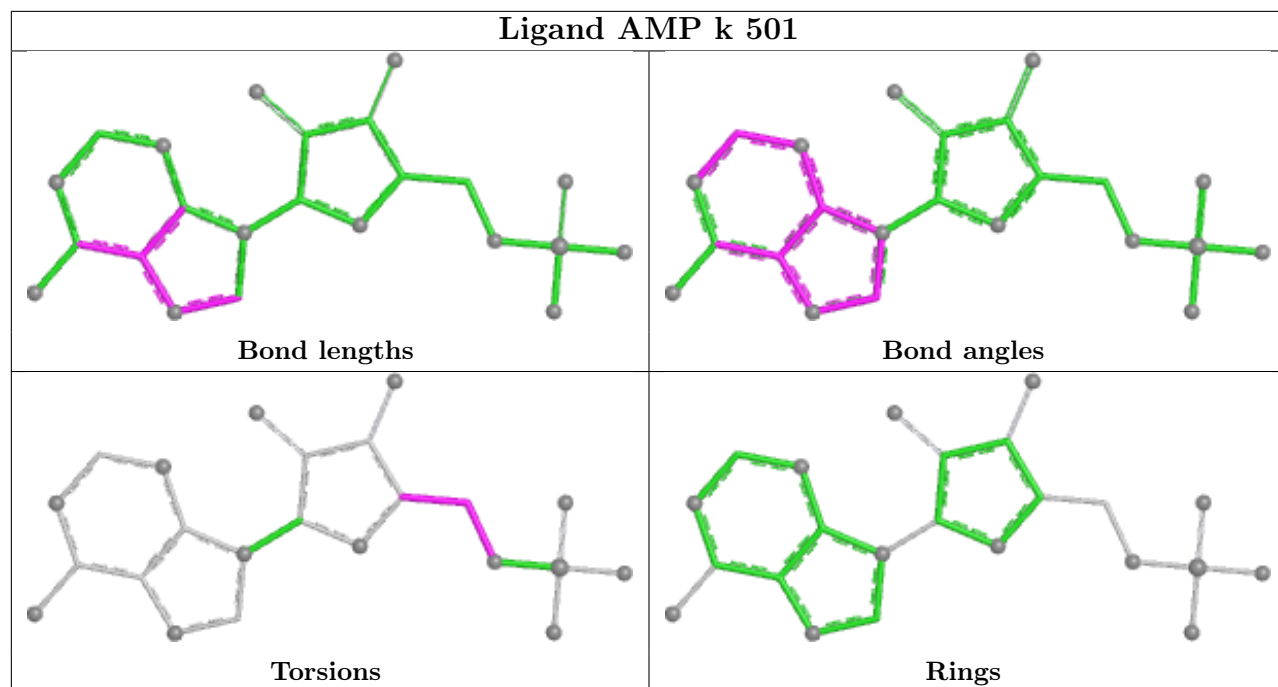


Ligand PC1 M 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ZMP j 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PC1 H 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PC1 d 401	
	
Bond lengths	Bond angles
	
Torsions	Rings



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.

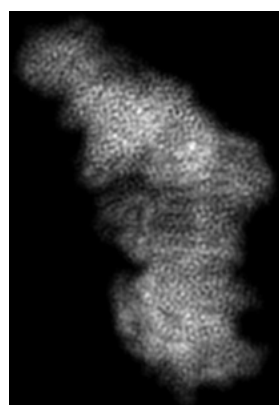
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14688. These allow visual inspection of the internal detail of the map and identification of artifacts.

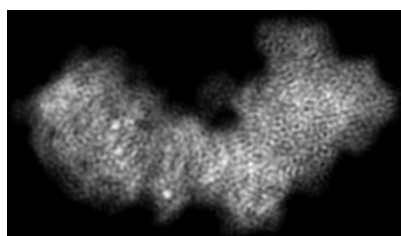
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

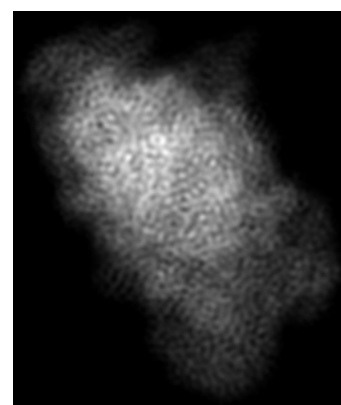
6.1.1 Primary map



X



Y



Z

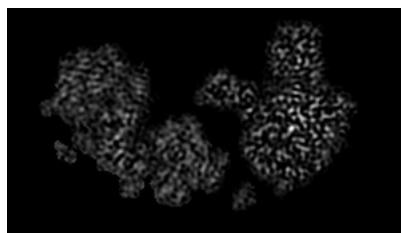
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 68



Y Index: 80



Z Index: 118

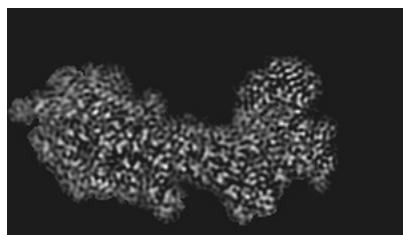
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

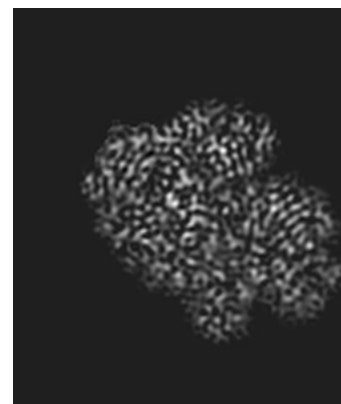
6.3.1 Primary map



X Index: 60



Y Index: 104



Z Index: 172

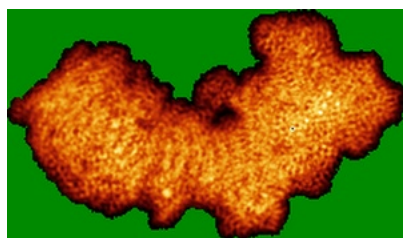
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

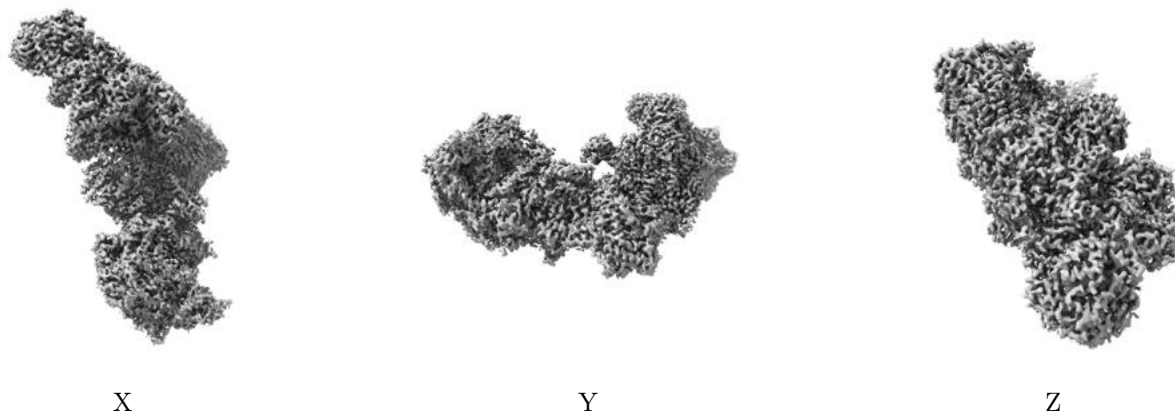


Z

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

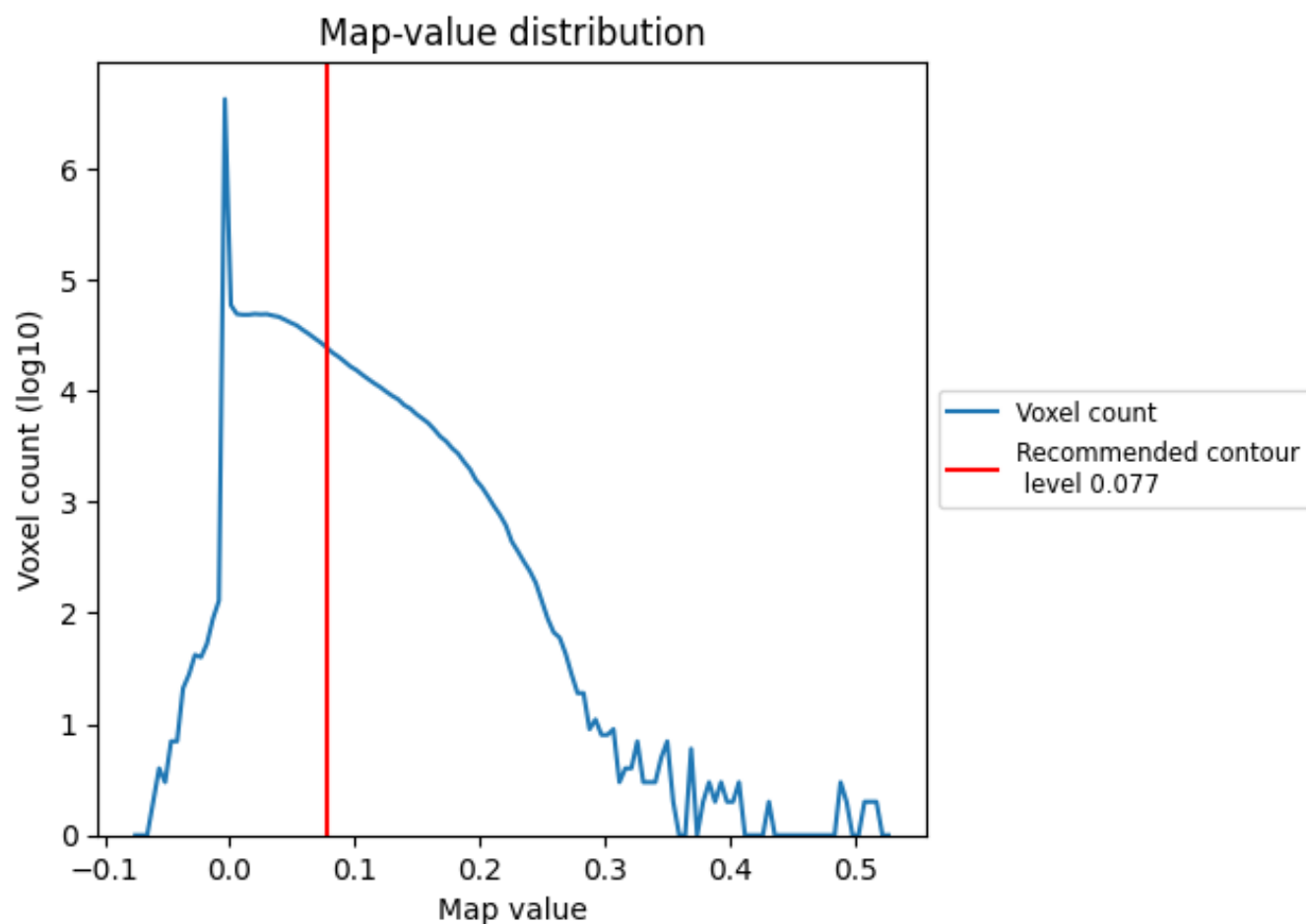
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

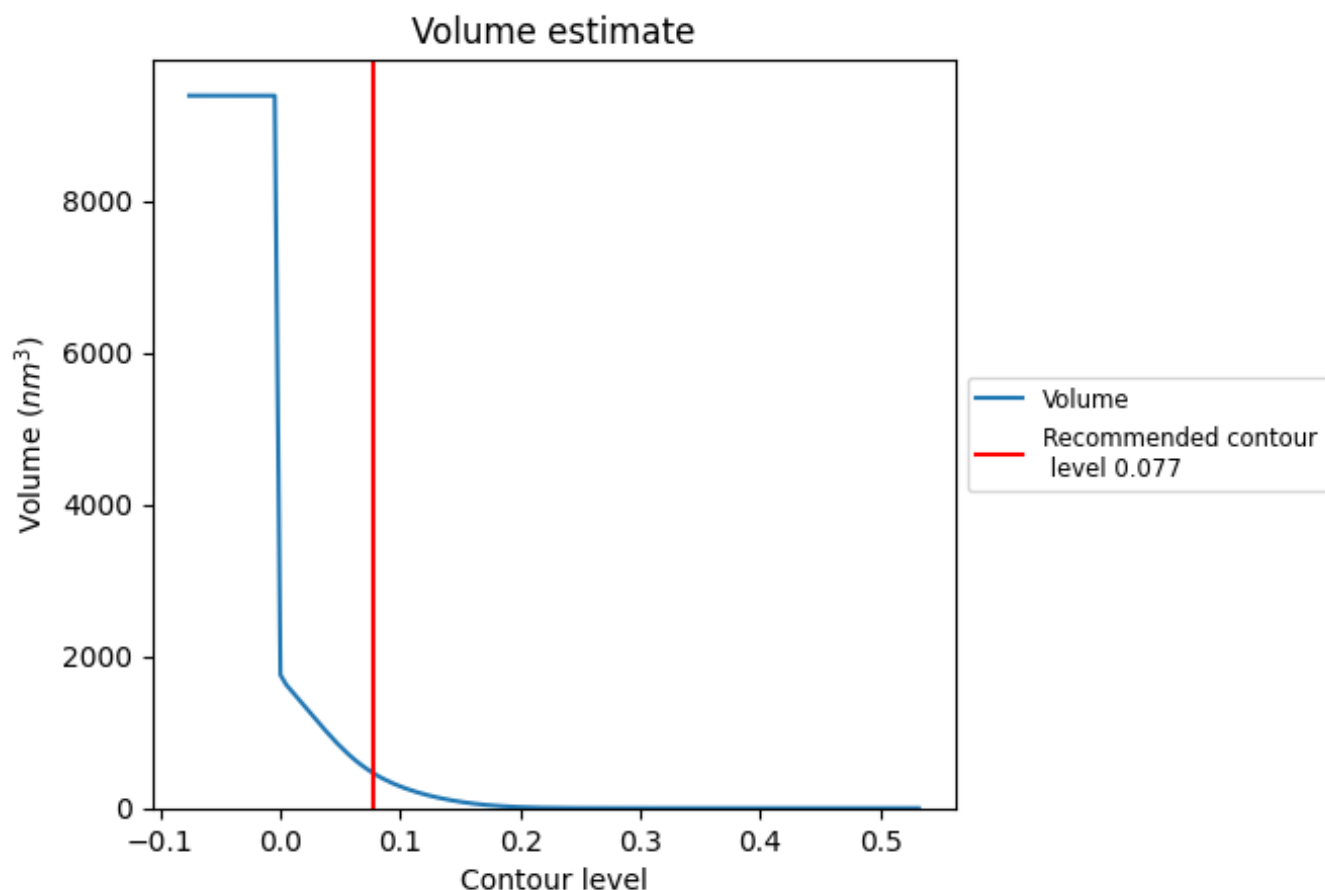
This section contains the results of statistical analysis of the map.

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 467 nm³; this corresponds to an approximate mass of 422 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.

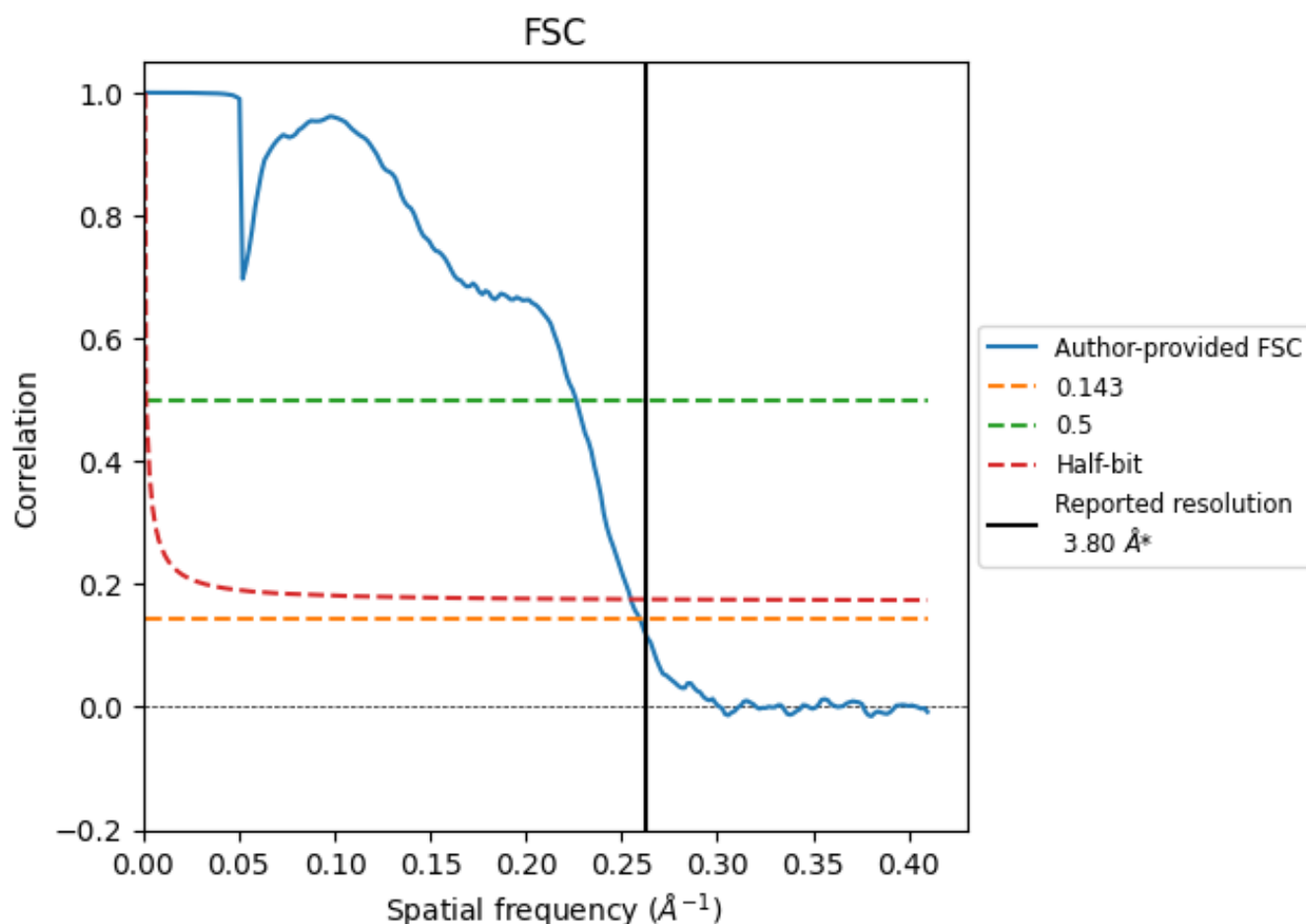
7.3 Rotationally averaged power spectrum [i](#)

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 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

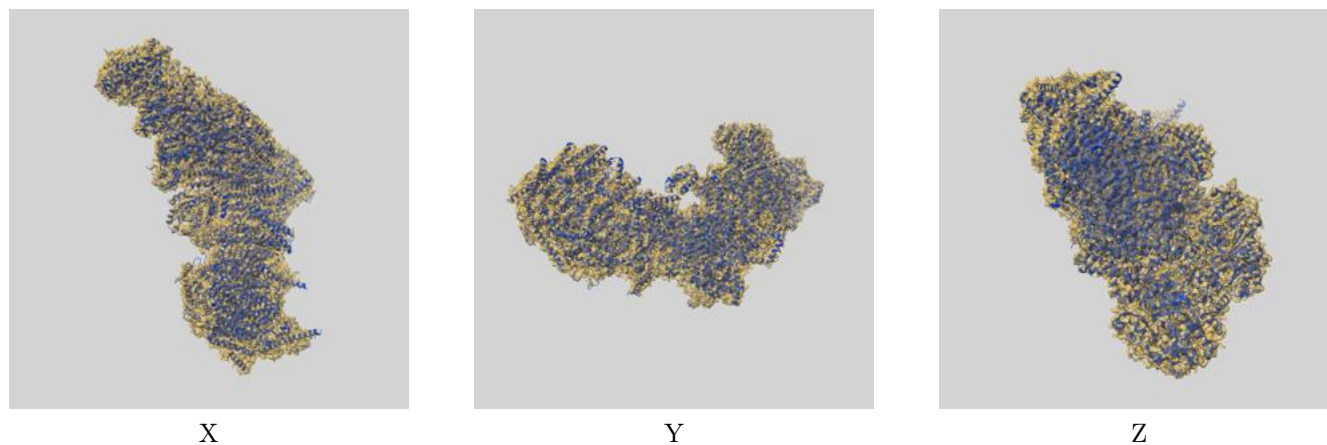
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.85	4.42	3.92
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

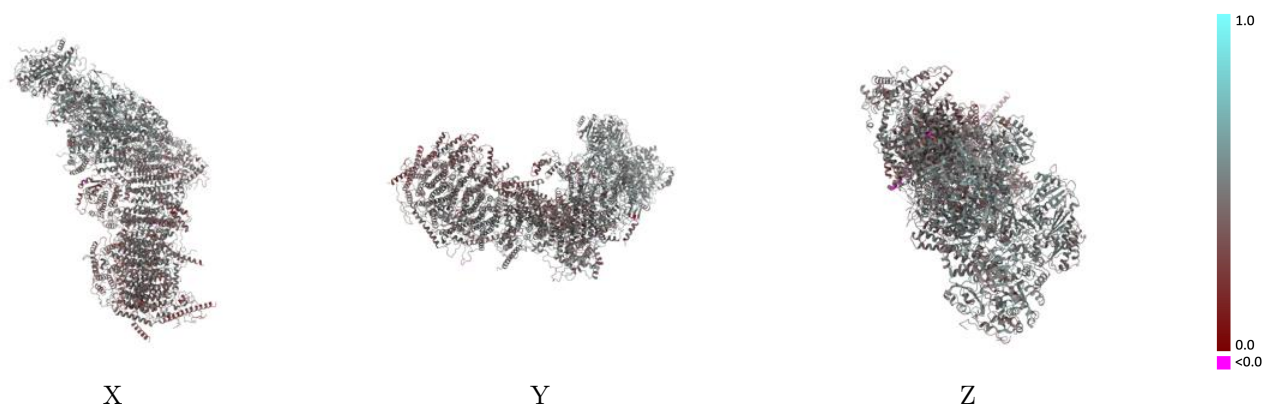
This section contains information regarding the fit between EMDB map EMD-14688 and PDB model 7ZEB. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



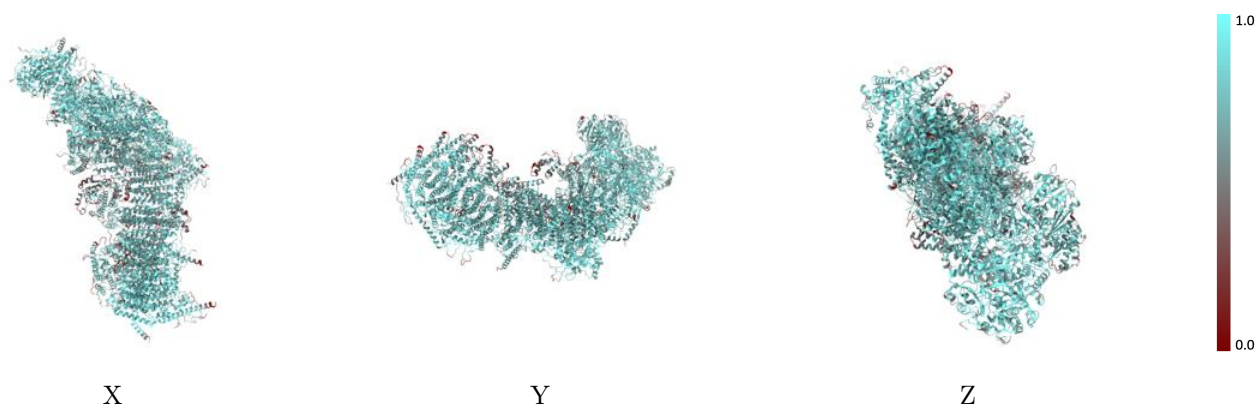
The images above show the 3D surface view of the map at the recommended contour level 0.077 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



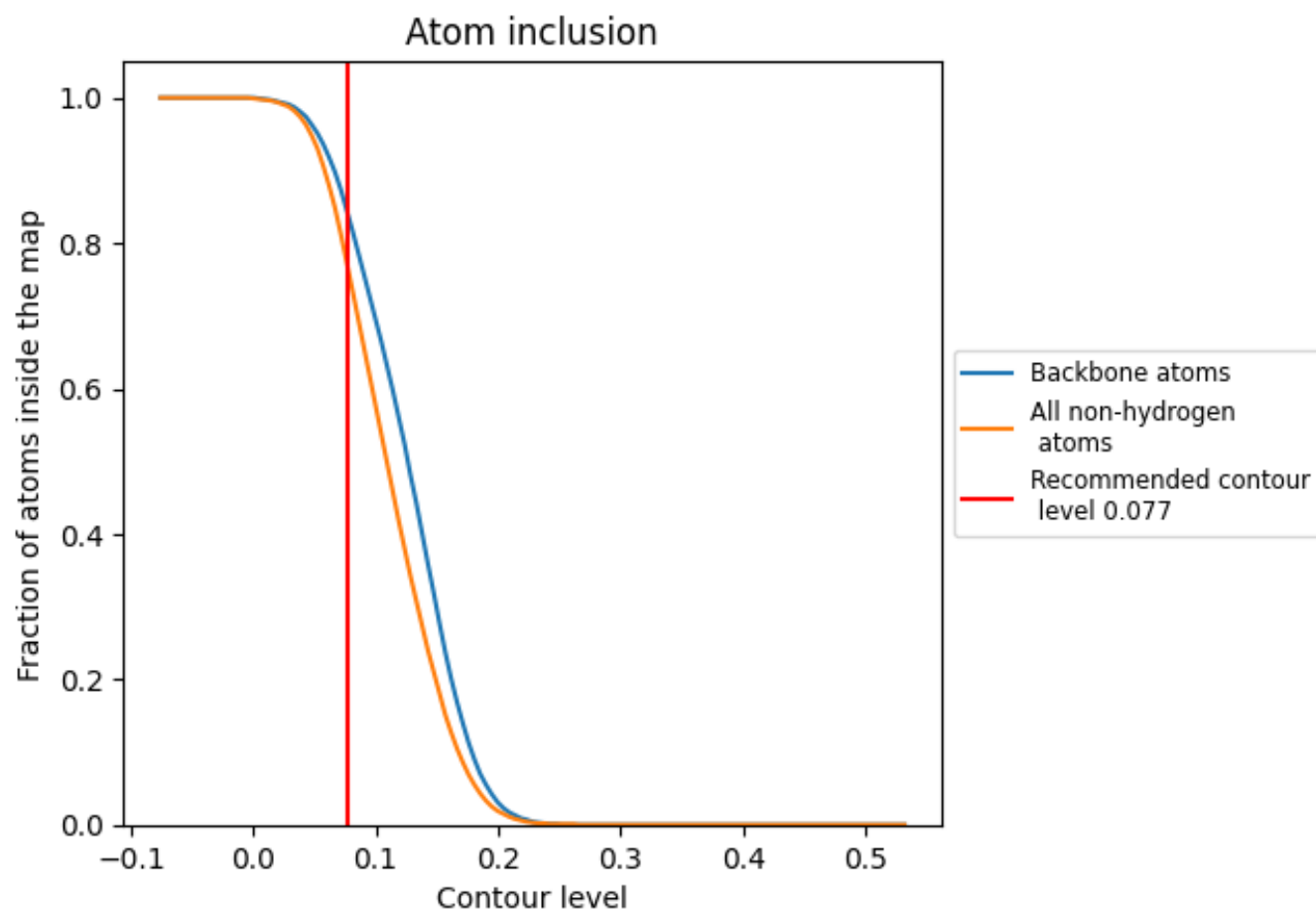
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.077).

9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 77% 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 (0.077) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.4520
1	 0.7980	 0.4800
2	 0.7770	 0.4780
3	 0.7820	 0.4990
4	 0.7940	 0.4910
5	 0.8120	 0.5140
6	 0.8580	 0.5100
9	 0.8280	 0.4820
A	 0.7690	 0.4330
H	 0.8400	 0.4570
J	 0.7590	 0.4070
K	 0.7860	 0.4270
L	 0.8390	 0.4280
M	 0.8510	 0.4680
N	 0.8290	 0.4590
V	 0.5880	 0.3810
W	 0.8180	 0.4530
X	 0.6310	 0.3730
Y	 0.7910	 0.4570
Z	 0.8070	 0.4370
a	 0.8040	 0.4880
b	 0.7670	 0.5100
c	 0.7590	 0.5070
d	 0.7180	 0.4690
e	 0.6860	 0.4850
f	 0.6640	 0.4570
g	 0.7050	 0.4890
h	 0.7390	 0.4980
i	 0.7700	 0.5000
j	 0.4520	 0.3800
k	 0.6100	 0.3700
l	 0.7610	 0.4400
m	 0.7540	 0.4320
n	 0.6780	 0.3680
o	 0.7920	 0.4460



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Chain	Atom inclusion	Q-score
p	 0.6900	 0.3950
q	 0.8020	 0.4510
r	 0.7210	 0.4140
s	 0.7300	 0.3510
t	 0.6930	 0.3920
u	 0.8030	 0.3960
v	 0.7390	 0.4100
w	 0.7390	 0.4440
x	 0.6870	 0.4190
y	 0.7050	 0.4120
z	 0.8640	 0.4520