



## Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 12:18 PM UTC

PDB ID : 9CD6 / pdb\_00009cd6  
EMDB ID : EMD-45463  
Title : Cryo-EM structure of respiratory supercomplex I in open state  
Authors : Zhang, Z.; Maharjan, R.; Tringides, M.  
Deposited on : 2024-06-24  
Resolution : 3.20 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

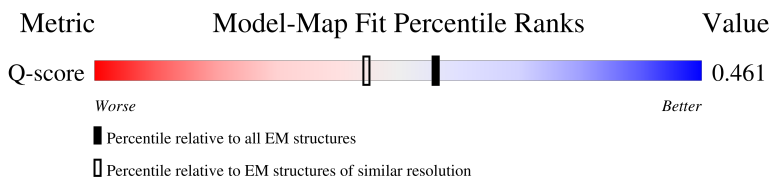
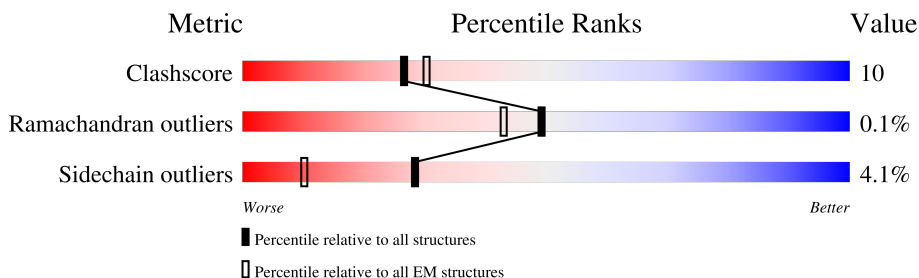
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 3.20 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.














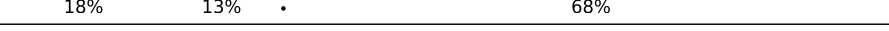







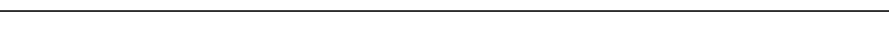

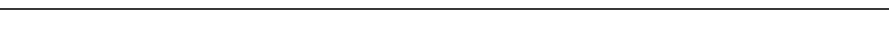
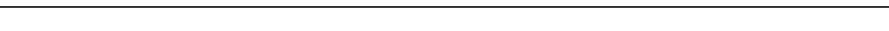


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 ( 2.70 - 3.70 )

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  $\geq 3$ , 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	B	464	
2	C	469	
3	D	264	
4	E	249	

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Mol	Chain	Length	Quality of chain
5	F	123	
6	H	212	
7	I	196	
8	J	175	
9	K	145	
10	L	372	
11	N	116	
12	O	156	
12	X	156	
13	P	99	
14	Q	154	
15	R	110	
16	S	70	
17	T	169	
18	U	357	
19	V	141	
20	W	144	
21	Y	105	
22	Z	114	
23	a	189	
24	c	186	
25	d	176	
26	e	154	
27	f	76	
28	g	122	

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Mol	Chain	Length	Quality of chain
29	h	106	
30	i	347	
31	j	115	
32	k	98	
33	l	606	
34	m	175	
35	n	58	
36	o	129	
37	p	221	
38	q	459	
39	r	318	
40	s	249	
41	t	137	
42	G	727	
43	M	113	
44	b	128	

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
46	SF4	B	502	-	-	X	-
46	SF4	I	301	-	-	X	-

## 2 Entry composition [i](#)

There are 49 unique types of molecules in this entry. The entry contains 65688 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	429	Total	C	N	O	S	0	0
			3300	2084	587	609	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	430	Total	C	N	O	S	0	0
			3453	2207	592	630	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	208	Total	C	N	O	S	0	0
			1737	1123	298	314	2		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	93	Total	C	N	O	S	0	0
			720	439	135	143	3		

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	118	Total	C	N	O	S	0	0
			963	608	173	179	3		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	144	Total	C	N	O	S	0	0
			1203	769	217	212	5		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	328	Total	C	N	O	S	0	0
			2625	1696	458	463	8		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	112	Total	C	N	O	S	0	0
			911	588	154	166	3		

- Molecule 12 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	83	Total	C	N	O	S	0	0
			668	431	99	133	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	85	Total	C	N	O	S	0	0
			689	445	101	138	5		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	83	Total	C	N	O	S	0	0
			669	419	125	123	2		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	112	Total	C	N	O	S	0	0
			955	610	176	164	5		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	35	Total	C	N	O	S	0	0
			295	185	55	54	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	82	Total	C	N	O	S	0	0
			638	414	109	114	1		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	318	Total	C	N	O	S	0	0
			2573	1638	437	488	10		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	140	Total	C	N	O	S	0	0
			1162	749	201	203	9		

- Molecule 21 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	66	Total	C	N	O	S	0	0
			571	378	94	98	1		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	77	Total	C	N	O	S	0	0
			620	407	104	108	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	c	153	Total	C	N	O	S	0	0
			1291	838	208	237	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	d	169	Total	C	N	O	S	0	0
			1426	895	259	264	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	e	99	Total	C	N	O	S	0	0
			826	530	137	155	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	f	46	Total	C	N	O	0	0
			391	259	67	65		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 30 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 31 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	106	Total	C	N	O	S	0	0
			845	573	122	144	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	603	Total	C	N	O	S	0	0
			4785	3174	741	819	51		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	m	173	Total	C	N	O	S	0	0
			1321	888	187	234	12		

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

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

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	o	126	Total	C	N	O		0	0
			1041	677	179	185			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	p	177	Total	C	N	O	S	0	0
			1529	979	278	264	8		

- Molecule 38 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q	459	Total	C	N	O	S	0	0
			3630	2410	572	609	39		

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	r	309	Total	C	N	O	S	0	0
			2437	1632	376	408	21		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	s	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	117	Total	C	N	O	S	0	0
			1014	632	193	180	9		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	G	684	Total	C	N	O	S	0	0
			5260	3298	917	1006	39		

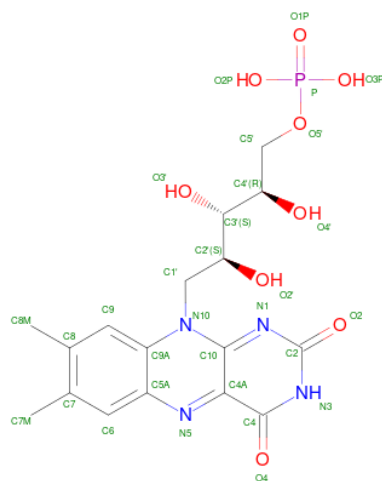
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	M	96	Total	C	N	O	S	0	0
			774	487	146	138	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

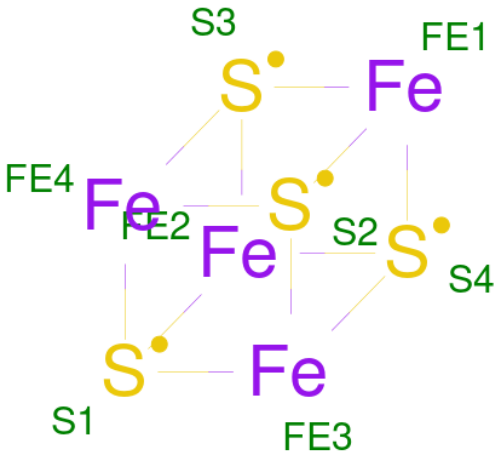
Mol	Chain	Residues	Atoms					AltConf	Trace
44	b	111	Total	C	N	O	S	0	0
			946	623	163	159	1		

- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



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

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



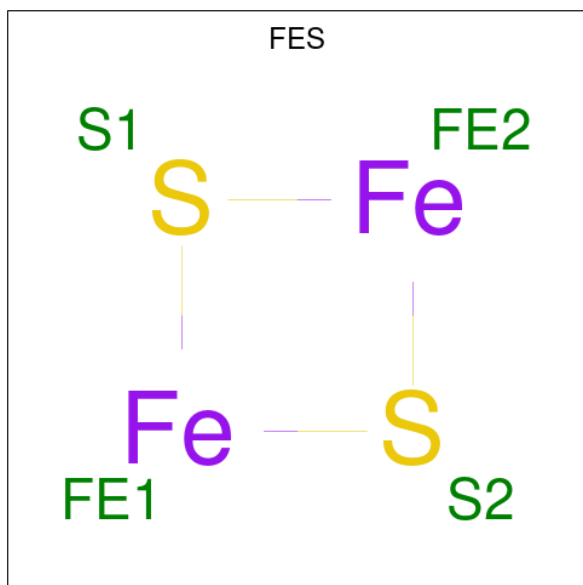
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total 8	Fe 4	S 4	0
46	H	1	Total 8	Fe 4	S 4	0
46	H	1	Total 8	Fe 4	S 4	0

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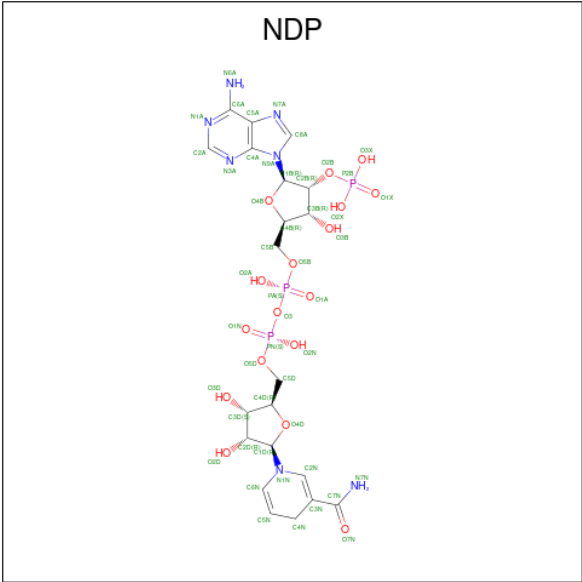
Mol	Chain	Residues	Atoms			AltConf
46	I	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



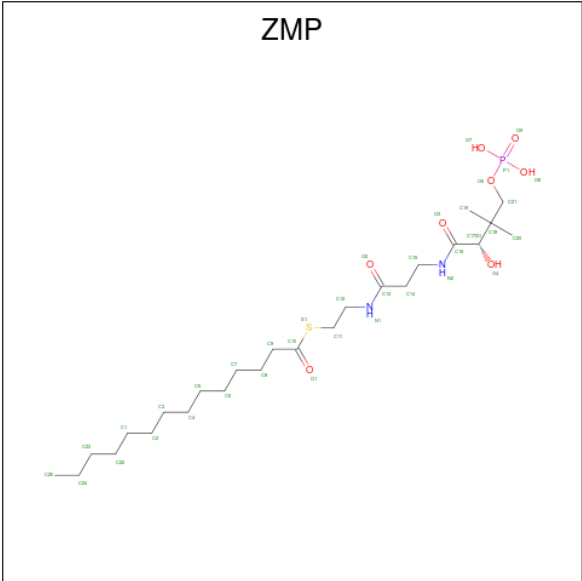
Mol	Chain	Residues	Atoms			AltConf
47	E	1	Total	Fe	S	0
			4	2	2	
47	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula:  $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$ ).



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

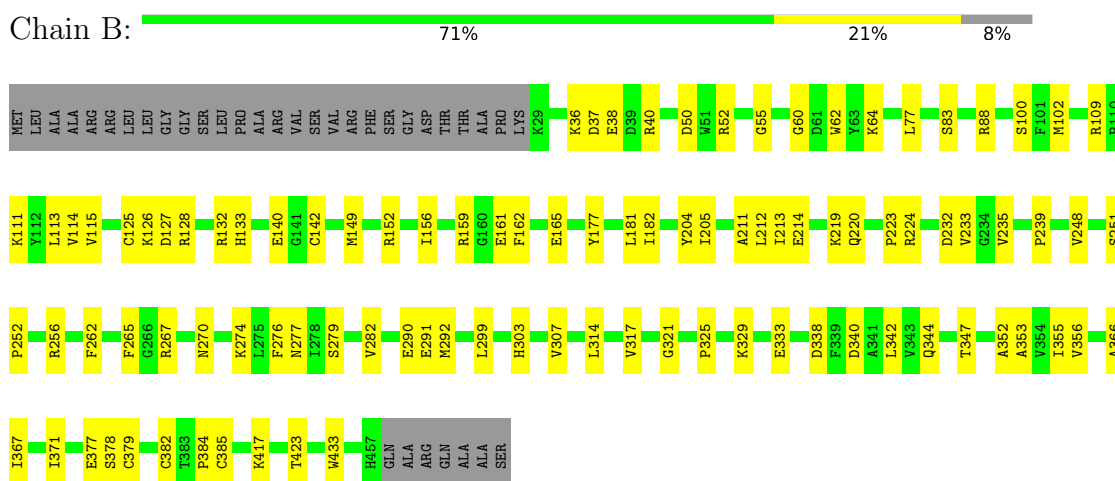
- Molecule 49 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C<sub>25</sub>H<sub>49</sub>N<sub>2</sub>O<sub>8</sub>PS).



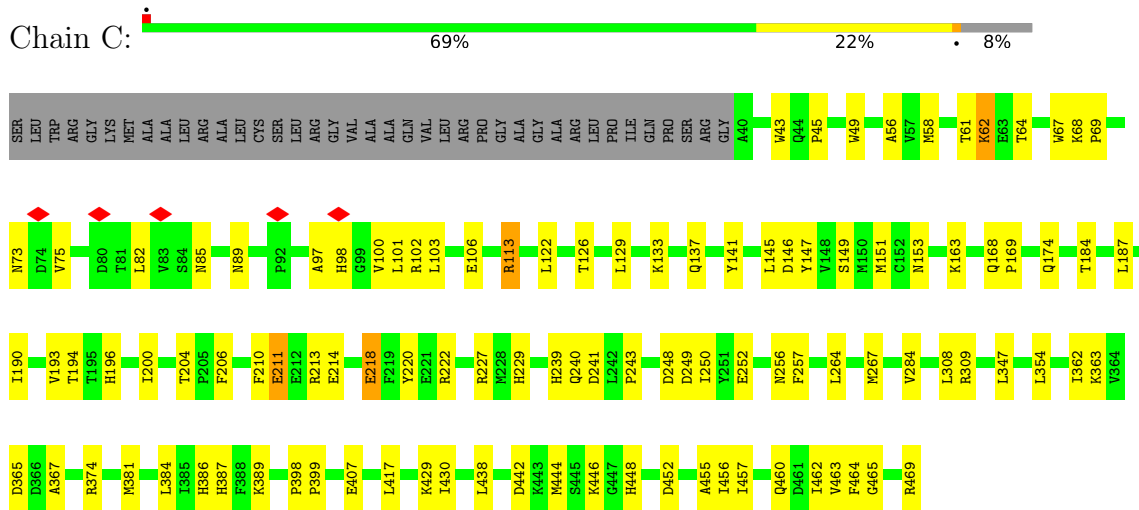
### 3 Residue-property plots

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

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

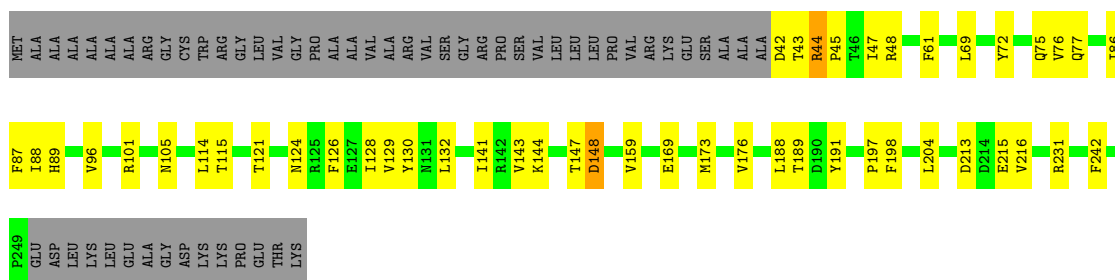


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

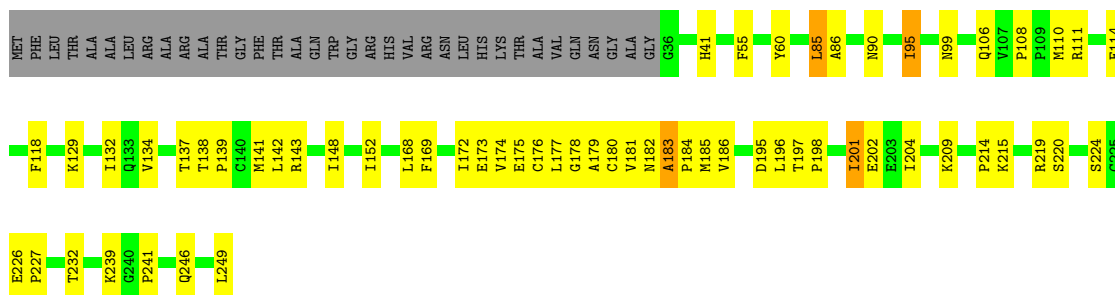


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

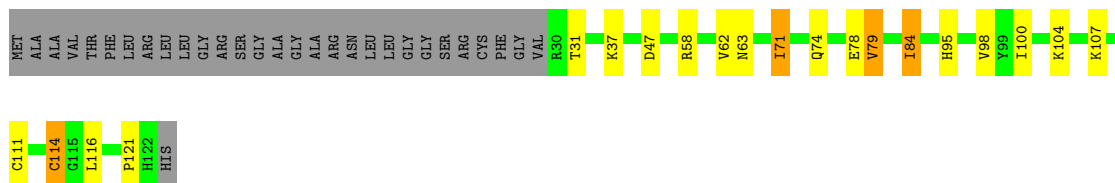




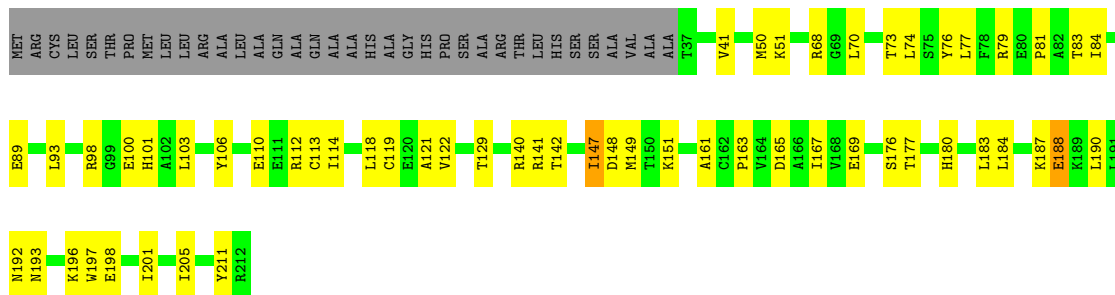
- Molecule 4: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



- Molecule 5: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

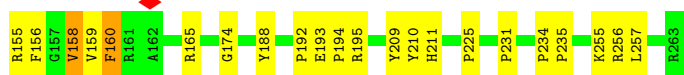
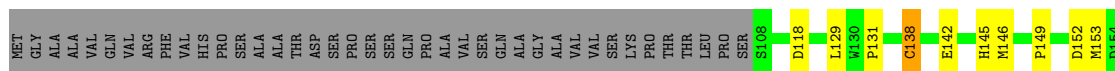


- Molecule 6: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

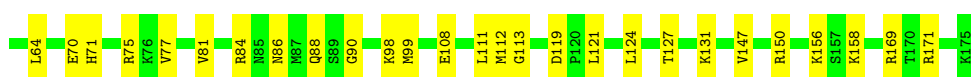
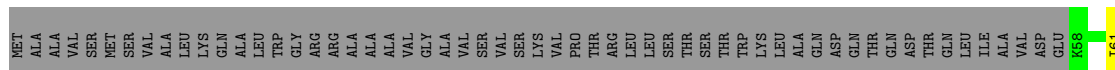


- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

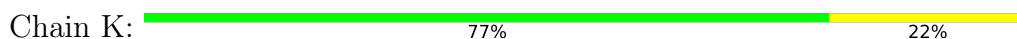




- Molecule 8: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



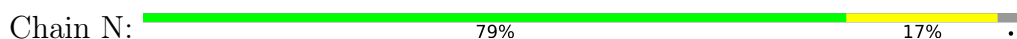
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



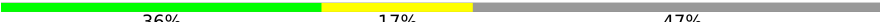
- Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

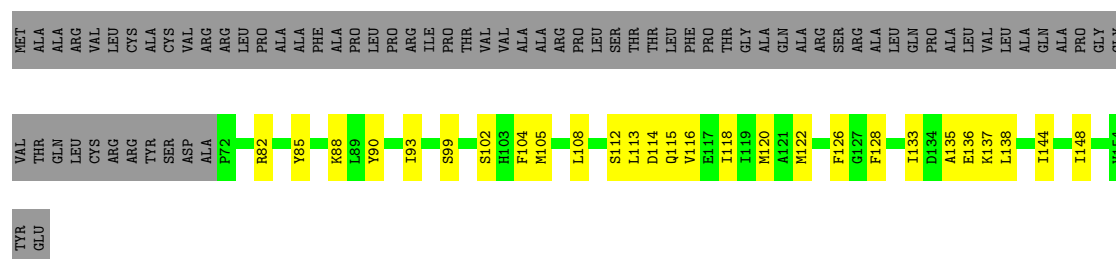


- Molecule 11: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1




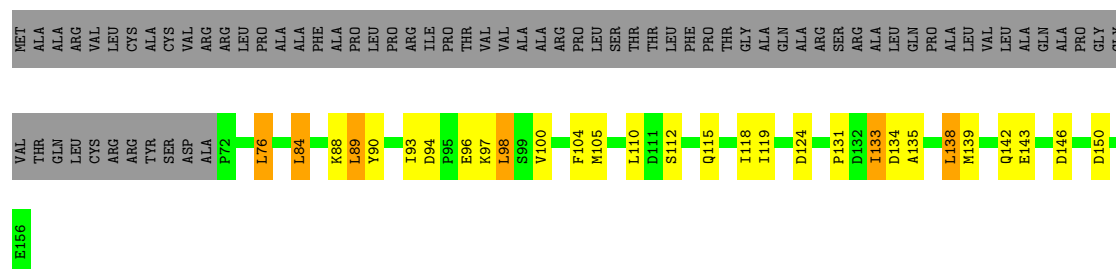
- Molecule 12: Acyl carrier protein

Chain O:  36% 17% 47%



- Molecule 12: Acyl carrier protein

Chain X:  36% 15% 46%



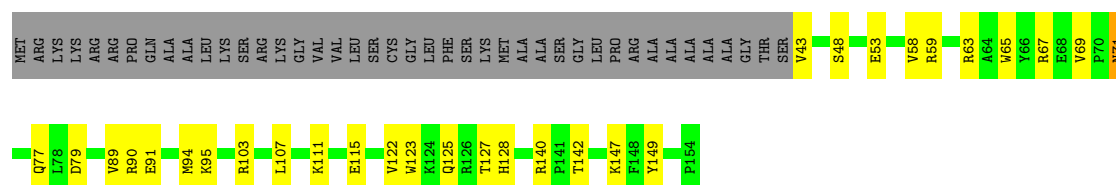
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P:  65% 17% 16%



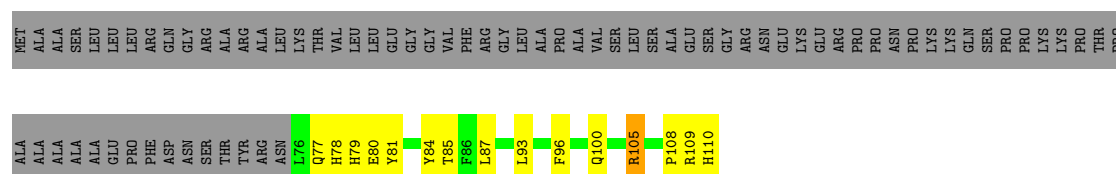
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Q:  53% 19% 27%



- Molecule 15: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain R:  18% 13% 68%




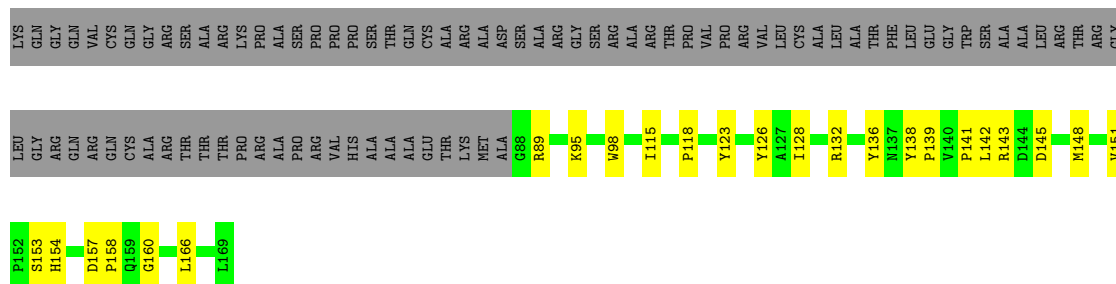
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:  74% 23% .



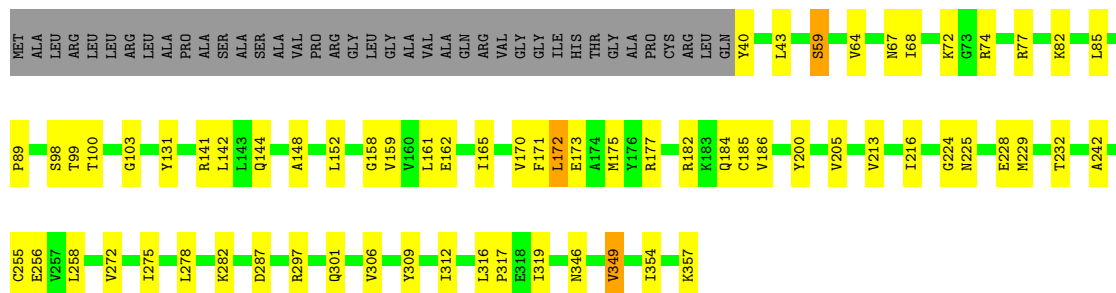
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain T:  34% 14% 51%




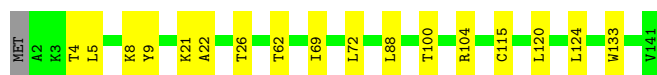
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain U:  70% 18% 11%



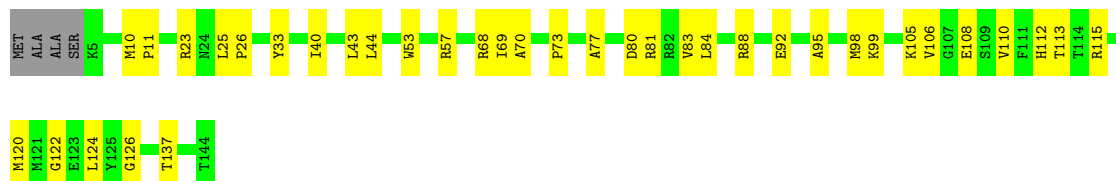
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:  87% 12% .



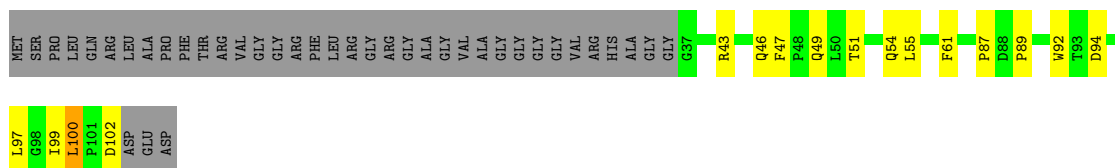
- Molecule 20: NADH:ubiquinone oxidoreductase subunit A13

Chain W:  72% 26% .



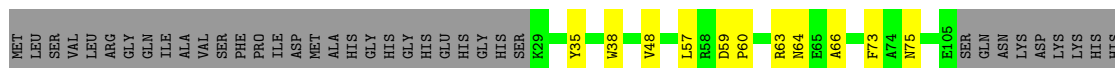
- Molecule 21: NADH:ubiquinone oxidoreductase subunit B2

Chain Y: 



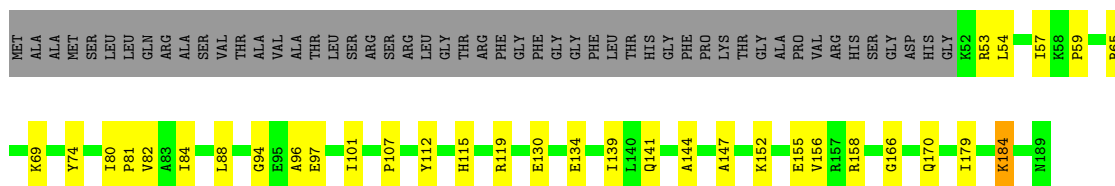
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z: 



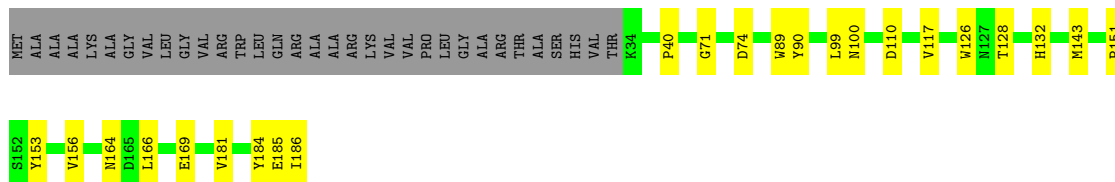
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a: 



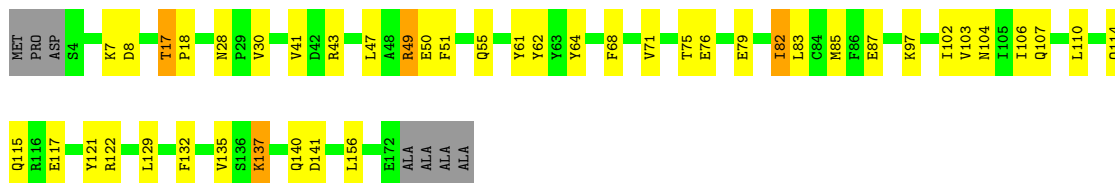
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 



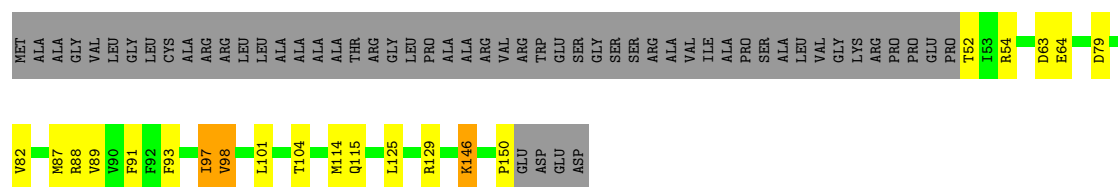
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 



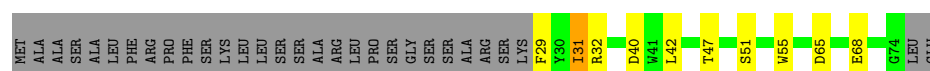
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 




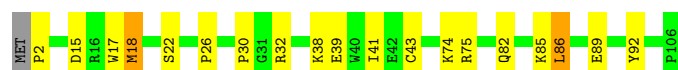
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 



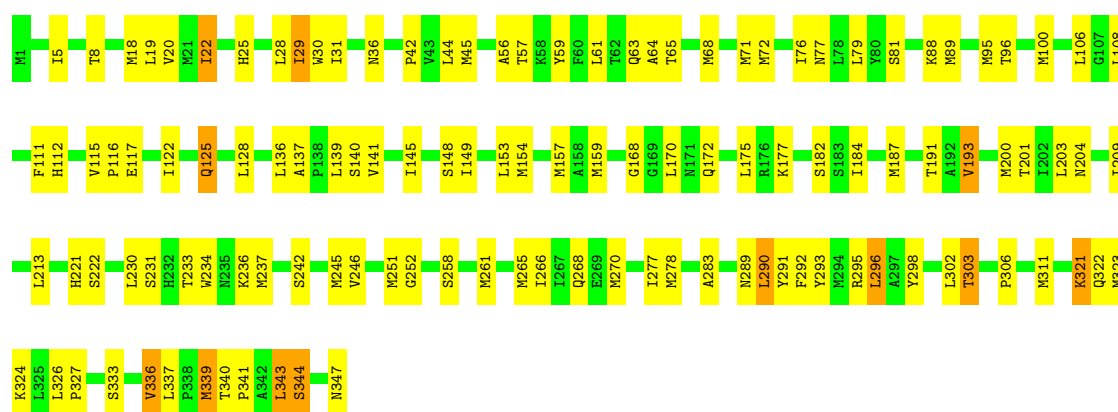
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 



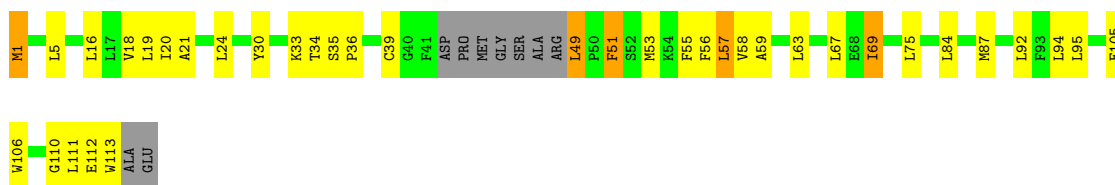
- Molecule 30: NADH-ubiquinone oxidoreductase chain 2

Chain i: 



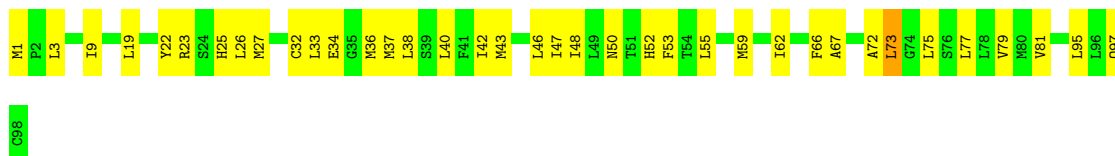
- Molecule 31: NADH-ubiquinone oxidoreductase chain 3

Chain j: 



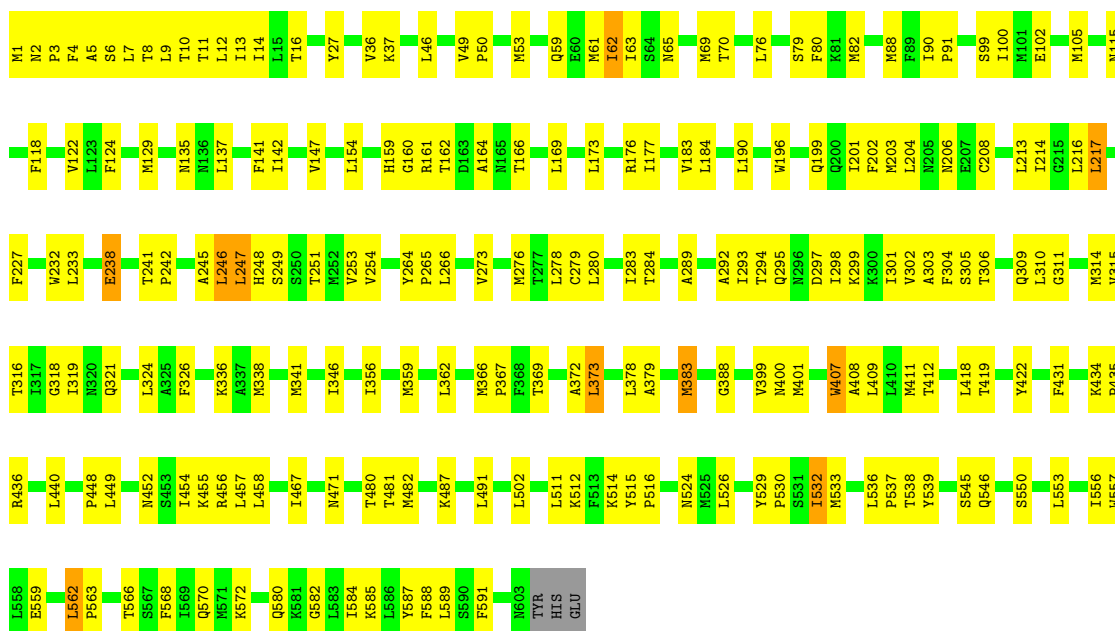
- Molecule 32: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 62% 37%



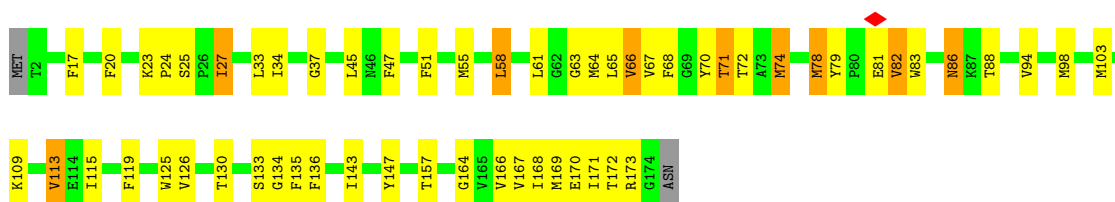
- Molecule 33: NADH-ubiquinone oxidoreductase chain 5

Chain l: 65% 33%



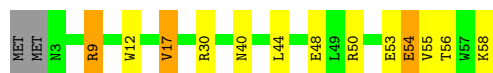
- Molecule 34: NADH-ubiquinone oxidoreductase chain 6

Chain m: 66% 28% 5%



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

Chain n:  74% 17% 5% .



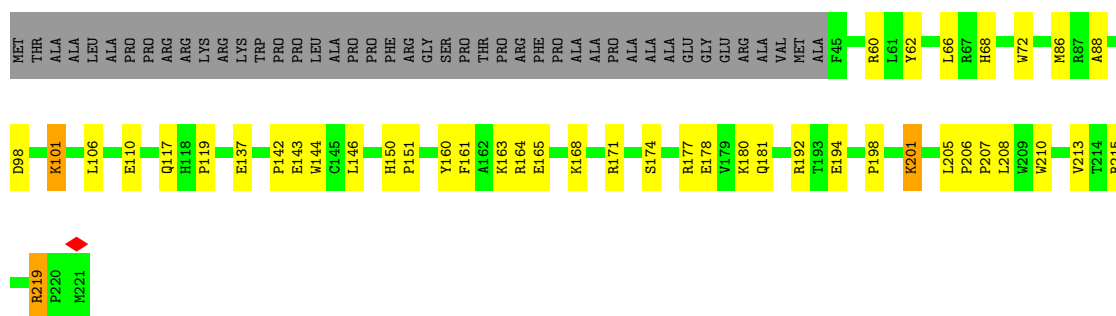
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:  74% 22% . .



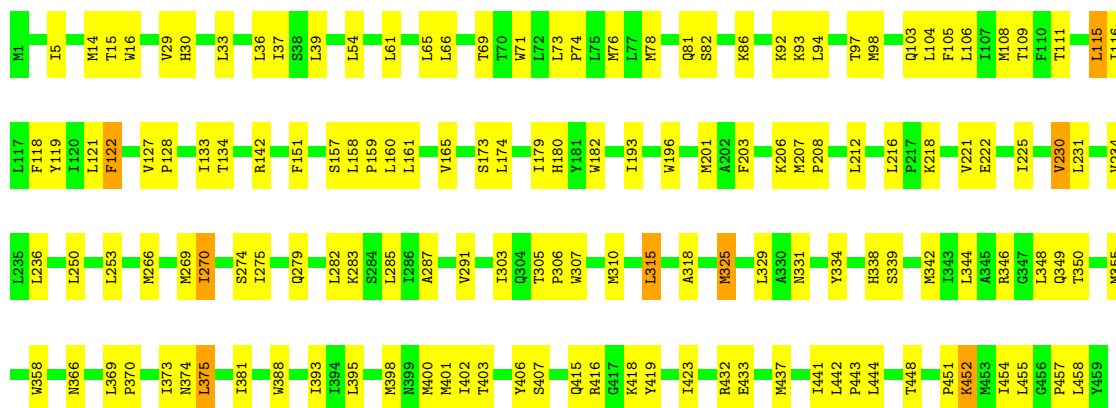
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:  60% 19% . 20%



- Molecule 38: NADH-ubiquinone oxidoreductase chain 4

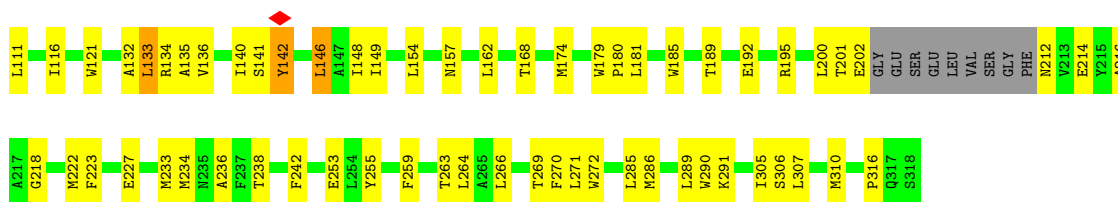
Chain q:  68% 30% .



- Molecule 39: NADH-ubiquinone oxidoreductase chain 1

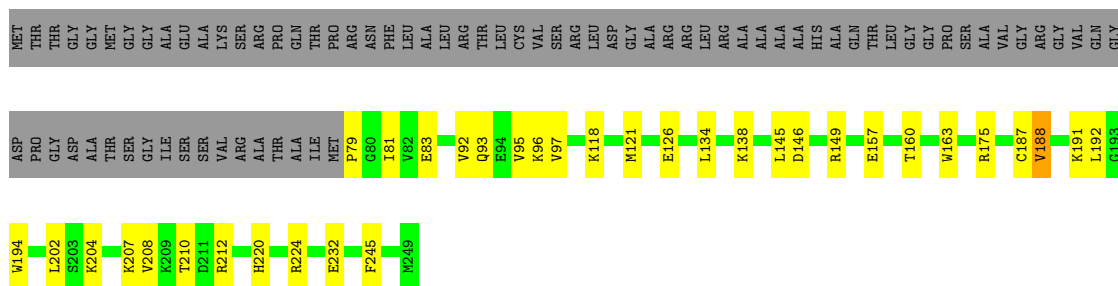
Chain r:  66% 29% . .





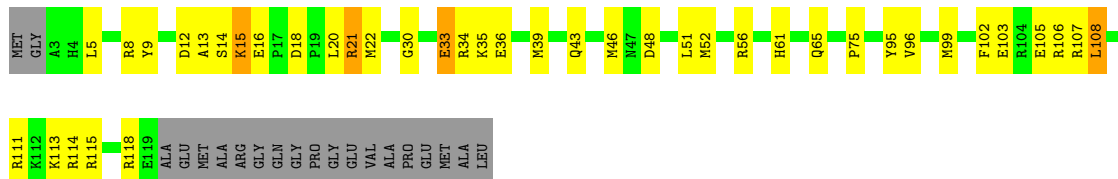
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain s:



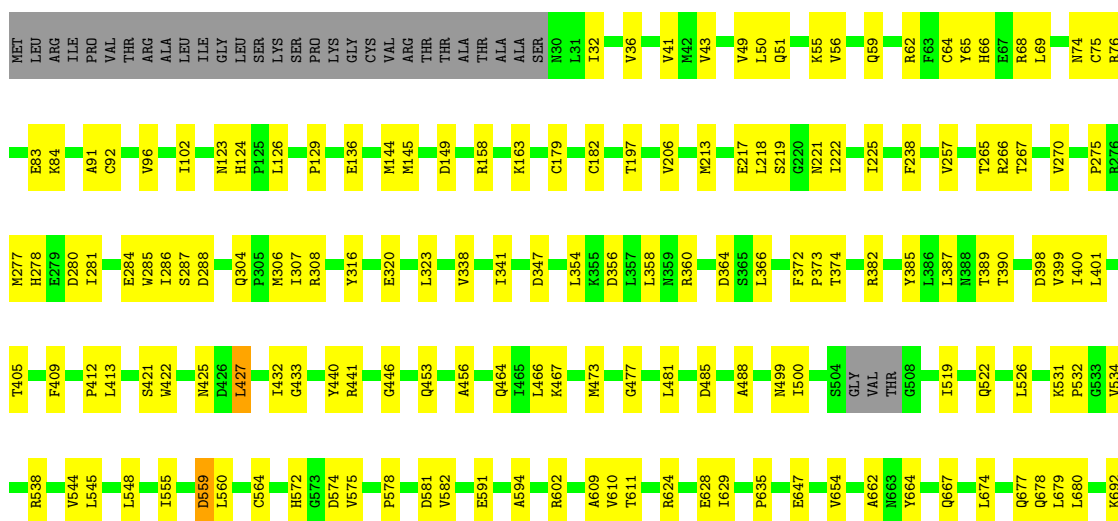
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain t:



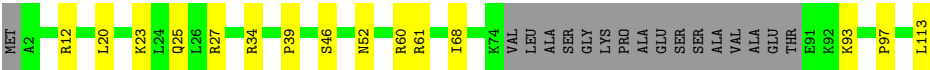
- Molecule 42: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:

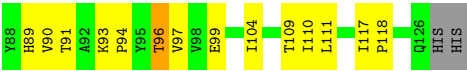
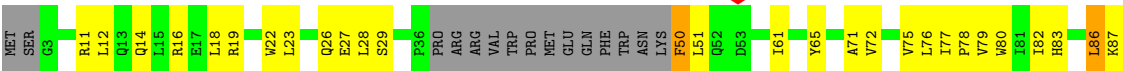




- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16982	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.035	Depositor
Minimum map value	-0.637	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, NDP, FES, ZMP, FMN

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	B	0.22	0/3375	0.36	0/4561
2	C	0.27	0/3545	0.39	0/4805
3	D	0.12	0/1788	0.28	0/2435
4	E	0.30	0/1698	0.45	0/2311
5	F	0.11	0/733	0.23	0/988
6	H	0.15	0/1443	0.30	0/1952
7	I	0.28	0/1280	0.45	0/1730
8	J	0.10	0/986	0.25	0/1329
9	K	0.11	0/1244	0.25	0/1693
10	L	0.35	0/2694	0.47	0/3649
11	N	0.13	0/930	0.27	0/1258
12	O	0.11	0/679	0.25	0/916
12	X	0.14	0/701	0.30	0/946
13	P	0.13	0/680	0.33	0/916
14	Q	0.10	0/979	0.23	0/1317
15	R	0.48	0/304	0.58	0/410
16	S	0.14	0/577	0.32	0/777
17	T	0.13	0/659	0.29	0/905
18	U	0.31	0/2633	0.42	0/3565
19	V	0.12	0/1042	0.26	0/1411
20	W	0.14	0/1193	0.28	0/1609
21	Y	0.13	0/597	0.32	0/818
22	Z	0.09	0/639	0.23	0/864
23	a	0.22	0/1184	0.36	0/1603
24	c	0.20	0/1346	0.35	0/1840
25	d	0.13	0/1458	0.27	0/1965
26	e	0.30	0/849	0.45	0/1153
27	f	0.14	0/404	0.29	0/547
28	g	0.12	0/1031	0.27	0/1394
29	h	0.12	0/889	0.25	0/1190
30	i	0.16	0/2773	0.32	0/3768
31	j	0.52	0/866	0.67	0/1183

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	k	0.40	0/759	0.61	0/1029
33	l	0.24	0/4914	0.43	0/6683
34	m	0.48	0/1356	0.66	0/1839
35	n	0.55	0/491	0.77	0/663
36	o	0.17	0/1070	0.31	0/1451
37	p	0.20	0/1585	0.32	0/2148
38	q	0.15	0/3721	0.31	0/5073
39	r	0.43	0/2507	0.62	1/3428 (0.0%)
40	s	0.11	0/1436	0.28	0/1938
41	t	0.22	0/1038	0.34	0/1389
42	G	0.12	0/5347	0.28	0/7243
43	M	0.12	0/792	0.30	0/1069
44	b	0.20	0/976	0.44	0/1328
All	All	0.24	0/67191	0.38	1/91089 (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
2	C	0	1
7	I	0	1
26	e	0	1
35	n	0	2
37	p	0	2
39	r	0	1
All	All	0	8

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	r	91	MET	N-CA-C	-6.05	99.84	109.04

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	113	ARG	Sidechain
7	I	165	ARG	Sidechain

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Mol	Chain	Res	Type	Group
26	e	88	ARG	Sidechain
35	n	30	ARG	Sidechain
35	n	9	ARG	Sidechain
37	p	215	ARG	Sidechain
37	p	219	ARG	Sidechain
39	r	91	MET	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3300	0	3258	70	0
2	C	3453	0	3389	75	0
3	D	1737	0	1691	38	0
4	E	1658	0	1662	49	0
5	F	720	0	683	13	0
6	H	1412	0	1363	45	0
7	I	1249	0	1254	30	0
8	J	963	0	962	23	0
9	K	1203	0	1161	24	0
10	L	2625	0	2640	65	0
11	N	911	0	950	13	0
12	O	668	0	672	18	0
12	X	689	0	687	24	0
13	P	669	0	675	14	0
14	Q	955	0	960	25	0
15	R	295	0	279	13	0
16	S	562	0	557	12	0
17	T	638	0	637	20	0
18	U	2573	0	2534	44	0
19	V	1021	0	1025	9	0
20	W	1162	0	1156	31	0
21	Y	571	0	522	17	0
22	Z	620	0	602	9	0
23	a	1151	0	1164	31	0
24	c	1291	0	1185	21	0
25	d	1426	0	1394	37	0
26	e	826	0	788	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	f	391	0	392	9	0
28	g	1000	0	994	21	0
29	h	867	0	871	17	0
30	i	2710	0	2874	88	0
31	j	845	0	886	42	0
32	k	748	0	799	36	0
33	l	4785	0	4935	150	0
34	m	1321	0	1320	53	0
35	n	479	0	486	9	0
36	o	1041	0	1053	19	0
37	p	1529	0	1465	30	0
38	q	3630	0	3837	91	0
39	r	2437	0	2542	83	0
40	s	1398	0	1374	29	0
41	t	1014	0	983	33	0
42	G	5260	0	5287	106	0
43	M	774	0	801	16	0
44	b	946	0	963	34	0
45	B	31	0	19	0	0
46	B	8	0	0	2	0
46	G	16	0	0	0	0
46	H	16	0	0	1	0
46	I	8	0	0	2	0
47	E	4	0	0	1	0
47	G	4	0	0	0	0
48	L	48	0	26	5	0
49	Q	30	0	30	2	0
All	All	65688	0	65787	1310	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 10.

All (1310) 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)
1:B:385:CYS:HB2	46:B:502:SF4:S3	2.08	0.93
6:H:101:HIS:H	6:H:149:MET:HE1	1.42	0.85
10:L:357:LEU:HD13	10:L:357:LEU:H	1.42	0.84
1:B:385:CYS:HB3	46:B:502:SF4:S1	2.19	0.83
23:a:130:GLU:HB2	35:n:58:LYS:HD2	1.59	0.83
33:l:253:VAL:HB	33:l:310:LEU:HD11	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:l:562:LEU:HB2	33:l:563:PRO:HD3	1.61	0.80
34:m:113:VAL:HG13	34:m:119:PHE:HB2	1.63	0.80
4:E:183:ALA:HB3	4:E:195:ASP:HA	1.65	0.79
33:l:227:PHE:H	33:l:284:THR:HG22	1.47	0.79
5:F:111:CYS:SG	5:F:114:CYS:N	2.56	0.79
25:d:68:PHE:HB3	35:n:44:LEU:HD11	1.64	0.78
31:j:55:PHE:HB2	34:m:74:MET:HE1	1.66	0.78
2:C:367:ALA:HB3	42:G:149:ASP:HB2	1.65	0.77
10:L:226:LEU:HD11	10:L:285:PRO:HB2	1.67	0.76
10:L:215:MET:HG3	10:L:222:PRO:HD2	1.68	0.75
4:E:214:PRO:HB2	4:E:219:ARG:HH12	1.48	0.75
31:j:56:PHE:HZ	32:k:75:LEU:HB3	1.51	0.75
2:C:146:ASP:HB3	2:C:153:ASN:HD21	1.52	0.75
31:j:59:ALA:HB1	34:m:67:VAL:HG23	1.69	0.75
33:l:100:ILE:HG21	33:l:246:LEU:HB2	1.67	0.74
2:C:308:LEU:HB2	2:C:407:GLU:HB2	1.70	0.74
18:U:256:GLU:HG2	18:U:282:LYS:HG3	1.70	0.73
31:j:58:VAL:HG22	31:j:113:TRP:CE3	2.24	0.73
33:l:5:ALA:HB2	33:l:61:MET:HE1	1.70	0.73
23:a:152:LYS:HE2	28:g:96:VAL:HG21	1.70	0.72
30:i:42:PRO:HG3	34:m:167:VAL:HG22	1.71	0.72
30:i:128:LEU:HD11	30:i:213:LEU:HD23	1.72	0.71
30:i:88:LYS:HD2	30:i:148:SER:HB3	1.72	0.71
6:H:198:GLU:HG2	9:K:108:TYR:HE1	1.55	0.71
2:C:381:MET:HE2	42:G:124:HIS:HD2	1.54	0.71
28:g:27:LYS:HG2	28:g:29:THR:H	1.56	0.70
33:l:214:ILE:HG12	33:l:276:MET:HE1	1.72	0.70
19:V:69:ILE:HG13	19:V:100:THR:HG21	1.72	0.70
23:a:179:ILE:HG21	29:h:38:LYS:HG3	1.74	0.70
5:F:104:LYS:HD3	5:F:107:LYS:HD2	1.74	0.70
37:p:207:PRO:O	44:b:11:ARG:NH2	2.24	0.69
10:L:201:ILE:HG13	48:L:401:NDP:H42N	1.73	0.69
21:Y:87:PRO:HG3	41:t:96:VAL:HG22	1.75	0.69
1:B:279:SER:HB3	4:E:181:VAL:HG12	1.75	0.69
30:i:268:GLN:HA	38:q:165:VAL:HG11	1.75	0.69
12:X:90:TYR:HE1	22:Z:60:PRO:HB2	1.58	0.69
27:f:68:GLU:HG2	28:g:21:ARG:HE	1.57	0.69
33:l:346:ILE:HG12	33:l:366:MET:HE1	1.74	0.69
39:r:185:TRP:HE1	39:r:238:THR:HG22	1.56	0.69
17:T:154:HIS:CE1	17:T:157:ASP:HB2	2.28	0.68
33:l:10:THR:HG21	44:b:79:VAL:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:n:54:GLU:HG2	35:n:55:VAL:HG22	1.73	0.68
25:d:71:VAL:HG11	25:d:87:GLU:HB3	1.75	0.68
39:r:63:PRO:HB3	39:r:214:GLU:HB3	1.75	0.68
15:R:84:TYR:HD1	15:R:87:LEU:HD12	1.59	0.68
3:D:88:ILE:HD13	3:D:143:VAL:HG13	1.77	0.67
33:l:280:LEU:O	33:l:284:THR:HG23	1.95	0.67
10:L:122:ILE:HG23	10:L:160:ILE:HB	1.76	0.66
1:B:132:ARG:HB2	1:B:165:GLU:HG3	1.78	0.66
42:G:574:ASP:OD2	42:G:702:ARG:NE	2.29	0.66
42:G:83:GLU:HG2	42:G:84:LYS:HG3	1.78	0.65
42:G:36:VAL:HG22	42:G:102:ILE:HD12	1.76	0.65
18:U:98:SER:HA	18:U:103:GLY:HA2	1.77	0.65
1:B:265:PHE:HB3	1:B:291:GLU:HG3	1.79	0.65
2:C:89:ASN:HD21	2:C:102:ARG:HE	1.45	0.65
1:B:325:PRO:HD2	1:B:347:THR:HA	1.78	0.65
31:j:58:VAL:HG22	31:j:113:TRP:HE3	1.61	0.64
32:k:25:HIS:CE1	34:m:78:MET:HB2	2.32	0.64
39:r:61:LEU:HD13	39:r:216:ALA:HB2	1.80	0.64
6:H:70:LEU:HG	39:r:272:TRP:CE2	2.33	0.64
7:I:192:PRO:HG2	39:r:58:LYS:NZ	2.12	0.64
33:l:372:ALA:HA	33:l:458:LEU:HD21	1.79	0.64
12:O:128:PHE:HZ	12:O:148:ILE:HG12	1.63	0.64
34:m:27:ILE:HB	39:r:121:TRP:CZ3	2.33	0.64
33:l:306:THR:HG22	33:l:336:LYS:HG2	1.79	0.64
37:p:174:SER:HA	37:p:177:ARG:HE	1.63	0.64
30:i:96:THR:O	30:i:100:MET:HG2	1.98	0.64
5:F:78:GLU:HB3	5:F:121:PRO:HG3	1.77	0.64
4:E:204:ILE:HG23	4:E:214:PRO:HG3	1.80	0.64
12:X:89:LEU:HD23	22:Z:64:ASN:HA	1.80	0.64
10:L:168:ASP:HB3	10:L:171:SER:HB3	1.80	0.63
2:C:438:LEU:HD13	2:C:462:ILE:HD13	1.80	0.63
30:i:170:LEU:HD22	30:i:291:TYR:HD2	1.63	0.63
33:l:378:LEU:HB3	33:l:383:MET:HG3	1.81	0.63
9:K:44:TYR:HE2	9:K:83:PRO:HB3	1.63	0.63
31:j:57:LEU:HD22	31:j:112:GLU:HG2	1.81	0.63
42:G:213:MET:HE1	42:G:713:ALA:HB1	1.80	0.63
39:r:157:ASN:HA	39:r:168:THR:HG21	1.81	0.63
1:B:113:LEU:HD13	1:B:149:MET:HE1	1.81	0.63
16:S:43:TYR:HB2	34:m:134:GLY:HA2	1.80	0.63
23:a:82:VAL:HG11	26:e:104:THR:HG21	1.79	0.63
38:q:339:SER:HB3	38:q:344:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:119:CYS:HB3	46:H:302:SF4:S3	2.38	0.62
23:a:155:GLU:OE2	23:a:158:ARG:NH2	2.32	0.62
24:c:184:TYR:HA	41:t:36:GLU:HA	1.81	0.62
13:P:24:CYS:N	13:P:58:CYS:SG	2.72	0.62
22:Z:57:LEU:HD21	37:p:88:ALA:HB2	1.82	0.62
26:e:115:GLN:HE22	38:q:452:LYS:HE2	1.64	0.62
30:i:65:THR:HG22	32:k:19:LEU:HD21	1.80	0.62
31:j:1:MET:SD	31:j:1:MET:N	2.67	0.62
39:r:236:ALA:HA	39:r:263:THR:HG22	1.80	0.62
30:i:136:LEU:HD21	30:i:209:ILE:HD11	1.82	0.62
8:J:158:LYS:NZ	42:G:69:LEU:O	2.32	0.62
39:r:91:MET:O	39:r:93:TYR:N	2.32	0.62
17:T:157:ASP:HB3	17:T:158:PRO:HD2	1.81	0.62
39:r:132:ALA:O	39:r:136:VAL:HG23	1.99	0.62
40:s:188:VAL:HG13	40:s:194:TRP:HB2	1.82	0.62
7:I:193:GLU:HG2	7:I:195:ARG:HG2	1.82	0.62
24:c:71:GLY:HA2	36:o:79:ASN:HB2	1.82	0.61
34:m:170:GLU:OE1	34:m:173:ARG:NH1	2.33	0.61
39:r:24:GLU:HA	39:r:271:LEU:HD13	1.82	0.61
39:r:100:LEU:HD23	39:r:103:LEU:HD12	1.82	0.61
1:B:38:GLU:HA	4:E:239:LYS:HD2	1.82	0.61
37:p:98:ASP:HB3	37:p:101:LYS:HB2	1.82	0.61
7:I:138:CYS:HB2	46:I:301:SF4:S2	2.41	0.61
18:U:258:LEU:HD21	18:U:278:LEU:HD21	1.81	0.61
17:T:118:PRO:HG3	39:r:306:SER:HB2	1.83	0.61
18:U:170:VAL:HG13	18:U:242:ALA:HB3	1.82	0.61
42:G:453:GLN:HE21	42:G:679:LEU:HD12	1.65	0.61
10:L:206:ASP:CG	10:L:208:PHE:H	2.09	0.61
30:i:289:ASN:HA	30:i:292:PHE:CE2	2.36	0.61
39:r:102:VAL:HG21	39:r:154:LEU:HD11	1.83	0.61
2:C:85:ASN:HD21	2:C:106:GLU:HB3	1.66	0.60
17:T:151:VAL:HB	40:s:207:LYS:HD3	1.81	0.60
33:l:37:LYS:HD2	33:l:105:MET:HE1	1.82	0.60
23:a:156:VAL:HG21	28:g:92:MET:HG3	1.84	0.60
15:R:78:HIS:HA	15:R:81:TYR:CD2	2.35	0.60
33:l:399:VAL:HG12	33:l:409:LEU:HG	1.84	0.60
38:q:208:PRO:HG3	38:q:216:LEU:HD22	1.84	0.60
39:r:185:TRP:NE1	39:r:238:THR:HG22	2.17	0.60
10:L:78:PRO:HB3	10:L:114:VAL:HG21	1.82	0.60
10:L:357:LEU:H	10:L:357:LEU:CD1	2.13	0.60
41:t:22:MET:HG3	41:t:105:GLU:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:141:GLN:HB2	25:d:83:LEU:HD21	1.83	0.60
10:L:183:GLU:HG3	10:L:195:ILE:HD13	1.82	0.60
38:q:134:THR:O	38:q:142:ARG:NH1	2.34	0.60
12:O:90:TYR:HD2	12:O:93:ILE:HG13	1.67	0.60
13:P:18:GLU:HG2	13:P:68:ARG:HB3	1.83	0.60
38:q:307:TRP:HA	38:q:310:MET:HE2	1.83	0.60
19:V:62:THR:HG22	19:V:104:ARG:HE	1.67	0.59
21:Y:55:LEU:HD23	33:l:367:PRO:HG3	1.83	0.59
30:i:193:VAL:HG23	30:i:201:THR:HG22	1.84	0.59
44:b:72:VAL:HG22	44:b:76:LEU:HD12	1.83	0.59
30:i:108:LEU:HD11	30:i:191:THR:HG21	1.85	0.59
31:j:58:VAL:CG1	39:r:286:MET:HE1	2.32	0.59
13:P:42:VAL:HG12	13:P:46:LYS:HE3	1.84	0.59
29:h:15:ASP:HB2	30:i:25:HIS:HB2	1.84	0.59
32:k:23:ARG:HD3	34:m:23:LYS:HB2	1.85	0.59
33:l:176:ARG:HG2	38:q:401:MET:HA	1.84	0.59
33:l:559:GLU:O	33:l:563:PRO:HD2	2.02	0.59
1:B:140:GLU:OE2	1:B:256:ARG:NH1	2.35	0.59
6:H:118:LEU:HD11	6:H:163:PRO:HD3	1.82	0.59
10:L:213:ALA:HA	10:L:276:PHE:HE1	1.67	0.59
42:G:341:ILE:HG13	42:G:545:LEU:HD11	1.85	0.59
10:L:281:ARG:HE	10:L:282:PRO:HD2	1.67	0.59
19:V:4:THR:HG22	19:V:8:LYS:HE3	1.83	0.59
42:G:266:ARG:HG2	42:G:267:THR:HG23	1.84	0.59
10:L:274:TYR:HB2	10:L:367:ALA:HB2	1.85	0.59
18:U:225:ASN:HB3	18:U:228:GLU:HB2	1.84	0.59
30:i:112:HIS:HB2	30:i:184:ILE:HD13	1.84	0.59
11:N:40:LYS:HA	11:N:45:ARG:HD3	1.84	0.59
29:h:86:LEU:HD23	29:h:92:TYR:HB2	1.85	0.59
38:q:403:THR:HA	38:q:406:TYR:CE2	2.38	0.59
31:j:111:LEU:HD22	31:j:113:TRP:CZ2	2.38	0.58
2:C:213:ARG:HH11	7:I:145:HIS:HE1	1.50	0.58
7:I:194:PRO:HD2	39:r:58:LYS:HD2	1.86	0.58
12:O:99:SER:HB3	12:O:102:SER:HB3	1.85	0.58
12:X:115:GLN:NE2	12:X:138:LEU:O	2.37	0.58
34:m:37:GLY:HA3	34:m:61:LEU:HD21	1.84	0.58
42:G:64:CYS:HB3	42:G:75:CYS:HB3	1.84	0.58
6:H:142:THR:O	6:H:187:LYS:NZ	2.34	0.58
13:P:17:ARG:HB2	13:P:68:ARG:HG2	1.85	0.58
23:a:57:ILE:HG12	37:p:146:LEU:HD11	1.83	0.58
42:G:400:ILE:HG13	42:G:427:LEU:HD11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:169:ARG:HG2	15:R:105:ARG:HH22	1.67	0.58
30:i:159:MET:HB2	30:i:278:MET:HE1	1.84	0.58
33:l:293:ILE:HD11	33:l:418:LEU:HD22	1.85	0.58
23:a:130:GLU:O	23:a:134:GLU:HG2	2.03	0.58
23:a:139:ILE:HG23	38:q:54:LEU:HD23	1.86	0.58
37:p:164:ARG:HG2	37:p:168:LYS:HE3	1.85	0.58
44:b:61:ILE:HB	44:b:65:TYR:HB3	1.85	0.58
30:i:44:LEU:HD22	30:i:122:ILE:HG21	1.84	0.58
1:B:88:ARG:HD2	1:B:274:LYS:HD3	1.86	0.58
4:E:85:LEU:HG	15:R:87:LEU:HD13	1.85	0.58
25:d:106:ILE:HG13	25:d:135:VAL:HG21	1.86	0.58
30:i:57:THR:HG22	32:k:77:LEU:HB3	1.85	0.58
38:q:269:MET:HG3	38:q:270:ILE:HD12	1.84	0.58
25:d:17:THR:HG23	44:b:110:ILE:HB	1.84	0.58
30:i:252:GLY:HA3	30:i:290:LEU:HD23	1.86	0.58
39:r:63:PRO:HG2	39:r:71:PHE:CE2	2.39	0.58
2:C:149:SER:O	2:C:153:ASN:ND2	2.36	0.58
13:P:38:GLU:HA	42:G:667:GLN:HE21	1.67	0.57
34:m:17:PHE:HA	34:m:20:PHE:CE2	2.39	0.57
29:h:26:PRO:HD3	32:k:55:LEU:HD13	1.86	0.57
33:l:356:ILE:HA	33:l:359:MET:HE2	1.85	0.57
10:L:190:PHE:HB3	10:L:193:ALA:HB2	1.87	0.57
31:j:21:ALA:HB1	39:r:218:GLY:HA3	1.85	0.57
3:D:148:ASP:N	3:D:148:ASP:OD1	2.36	0.57
20:W:108:GLU:H	29:h:75:ARG:HH12	1.52	0.57
25:d:122:ARG:HH21	33:l:206:ASN:HD21	1.52	0.57
30:i:30:TRP:HZ2	32:k:37:MET:HE1	1.70	0.57
30:i:72:MET:HE3	30:i:76:ILE:HD11	1.85	0.57
2:C:218:GLU:OE2	43:M:34:ARG:NH2	2.38	0.57
30:i:61:LEU:HD11	32:k:26:LEU:HD11	1.86	0.57
33:l:295:GLN:HB2	33:l:301:ILE:HG12	1.86	0.57
21:Y:54:GLN:HG2	33:l:367:PRO:HG2	1.86	0.57
24:c:186:ILE:HD11	41:t:34:ARG:CZ	2.35	0.57
30:i:79:LEU:HD23	32:k:47:ILE:HG12	1.86	0.57
33:l:2:ASN:ND2	44:b:83:HIS:HE1	2.03	0.57
3:D:215:GLU:HG3	10:L:66:ASN:HD22	1.70	0.57
40:s:187:CYS:SG	40:s:188:VAL:N	2.78	0.57
33:l:362:LEU:HB2	33:l:431:PHE:HA	1.86	0.57
36:o:31:LYS:O	36:o:35:GLU:HG2	2.05	0.57
10:L:352:ARG:HB3	10:L:357:LEU:HD12	1.86	0.56
2:C:444:MET:SD	2:C:460:GLN:NE2	2.78	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:101:HIS:HB3	6:H:167:ILE:HD11	1.87	0.56
33:l:373:LEU:HG	33:l:431:PHE:HE2	1.70	0.56
35:n:50:ARG:HG2	35:n:53:GLU:HB2	1.87	0.56
4:E:198:PRO:O	4:E:202:GLU:HG2	2.06	0.56
20:W:122:GLY:HA3	34:m:126:VAL:HG13	1.86	0.56
23:a:65:ARG:HG2	23:a:69:LYS:HE3	1.87	0.56
38:q:196:TRP:CD1	38:q:250:LEU:HB3	2.39	0.56
37:p:143:GLU:HB2	37:p:164:ARG:HH12	1.71	0.56
41:t:33:GLU:OE1	41:t:35:LYS:NZ	2.38	0.56
2:C:68:LYS:HD2	2:C:69:PRO:HD2	1.88	0.56
12:O:120:MET:HG2	14:Q:67:ARG:HH21	1.71	0.56
18:U:148:ALA:HB1	18:U:159:VAL:HG11	1.88	0.56
23:a:53:ARG:HB3	44:b:28:LEU:HD12	1.86	0.56
5:F:63:ASN:H	6:H:188:GLU:HG3	1.70	0.56
20:W:88:ARG:O	20:W:92:GLU:HG2	2.05	0.56
31:j:75:LEU:HD13	39:r:305:ILE:HD11	1.88	0.56
33:l:202:PHE:HA	33:l:266:LEU:HD21	1.86	0.56
33:l:8:THR:HB	33:l:82:MET:HE3	1.87	0.56
6:H:76:TYR:HA	6:H:79:ARG:HD2	1.87	0.56
21:Y:43:ARG:HH22	21:Y:49:GLN:HB2	1.69	0.56
25:d:110:LEU:HD11	33:l:203:MET:HG2	1.88	0.56
31:j:33:LYS:O	31:j:35:SER:N	2.39	0.56
32:k:27:MET:HG2	34:m:72:THR:HG22	1.88	0.56
33:l:184:LEU:HD12	38:q:393:ILE:HG21	1.87	0.56
40:s:160:THR:HA	40:s:163:TRP:CD1	2.41	0.56
12:X:94:ASP:OD1	12:X:94:ASP:N	2.39	0.56
30:i:45:MET:HE1	34:m:171:ILE:HG23	1.88	0.56
9:K:78:ASP:HB3	9:K:81:MET:HG3	1.88	0.55
31:j:56:PHE:CE1	34:m:71:THR:HG22	2.40	0.55
33:l:177:ILE:HG12	38:q:401:MET:HE2	1.88	0.55
44:b:93:LYS:HD2	44:b:94:PRO:HD2	1.87	0.55
7:I:149:PRO:HA	39:r:34:ARG:HG2	1.88	0.55
7:I:194:PRO:HB3	7:I:256:ARG:HH12	1.71	0.55
21:Y:54:GLN:NE2	33:l:367:PRO:HD2	2.22	0.55
27:f:47:THR:HG23	28:g:65:LEU:HD22	1.88	0.55
33:l:419:THR:HA	33:l:422:TYR:CE2	2.42	0.55
1:B:220:GLN:HE21	4:E:118:PHE:HB2	1.72	0.55
12:O:115:GLN:NE2	12:O:135:ALA:O	2.32	0.55
33:l:13:ILE:HG13	44:b:82:ILE:HD11	1.87	0.55
33:l:553:LEU:HD21	36:o:94:GLY:HA2	1.89	0.55
1:B:314:LEU:HD23	1:B:329:LYS:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:62:LYS:H	2:C:62:LYS:HD3	1.71	0.55
42:G:145:MET:O	43:M:61:ARG:NH1	2.39	0.55
43:M:12:ARG:HG2	43:M:20:LEU:HD12	1.87	0.55
3:D:173:MET:HE3	3:D:188:LEU:HB2	1.89	0.55
25:d:28:ASN:HA	41:t:75:PRO:HG3	1.89	0.55
21:Y:92:TRP:HZ3	41:t:103:GLU:HG3	1.72	0.55
2:C:98:HIS:HB2	2:C:464:PHE:HE2	1.72	0.55
39:r:90:PRO:HD3	39:r:162:LEU:HB3	1.89	0.55
42:G:275:PRO:HG3	42:G:286:ILE:HG12	1.89	0.55
18:U:182:ARG:HH22	18:U:317:PRO:HD2	1.71	0.55
18:U:255:CYS:HA	18:U:282:LYS:HB3	1.87	0.55
21:Y:100:LEU:HD23	41:t:30:GLY:HA2	1.88	0.55
27:f:31:ILE:HD12	27:f:32:ARG:HG3	1.89	0.55
30:i:89:MET:HB2	30:i:95:MET:HG2	1.88	0.55
12:O:133:ILE:HG22	12:O:137:LYS:HE3	1.89	0.54
5:F:62:VAL:HA	6:H:188:GLU:HG2	1.88	0.54
2:C:73:ASN:C	2:C:75:VAL:H	2.14	0.54
12:O:113:LEU:HD12	14:Q:94:MET:HE2	1.88	0.54
24:c:166:LEU:HB3	24:c:169:GLU:HB2	1.90	0.54
30:i:177:LYS:HB3	30:i:177:LYS:HZ2	1.72	0.54
33:l:341:MET:HE2	33:l:457:LEU:HD12	1.88	0.54
42:G:308:ARG:NH2	42:G:578:PRO:O	2.40	0.54
42:G:354:LEU:HD22	42:G:548:LEU:HD22	1.90	0.54
2:C:429:LYS:HG2	3:D:115:THR:HB	1.89	0.54
11:N:50:GLN:HE22	43:M:93:LYS:HG2	1.72	0.54
11:N:59:VAL:HG22	11:N:68:LEU:HD21	1.89	0.54
12:X:93:ILE:HD11	12:X:110:LEU:HD11	1.89	0.54
33:l:526:LEU:HD12	33:l:530:PRO:HG3	1.90	0.54
42:G:66:HIS:HB3	42:G:69:LEU:HB2	1.90	0.54
3:D:87:PHE:HE1	3:D:144:LYS:HD2	1.73	0.54
10:L:356:TRP:CZ2	10:L:362:GLU:HB3	2.43	0.54
18:U:182:ARG:HE	18:U:184:GLN:HB2	1.73	0.54
30:i:283:ALA:HB1	38:q:158:LEU:HD13	1.90	0.54
2:C:374:ARG:NH2	6:H:165:ASP:OD1	2.40	0.54
6:H:74:LEU:HB2	39:r:272:TRP:CZ2	2.43	0.54
10:L:163:SER:HB2	10:L:197:LYS:HG2	1.90	0.54
30:i:68:MET:HE2	32:k:36:MET:HB3	1.90	0.54
8:J:111:LEU:HD11	9:K:126:PRO:HG2	1.88	0.54
9:K:106:ARG:HB2	9:K:109:ILE:HG13	1.88	0.54
30:i:298:TYR:HA	30:i:302:LEU:HB2	1.90	0.54
34:m:58:LEU:HD11	39:r:106:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:o:49:LEU:HD23	37:p:208:LEU:HD21	1.90	0.54
42:G:374:THR:HG22	42:G:532:PRO:HG2	1.90	0.54
17:T:128:ILE:HG12	31:j:84:LEU:HB2	1.90	0.54
1:B:378:SER:OG	1:B:385:CYS:SG	2.61	0.54
3:D:72:TYR:HB3	3:D:88:ILE:HG23	1.89	0.54
3:D:75:GLN:HB3	3:D:87:PHE:HD2	1.73	0.54
3:D:242:PHE:HE1	43:M:60:ARG:HG2	1.73	0.54
7:I:142:GLU:HG2	7:I:235:PRO:O	2.07	0.54
13:P:68:ARG:HH22	42:G:364:ASP:HB3	1.73	0.54
33:l:539:TYR:OH	36:o:10:ARG:NH2	2.40	0.54
39:r:69:SER:O	39:r:73:ILE:HG12	2.08	0.54
39:r:141:SER:HB2	39:r:289:LEU:HB3	1.90	0.54
2:C:67:TRP:HZ3	33:l:580:GLN:HB3	1.73	0.53
42:G:466:LEU:HD13	42:G:500:ILE:HD11	1.90	0.53
33:l:69:MET:HE3	33:l:76:LEU:HD12	1.90	0.53
34:m:103:MET:HE1	34:m:115:ILE:HG21	1.90	0.53
43:M:46:SER:O	43:M:52:ASN:ND2	2.36	0.53
1:B:109:ARG:NH2	1:B:232:ASP:O	2.42	0.53
2:C:229:HIS:CD2	7:I:234:PRO:HD3	2.43	0.53
12:O:114:ASP:OD1	14:Q:90:ARG:NH1	2.41	0.53
33:l:315:VAL:HG11	33:l:412:THR:HG21	1.90	0.53
39:r:149:ILE:HG12	39:r:181:LEU:HD22	1.90	0.53
8:J:108:GLU:HG3	8:J:113:GLY:HA2	1.91	0.53
38:q:108:MET:HB3	38:q:121:LEU:HD13	1.90	0.53
38:q:133:ILE:HD11	38:q:231:LEU:HD11	1.89	0.53
42:G:485:ASP:HB3	42:G:680:LEU:HG	1.89	0.53
19:V:22:ALA:O	19:V:26:THR:OG1	2.26	0.53
42:G:389:THR:O	42:G:390:THR:OG1	2.25	0.53
9:K:65:THR:O	9:K:73:THR:OG1	2.20	0.53
13:P:37:ILE:HD13	13:P:55:ILE:HD13	1.90	0.53
31:j:87:MET:HG2	34:m:147:TYR:HB3	1.91	0.53
1:B:128:ARG:HD2	4:E:178:GLY:HA3	1.90	0.53
2:C:196:HIS:HE1	2:C:455:ALA:HA	1.74	0.53
31:j:55:PHE:HB3	34:m:70:TYR:HE2	1.73	0.53
33:l:278:LEU:HB2	33:l:318:GLY:HA3	1.91	0.53
3:D:43:THR:O	3:D:44:ARG:HB2	2.08	0.53
33:l:467:ILE:O	33:l:471:ASN:ND2	2.36	0.53
38:q:15:THR:O	38:q:93:LYS:NZ	2.41	0.53
18:U:82:LYS:HB2	18:U:272:VAL:HG21	1.90	0.53
23:a:97:GLU:HB2	25:d:62:TYR:HD1	1.74	0.53
31:j:105:GLU:HG2	31:j:110:GLY:HA3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:r:142:TYR:HE1	39:r:146:LEU:HD22	1.73	0.53
31:j:53:MET:HE2	34:m:172:THR:HB	1.91	0.53
33:l:124:PHE:HE1	33:l:147:VAL:HG13	1.74	0.53
36:o:25:ILE:HG23	36:o:30:ARG:NH2	2.24	0.53
42:G:182:CYS:HA	42:G:225:ILE:HD11	1.90	0.53
10:L:167:ALA:HA	10:L:176:LEU:HB3	1.91	0.52
12:X:105:MET:HB2	12:X:139:MET:HE3	1.91	0.52
32:k:23:ARG:HG3	34:m:23:LYS:HD3	1.91	0.52
17:T:153:SER:HB3	40:s:207:LYS:HB2	1.90	0.52
33:l:545:SER:OG	38:q:274:SER:O	2.22	0.52
10:L:349:ARG:NH1	14:Q:77:GLN:O	2.42	0.52
18:U:205:VAL:HG21	18:U:275:ILE:HG23	1.90	0.52
22:Z:73:PHE:CG	33:l:435:PRO:HG3	2.45	0.52
2:C:457:ILE:HG23	2:C:462:ILE:HD12	1.92	0.52
12:X:115:GLN:O	12:X:118:ILE:HG13	2.09	0.52
39:r:134:ARG:HB3	39:r:200:LEU:HD13	1.92	0.52
30:i:18:MET:O	30:i:22:ILE:HB	2.09	0.52
33:l:65:ASN:HA	44:b:89:HIS:NE2	2.24	0.52
33:l:99:SER:HA	33:l:456:ARG:HH21	1.74	0.52
31:j:58:VAL:HG13	39:r:286:MET:HE1	1.92	0.52
2:C:194:THR:HB	2:C:206:PHE:HA	1.91	0.52
7:I:192:PRO:HG2	39:r:58:LYS:HZ3	1.74	0.52
16:S:54:ILE:HD12	40:s:96:LYS:HA	1.92	0.52
18:U:59:SER:HB3	18:U:152:LEU:HD11	1.91	0.52
42:G:219:SER:OG	42:G:288:ASP:OD2	2.26	0.52
12:O:138:LEU:HB3	12:O:144:ILE:HG12	1.92	0.52
16:S:54:ILE:HG22	16:S:64:LYS:HG3	1.90	0.52
30:i:64:ALA:O	30:i:68:MET:HG2	2.10	0.52
6:H:68:ARG:NH2	20:W:26:PRO:O	2.43	0.52
6:H:100:GLU:OE2	6:H:193:ASN:ND2	2.43	0.52
18:U:182:ARG:HH21	18:U:316:LEU:HD22	1.75	0.52
21:Y:102:ASP:OD2	41:t:118:ARG:NH2	2.39	0.52
38:q:285:LEU:HD13	38:q:342:MET:HE1	1.92	0.52
39:r:74:ALA:HB3	39:r:75:PRO:HD3	1.90	0.52
1:B:109:ARG:HH12	1:B:233:VAL:HG22	1.75	0.51
2:C:56:ALA:HB1	33:l:580:GLN:HE22	1.75	0.51
25:d:114:GLN:HG2	33:l:199:GLN:HA	1.90	0.51
38:q:106:LEU:HD13	38:q:234:VAL:HG11	1.92	0.51
2:C:137:GLN:NE2	6:H:121:ALA:O	2.43	0.51
8:J:64:LEU:HD13	14:Q:107:LEU:HD23	1.93	0.51
17:T:141:PRO:HG3	40:s:118:LYS:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:LEU:HD13	2:C:430:ILE:HG21	1.91	0.51
10:L:165:LEU:HD12	10:L:199:SER:HB2	1.91	0.51
33:l:452:ASN:HA	33:l:455:LYS:HE3	1.91	0.51
42:G:278:HIS:CE1	42:G:280:ASP:HB2	2.46	0.51
2:C:151:MET:HG3	2:C:220:TYR:CE2	2.46	0.51
7:I:118:ASP:HB2	7:I:257:LEU:HB2	1.92	0.51
23:a:147:ALA:HB2	38:q:173:SER:HB2	1.92	0.51
31:j:56:PHE:CZ	32:k:75:LEU:HB3	2.39	0.51
38:q:116:ILE:HG21	40:s:245:PHE:HB3	1.93	0.51
38:q:358:TRP:HE3	38:q:441:ILE:HD12	1.74	0.51
42:G:456:ALA:O	42:G:499:ASN:ND2	2.43	0.51
10:L:339:PRO:HG2	10:L:342:LEU:HG	1.92	0.51
12:X:105:MET:HE1	12:X:112:SER:HA	1.91	0.51
31:j:55:PHE:CB	34:m:74:MET:HE1	2.36	0.51
39:r:68:ILE:O	39:r:69:SER:C	2.53	0.51
39:r:92:PRO:HD3	39:r:255:TYR:CD1	2.45	0.51
20:W:70:ALA:HB2	40:s:202:LEU:HD13	1.92	0.51
30:i:344:SER:HA	30:i:347:ASN:HD22	1.75	0.51
37:p:160:TYR:HA	37:p:163:LYS:HZ2	1.75	0.51
42:G:49:VAL:HB	42:G:91:ALA:HA	1.92	0.51
1:B:114:VAL:HG11	1:B:212:LEU:HD22	1.93	0.51
6:H:140:ARG:HG2	42:G:238:PHE:CG	2.46	0.51
8:J:81:VAL:HG21	8:J:150:ARG:HD2	1.93	0.51
9:K:14:VAL:HA	9:K:23:TYR:CD1	2.46	0.51
20:W:137:THR:HG21	34:m:125:TRP:HB2	1.93	0.51
27:f:65:ASP:HB3	28:g:25:PRO:HB3	1.92	0.51
31:j:55:PHE:HB2	34:m:74:MET:CE	2.38	0.51
1:B:37:ASP:O	4:E:239:LYS:NZ	2.40	0.51
1:B:274:LYS:HZ2	1:B:352:ALA:HB3	1.75	0.51
6:H:84:ILE:O	7:I:155:ARG:NH2	2.44	0.51
16:S:44:GLN:HE21	34:m:135:PHE:HE1	1.59	0.51
2:C:384:LEU:HD21	42:G:129:PRO:HD3	1.93	0.51
4:E:143:ARG:HB3	4:E:184:PRO:HD3	1.92	0.51
18:U:72:LYS:HE2	18:U:162:GLU:HB3	1.93	0.51
22:Z:48:VAL:HG22	33:l:511:LEU:HD21	1.91	0.51
33:l:302:VAL:O	33:l:306:THR:HG23	2.10	0.51
38:q:36:LEU:HD22	38:q:39:LEU:HD12	1.92	0.51
14:Q:71:ASN:OD1	14:Q:71:ASN:N	2.42	0.50
23:a:74:TYR:CD2	26:e:91:PHE:HB3	2.46	0.50
38:q:94:LEU:O	38:q:98:MET:HG2	2.11	0.50
38:q:325:MET:SD	38:q:441:ILE:HG13	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LYS:HD3	4:E:249:LEU:HD21	1.94	0.50
4:E:196:LEU:HD13	4:E:201:ILE:HG12	1.93	0.50
10:L:80:ARG:HH21	10:L:127:ARG:HH21	1.58	0.50
40:s:146:ASP:OD1	40:s:149:ARG:NH1	2.44	0.50
42:G:338:VAL:HG22	42:G:544:VAL:HB	1.92	0.50
44:b:22:TRP:O	44:b:26:GLN:HG2	2.11	0.50
2:C:250:ILE:HG22	2:C:354:LEU:HD11	1.92	0.50
4:E:132:ILE:HD11	4:E:169:PHE:HD1	1.76	0.50
14:Q:48:SER:HB2	14:Q:53:GLU:HB2	1.92	0.50
20:W:10:MET:HE3	20:W:11:PRO:HD2	1.93	0.50
20:W:120:MET:HE2	34:m:126:VAL:HG12	1.93	0.50
20:W:126:GLY:HA2	34:m:125:TRP:HH2	1.76	0.50
2:C:122:LEU:HD23	2:C:465:GLY:HA2	1.93	0.50
3:D:69:LEU:HD21	11:N:94:MET:HE1	1.92	0.50
36:o:39:ILE:HG23	36:o:42:ARG:HH21	1.75	0.50
38:q:119:TYR:CZ	38:q:161:LEU:HB2	2.47	0.50
1:B:159:ARG:NH1	4:E:176:CYS:O	2.45	0.50
5:F:114:CYS:HB2	5:F:116:LEU:HG	1.94	0.50
38:q:369:LEU:HD12	38:q:370:PRO:HD2	1.93	0.50
41:t:22:MET:HE1	41:t:102:PHE:CD2	2.47	0.50
42:G:308:ARG:HD2	42:G:581:ASP:HA	1.94	0.50
7:I:131:PRO:HD3	7:I:158:VAL:HG12	1.93	0.50
7:I:225:PRO:HB2	10:L:87:MET:HG3	1.92	0.50
23:a:94:GLY:O	25:d:61:TYR:OH	2.27	0.50
33:l:14:ILE:HD13	44:b:75:VAL:HG12	1.93	0.50
33:l:546:GLN:O	33:l:550:SER:HB2	2.11	0.50
42:G:222:ILE:HA	42:G:225:ILE:HG12	1.93	0.50
11:N:72:LEU:HD13	11:N:80:VAL:HG11	1.92	0.50
25:d:137:LYS:NZ	25:d:141:ASP:OD1	2.45	0.50
27:f:55:TRP:NE1	28:g:68:THR:HG22	2.26	0.50
42:G:123:ASN:HB3	42:G:158:ARG:HG2	1.93	0.50
1:B:325:PRO:HG3	1:B:433:TRP:HB3	1.94	0.50
11:N:25:LYS:HE2	11:N:60:LYS:HG2	1.93	0.50
14:Q:149:TYR:CZ	42:G:320:GLU:HG3	2.47	0.50
19:V:5:LEU:HD23	19:V:8:LYS:HD2	1.93	0.50
40:s:208:VAL:HG12	40:s:210:THR:HG23	1.94	0.50
4:E:137:THR:HB	47:E:301:FES:S1	2.52	0.49
18:U:255:CYS:HA	18:U:282:LYS:HD2	1.93	0.49
33:l:161:ARG:HG2	33:l:164:ALA:H	1.77	0.49
42:G:307:ILE:HG22	42:G:582:VAL:HG22	1.94	0.49
42:G:526:LEU:HD21	42:G:532:PRO:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:103:LEU:HD11	2:C:457:ILE:HD11	1.94	0.49
8:J:84:ARG:NH2	42:G:284:GLU:OE2	2.44	0.49
19:V:9:TYR:CZ	19:V:21:LYS:HE3	2.47	0.49
20:W:113:THR:HG22	20:W:115:ARG:H	1.77	0.49
29:h:17:TRP:CD1	29:h:17:TRP:H	2.30	0.49
33:l:49:VAL:HB	33:l:50:PRO:HD3	1.94	0.49
38:q:127:VAL:HB	38:q:128:PRO:HD3	1.94	0.49
16:S:50:ARG:O	16:S:54:ILE:HG12	2.12	0.49
33:l:292:ALA:HB2	33:l:304:PHE:HB3	1.93	0.49
2:C:241:ASP:HA	2:C:362:ILE:HG21	1.94	0.49
4:E:179:ALA:HB1	4:E:182:ASN:HB2	1.94	0.49
5:F:95:HIS:HE1	5:F:98:VAL:HG22	1.78	0.49
24:c:156:VAL:HG11	41:t:95:TYR:CZ	2.47	0.49
37:p:146:LEU:HB3	37:p:161:PHE:HE1	1.78	0.49
42:G:43:VAL:HG12	42:G:55:LYS:HD2	1.93	0.49
6:H:196:LYS:HD3	9:K:113:HIS:CE1	2.48	0.49
39:r:87:VAL:HG13	39:r:95:LEU:HD23	1.95	0.49
42:G:433:GLY:N	42:G:446:GLY:O	2.45	0.49
4:E:138:THR:HA	4:E:141:MET:HE2	1.95	0.49
9:K:34:ARG:NH2	9:K:58:ARG:O	2.46	0.49
12:X:138:LEU:HD12	12:X:143:GLU:HB3	1.94	0.49
33:l:319:ILE:HG13	33:l:399:VAL:HG22	1.94	0.49
2:C:222:ARG:NH1	2:C:249:ASP:OD2	2.46	0.49
2:C:389:LYS:HG3	42:G:144:MET:HG3	1.94	0.49
18:U:67:ASN:OD1	18:U:68:ILE:N	2.42	0.49
23:a:179:ILE:HD11	29:h:41:ILE:HB	1.94	0.49
33:l:302:VAL:O	33:l:305:SER:OG	2.22	0.49
39:r:146:LEU:HG	39:r:185:TRP:CZ3	2.48	0.49
42:G:624:ARG:NH1	42:G:628:GLU:HB2	2.27	0.49
9:K:144:TYR:CE1	42:G:308:ARG:HD3	2.48	0.49
10:L:345:ILE:HG13	10:L:349:ARG:HB2	1.95	0.49
14:Q:91:GLU:HG2	14:Q:95:LYS:HE3	1.94	0.49
35:n:12:TRP:HE3	35:n:12:TRP:H	1.59	0.49
38:q:105:PHE:O	38:q:109:THR:HG23	2.11	0.49
38:q:287:ALA:O	38:q:291:VAL:HG23	2.13	0.49
40:s:95:VAL:HG12	40:s:97:VAL:HG22	1.94	0.49
18:U:317:PRO:HB3	26:e:52:THR:O	2.12	0.49
33:l:289:ALA:O	33:l:293:ILE:HG13	2.13	0.49
33:l:305:SER:O	33:l:309:GLN:HG2	2.13	0.49
10:L:165:LEU:HD11	10:L:261:VAL:HG12	1.95	0.49
12:X:119:ILE:HG21	12:X:135:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:h:32:ARG:HB2	32:k:52:HIS:HD2	1.78	0.49
38:q:231:LEU:O	38:q:236:LEU:HG	2.13	0.49
39:r:67:SER:O	39:r:68:ILE:C	2.56	0.49
39:r:142:TYR:CE1	39:r:192:GLU:HB2	2.48	0.49
42:G:401:LEU:HD11	42:G:432:ILE:HG13	1.95	0.49
4:E:134:VAL:O	4:E:173:GLU:HA	2.13	0.48
6:H:50:MET:HE2	17:T:95:LYS:HE2	1.95	0.48
33:l:273:VAL:HA	33:l:276:MET:HE2	1.95	0.48
39:r:63:PRO:CB	39:r:214:GLU:HB3	2.41	0.48
42:G:559:ASP:OD1	42:G:559:ASP:N	2.45	0.48
32:k:1:MET:HE1	32:k:9:ILE:HD12	1.94	0.48
33:l:12:LEU:HD22	33:l:129:MET:HB3	1.94	0.48
42:G:68:ARG:HE	42:G:284:GLU:HB2	1.78	0.48
8:J:71:HIS:CE1	8:J:75:ARG:HH21	2.31	0.48
8:J:77:VAL:HG13	8:J:99:MET:HG3	1.95	0.48
10:L:126:GLY:O	48:L:401:NDP:H52A	2.13	0.48
39:r:234:MET:O	39:r:238:THR:HG23	2.14	0.48
42:G:366:LEU:O	42:G:531:LYS:N	2.46	0.48
9:K:1:MET:SD	9:K:1:MET:N	2.78	0.48
9:K:42:ASP:OD1	9:K:46:ASN:N	2.47	0.48
18:U:40:TYR:HB3	18:U:301:GLN:HE22	1.79	0.48
2:C:169:PRO:HG2	2:C:174:GLN:HE21	1.77	0.48
10:L:112:ARG:HH12	10:L:153:GLU:HB2	1.78	0.48
25:d:43:ARG:O	25:d:47:LEU:HG	2.14	0.48
30:i:100:MET:HE3	30:i:111:PHE:HZ	1.78	0.48
33:l:315:VAL:O	33:l:319:ILE:HG12	2.14	0.48
42:G:32:ILE:HD11	42:G:96:VAL:HG23	1.95	0.48
3:D:231:ARG:HH12	6:H:129:THR:HA	1.78	0.48
14:Q:142:THR:HA	14:Q:147:LYS:HE3	1.95	0.48
15:R:93:LEU:HA	15:R:96:PHE:HD2	1.79	0.48
16:S:16:LEU:O	16:S:19:PRO:HD2	2.12	0.48
20:W:115:ARG:HA	40:s:220:HIS:HD2	1.78	0.48
33:l:584:ILE:HA	33:l:587:TYR:CZ	2.49	0.48
16:S:14:ALA:O	16:S:18:ILE:HG13	2.14	0.48
30:i:236:LYS:HG2	30:i:237:MET:HG3	1.96	0.48
38:q:398:MET:O	38:q:402:ILE:HG13	2.14	0.48
11:N:31:ILE:O	11:N:35:LEU:HG	2.14	0.48
25:d:41:VAL:HG13	44:b:80:TRP:HD1	1.77	0.48
27:f:40:ASP:O	27:f:42:LEU:N	2.44	0.48
31:j:58:VAL:HG11	39:r:286:MET:HE1	1.94	0.48
38:q:71:TRP:O	38:q:74:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:q:334:TYR:O	38:q:338:HIS:N	2.44	0.48
1:B:50:ASP:HB3	1:B:55:GLY:HA3	1.95	0.48
6:H:148:ASP:OD1	6:H:148:ASP:N	2.42	0.48
11:N:110:ASN:HD22	11:N:113:LYS:HD2	1.79	0.48
17:T:115:ILE:HG12	31:j:92:LEU:HD13	1.95	0.48
18:U:89:PRO:O	18:U:144:GLN:NE2	2.45	0.48
12:X:133:ILE:HD13	12:X:133:ILE:H	1.79	0.48
30:i:20:VAL:HG11	30:i:137:ALA:HB1	1.96	0.48
39:r:92:PRO:HD3	39:r:255:TYR:HD1	1.78	0.48
42:G:43:VAL:HG21	42:G:96:VAL:HG21	1.96	0.48
7:I:152:ASP:OD2	39:r:34:ARG:HB3	2.14	0.48
10:L:60:LEU:HA	10:L:237:ILE:HD11	1.96	0.48
13:P:36:PHE:HZ	13:P:44:LEU:HD12	1.79	0.48
20:W:43:LEU:HG	39:r:179:TRP:HE1	1.78	0.48
24:c:153:TYR:H	41:t:5:LEU:HD21	1.79	0.48
38:q:193:ILE:HA	38:q:253:LEU:HD21	1.94	0.48
8:J:156:LYS:O	42:G:51:GLN:NE2	2.44	0.47
17:T:138:TYR:CZ	40:s:121:MET:HG3	2.49	0.47
12:X:100:VAL:HG12	12:X:142:GLN:HB2	1.95	0.47
32:k:38:LEU:HD21	34:m:37:GLY:HA2	1.96	0.47
39:r:174:MET:HB3	39:r:242:PHE:HA	1.94	0.47
42:G:398:ASP:C	42:G:427:LEU:HD12	2.39	0.47
2:C:61:THR:N	2:C:64:THR:OG1	2.45	0.47
4:E:132:ILE:HG21	4:E:152:ILE:HD13	1.95	0.47
10:L:62:ARG:HB3	10:L:92:MET:HE1	1.96	0.47
13:P:65:LEU:HB2	13:P:79:LEU:HD11	1.96	0.47
31:j:105:GLU:HG3	34:m:169:MET:SD	2.54	0.47
33:l:341:MET:HE3	33:l:454:ILE:HG12	1.96	0.47
38:q:275:ILE:O	38:q:279:GLN:HG2	2.14	0.47
3:D:101:ARG:NH1	3:D:159:VAL:O	2.47	0.47
10:L:125:VAL:HG13	48:L:401:NDP:C4A	2.44	0.47
13:P:16:LEU:HD22	13:P:94:VAL:HG12	1.96	0.47
19:V:72:LEU:HD23	19:V:72:LEU:HA	1.76	0.47
30:i:291:TYR:HA	38:q:151:PHE:HZ	1.79	0.47
2:C:384:LEU:HD22	42:G:126:LEU:HB3	1.96	0.47
8:J:131:LYS:HE3	8:J:147:VAL:HG11	1.96	0.47
8:J:169:ARG:HG2	15:R:105:ARG:NH2	2.28	0.47
36:o:48:LEU:HB3	37:p:208:LEU:HD13	1.96	0.47
39:r:26:LYS:HA	39:r:36:GLY:HA3	1.96	0.47
39:r:81:LEU:O	39:r:85:MET:HG3	2.14	0.47
41:t:8:ARG:HG3	41:t:13:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ILE:O	1:B:371:ILE:HG12	2.14	0.47
3:D:128:ILE:HD11	3:D:176:VAL:HG11	1.95	0.47
4:E:137:THR:HG22	4:E:138:THR:H	1.80	0.47
10:L:196:ILE:HG22	10:L:198:PRO:HD3	1.97	0.47
14:Q:43:VAL:HG11	14:Q:103:ARG:NH1	2.30	0.47
18:U:64:VAL:HG12	18:U:72:LYS:HB2	1.96	0.47
20:W:105:LYS:HB3	40:s:81:ILE:HD11	1.96	0.47
22:Z:38:TRP:HB3	22:Z:66:ALA:HB3	1.96	0.47
24:c:128:THR:HG22	24:c:132:HIS:CD2	2.50	0.47
30:i:29:ILE:HD13	30:i:141:VAL:HG22	1.96	0.47
33:l:208:CYS:SG	33:l:266:LEU:HB3	2.54	0.47
33:l:278:LEU:HD12	33:l:315:VAL:HG13	1.97	0.47
2:C:214:GLU:OE1	2:C:227:ARG:NH2	2.47	0.47
3:D:105:ASN:O	43:M:97:PRO:HD3	2.14	0.47
6:H:77:LEU:HB2	39:r:31:MET:HG2	1.96	0.47
6:H:83:THR:HG21	39:r:35:LYS:H	1.80	0.47
6:H:148:ASP:HA	6:H:184:LEU:HA	1.96	0.47
29:h:85:LYS:O	29:h:89:GLU:HG2	2.15	0.47
30:i:258:SER:OG	30:i:333:SER:O	2.31	0.47
33:l:227:PHE:N	33:l:284:THR:HG22	2.22	0.47
37:p:201:LYS:H	37:p:201:LYS:HD2	1.79	0.47
39:r:185:TRP:O	39:r:189:THR:HG23	2.15	0.47
3:D:88:ILE:HG12	3:D:96:VAL:HG21	1.95	0.47
12:X:143:GLU:HA	12:X:146:ASP:OD2	2.15	0.47
26:e:79:ASP:HB3	26:e:82:VAL:HG12	1.96	0.47
38:q:82:SER:HB3	38:q:432:ARG:NH2	2.30	0.47
38:q:122:PHE:HE1	38:q:206:LYS:HG3	1.79	0.47
41:t:43:GLN:HA	41:t:46:MET:HE2	1.97	0.47
42:G:304:GLN:HB2	42:G:316:TYR:CD1	2.49	0.47
42:G:372:PHE:H	42:G:532:PRO:HB2	1.78	0.47
42:G:488:ALA:HB2	42:G:677:GLN:HB3	1.97	0.47
20:W:124:LEU:HD12	34:m:130:THR:HG21	1.97	0.47
33:l:213:LEU:HD23	33:l:216:LEU:HD12	1.97	0.47
41:t:18:ASP:OD2	41:t:21:ARG:NH1	2.48	0.47
42:G:265:THR:HG22	42:G:270:VAL:HA	1.97	0.47
4:E:41:HIS:CD2	4:E:95:ILE:HD12	2.49	0.47
4:E:55:PHE:HB2	4:E:60:TYR:CZ	2.50	0.47
25:d:82:ILE:H	25:d:82:ILE:HG13	1.43	0.47
26:e:125:LEU:O	26:e:129:ARG:HG2	2.15	0.47
32:k:32:CYS:HA	34:m:20:PHE:HE1	1.80	0.47
33:l:379:ALA:O	33:l:388:GLY:HA3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:l:400:ASN:HA	33:l:409:LEU:HD11	1.97	0.47
38:q:266:MET:HE2	38:q:395:LEU:HD12	1.97	0.47
1:B:83:SER:HB2	1:B:262:PHE:HB3	1.96	0.47
4:E:183:ALA:HB1	4:E:184:PRO:HD2	1.96	0.47
7:I:131:PRO:HD2	7:I:159:VAL:O	2.15	0.47
8:J:90:GLY:HA2	42:G:59:GLN:HE22	1.80	0.47
20:W:112:HIS:HA	40:s:79:PRO:HG2	1.96	0.47
25:d:132:PHE:HE2	33:l:204:LEU:HD11	1.80	0.47
33:l:61:MET:HG2	44:b:99:GLU:HA	1.96	0.47
34:m:86:ASN:ND2	34:m:88:THR:OG1	2.47	0.47
42:G:257:VAL:HG11	42:G:413:LEU:HB2	1.96	0.47
2:C:126:THR:HG22	7:I:210:TYR:HE1	1.80	0.46
4:E:138:THR:O	4:E:142:LEU:HG	2.14	0.46
9:K:50:GLU:HB2	9:K:89:TRP:HZ2	1.80	0.46
11:N:94:MET:SD	11:N:99:PRO:HG3	2.56	0.46
24:c:143:MET:HB3	33:l:407:TRP:CD2	2.50	0.46
33:l:102:GLU:HG2	33:l:449:LEU:HB3	1.97	0.46
38:q:74:PRO:O	38:q:78:MET:HG3	2.15	0.46
1:B:126:LYS:HG3	1:B:127:ASP:H	1.79	0.46
1:B:213:ILE:HG23	1:B:235:VAL:HA	1.97	0.46
2:C:126:THR:HG22	7:I:210:TYR:CE1	2.50	0.46
8:J:75:ARG:NH2	8:J:119:ASP:OD1	2.49	0.46
8:J:88:GLN:HE21	42:G:136:GLU:HA	1.80	0.46
18:U:172:LEU:HD21	18:U:186:VAL:HG13	1.97	0.46
33:l:183:VAL:HG21	38:q:400:MET:HE1	1.96	0.46
33:l:190:LEU:HB2	33:l:196:TRP:NE1	2.31	0.46
37:p:177:ARG:HA	37:p:180:LYS:HE3	1.96	0.46
38:q:76:MET:SD	38:q:230:VAL:HG13	2.56	0.46
2:C:101:LEU:HB2	2:C:464:PHE:CZ	2.50	0.46
4:E:108:PRO:HB2	4:E:111:ARG:HG2	1.97	0.46
25:d:49:ARG:HA	25:d:49:ARG:HD3	1.62	0.46
25:d:122:ARG:NH2	33:l:206:ASN:HD21	2.14	0.46
33:l:65:ASN:HA	44:b:89:HIS:CD2	2.50	0.46
1:B:161:GLU:HG2	4:E:177:LEU:HD22	1.97	0.46
1:B:329:LYS:O	1:B:333:GLU:HG3	2.16	0.46
2:C:129:LEU:HD23	3:D:204:LEU:HD11	1.97	0.46
12:O:82:ARG:HB2	12:O:126:PHE:CZ	2.50	0.46
15:R:81:TYR:CD1	15:R:85:THR:HG21	2.50	0.46
18:U:256:GLU:HB2	18:U:278:LEU:HD13	1.98	0.46
25:d:122:ARG:HH22	33:l:203:MET:HA	1.81	0.46
32:k:66:PHE:CE2	34:m:157:THR:HG22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:l:247:LEU:HD12	33:l:248:HIS:HE1	1.80	0.46
38:q:358:TRP:CE3	38:q:441:ILE:HD12	2.50	0.46
39:r:259:PHE:O	39:r:263:THR:HG23	2.15	0.46
41:t:12:ASP:HB2	41:t:15:LYS:HG2	1.96	0.46
1:B:60:GLY:HA2	4:E:241:PRO:HA	1.98	0.46
21:Y:99:ILE:HG13	41:t:108:LEU:HD22	1.97	0.46
30:i:337:LEU:O	30:i:340:THR:HG23	2.16	0.46
33:l:161:ARG:HE	33:l:238:GLU:HG3	1.80	0.46
33:l:284:THR:OG1	33:l:311:GLY:HA3	2.15	0.46
37:p:181:GLN:NE2	37:p:198:PRO:O	2.48	0.46
38:q:118:PHE:O	38:q:122:PHE:HB3	2.15	0.46
42:G:389:THR:HB	42:G:473:MET:HE3	1.98	0.46
2:C:184:THR:HA	2:C:187:LEU:HD12	1.98	0.46
16:S:59:ARG:HB3	16:S:61:HIS:CD2	2.51	0.46
17:T:160:GLY:HA3	40:s:204:LYS:HE3	1.98	0.46
25:d:85:MET:HE1	38:q:182:TRP:CD1	2.51	0.46
30:i:71:MET:HG3	32:k:40:LEU:HD13	1.98	0.46
32:k:38:LEU:O	32:k:42:ILE:HG12	2.16	0.46
42:G:400:ILE:HD12	42:G:427:LEU:HD21	1.98	0.46
2:C:248:ASP:O	2:C:252:GLU:HG2	2.16	0.46
10:L:263:PRO:HG3	10:L:339:PRO:HA	1.97	0.46
21:Y:99:ILE:HD13	41:t:107:ARG:HD3	1.97	0.46
23:a:96:ALA:HB2	25:d:61:TYR:CE2	2.50	0.46
25:d:18:PRO:HA	44:b:109:THR:HA	1.96	0.46
33:l:536:LEU:HB3	33:l:537:PRO:HD3	1.98	0.46
38:q:78:MET:HA	38:q:81:GLN:HE21	1.81	0.46
40:s:92:VAL:HG21	40:s:138:LYS:HG2	1.97	0.46
42:G:591:GLU:HG2	42:G:610:VAL:HG23	1.98	0.46
2:C:133:LYS:HD2	2:C:141:TYR:HE2	1.81	0.46
30:i:298:TYR:O	30:i:303:THR:HG22	2.15	0.46
34:m:67:VAL:O	34:m:71:THR:HG23	2.16	0.46
32:k:34:GLU:HG2	34:m:68:PHE:CZ	2.50	0.46
33:l:2:ASN:HB3	33:l:3:PRO:HD3	1.98	0.46
39:r:116:ILE:HG21	39:r:135:ALA:HB3	1.97	0.46
2:C:309:ARG:HG3	2:C:407:GLU:HB3	1.98	0.46
9:K:48:TYR:OH	9:K:83:PRO:HD2	2.16	0.46
9:K:64:TYR:HB2	9:K:77:VAL:HG12	1.98	0.46
10:L:346:GLU:HG2	14:Q:79:ASP:CG	2.41	0.46
20:W:83:VAL:HG13	20:W:124:LEU:HD21	1.98	0.46
12:X:104:PHE:HB3	12:X:110:LEU:HD12	1.96	0.46
23:a:101:ILE:HG12	25:d:64:TYR:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:h:2:PRO:HD2	30:i:140:SER:HA	1.98	0.46
31:j:63:LEU:O	31:j:67:LEU:HG	2.15	0.46
39:r:179:TRP:CG	39:r:180:PRO:HD3	2.51	0.46
1:B:276:PHE:CD1	1:B:352:ALA:HB1	2.51	0.45
4:E:137:THR:OG1	4:E:175:GLU:OE1	2.27	0.45
15:R:79:HIS:CD2	15:R:80:GLU:HG2	2.51	0.45
25:d:104:ASN:HA	25:d:107:GLN:HE21	1.81	0.45
26:e:93:PHE:O	26:e:98:VAL:HG22	2.16	0.45
33:l:303:ALA:O	33:l:306:THR:OG1	2.24	0.45
34:m:24:PRO:HG3	34:m:83:TRP:CD1	2.51	0.45
39:r:201:THR:HG22	39:r:202:GLU:HG2	1.96	0.45
39:r:266:LEU:O	39:r:269:THR:OG1	2.27	0.45
41:t:8:ARG:HB2	41:t:16:GLU:HG2	1.98	0.45
42:G:647:GLU:HB2	42:G:654:VAL:HG11	1.98	0.45
1:B:152:ARG:NH2	15:R:100:GLN:HA	2.31	0.45
3:D:124:ASN:HD21	11:N:108:PRO:HG2	1.80	0.45
6:H:151:LYS:HE2	7:I:211:HIS:CD2	2.52	0.45
33:l:88:MET:HE2	33:l:326:PHE:CE2	2.51	0.45
33:l:279:CYS:O	33:l:283:ILE:HG13	2.16	0.45
3:D:87:PHE:CE1	3:D:144:LYS:HD2	2.51	0.45
4:E:172:ILE:HG12	4:E:173:GLU:H	1.81	0.45
10:L:231:VAL:O	10:L:265:ARG:NH2	2.49	0.45
10:L:357:LEU:HD23	14:Q:77:GLN:HE22	1.81	0.45
20:W:80:ASP:OD1	20:W:81:ARG:N	2.49	0.45
30:i:30:TRP:CZ2	32:k:37:MET:HE1	2.51	0.45
30:i:168:GLY:O	30:i:172:GLN:HG2	2.15	0.45
30:i:221:HIS:HA	30:i:321:LYS:HZ1	1.82	0.45
33:l:245:ALA:O	33:l:249:SER:HB3	2.15	0.45
33:l:401:MET:SD	33:l:482:MET:HG3	2.56	0.45
34:m:166:VAL:O	34:m:170:GLU:HG2	2.16	0.45
41:t:18:ASP:HB3	41:t:21:ARG:HB2	1.99	0.45
2:C:444:MET:HE2	2:C:456:ILE:HG23	1.98	0.45
48:L:401:NDP:H2N	48:L:401:NDP:H2D	1.75	0.45
16:S:12:MET:HE3	39:r:264:LEU:HD22	1.97	0.45
18:U:171:PHE:O	18:U:175:MET:HG3	2.16	0.45
25:d:140:GLN:HB2	36:o:127:ILE:HG22	1.99	0.45
37:p:142:PRO:HB2	37:p:144:TRP:CD1	2.51	0.45
38:q:16:TRP:NE1	38:q:97:THR:HG21	2.32	0.45
44:b:87:LYS:HE2	44:b:87:LYS:HB2	1.74	0.45
1:B:115:VAL:HG21	1:B:142:CYS:SG	2.57	0.45
2:C:45:PRO:HB3	2:C:49:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:84:ILE:HD12	5:F:100:ILE:HB	1.98	0.45
11:N:38:ILE:O	11:N:45:ARG:NH1	2.45	0.45
28:g:64:LEU:O	28:g:68:THR:HG23	2.16	0.45
30:i:261:MET:HG2	30:i:340:THR:HG22	1.99	0.45
36:o:23:TYR:OH	37:p:110:GLU:HG3	2.17	0.45
38:q:106:LEU:O	38:q:109:THR:OG1	2.27	0.45
1:B:62:TRP:CD2	1:B:181:LEU:HD13	2.51	0.45
6:H:113:CYS:O	6:H:141:ARG:NH1	2.50	0.45
28:g:106:LYS:O	28:g:108:LYS:NZ	2.47	0.45
30:i:222:SER:HB2	30:i:233:THR:HG21	1.98	0.45
30:i:251:MET:HE2	30:i:293:TYR:OH	2.16	0.45
33:l:2:ASN:HD21	44:b:83:HIS:HE1	1.65	0.45
33:l:79:SER:OG	33:l:135:ASN:HB3	2.17	0.45
38:q:373:ILE:HD11	38:q:444:LEU:HG	1.98	0.45
39:r:31:MET:HE1	39:r:272:TRP:HA	1.99	0.45
4:E:129:LYS:HB3	4:E:168:LEU:HD23	1.99	0.45
9:K:95:ASP:OD2	43:M:34:ARG:N	2.50	0.45
13:P:16:LEU:HA	13:P:69:TYR:HA	1.99	0.45
33:l:160:GLY:HA3	37:p:137:GLU:HB3	1.98	0.45
38:q:315:LEU:HD12	38:q:381:ILE:HD12	1.99	0.45
2:C:168:GLN:HB3	3:D:45:PRO:O	2.17	0.45
2:C:239:HIS:CD2	2:C:240:GLN:HG3	2.52	0.45
8:J:121:LEU:HD22	8:J:124:LEU:HD12	1.99	0.45
10:L:43:ARG:NH2	10:L:93:GLY:O	2.50	0.45
18:U:131:TYR:CD1	18:U:185:CYS:HB3	2.51	0.45
23:a:166:GLY:O	23:a:170:GLN:NE2	2.50	0.45
25:d:76:GLU:HB3	26:e:146:LYS:HD3	1.98	0.45
30:i:340:THR:N	30:i:341:PRO:HD2	2.32	0.45
33:l:88:MET:HE2	33:l:326:PHE:HE2	1.81	0.45
33:l:173:LEU:O	33:l:177:ILE:HG13	2.17	0.45
38:q:65:LEU:O	38:q:69:THR:HG23	2.17	0.45
39:r:133:LEU:HD13	39:r:133:LEU:HA	1.82	0.45
42:G:464:GLN:HA	42:G:467:LYS:HD2	1.99	0.45
1:B:62:TRP:CZ3	1:B:181:LEU:HB3	2.51	0.45
1:B:342:LEU:HB3	1:B:347:THR:HG23	1.99	0.45
4:E:95:ILE:HG12	4:E:99:ASN:HD21	1.82	0.45
6:H:41:VAL:HA	43:M:113:LEU:HB3	1.98	0.45
6:H:188:GLU:O	6:H:192:ASN:ND2	2.50	0.45
17:T:151:VAL:O	40:s:207:LYS:NZ	2.47	0.45
21:Y:87:PRO:HB2	21:Y:92:TRP:CZ2	2.52	0.45
29:h:15:ASP:OD1	29:h:15:ASP:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:n:54:GLU:N	35:n:54:GLU:OE1	2.49	0.45
42:G:74:ASN:HD21	42:G:179:CYS:HA	1.81	0.45
42:G:421:SER:O	42:G:425:ASN:N	2.49	0.45
42:G:575:VAL:O	42:G:578:PRO:HD2	2.17	0.45
8:J:112:MET:SD	9:K:126:PRO:HB2	2.57	0.45
23:a:184:LYS:HD3	29:h:30:PRO:HB3	1.98	0.45
25:d:117:GLU:HB2	25:d:121:TYR:HA	1.99	0.45
30:i:182:SER:HB2	30:i:293:TYR:OH	2.16	0.45
31:j:20:ILE:HG23	31:j:24:LEU:HD13	1.98	0.45
33:l:529:TYR:O	33:l:533:MET:HB2	2.16	0.45
34:m:82:VAL:HG12	34:m:83:TRP:H	1.82	0.45
1:B:270:ASN:HB3	1:B:338:ASP:HB2	1.98	0.44
10:L:213:ALA:HA	10:L:276:PHE:CE1	2.50	0.44
10:L:272:VAL:HG12	10:L:283:PHE:HE1	1.82	0.44
18:U:99:THR:O	27:f:31:ILE:HD11	2.17	0.44
12:X:150:ASP:OD2	44:b:16:ARG:HD2	2.17	0.44
24:c:110:ASP:OD1	24:c:110:ASP:N	2.47	0.44
33:l:201:ILE:HG22	33:l:266:LEU:HD11	1.99	0.44
33:l:294:THR:O	33:l:524:ASN:ND2	2.44	0.44
38:q:33:LEU:O	38:q:37:ILE:HG13	2.16	0.44
5:F:71:ILE:HG23	6:H:110:GLU:HB2	1.99	0.44
6:H:119:CYS:HA	6:H:122:VAL:HG12	2.00	0.44
18:U:74:ARG:HA	18:U:77:ARG:HE	1.83	0.44
30:i:65:THR:HG21	33:l:588:PHE:HE2	1.81	0.44
10:L:53:VAL:HG22	10:L:122:ILE:HD12	1.99	0.44
10:L:57:THR:HG21	10:L:86:THR:HG22	1.99	0.44
20:W:57:ARG:HB3	39:r:316:PRO:HG3	1.99	0.44
21:Y:61:PHE:CZ	33:l:455:LYS:HG3	2.53	0.44
28:g:51:ARG:HD3	30:i:322:GLN:HE21	1.82	0.44
32:k:97:GLN:HA	33:l:582:GLY:HA3	2.00	0.44
33:l:118:PHE:O	33:l:122:VAL:HG23	2.17	0.44
33:l:248:HIS:HA	33:l:253:VAL:HG13	1.99	0.44
37:p:171:ARG:HD2	37:p:210:TRP:CD2	2.52	0.44
42:G:409:PHE:HB3	42:G:694:PHE:HB2	1.98	0.44
2:C:43:TRP:O	38:q:142:ARG:NH2	2.50	0.44
4:E:143:ARG:CB	4:E:184:PRO:HD3	2.48	0.44
6:H:211:TYR:CZ	43:M:39:PRO:HG3	2.51	0.44
13:P:37:ILE:HA	13:P:41:TYR:HB2	2.00	0.44
18:U:142:LEU:HD12	18:U:165:ILE:HG21	1.99	0.44
18:U:213:VAL:HA	18:U:216:ILE:HD12	2.00	0.44
32:k:73:LEU:HD23	32:k:73:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:l:491:LEU:HD12	33:l:491:LEU:H	1.83	0.44
37:p:205:LEU:HD13	44:b:18:LEU:HD21	2.00	0.44
1:B:111:LYS:HG2	1:B:239:PRO:HB2	2.00	0.44
1:B:133:HIS:HE1	4:E:224:SER:HB3	1.82	0.44
6:H:196:LYS:HD2	6:H:197:TRP:NE1	2.33	0.44
10:L:59:PHE:HD1	10:L:205:GLU:HG2	1.81	0.44
16:S:4:GLU:HG2	39:r:26:LYS:HE2	1.99	0.44
17:T:123:TYR:HA	17:T:126:TYR:HD2	1.82	0.44
18:U:85:LEU:HD22	18:U:158:GLY:HA3	1.99	0.44
23:a:115:HIS:O	23:a:119:ARG:HG3	2.18	0.44
28:g:109:LYS:HE3	28:g:114:ILE:HG22	1.98	0.44
31:j:16:LEU:O	31:j:20:ILE:HG13	2.17	0.44
31:j:69:ILE:HD11	39:r:148:ILE:HG12	2.00	0.44
39:r:142:TYR:CE1	39:r:146:LEU:HD22	2.50	0.44
42:G:197:THR:HG22	42:G:206:VAL:HG22	2.00	0.44
42:G:677:GLN:HG2	42:G:678:GLN:H	1.82	0.44
2:C:102:ARG:HH22	14:Q:123:TRP:HA	1.83	0.44
2:C:145:LEU:HD11	2:C:430:ILE:HD13	2.00	0.44
6:H:81:PRO:HG3	39:r:30:TYR:HE1	1.81	0.44
6:H:89:GLU:HG2	9:K:61:TRP:HB3	1.99	0.44
6:H:93:LEU:HD23	9:K:93:MET:HE3	1.99	0.44
10:L:84:TYR:HA	10:L:87:MET:HE2	1.99	0.44
20:W:84:LEU:HD12	40:s:134:LEU:HD21	2.00	0.44
23:a:59:PRO:HG3	38:q:350:THR:O	2.17	0.44
30:i:266:ILE:O	30:i:270:MET:HG3	2.18	0.44
33:l:6:SER:O	33:l:10:THR:HG23	2.17	0.44
33:l:63:ILE:HG23	44:b:97:VAL:HG22	1.98	0.44
33:l:298:ILE:O	33:l:302:VAL:HG23	2.17	0.44
34:m:63:GLY:O	34:m:66:VAL:HG12	2.17	0.44
44:b:87:LYS:O	44:b:91:THR:OG1	2.36	0.44
1:B:314:LEU:HD11	1:B:317:VAL:HG23	2.00	0.44
2:C:73:ASN:C	2:C:75:VAL:N	2.76	0.44
2:C:163:LYS:HG3	3:D:48:ARG:NH1	2.33	0.44
8:J:158:LYS:HD3	42:G:65:TYR:HE1	1.81	0.44
12:O:104:PHE:HD1	12:O:108:LEU:HD12	1.82	0.44
14:Q:59:ARG:O	14:Q:63:ARG:HG3	2.18	0.44
24:c:151:PRO:O	41:t:9:TYR:OH	2.33	0.44
24:c:156:VAL:HG12	41:t:99:MET:HG3	2.00	0.44
30:i:203:LEU:HD22	30:i:343:LEU:HD21	1.98	0.44
31:j:111:LEU:HD22	31:j:113:TRP:HZ2	1.79	0.44
33:l:247:LEU:HD12	33:l:248:HIS:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:n:17:VAL:HG11	38:q:30:HIS:CG	2.52	0.44
37:p:180:LYS:HE3	37:p:180:LYS:HB3	1.90	0.44
1:B:211:ALA:HB2	1:B:223:PRO:HG3	1.99	0.44
10:L:357:LEU:HD23	14:Q:77:GLN:NE2	2.33	0.44
25:d:75:THR:O	28:g:110:THR:OG1	2.33	0.44
25:d:115:GLN:HG2	33:l:62:ILE:HG22	1.99	0.44
30:i:193:VAL:HG13	30:i:266:ILE:HG23	2.00	0.44
38:q:306:PRO:HA	38:q:458:LEU:HD22	1.99	0.44
38:q:366:ASN:HD22	38:q:407:SER:HB3	1.82	0.44
39:r:307:LEU:HA	39:r:310:MET:HG2	2.00	0.44
42:G:281:ILE:HD11	42:G:602:ARG:HD2	2.00	0.44
2:C:147:TYR:CZ	2:C:463:VAL:HG13	2.53	0.44
3:D:42:ASP:OD1	3:D:43:THR:N	2.44	0.44
13:P:46:LYS:HE2	42:G:674:LEU:HD11	1.99	0.44
14:Q:89:VAL:HG22	49:Q:201:ZMP:H7	1.99	0.44
18:U:182:ARG:NH2	18:U:317:PRO:HD2	2.32	0.44
25:d:51:PHE:O	25:d:55:GLN:HG2	2.17	0.44
33:l:159:HIS:HB3	38:q:416:ARG:HG2	1.99	0.44
37:p:174:SER:O	37:p:178:GLU:HG3	2.18	0.44
38:q:349:GLN:HB2	38:q:415:GLN:O	2.18	0.44
42:G:49:VAL:HG13	42:G:102:ILE:HD13	1.98	0.44
44:b:117:ILE:HD12	44:b:118:PRO:HD2	2.00	0.44
4:E:148:ILE:HG23	4:E:201:ILE:HG13	2.00	0.43
6:H:147:ILE:HG22	6:H:190:LEU:HD11	1.99	0.43
6:H:180:HIS:CE1	10:L:95:LEU:HD21	2.53	0.43
8:J:171:ARG:NE	15:R:108:PRO:HG2	2.33	0.43
20:W:53:TRP:CE2	20:W:57:ARG:HD2	2.53	0.43
20:W:98:MET:HG2	29:h:82:GLN:HG2	1.99	0.43
23:a:80:ILE:HB	23:a:81:PRO:HD3	1.99	0.43
24:c:185:GLU:C	24:c:186:ILE:HD12	2.42	0.43
25:d:103:VAL:HG22	25:d:135:VAL:HG12	1.99	0.43
29:h:39:GLU:OE1	40:s:224:ARG:NH2	2.47	0.43
33:l:142:ILE:HA	38:q:370:PRO:HB2	2.00	0.43
33:l:297:ASP:O	33:l:301:ILE:HG13	2.18	0.43
33:l:419:THR:HA	33:l:422:TYR:CZ	2.52	0.43
38:q:451:PRO:O	38:q:455:LEU:HG	2.18	0.43
2:C:196:HIS:O	2:C:200:ILE:HG12	2.18	0.43
5:F:58:ARG:HD3	9:K:123:GLN:HE21	1.83	0.43
7:I:118:ASP:OD2	7:I:255:LYS:HA	2.19	0.43
7:I:156:PHE:HB2	7:I:158:VAL:HG23	2.00	0.43
15:R:110:HIS:HA	42:G:441:ARG:HE	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:T:128:ILE:O	17:T:132:ARG:HG3	2.18	0.43
30:i:242:SER:O	30:i:246:VAL:HG23	2.18	0.43
39:r:86:TRP:NE1	39:r:233:MET:HB2	2.33	0.43
42:G:398:ASP:OD1	42:G:399:VAL:N	2.52	0.43
1:B:204:TYR:HB3	1:B:377:GLU:HB3	1.99	0.43
3:D:132:LEU:HB2	3:D:141:ILE:HG22	2.00	0.43
18:U:349:VAL:HB	27:f:29:PHE:CD1	2.53	0.43
12:X:90:TYR:CE1	22:Z:60:PRO:HB2	2.47	0.43
32:k:33:LEU:HA	32:k:36:MET:HE2	2.00	0.43
33:l:264:TYR:N	33:l:265:PRO:HD2	2.33	0.43
38:q:433:GLU:O	38:q:437:MET:HG2	2.19	0.43
1:B:276:PHE:CE2	1:B:290:GLU:HB3	2.52	0.43
3:D:173:MET:HB3	3:D:198:PHE:HB2	1.99	0.43
4:E:185:MET:HE3	4:E:185:MET:HB3	1.81	0.43
14:Q:58:VAL:HG21	49:Q:201:ZMP:H20B	2.00	0.43
20:W:53:TRP:NE1	20:W:57:ARG:HD2	2.33	0.43
30:i:175:LEU:HD22	30:i:296:LEU:HD11	2.00	0.43
42:G:356:ASP:O	42:G:360:ARG:HG2	2.18	0.43
42:G:382:ARG:HA	42:G:385:TYR:CE1	2.53	0.43
1:B:52:ARG:NH2	15:R:77:GLN:HG2	2.34	0.43
1:B:299:LEU:HD12	1:B:303:HIS:HD2	1.83	0.43
1:B:366:ALA:HA	4:E:141:MET:HE1	2.00	0.43
7:I:131:PRO:HG2	7:I:160:PHE:HD1	1.83	0.43
7:I:146:MET:HE3	7:I:153:MET:SD	2.58	0.43
12:O:128:PHE:CZ	12:O:148:ILE:HG12	2.48	0.43
17:T:139:PRO:HD3	20:W:69:ILE:HD13	2.00	0.43
18:U:224:GLY:HA2	18:U:229:MET:HE3	2.01	0.43
30:i:28:LEU:HD23	30:i:31:ILE:HD12	2.00	0.43
42:G:217:GLU:HG3	42:G:412:PRO:HB3	2.00	0.43
42:G:360:ARG:NH2	42:G:635:PRO:HD3	2.33	0.43
1:B:214:GLU:OE2	1:B:224:ARG:NE	2.31	0.43
1:B:307:VAL:HG21	1:B:314:LEU:HB2	2.00	0.43
2:C:222:ARG:O	2:C:243:PRO:HG3	2.19	0.43
3:D:213:ASP:HB3	3:D:216:VAL:HG22	2.00	0.43
5:F:79:VAL:HG21	5:F:84:ILE:HG12	1.99	0.43
12:X:84:LEU:HD12	12:X:98:LEU:HD13	2.01	0.43
21:Y:94:ASP:O	21:Y:99:ILE:N	2.52	0.43
28:g:36:MET:HG2	30:i:339:MET:HE2	2.01	0.43
38:q:355:MET:HA	38:q:358:TRP:HD1	1.84	0.43
2:C:256:ASN:HA	43:M:23:LYS:HD3	2.01	0.43
18:U:148:ALA:HB2	18:U:161:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:i:111:PHE:HA	33:l:591:PHE:CE1	2.53	0.43
30:i:231:SER:O	30:i:234:TRP:HD1	2.01	0.43
30:i:258:SER:HB2	30:i:336:VAL:HG12	2.00	0.43
30:i:296:LEU:HD23	30:i:296:LEU:HA	1.79	0.43
32:k:48:ILE:HG23	32:k:53:PHE:HB3	2.01	0.43
37:p:62:TYR:CZ	37:p:66:LEU:HD11	2.54	0.43
42:G:278:HIS:HE1	42:G:280:ASP:HB2	1.82	0.43
3:D:173:MET:HE1	3:D:189:THR:HG23	1.99	0.43
4:E:138:THR:HB	4:E:139:PRO:HD3	2.00	0.43
7:I:160:PHE:HD1	7:I:160:PHE:HA	1.74	0.43
10:L:311:ARG:O	10:L:315:GLU:HG2	2.19	0.43
10:L:350:ARG:HA	31:j:36:PRO:HB3	2.01	0.43
30:i:125:GLN:H	30:i:125:GLN:HG2	1.51	0.43
38:q:66:LEU:HD21	38:q:111:THR:HG23	2.01	0.43
38:q:218:LYS:O	38:q:222:GLU:HG2	2.18	0.43
39:r:149:ILE:HG21	39:r:185:TRP:HB2	2.00	0.43
41:t:14:SER:CB	41:t:113:LYS:HZ1	2.32	0.43
42:G:50:LEU:HD11	42:G:62:ARG:HD3	2.01	0.43
42:G:218:LEU:HD23	42:G:287:SER:HA	2.00	0.43
44:b:77:ILE:HB	44:b:78:PRO:HD3	2.00	0.43
1:B:77:LEU:HD13	1:B:100:SER:HA	2.00	0.43
2:C:257:PHE:HD2	2:C:347:LEU:HD11	1.83	0.43
3:D:173:MET:HA	3:D:197:PRO:HD2	2.00	0.43
6:H:106:TYR:CE2	6:H:112:ARG:HA	2.53	0.43
18:U:173:GLU:OE2	18:U:177:ARG:NH2	2.52	0.43
21:Y:89:PRO:HA	21:Y:92:TRP:CE3	2.54	0.43
29:h:17:TRP:CH2	29:h:18:MET:HE2	2.54	0.43
31:j:30:TYR:CD2	39:r:59:GLU:HB2	2.54	0.43
31:j:56:PHE:CD2	32:k:79:VAL:HG11	2.54	0.43
33:l:154:LEU:HD12	33:l:247:LEU:HD11	1.99	0.43
33:l:514:LYS:HB3	33:l:514:LYS:HE3	1.79	0.43
44:b:71:ALA:O	44:b:75:VAL:HG22	2.18	0.43
12:O:115:GLN:NE2	12:O:138:LEU:O	2.47	0.43
17:T:136:TYR:HB3	34:m:136:PHE:CZ	2.54	0.43
26:e:97:ILE:O	26:e:98:VAL:C	2.61	0.43
30:i:5:ILE:O	30:i:8:THR:OG1	2.32	0.43
33:l:90:ILE:HB	33:l:91:PRO:HD3	2.00	0.43
33:l:524:ASN:OD1	37:p:119:PRO:HB2	2.19	0.43
34:m:78:MET:HG2	34:m:79:TYR:N	2.32	0.43
3:D:88:ILE:HG22	3:D:89:HIS:O	2.19	0.42
3:D:129:VAL:HG13	3:D:144:LYS:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:158:LYS:NZ	10:L:247:ALA:O	2.52	0.42
11:N:90:LEU:O	11:N:94:MET:HG2	2.19	0.42
17:T:143:ARG:NH2	40:s:126:GLU:OE1	2.45	0.42
20:W:77:ALA:HA	20:W:80:ASP:OD2	2.18	0.42
23:a:107:PRO:HB2	23:a:112:TYR:CZ	2.54	0.42
23:a:144:ALA:HB2	25:d:82:ILE:HG12	2.00	0.42
33:l:162:THR:O	33:l:166:THR:HG23	2.19	0.42
42:G:65:TYR:HB2	42:G:92:CYS:HB2	2.01	0.42
1:B:128:ARG:NE	1:B:165:GLU:OE2	2.50	0.42
1:B:205:ILE:HG12	1:B:379:CYS:HB3	2.01	0.42
1:B:251:SER:OG	1:B:252:PRO:HD3	2.19	0.42
1:B:314:LEU:HD13	1:B:356:VAL:HG13	2.01	0.42
4:E:186:VAL:HG13	4:E:196:LEU:HD12	2.01	0.42
9:K:23:TYR:CE1	9:K:33:VAL:HB	2.54	0.42
20:W:40:ILE:O	20:W:44:LEU:HG	2.19	0.42
20:W:57:ARG:NH1	39:r:168:THR:HG22	2.34	0.42
20:W:95:ALA:HA	20:W:106:VAL:HG11	2.01	0.42
12:X:131:PRO:HG3	24:c:89:TRP:CE3	2.53	0.42
24:c:40:PRO:O	24:c:74:ASP:HB3	2.18	0.42
30:i:106:LEU:HD22	30:i:187:MET:HE2	1.99	0.42
33:l:9:LEU:HD11	33:l:63:ILE:HG21	2.00	0.42
33:l:316:THR:HG22	33:l:321:GLN:HB3	2.01	0.42
39:r:61:LEU:C	39:r:61:LEU:HD22	2.44	0.42
42:G:59:GLN:HE21	42:G:62:ARG:NH2	2.17	0.42
1:B:177:TYR:CD1	1:B:182:ILE:HG13	2.54	0.42
2:C:113:ARG:HE	2:C:113:ARG:HA	1.83	0.42
10:L:68:LEU:HA	10:L:71:MET:HE2	2.01	0.42
10:L:168:ASP:OD2	10:L:170:LYS:NZ	2.38	0.42
10:L:276:PHE:CZ	10:L:281:ARG:HD3	2.54	0.42
33:l:408:ALA:O	33:l:412:THR:HG23	2.18	0.42
39:r:185:TRP:CD1	39:r:238:THR:HG22	2.55	0.42
10:L:206:ASP:O	10:L:210:ASN:ND2	2.45	0.42
18:U:316:LEU:HB2	18:U:319:ILE:HG12	2.00	0.42
18:U:346:ASN:O	18:U:349:VAL:HG22	2.19	0.42
31:j:106:TRP:CE2	39:r:291:LYS:HD2	2.55	0.42
37:p:213:VAL:O	44:b:19:ARG:HD2	2.20	0.42
41:t:46:MET:HE3	41:t:56:ARG:HD3	2.00	0.42
1:B:384:PRO:HB2	1:B:423:THR:HG22	2.00	0.42
2:C:218:GLU:OE1	43:M:27:ARG:NH1	2.50	0.42
19:V:120:LEU:O	19:V:124:LEU:HG	2.18	0.42
24:c:117:VAL:HG22	33:l:538:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:164:ASN:HA	24:c:181:VAL:HB	2.01	0.42
25:d:82:ILE:HD12	25:d:83:LEU:HG	2.01	0.42
30:i:200:MET:SD	30:i:265:MET:HB3	2.60	0.42
31:j:49:LEU:HB3	31:j:51:PHE:CE2	2.55	0.42
31:j:63:LEU:HD23	32:k:72:ALA:HB2	2.02	0.42
32:k:22:TYR:HA	34:m:23:LYS:HE2	2.01	0.42
32:k:46:LEU:HD22	34:m:47:PHE:CG	2.54	0.42
33:l:566:THR:O	33:l:570:GLN:HG2	2.19	0.42
38:q:203:PHE:O	38:q:207:MET:HG2	2.19	0.42
42:G:534:VAL:HG23	42:G:538:ARG:HE	1.84	0.42
1:B:256:ARG:O	4:E:246:GLN:N	2.44	0.42
1:B:267:ARG:HH21	1:B:338:ASP:CG	2.27	0.42
2:C:97:ALA:HB1	2:C:101:LEU:HB3	2.01	0.42
3:D:76:VAL:HG22	3:D:86:ILE:HG23	2.01	0.42
5:F:47:ASP:OD1	5:F:47:ASP:N	2.52	0.42
10:L:187:ARG:HG2	10:L:195:ILE:HD11	2.01	0.42
18:U:256:GLU:HG3	18:U:278:LEU:HD22	2.00	0.42
23:a:144:ALA:CB	25:d:82:ILE:HG12	2.49	0.42
25:d:97:LYS:HE2	26:e:114:MET:HB2	2.01	0.42
32:k:37:MET:HE3	32:k:67:ALA:HA	2.01	0.42
32:k:75:LEU:HD11	34:m:68:PHE:CD1	2.54	0.42
33:l:141:PHE:HE2	38:q:375:LEU:HD11	1.84	0.42
38:q:115:LEU:HB2	38:q:174:LEU:HB3	2.02	0.42
39:r:238:THR:OG1	39:r:266:LEU:HD13	2.18	0.42
1:B:126:LYS:HG2	1:B:277:ASN:HD21	1.84	0.42
2:C:442:ASP:O	2:C:446:LYS:HG3	2.19	0.42
10:L:365:LYS:H	10:L:365:LYS:HD3	1.85	0.42
20:W:23:ARG:HG3	20:W:25:LEU:HD13	2.02	0.42
20:W:73:PRO:HA	40:s:121:MET:HE3	2.02	0.42
26:e:54:ARG:HH21	30:i:306:PRO:HB3	1.85	0.42
30:i:77:ASN:O	30:i:81:SER:OG	2.31	0.42
33:l:516:PRO:HB3	37:p:72:TRP:CH2	2.53	0.42
37:p:206:PRO:HG3	44:b:14:GLN:OE1	2.19	0.42
38:q:158:LEU:HB2	38:q:159:PRO:HD3	2.02	0.42
39:r:72:ILE:O	39:r:75:PRO:HD2	2.20	0.42
41:t:61:HIS:O	41:t:65:GLN:NE2	2.52	0.42
4:E:106:GLN:O	15:R:109:ARG:NH2	2.52	0.42
18:U:200:TYR:OH	18:U:306:VAL:HG13	2.19	0.42
28:g:106:LYS:HE2	28:g:106:LYS:HB3	1.90	0.42
30:i:115:VAL:HB	30:i:116:PRO:HD3	2.02	0.42
34:m:25:SER:OG	34:m:78:MET:SD	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:q:346:ARG:O	38:q:419:TYR:HA	2.20	0.42
39:r:61:LEU:HD13	39:r:61:LEU:H	1.85	0.42
43:M:25:GLN:H	43:M:25:GLN:HG2	1.59	0.42
44:b:89:HIS:NE2	44:b:96:THR:HB	2.34	0.42
1:B:321:GLY:HA2	1:B:353:ALA:HB3	2.01	0.42
2:C:387:HIS:HE1	6:H:161:ALA:O	2.03	0.42
3:D:69:LEU:HD13	3:D:96:VAL:HG22	2.01	0.42
3:D:126:PHE:HB2	3:D:147:THR:HG23	2.01	0.42
6:H:98:ARG:HB3	6:H:169:GLU:OE1	2.20	0.42
14:Q:111:LYS:O	14:Q:115:GLU:HG2	2.20	0.42
30:i:45:MET:HG3	30:i:56:ALA:HB2	2.01	0.42
31:j:95:LEU:HD11	39:r:305:ILE:HD12	2.02	0.42
34:m:51:PHE:HD2	34:m:143:ILE:HD13	1.85	0.42
37:p:161:PHE:O	37:p:165:GLU:HG2	2.20	0.42
39:r:105:MET:HE3	39:r:105:MET:HB3	1.89	0.42
41:t:111:ARG:HH12	41:t:115:ARG:NE	2.18	0.42
42:G:323:LEU:HB3	42:G:629:ILE:HD12	2.01	0.42
2:C:211:GLU:HG2	7:I:149:PRO:HG2	2.00	0.42
2:C:398:PRO:HA	2:C:399:PRO:HD3	1.97	0.42
10:L:358:THR:HB	31:j:39:CYS:O	2.19	0.42
19:V:133:TRP:HB3	30:i:277:ILE:HD11	2.01	0.42
23:a:54:LEU:HA	44:b:27:GLU:HA	2.02	0.42
33:l:124:PHE:CD2	33:l:247:LEU:HD22	2.55	0.42
33:l:366:MET:HB3	33:l:369:THR:OG1	2.20	0.42
1:B:115:VAL:HB	1:B:156:ILE:HG12	2.01	0.41
14:Q:65:TRP:O	14:Q:69:VAL:HG23	2.20	0.41
18:U:131:TYR:CG	18:U:185:CYS:HB3	2.54	0.41
23:a:179:ILE:HG23	29:h:22:SER:HB3	2.02	0.41
33:l:7:LEU:HA	33:l:10:THR:OG1	2.20	0.41
37:p:150:HIS:CD2	37:p:151:PRO:HD2	2.54	0.41
38:q:5:ILE:HG23	38:q:104:LEU:HD11	2.02	0.41
38:q:329:LEU:HD23	38:q:437:MET:HE3	2.02	0.41
39:r:61:LEU:HD13	39:r:216:ALA:CB	2.47	0.41
39:r:142:TYR:CD1	39:r:192:GLU:HB2	2.55	0.41
40:s:126:GLU:HB2	40:s:212:ARG:HH22	1.85	0.41
42:G:221:ASN:ND2	42:G:285:TRP:HB3	2.35	0.41
42:G:265:THR:HG21	42:G:609:ALA:HB1	2.02	0.41
44:b:12:LEU:C	44:b:16:ARG:HE	2.28	0.41
4:E:195:ASP:HB3	4:E:220:SER:HB3	2.02	0.41
8:J:70:GLU:OE1	14:Q:140:ARG:NH1	2.53	0.41
8:J:111:LEU:HD13	10:L:96:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:O:105:MET:HE2	12:O:112:SER:HA	2.01	0.41
12:X:97:LYS:HE3	12:X:97:LYS:HB2	1.91	0.41
24:c:184:TYR:HD2	41:t:34:ARG:HH21	1.67	0.41
30:i:59:TYR:O	30:i:63:GLN:HG2	2.20	0.41
30:i:193:VAL:HG21	30:i:266:ILE:HG12	2.01	0.41
32:k:62:ILE:HG13	34:m:157:THR:HG21	2.02	0.41
36:o:40:ARG:HD3	37:p:194:GLU:OE2	2.20	0.41
36:o:112:LYS:NZ	38:q:388:TRP:O	2.51	0.41
36:o:114:LYS:O	36:o:118:GLU:HG2	2.20	0.41
38:q:348:LEU:HD12	38:q:415:GLN:HE22	1.85	0.41
42:G:36:VAL:HB	42:G:56:VAL:HG11	2.01	0.41
42:G:662:ALA:HB1	42:G:664:TYR:CE2	2.54	0.41
2:C:193:VAL:HG11	2:C:264:LEU:HD21	2.03	0.41
8:J:84:ARG:NH1	8:J:88:GLN:O	2.52	0.41
10:L:206:ASP:OD1	10:L:207:ARG:N	2.53	0.41
26:e:150:PRO:HG2	28:g:115:LEU:HD22	2.01	0.41
30:i:117:GLU:HG2	32:k:97:GLN:O	2.19	0.41
30:i:326:LEU:HB3	30:i:327:PRO:HD3	2.03	0.41
31:j:112:GLU:O	31:j:113:TRP:C	2.63	0.41
38:q:303:ILE:HG22	38:q:305:THR:HG23	2.02	0.41
39:r:222:MET:HE3	39:r:222:MET:HB2	1.92	0.41
39:r:286:MET:HE2	39:r:290:TRP:HE1	1.85	0.41
42:G:422:TRP:CE3	42:G:440:TYR:HB2	2.56	0.41
42:G:572:HIS:CE1	42:G:700:ILE:HG12	2.55	0.41
42:G:695:TYR:HE2	42:G:714:VAL:HG11	1.85	0.41
44:b:50:PHE:HD1	44:b:50:PHE:HA	1.71	0.41
2:C:190:ILE:HD11	2:C:257:PHE:CZ	2.56	0.41
2:C:448:HIS:HB3	2:C:452:ASP:HB2	2.02	0.41
3:D:77:GLN:HE21	43:M:68:ILE:HG12	1.85	0.41
3:D:114:LEU:HD13	3:D:130:TYR:CD2	2.56	0.41
18:U:141:ARG:HH12	18:U:171:PHE:HE2	1.66	0.41
18:U:309:TYR:O	18:U:312:ILE:HG13	2.21	0.41
24:c:143:MET:HB3	33:l:407:TRP:CE2	2.55	0.41
28:g:4:MET:H	28:g:4:MET:HG2	1.61	0.41
30:i:323:MET:H	30:i:323:MET:HG2	1.61	0.41
33:l:80:PHE:HB3	33:l:82:MET:HE2	2.03	0.41
33:l:241:THR:HG22	33:l:299:LYS:HD2	2.02	0.41
33:l:556:ILE:HG22	33:l:557:TRP:N	2.35	0.41
36:o:5:LYS:HB2	36:o:5:LYS:HE2	1.80	0.41
38:q:109:THR:HG22	38:q:121:LEU:HB2	2.02	0.41
38:q:457:PRO:HG2	38:q:458:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:t:20:LEU:HB2	41:t:21:ARG:HH12	1.85	0.41
42:G:306:MET:HE2	42:G:316:TYR:CE1	2.55	0.41
3:D:61:PHE:CZ	43:M:97:PRO:HG3	2.55	0.41
10:L:191:PRO:HG2	10:L:192:GLU:OE1	2.20	0.41
14:Q:43:VAL:HG11	14:Q:103:ARG:HH11	1.86	0.41
16:S:4:GLU:O	16:S:7:PRO:HD2	2.20	0.41
18:U:40:TYR:HB3	18:U:301:GLN:NE2	2.34	0.41
24:c:126:TRP:CH2	33:l:532:ILE:HA	2.55	0.41
30:i:95:MET:HE2	30:i:149:ILE:HA	2.03	0.41
30:i:139:LEU:HD23	30:i:139:LEU:HA	1.79	0.41
31:j:87:MET:HE3	31:j:87:MET:HB3	1.93	0.41
33:l:27:TYR:O	33:l:115:ASN:ND2	2.46	0.41
33:l:338:MET:HB2	33:l:457:LEU:HB3	2.03	0.41
36:o:14:LEU:HD12	36:o:15:PRO:HD2	2.02	0.41
38:q:201:MET:HE1	38:q:212:LEU:HD11	2.03	0.41
38:q:221:VAL:HA	38:q:283:LYS:HD3	2.02	0.41
41:t:114:ARG:HB3	41:t:118:ARG:NH1	2.35	0.41
42:G:68:ARG:HH21	42:G:277:MET:HE2	1.84	0.41
42:G:560:LEU:HD13	42:G:564:CYS:SG	2.60	0.41
4:E:55:PHE:CZ	4:E:86:ALA:HB2	2.56	0.41
4:E:132:ILE:HD11	4:E:169:PHE:CD1	2.55	0.41
10:L:32:HIS:HD1	10:L:33:HIS:H	1.69	0.41
12:O:85:TYR:HA	12:O:88:LYS:HD2	2.03	0.41
28:g:51:ARG:HD3	30:i:322:GLN:HG2	2.02	0.41
37:p:68:HIS:CE1	37:p:117:GLN:HG3	2.56	0.41
39:r:68:ILE:HG23	39:r:69:SER:H	1.85	0.41
42:G:519:ILE:HG22	42:G:522:GLN:H	1.86	0.41
42:G:692:LYS:HD3	42:G:715:THR:HG22	2.03	0.41
1:B:248:VAL:O	1:B:251:SER:OG	2.30	0.41
1:B:292:MET:HE3	1:B:292:MET:HB3	1.98	0.41
2:C:267:MET:HE3	2:C:267:MET:HB3	1.88	0.41
6:H:176:SER:HA	7:I:231:PRO:HD3	2.02	0.41
8:J:98:LYS:HG2	8:J:127:THR:HG22	2.03	0.41
9:K:49:TYR:HB2	9:K:61:TRP:CE2	2.55	0.41
10:L:59:PHE:HB3	48:L:401:NDP:O2N	2.20	0.41
23:a:53:ARG:NH2	44:b:29:SER:O	2.54	0.41
25:d:102:ILE:O	25:d:106:ILE:HG12	2.21	0.41
26:e:146:LYS:HB2	26:e:146:LYS:NZ	2.36	0.41
33:l:568:PHE:O	33:l:572:LYS:HG2	2.21	0.41
36:o:59:VAL:HG22	38:q:423:ILE:HG12	2.02	0.41
40:s:83:GLU:CD	40:s:83:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:M:93:LYS:HB3	43:M:93:LYS:HE2	1.83	0.41
1:B:340:ASP:O	1:B:344:GLN:HG2	2.20	0.41
4:E:227:PRO:HG2	4:E:232:THR:H	1.85	0.41
6:H:89:GLU:OE2	9:K:34:ARG:NH2	2.45	0.41
12:O:118:ILE:O	12:O:122:MET:HG2	2.21	0.41
17:T:154:HIS:CD2	17:T:157:ASP:HB2	2.55	0.41
25:d:30:VAL:HG13	33:l:53:MET:HG2	2.03	0.41
28:g:84:MET:HB3	30:i:344:SER:HB3	2.03	0.41
34:m:164:GLY:O	34:m:168:ILE:HG12	2.21	0.41
35:n:40:ASN:HD21	35:n:56:THR:HG21	1.85	0.41
38:q:14:MET:HE2	38:q:14:MET:HB3	1.93	0.41
39:r:2:PHE:CE2	39:r:6:ILE:HD11	2.56	0.41
42:G:555:ILE:HG23	42:G:559:ASP:HB2	2.03	0.41
1:B:162:PHE:HE1	4:E:177:LEU:O	2.04	0.41
1:B:355:ILE:HD13	4:E:139:PRO:HG3	2.03	0.41
2:C:58:MET:HG2	30:i:295:ARG:NH1	2.36	0.41
2:C:239:HIS:HA	2:C:363:LYS:HE3	2.02	0.41
2:C:386:HIS:NE2	42:G:149:ASP:HA	2.36	0.41
4:E:110:MET:O	4:E:114:GLU:HG3	2.21	0.41
6:H:51:LYS:HG2	20:W:33:TYR:HE2	1.85	0.41
6:H:201:ILE:O	6:H:205:ILE:HG12	2.20	0.41
7:I:129:LEU:O	7:I:158:VAL:HA	2.21	0.41
10:L:202:PHE:CD2	10:L:234:PRO:HB2	2.56	0.41
12:O:116:VAL:HG12	12:O:120:MET:HE2	2.03	0.41
13:P:23:LEU:HD23	13:P:23:LEU:H	1.85	0.41
18:U:297:ARG:HG2	18:U:301:GLN:NE2	2.36	0.41
21:Y:51:THR:HG23	21:Y:54:GLN:H	1.85	0.41
24:c:90:TYR:HE2	24:c:100:ASN:HD21	1.68	0.41
29:h:43:CYS:HA	40:s:224:ARG:HD2	2.03	0.41
30:i:28:LEU:HD23	30:i:28:LEU:HA	1.80	0.41
30:i:61:LEU:O	30:i:65:THR:HG23	2.21	0.41
30:i:145:ILE:O	30:i:149:ILE:HG13	2.20	0.41
30:i:153:LEU:HD11	30:i:157:MET:HE3	2.02	0.41
31:j:111:LEU:HA	31:j:113:TRP:CE2	2.55	0.41
33:l:4:PHE:HD2	33:l:61:MET:HE2	1.85	0.41
38:q:73:LEU:HD22	38:q:103:GLN:OE1	2.20	0.41
40:s:157:GLU:O	40:s:160:THR:OG1	2.34	0.41
41:t:48:ASP:HB3	44:b:104:ILE:HB	2.03	0.41
1:B:214:GLU:OE1	1:B:219:LYS:HD2	2.21	0.41
2:C:284:VAL:HG22	2:C:444:MET:HG2	2.03	0.41
12:X:76:LEU:HD13	12:X:76:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:k:22:TYR:O	33:l:585:LYS:HE3	2.21	0.41
33:l:356:ILE:HG22	33:l:359:MET:HE2	2.02	0.41
34:m:133:SER:O	34:m:136:PHE:HB2	2.19	0.41
40:s:192:LEU:HD13	40:s:194:TRP:CH2	2.56	0.41
42:G:347:ASP:HB2	42:G:594:ALA:HB1	2.03	0.41
1:B:417:LYS:HD3	1:B:417:LYS:HA	1.85	0.40
3:D:191:TYR:HB2	14:Q:128:HIS:CD2	2.56	0.40
5:F:31:THR:HA	5:F:37:LYS:HA	2.03	0.40
30:i:261:MET:SD	30:i:336:VAL:HG13	2.61	0.40
32:k:95:LEU:H	32:k:95:LEU:HG	1.70	0.40
33:l:217:LEU:HD12	33:l:276:MET:HE3	2.02	0.40
33:l:448:PRO:O	33:l:452:ASN:ND2	2.53	0.40
38:q:225:ILE:HD13	38:q:331:ASN:HB2	2.03	0.40
39:r:67:SER:OG	39:r:69:SER:OG	2.38	0.40
41:t:5:LEU:H	41:t:5:LEU:HD12	1.87	0.40
1:B:162:PHE:HB3	1:B:165:GLU:HB2	2.02	0.40
12:O:136:GLU:OE2	14:Q:59:ARG:NH1	2.54	0.40
14:Q:123:TRP:O	14:Q:125:GLN:NE2	2.54	0.40
12:X:119:ILE:HD13	12:X:119:ILE:HA	1.96	0.40
23:a:84:ILE:O	23:a:88:LEU:HG	2.21	0.40
33:l:241:THR:OG1	33:l:242:PRO:HD3	2.21	0.40
34:m:94:VAL:O	34:m:98:MET:HG2	2.21	0.40
36:o:28:GLU:HG2	36:o:29:THR:N	2.36	0.40
36:o:89:LEU:HA	36:o:92:LEU:HG	2.03	0.40
38:q:442:LEU:HB2	38:q:443:PRO:HD3	2.03	0.40
44:b:86:LEU:O	44:b:90:VAL:HG12	2.21	0.40
1:B:36:LYS:O	1:B:40:ARG:HG3	2.21	0.40
3:D:121:THR:HG21	11:N:116:ILE:HG21	2.03	0.40
4:E:141:MET:HE2	4:E:141:MET:HB3	1.89	0.40
6:H:140:ARG:HG2	42:G:238:PHE:CD1	2.55	0.40
7:I:131:PRO:HG2	7:I:160:PHE:CD1	2.57	0.40
7:I:174:GLY:HA2	46:I:301:SF4:S3	2.61	0.40
7:I:188:TYR:CE1	7:I:195:ARG:HD2	2.56	0.40
10:L:163:SER:N	10:L:196:ILE:O	2.49	0.40
17:T:136:TYR:O	20:W:68:ARG:NH1	2.55	0.40
12:X:133:ILE:HG12	12:X:134:ASP:N	2.36	0.40
28:g:5:SER:HA	28:g:10:ARG:NH1	2.37	0.40
30:i:154:MET:SD	30:i:191:THR:HB	2.62	0.40
30:i:230:LEU:O	30:i:233:THR:OG1	2.32	0.40
34:m:70:TYR:O	34:m:74:MET:HG2	2.21	0.40
36:o:31:LYS:NZ	36:o:31:LYS:HB3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:q:444:LEU:O	38:q:448:THR:HG23	2.21	0.40
42:G:373:PRO:HD3	42:G:481:LEU:HB3	2.02	0.40
10:L:59:PHE:CZ	10:L:206:ASP:HB2	2.57	0.40
10:L:352:ARG:CB	10:L:357:LEU:HD12	2.51	0.40
16:S:41:PHE:HB3	34:m:134:GLY:O	2.22	0.40
17:T:145:ASP:OD1	17:T:148:MET:HG3	2.21	0.40
12:X:88:LYS:HB3	22:Z:35:TYR:CD2	2.56	0.40
24:c:99:LEU:HD23	24:c:99:LEU:HA	1.90	0.40
28:g:97:LYS:HE2	28:g:97:LYS:HB3	1.79	0.40
30:i:89:MET:HE3	30:i:89:MET:HB3	2.02	0.40
31:j:94:LEU:HD23	31:j:94:LEU:HA	1.83	0.40
33:l:13:ILE:O	33:l:16:THR:OG1	2.34	0.40
38:q:29:VAL:O	38:q:33:LEU:HG	2.22	0.40
38:q:157:SER:O	38:q:160:LEU:HB3	2.22	0.40
38:q:318:ALA:HB1	38:q:374:ASN:CG	2.46	0.40
40:s:145:LEU:O	40:s:149:ARG:HG3	2.21	0.40
1:B:384:PRO:HD2	42:G:76:ARG:HG3	2.04	0.40
2:C:469:ARG:NH1	3:D:169:GLU:OE2	2.54	0.40
9:K:50:GLU:HB2	9:K:89:TRP:CZ2	2.56	0.40
10:L:241:SER:O	10:L:245:ILE:HG12	2.22	0.40
18:U:354:ILE:HA	18:U:357:LYS:HB2	2.04	0.40
12:X:88:LYS:O	22:Z:63:ARG:NH2	2.55	0.40
21:Y:46:GLN:HG2	21:Y:47:PHE:N	2.36	0.40
21:Y:99:ILE:HG12	41:t:107:ARG:HB2	2.04	0.40
27:f:51:SER:HB2	28:g:68:THR:HG21	2.03	0.40
33:l:7:LEU:O	33:l:11:THR:HG23	2.22	0.40
33:l:137:LEU:HD23	33:l:137:LEU:HA	1.85	0.40
33:l:232:TRP:HZ3	33:l:248:HIS:CD2	2.39	0.40
34:m:34:ILE:HD13	34:m:65:LEU:HD12	2.03	0.40
35:n:48:GLU:OE1	35:n:48:GLU:N	2.49	0.40
38:q:208:PRO:HD3	38:q:236:LEU:HD22	2.04	0.40
41:t:52:MET:O	41:t:56:ARG:HG3	2.22	0.40
42:G:405:THR:HB	42:G:477:GLY:HA3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	427/464 (92%)	414 (97%)	13 (3%)	0	100	100
2	C	428/469 (91%)	417 (97%)	11 (3%)	0	100	100
3	D	206/264 (78%)	200 (97%)	6 (3%)	0	100	100
4	E	212/249 (85%)	204 (96%)	7 (3%)	1 (0%)	24	59
5	F	91/123 (74%)	90 (99%)	1 (1%)	0	100	100
6	H	174/212 (82%)	172 (99%)	2 (1%)	0	100	100
7	I	154/196 (79%)	149 (97%)	5 (3%)	0	100	100
8	J	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
9	K	142/145 (98%)	141 (99%)	1 (1%)	0	100	100
10	L	324/372 (87%)	312 (96%)	12 (4%)	0	100	100
11	N	110/116 (95%)	109 (99%)	1 (1%)	0	100	100
12	O	81/156 (52%)	80 (99%)	1 (1%)	0	100	100
12	X	83/156 (53%)	83 (100%)	0	0	100	100
13	P	81/99 (82%)	79 (98%)	2 (2%)	0	100	100
14	Q	110/154 (71%)	106 (96%)	3 (3%)	1 (1%)	14	47
15	R	33/110 (30%)	32 (97%)	1 (3%)	0	100	100
16	S	68/70 (97%)	68 (100%)	0	0	100	100
17	T	80/169 (47%)	78 (98%)	2 (2%)	0	100	100
18	U	316/357 (88%)	311 (98%)	4 (1%)	1 (0%)	36	68
19	V	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
20	W	138/144 (96%)	137 (99%)	1 (1%)	0	100	100
21	Y	64/105 (61%)	61 (95%)	3 (5%)	0	100	100
22	Z	75/114 (66%)	75 (100%)	0	0	100	100
23	a	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
24	c	151/186 (81%)	147 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	d	167/176 (95%)	167 (100%)	0	0	100	100
26	e	97/154 (63%)	90 (93%)	6 (6%)	1 (1%)	12	45
27	f	44/76 (58%)	43 (98%)	1 (2%)	0	100	100
28	g	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
29	h	103/106 (97%)	99 (96%)	4 (4%)	0	100	100
30	i	345/347 (99%)	334 (97%)	11 (3%)	0	100	100
31	j	102/115 (89%)	96 (94%)	5 (5%)	1 (1%)	12	45
32	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
33	l	601/606 (99%)	574 (96%)	26 (4%)	1 (0%)	43	73
34	m	171/175 (98%)	159 (93%)	12 (7%)	0	100	100
35	n	54/58 (93%)	52 (96%)	2 (4%)	0	100	100
36	o	124/129 (96%)	121 (98%)	3 (2%)	0	100	100
37	p	175/221 (79%)	173 (99%)	2 (1%)	0	100	100
38	q	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
39	r	305/318 (96%)	294 (96%)	10 (3%)	1 (0%)	36	68
40	s	169/249 (68%)	162 (96%)	7 (4%)	0	100	100
41	t	115/137 (84%)	115 (100%)	0	0	100	100
42	G	680/727 (94%)	666 (98%)	14 (2%)	0	100	100
43	M	92/113 (81%)	90 (98%)	2 (2%)	0	100	100
44	b	107/128 (84%)	96 (90%)	11 (10%)	0	100	100
All	All	8061/9449 (85%)	7842 (97%)	212 (3%)	7 (0%)	49	79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	j	34	THR
33	l	562	LEU
39	r	92	PRO
4	E	183	ALA
18	U	59	SER
26	e	97	ILE
14	Q	122	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	B	343/368 (93%)	339 (99%)	4 (1%)	63	79
2	C	370/398 (93%)	361 (98%)	9 (2%)	43	70
3	D	190/228 (83%)	187 (98%)	3 (2%)	55	75
4	E	183/207 (88%)	173 (94%)	10 (6%)	19	52
5	F	77/97 (79%)	72 (94%)	5 (6%)	15	47
6	H	151/176 (86%)	144 (95%)	7 (5%)	24	58
7	I	132/163 (81%)	128 (97%)	4 (3%)	36	66
8	J	107/152 (70%)	105 (98%)	2 (2%)	50	73
9	K	130/131 (99%)	128 (98%)	2 (2%)	57	76
10	L	283/320 (88%)	262 (93%)	21 (7%)	13	43
11	N	99/101 (98%)	98 (99%)	1 (1%)	68	80
12	O	77/132 (58%)	77 (100%)	0	100	100
12	X	79/132 (60%)	71 (90%)	8 (10%)	7	30
13	P	74/82 (90%)	72 (97%)	2 (3%)	39	68
14	Q	105/134 (78%)	103 (98%)	2 (2%)	50	73
15	R	34/92 (37%)	33 (97%)	1 (3%)	37	67
16	S	58/58 (100%)	53 (91%)	5 (9%)	10	36
17	T	69/134 (52%)	65 (94%)	4 (6%)	18	51
18	U	281/307 (92%)	275 (98%)	6 (2%)	47	71
19	V	101/102 (99%)	99 (98%)	2 (2%)	48	72
20	W	122/124 (98%)	120 (98%)	2 (2%)	55	75
21	Y	60/84 (71%)	58 (97%)	2 (3%)	33	65
22	Z	59/90 (66%)	57 (97%)	2 (3%)	32	64
23	a	121/158 (77%)	120 (99%)	1 (1%)	73	82
24	c	138/160 (86%)	138 (100%)	0	100	100
25	d	153/156 (98%)	143 (94%)	10 (6%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	e	91/129 (70%)	84 (92%)	7 (8%)	12	41
27	f	42/66 (64%)	41 (98%)	1 (2%)	43	70
28	g	108/109 (99%)	101 (94%)	7 (6%)	15	47
29	h	93/94 (99%)	90 (97%)	3 (3%)	34	65
30	i	311/311 (100%)	293 (94%)	18 (6%)	18	51
31	j	93/100 (93%)	85 (91%)	8 (9%)	10	36
32	k	85/85 (100%)	79 (93%)	6 (7%)	13	44
33	l	537/540 (99%)	506 (94%)	31 (6%)	18	51
34	m	139/141 (99%)	124 (89%)	15 (11%)	6	27
35	n	53/55 (96%)	50 (94%)	3 (6%)	18	51
36	o	110/114 (96%)	103 (94%)	7 (6%)	16	48
37	p	159/190 (84%)	152 (96%)	7 (4%)	25	59
38	q	409/409 (100%)	393 (96%)	16 (4%)	28	62
39	r	267/275 (97%)	247 (92%)	20 (8%)	12	42
40	s	153/206 (74%)	148 (97%)	5 (3%)	33	65
41	t	108/120 (90%)	101 (94%)	7 (6%)	15	47
42	G	576/610 (94%)	569 (99%)	7 (1%)	63	79
43	M	86/98 (88%)	86 (100%)	0	100	100
44	b	104/121 (86%)	98 (94%)	6 (6%)	18	51
All	All	7120/8059 (88%)	6831 (96%)	289 (4%)	28	60

All (289) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	102	MET
1	B	125	CYS
1	B	282	VAL
1	B	382	CYS
2	C	62	LYS
2	C	82	LEU
2	C	100	VAL
2	C	204	THR
2	C	210	PHE
2	C	211	GLU
2	C	218	GLU

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Mol	Chain	Res	Type
2	C	365	ASP
2	C	417	LEU
3	D	44	ARG
3	D	47	ILE
3	D	148	ASP
4	E	85	LEU
4	E	90	ASN
4	E	95	ILE
4	E	174	VAL
4	E	180	CYS
4	E	197	THR
4	E	201	ILE
4	E	209	LYS
4	E	215	LYS
4	E	226	GLU
5	F	71	ILE
5	F	74	GLN
5	F	79	VAL
5	F	84	ILE
5	F	114	CYS
6	H	73	THR
6	H	103	LEU
6	H	114	ILE
6	H	147	ILE
6	H	177	THR
6	H	183	LEU
6	H	188	GLU
7	I	138	CYS
7	I	158	VAL
7	I	160	PHE
7	I	209	TYR
8	J	61	ILE
8	J	86	ASN
9	K	59	HIS
9	K	125	VAL
10	L	32	HIS
10	L	50	VAL
10	L	101	MET
10	L	113	LYS
10	L	165	LEU
10	L	170	LYS
10	L	205	GLU

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Mol	Chain	Res	Type
10	L	206	ASP
10	L	215	MET
10	L	216	ARG
10	L	267	LEU
10	L	281	ARG
10	L	305	PHE
10	L	323	THR
10	L	335	ILE
10	L	350	ARG
10	L	352	ARG
10	L	355	ARG
10	L	356	TRP
10	L	357	LEU
10	L	365	LYS
11	N	5	LEU
13	P	42	VAL
13	P	44	LEU
14	Q	71	ASN
14	Q	127	THR
15	R	105	ARG
16	S	53	CYS
16	S	61	HIS
16	S	62	VAL
16	S	64	LYS
16	S	69	ILE
17	T	89	ARG
17	T	98	TRP
17	T	142	LEU
17	T	166	LEU
18	U	43	LEU
18	U	100	THR
18	U	172	LEU
18	U	232	THR
18	U	287	ASP
18	U	349	VAL
19	V	88	LEU
19	V	115	CYS
20	W	99	LYS
20	W	110	VAL
12	X	76	LEU
12	X	84	LEU
12	X	89	LEU

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Mol	Chain	Res	Type
12	X	96	GLU
12	X	98	LEU
12	X	124	ASP
12	X	133	ILE
12	X	138	LEU
21	Y	97	LEU
21	Y	100	LEU
22	Z	59	ASP
22	Z	75	ASN
23	a	184	LYS
25	d	7	LYS
25	d	8	ASP
25	d	17	THR
25	d	49	ARG
25	d	50	GLU
25	d	79	GLU
25	d	82	ILE
25	d	129	LEU
25	d	137	LYS
25	d	156	LEU
26	e	63	ASP
26	e	64	GLU
26	e	87	MET
26	e	89	VAL
26	e	98	VAL
26	e	101	LEU
26	e	146	LYS
27	f	31	ILE
28	g	2	THR
28	g	4	MET
28	g	16	LEU
28	g	29	THR
28	g	64	LEU
28	g	84	MET
28	g	101	GLU
29	h	18	MET
29	h	74	LYS
29	h	86	LEU
30	i	19	LEU
30	i	22	ILE
30	i	29	ILE
30	i	36	ASN

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Mol	Chain	Res	Type
30	i	125	GLN
30	i	193	VAL
30	i	204	ASN
30	i	245	MET
30	i	290	LEU
30	i	296	LEU
30	i	303	THR
30	i	311	MET
30	i	321	LYS
30	i	324	LYS
30	i	336	VAL
30	i	339	MET
30	i	343	LEU
30	i	344	SER
31	j	1	MET
31	j	5	LEU
31	j	18	VAL
31	j	19	LEU
31	j	49	LEU
31	j	51	PHE
31	j	57	LEU
31	j	69	ILE
32	k	3	LEU
32	k	43	MET
32	k	50	ASN
32	k	59	MET
32	k	73	LEU
32	k	81	VAL
33	l	1	MET
33	l	36	VAL
33	l	46	LEU
33	l	59	GLN
33	l	62	ILE
33	l	70	THR
33	l	169	LEU
33	l	217	LEU
33	l	233	LEU
33	l	238	GLU
33	l	246	LEU
33	l	247	LEU
33	l	251	THR
33	l	254	VAL

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Mol	Chain	Res	Type
33	l	314	MET
33	l	324	LEU
33	l	373	LEU
33	l	383	MET
33	l	407	TRP
33	l	411	MET
33	l	434	LYS
33	l	436	ARG
33	l	440	LEU
33	l	480	THR
33	l	481	THR
33	l	487	LYS
33	l	502	LEU
33	l	512	LYS
33	l	515	TYR
33	l	532	ILE
33	l	589	LEU
34	m	27	ILE
34	m	33	LEU
34	m	45	LEU
34	m	55	MET
34	m	58	LEU
34	m	64	MET
34	m	66	VAL
34	m	71	THR
34	m	74	MET
34	m	78	MET
34	m	81	GLU
34	m	82	VAL
34	m	86	ASN
34	m	109	LYS
34	m	113	VAL
35	n	9	ARG
35	n	17	VAL
35	n	54	GLU
36	o	5	LYS
36	o	7	LYS
36	o	31	LYS
36	o	44	LYS
36	o	57	LEU
36	o	93	PHE
36	o	95	ILE

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Mol	Chain	Res	Type
37	p	60	ARG
37	p	86	MET
37	p	101	LYS
37	p	106	LEU
37	p	192	ARG
37	p	201	LYS
37	p	219	ARG
38	q	61	LEU
38	q	86	LYS
38	q	92	LYS
38	q	115	LEU
38	q	122	PHE
38	q	179	ILE
38	q	180	HIS
38	q	230	VAL
38	q	270	ILE
38	q	282	LEU
38	q	315	LEU
38	q	325	MET
38	q	375	LEU
38	q	418	LYS
38	q	452	LYS
38	q	454	ILE
39	r	5	ASN
39	r	33	LEU
39	r	61	LEU
39	r	65	THR
39	r	68	ILE
39	r	91	MET
39	r	102	VAL
39	r	108	MET
39	r	111	LEU
39	r	133	LEU
39	r	140	ILE
39	r	142	TYR
39	r	146	LEU
39	r	195	ARG
39	r	212	ASN
39	r	223	PHE
39	r	227	GLU
39	r	253	GLU
39	r	270	PHE

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Mol	Chain	Res	Type
39	r	285	LEU
40	s	93	GLN
40	s	175	ARG
40	s	188	VAL
40	s	191	LYS
40	s	232	GLU
41	t	15	LYS
41	t	21	ARG
41	t	33	GLU
41	t	39	MET
41	t	51	LEU
41	t	106	ARG
41	t	108	LEU
42	G	41	VAL
42	G	163	LYS
42	G	358	LEU
42	G	387	LEU
42	G	427	LEU
42	G	559	ASP
42	G	611	THR
44	b	23	LEU
44	b	50	PHE
44	b	51	LEU
44	b	86	LEU
44	b	96	THR
44	b	111	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (138) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	220	GLN
1	B	244	ASN
1	B	281	HIS
1	B	313	ASN
2	C	42	GLN
2	C	85	ASN
2	C	89	ASN
2	C	93	GLN
2	C	153	ASN
2	C	166	ASN
2	C	174	GLN
2	C	196	HIS

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Mol	Chain	Res	Type
2	C	229	HIS
2	C	239	HIS
2	C	240	GLN
2	C	270	ASN
2	C	271	ASN
2	C	387	HIS
3	D	77	GLN
3	D	107	GLN
3	D	124	ASN
3	D	181	HIS
3	D	196	HIS
4	E	41	HIS
4	E	87	GLN
4	E	99	ASN
4	E	123	ASN
4	E	133	GLN
4	E	153	GLN
5	F	63	ASN
5	F	74	GLN
5	F	101	ASN
6	H	159	GLN
6	H	192	ASN
7	I	145	HIS
8	J	88	GLN
8	J	92	ASN
8	J	109	ASN
9	K	123	GLN
10	L	74	GLN
11	N	50	GLN
11	N	86	ASN
11	N	110	ASN
11	N	111	GLN
13	P	22	HIS
13	P	76	ASN
14	Q	77	GLN
14	Q	121	ASN
16	S	40	HIS
17	T	147	ASN
18	U	188	HIS
18	U	301	GLN
18	U	302	ASN
18	U	325	GLN

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Mol	Chain	Res	Type
20	W	61	GLN
20	W	76	GLN
20	W	112	HIS
12	X	115	GLN
21	Y	46	GLN
21	Y	54	GLN
21	Y	57	GLN
23	a	170	GLN
23	a	189	ASN
24	c	83	GLN
24	c	132	HIS
24	c	154	GLN
24	c	183	HIS
25	d	55	GLN
25	d	161	GLN
26	e	74	HIS
26	e	86	ASN
26	e	115	GLN
27	f	36	HIS
28	g	81	GLN
29	h	21	GLN
30	i	171	ASN
30	i	204	ASN
30	i	289	ASN
30	i	322	GLN
30	i	347	ASN
31	j	26	GLN
32	k	7	ASN
32	k	25	HIS
32	k	52	HIS
33	l	2	ASN
33	l	72	GLN
33	l	170	GLN
33	l	205	ASN
33	l	206	ASN
33	l	354	GLN
33	l	452	ASN
33	l	470	ASN
33	l	505	ASN
33	l	518	GLN
33	l	580	GLN
34	m	86	ASN

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Mol	Chain	Res	Type
35	n	3	ASN
35	n	40	ASN
36	o	126	ASN
37	p	75	HIS
37	p	93	HIS
37	p	108	GLN
37	p	211	HIS
38	q	30	HIS
38	q	51	ASN
38	q	81	GLN
38	q	180	HIS
38	q	184	HIS
38	q	279	GLN
38	q	366	ASN
38	q	374	ASN
38	q	415	GLN
38	q	434	ASN
38	q	440	HIS
38	q	450	ASN
39	r	38	ASN
39	r	138	GLN
39	r	169	GLN
39	r	194	ASN
39	r	212	ASN
39	r	230	ASN
39	r	304	HIS
40	s	150	GLN
40	s	220	HIS
41	t	44	GLN
41	t	47	ASN
41	t	65	GLN
41	t	92	HIS
42	G	74	ASN
42	G	142	GLN
42	G	278	HIS
42	G	453	GLN
42	G	569	GLN
42	G	669	ASN
42	G	688	GLN
43	M	110	GLN
44	b	83	HIS
44	b	126	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

11 ligands 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	$\# Z  > 2$
46	SF4	H	301	6	0,12,12	-	-	-		
46	SF4	B	502	1	0,12,12	-	-	-		
46	SF4	H	302	6	0,12,12	-	-	-		
45	FMN	B	501	-	33,33,33	1.02	2 (6%)	48,50,50	1.21	8 (16%)
46	SF4	G	802	42	0,12,12	-	-	-		
49	ZMP	Q	201	-	27,29,36	1.72	4 (14%)	34,38,45	1.67	5 (14%)
47	FES	G	803	42	0,4,4	-	-	-		
48	NDP	L	401	-	51,52,52	0.49	0	71,80,80	0.80	1 (1%)
46	SF4	G	801	42	0,12,12	-	-	-		
47	FES	E	301	4	0,4,4	-	-	-		
46	SF4	I	301	7	0,12,12	-	-	-		

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
47	FES	E	301	4	-	-	0/1/1/1
46	SF4	H	301	6	-	-	0/6/5/5
46	SF4	B	502	1	-	-	0/6/5/5
46	SF4	H	302	6	-	-	0/6/5/5
45	FMN	B	501	-	-	7/18/18/18	0/3/3/3
46	SF4	G	802	42	-	-	0/6/5/5
49	ZMP	Q	201	-	-	9/36/36/43	-
47	FES	G	803	42	-	-	0/1/1/1
46	SF4	G	801	42	-	-	0/6/5/5
48	NDP	L	401	-	-	7/34/77/77	0/5/5/5
46	SF4	I	301	7	-	-	0/6/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	Q	201	ZMP	C13-N1	5.39	1.46	1.33
49	Q	201	ZMP	C16-N2	4.92	1.45	1.33
45	B	501	FMN	C4A-N5	3.30	1.37	1.30
45	B	501	FMN	C10-N1	2.33	1.37	1.33
49	Q	201	ZMP	C10-S1	2.31	1.81	1.76
49	Q	201	ZMP	O3-C16	-2.16	1.19	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	Q	201	ZMP	C9-C10-S1	5.46	119.91	113.40
48	L	401	NDP	P2B-O2B-C2B	-5.39	109.03	123.43
49	Q	201	ZMP	O1-C10-C9	-3.57	119.86	123.98
45	B	501	FMN	C4-N3-C2	-3.29	119.79	125.64
45	B	501	FMN	O4-C4-C4A	-2.64	119.55	126.53
45	B	501	FMN	C4A-C4-N3	2.60	119.87	113.25
49	Q	201	ZMP	C14-C15-N2	-2.56	106.55	112.00
49	Q	201	ZMP	C11-S1-C10	2.55	109.39	101.84
45	B	501	FMN	C4A-C10-N10	2.47	120.01	116.48
49	Q	201	ZMP	O3-C16-N2	-2.37	117.97	122.98
45	B	501	FMN	C4'-C3'-C2'	-2.32	109.71	113.57
45	B	501	FMN	C10-C4A-N5	-2.16	120.39	124.81
45	B	501	FMN	C5A-C9A-N10	2.09	119.86	117.97
45	B	501	FMN	C9A-C5A-N5	-2.01	120.32	122.45

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	B	501	FMN	N10-C1'-C2'-O2'
45	B	501	FMN	C3'-C4'-C5'-O5'
45	B	501	FMN	O4'-C4'-C5'-O5'
45	B	501	FMN	C5'-O5'-P-O2P
45	B	501	FMN	C5'-O5'-P-O3P
48	L	401	NDP	C5D-O5D-PN-O1N
49	Q	201	ZMP	C17-C16-N2-C15
49	Q	201	ZMP	S1-C11-C12-N1
49	Q	201	ZMP	C9-C10-S1-C11
49	Q	201	ZMP	O3-C16-N2-C15
48	L	401	NDP	C2D-C1D-N1N-C6N
48	L	401	NDP	C2D-C1D-N1N-C2N
45	B	501	FMN	C5'-O5'-P-O1P
48	L	401	NDP	C4B-C5B-O5B-PA
49	Q	201	ZMP	N2-C16-C17-C18
49	Q	201	ZMP	O1-C10-S1-C11
48	L	401	NDP	O4D-C1D-N1N-C6N
48	L	401	NDP	O4D-C4D-C5D-O5D
49	Q	201	ZMP	O3-C16-C17-O4
48	L	401	NDP	O4D-C1D-N1N-C2N
49	Q	201	ZMP	O3-C16-C17-C18
49	Q	201	ZMP	N2-C16-C17-O4
45	B	501	FMN	N10-C1'-C2'-C3'

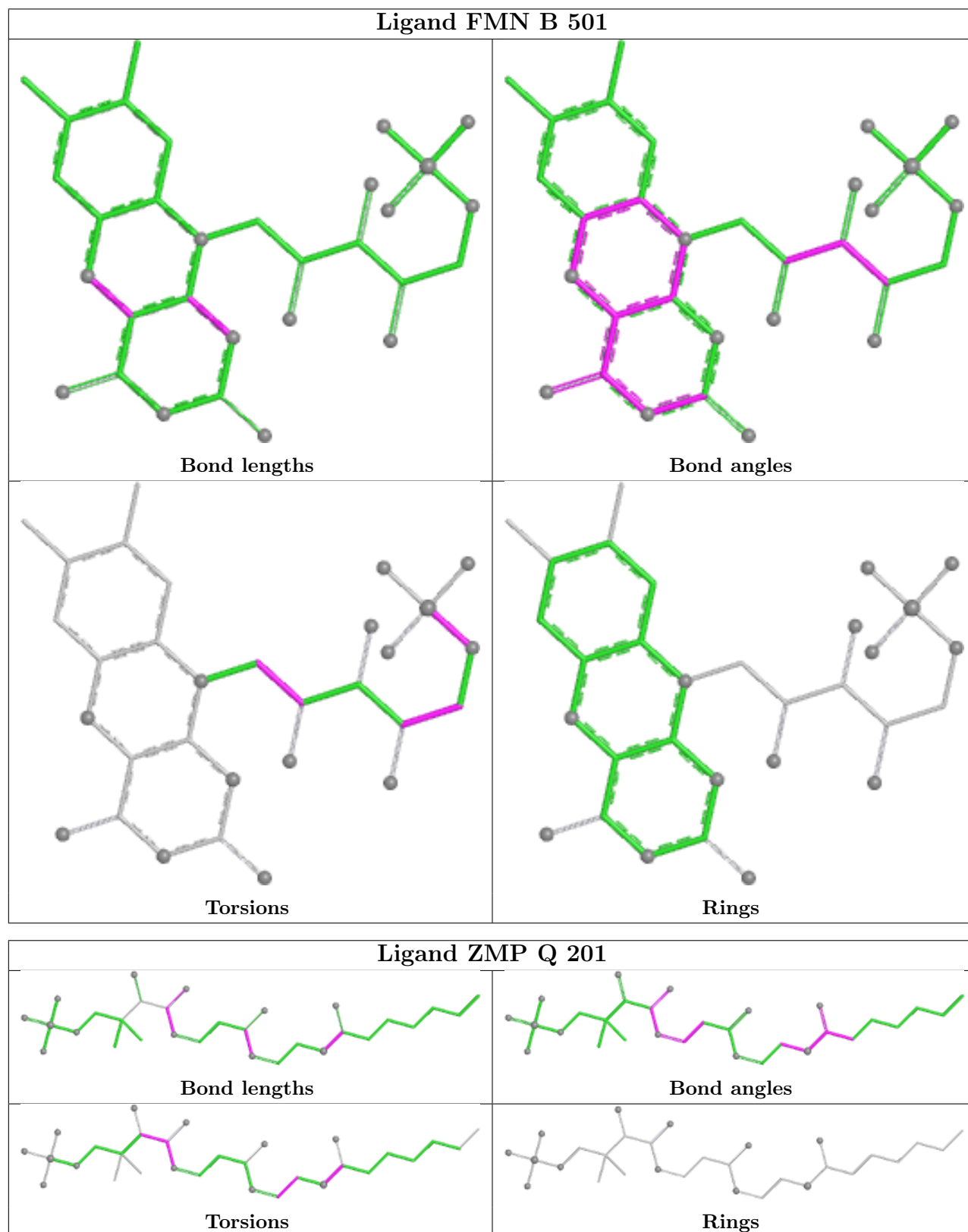
There are no ring outliers.

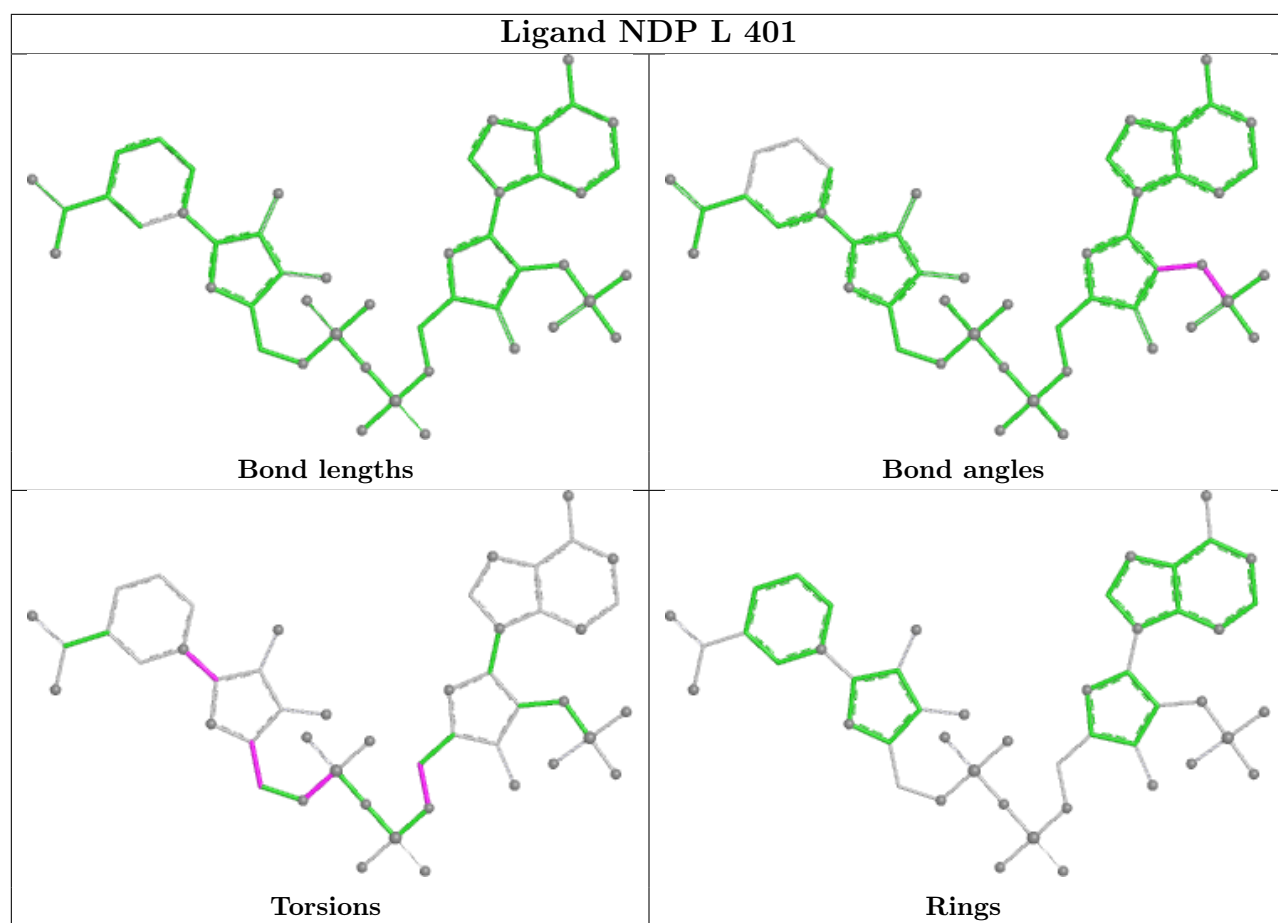
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	B	502	SF4	2	0
46	H	302	SF4	1	0
49	Q	201	ZMP	2	0
48	L	401	NDP	5	0
47	E	301	FES	1	0
46	I	301	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

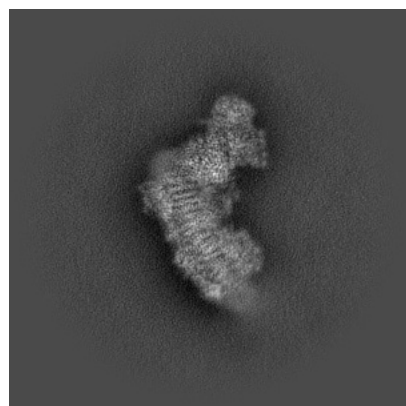
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45463. These allow visual inspection of the internal detail of the map and identification of artifacts.

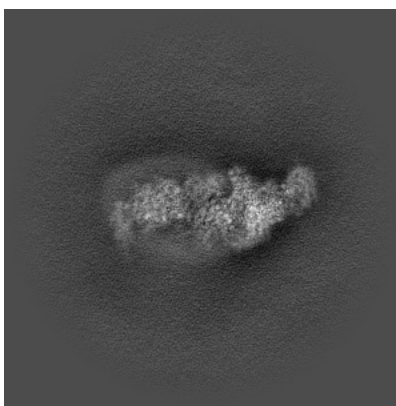
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

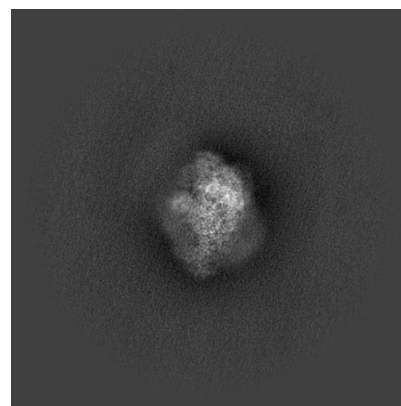
#### 6.1.1 Primary map



X

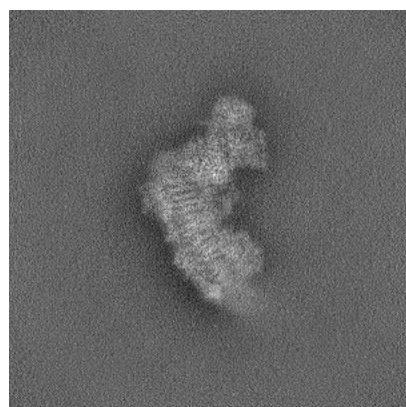


Y

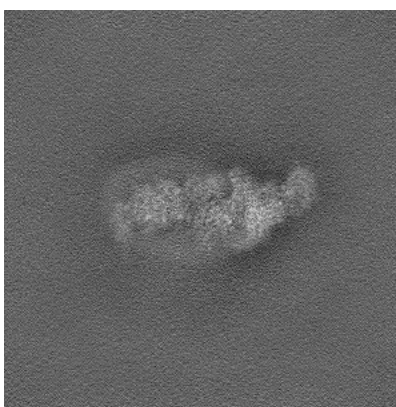


Z

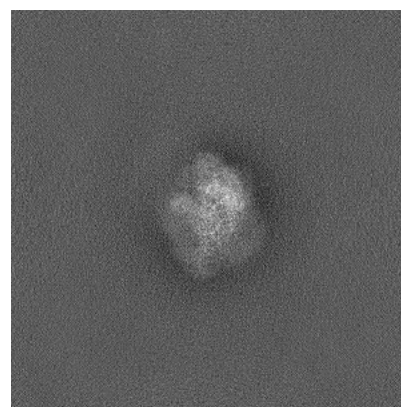
#### 6.1.2 Raw map



X



Y

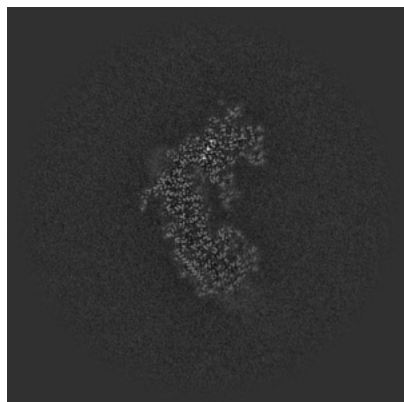


Z

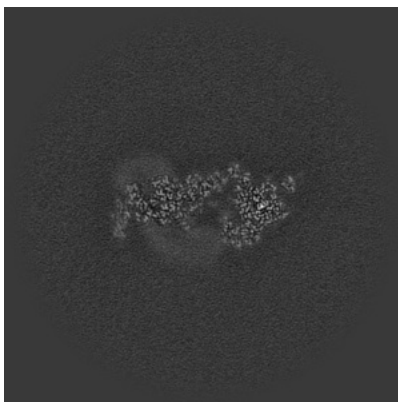
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

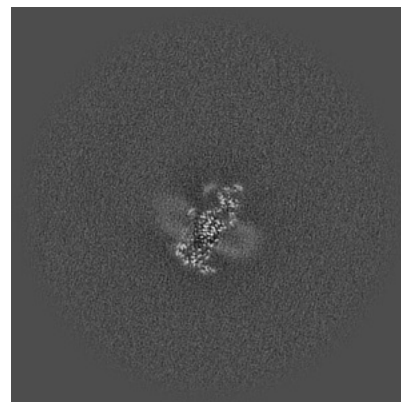
### 6.2.1 Primary map



X Index: 256

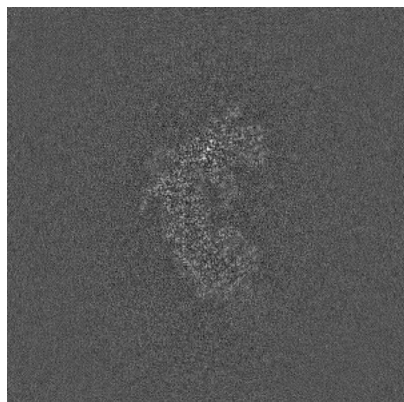


Y Index: 256

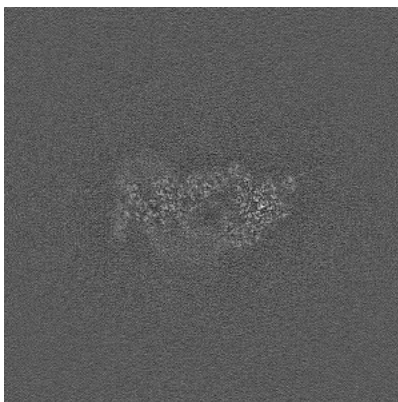


Z Index: 256

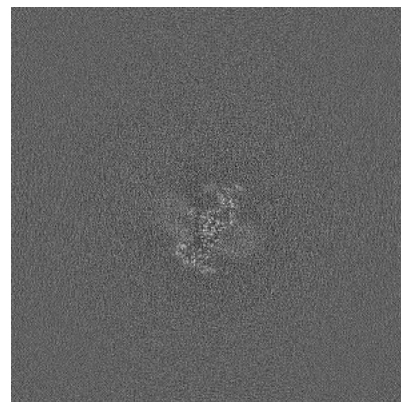
### 6.2.2 Raw map



X Index: 256



Y Index: 256

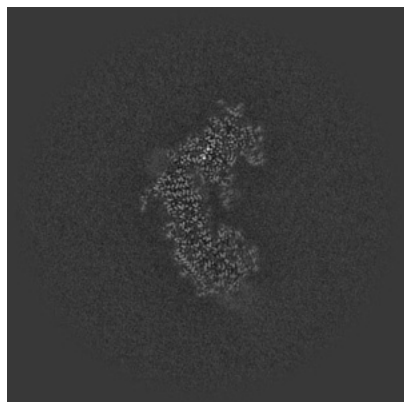


Z Index: 256

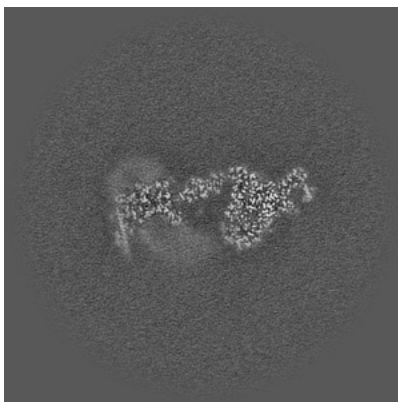
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

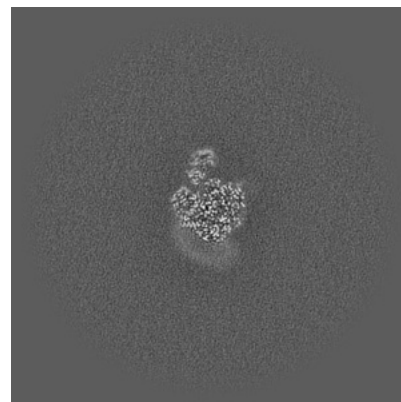
### 6.3.1 Primary map



X Index: 257

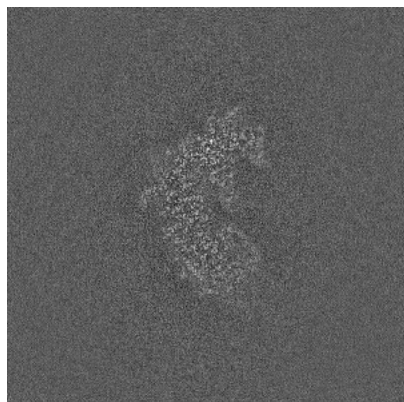


Y Index: 265

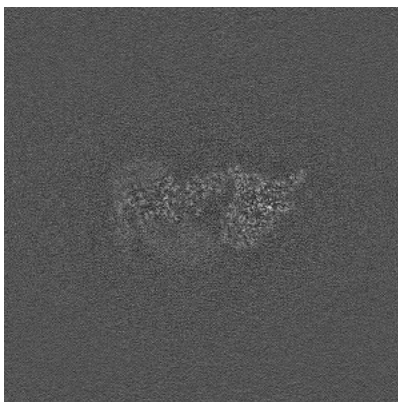


Z Index: 313

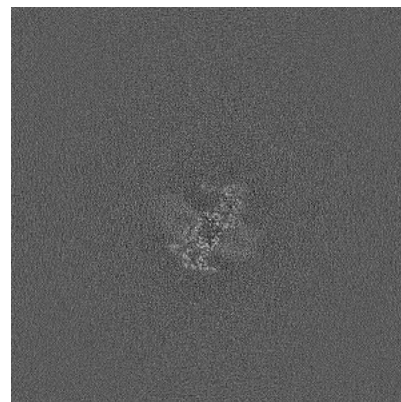
### 6.3.2 Raw map



X Index: 255



Y Index: 261

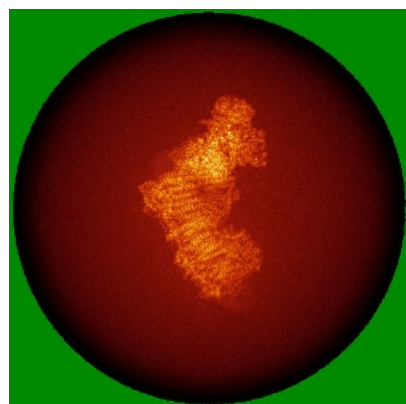


Z Index: 260

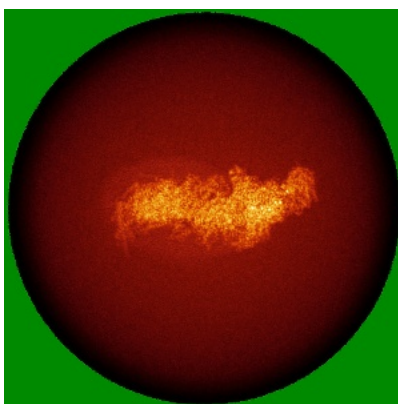
The images above show the largest variance slices of the map in three orthogonal directions.

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

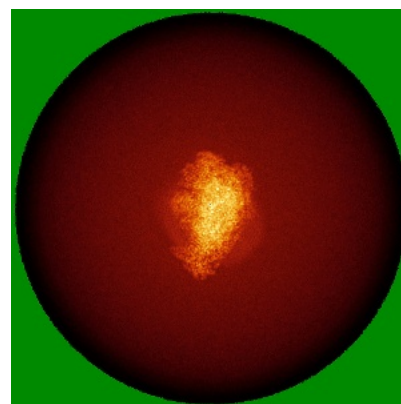
### 6.4.1 Primary map



X

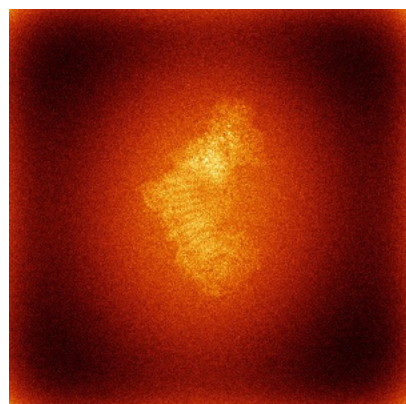


Y

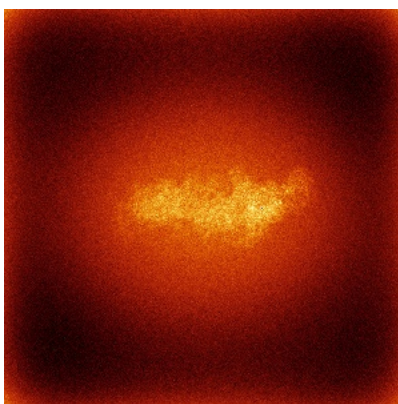


Z

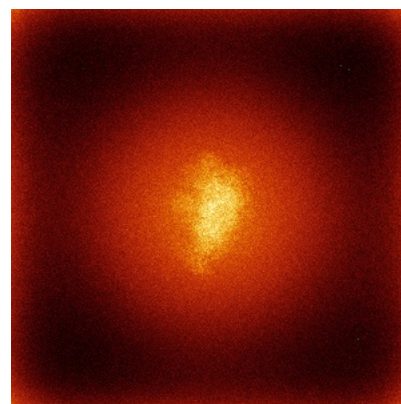
### 6.4.2 Raw map



X



Y

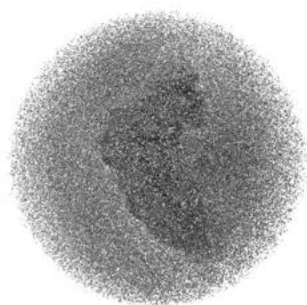


Z

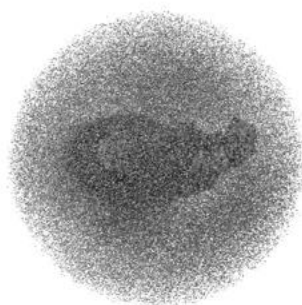
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

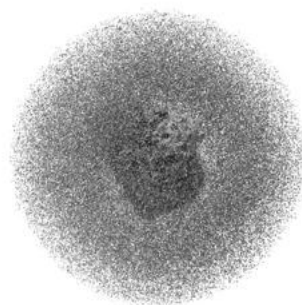
### 6.5.1 Primary map



X



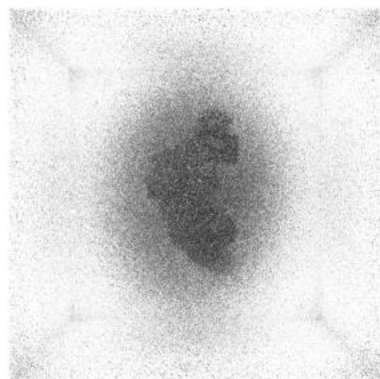
Y



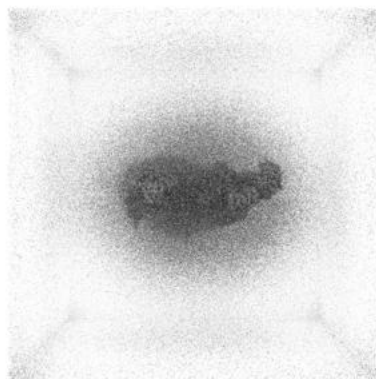
Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

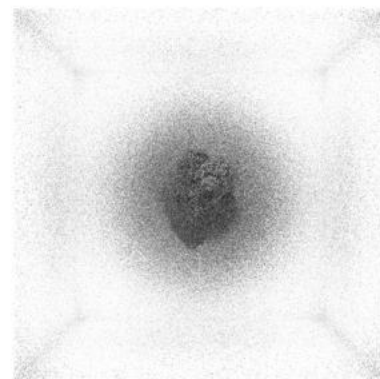
### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

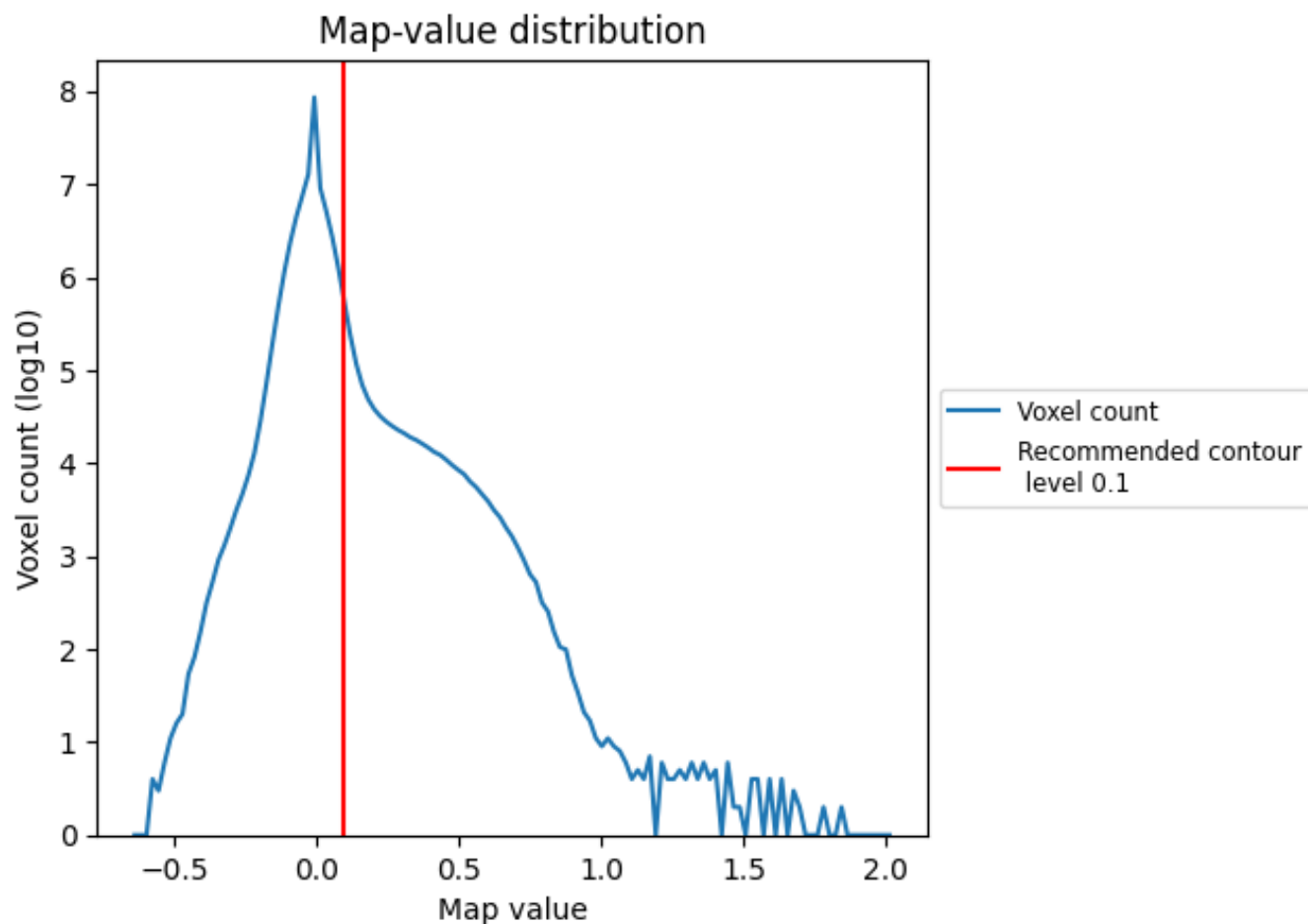
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

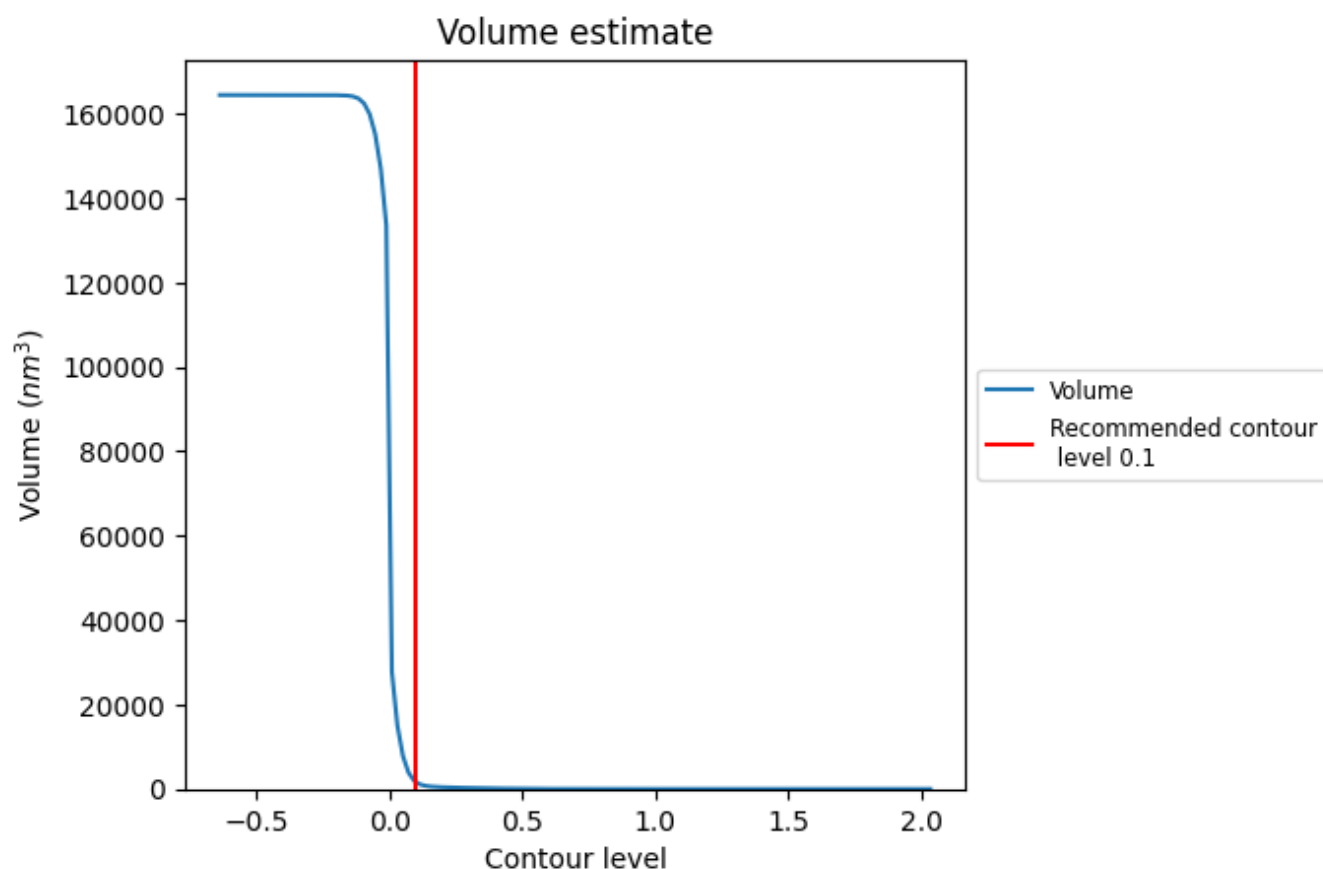
This section contains the results of statistical analysis of the map.

### 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.

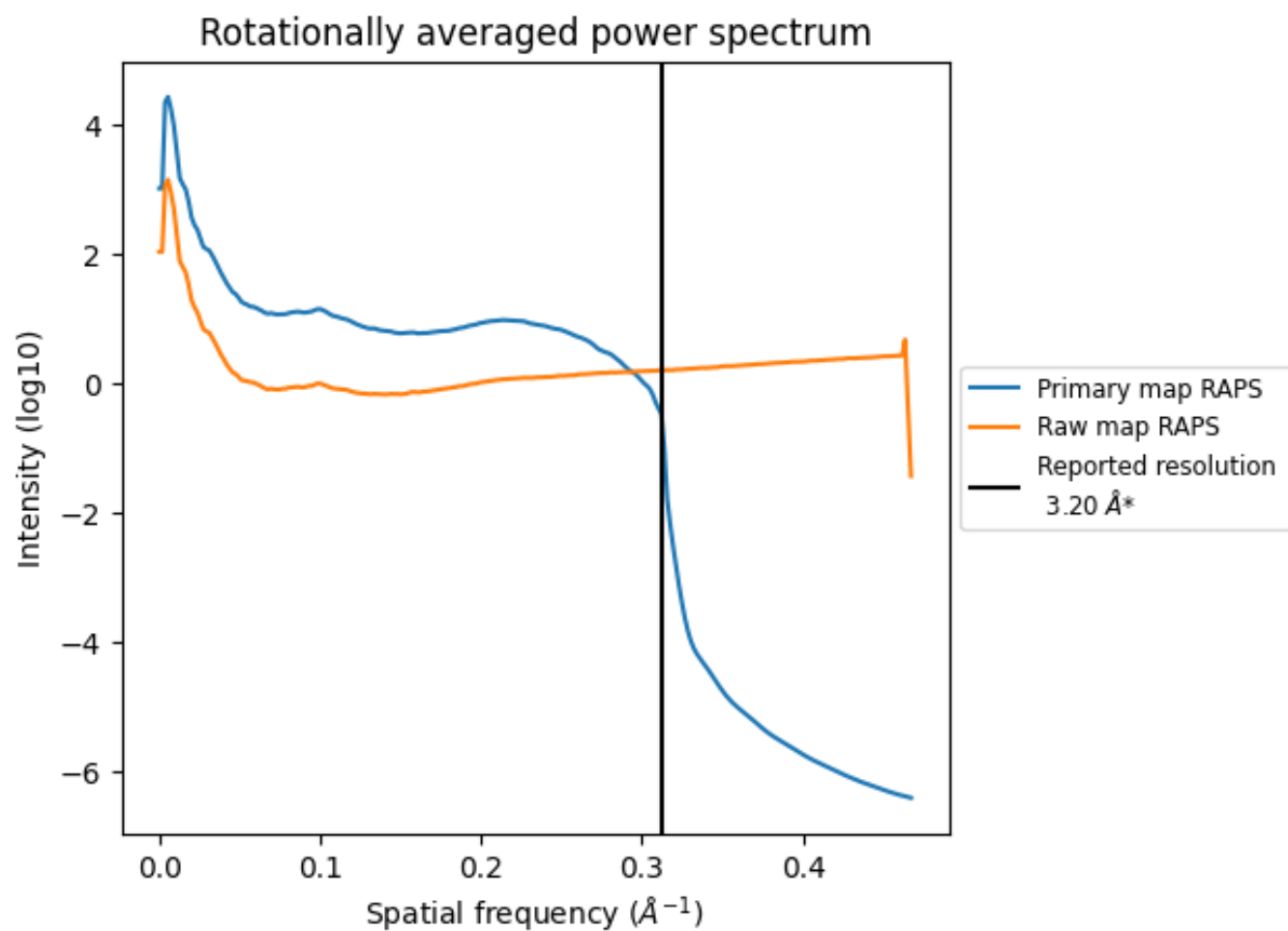
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1706  $\text{nm}^3$ ; this corresponds to an approximate mass of 1541 kDa.

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

### 7.3 Rotationally averaged power spectrum ⓘ

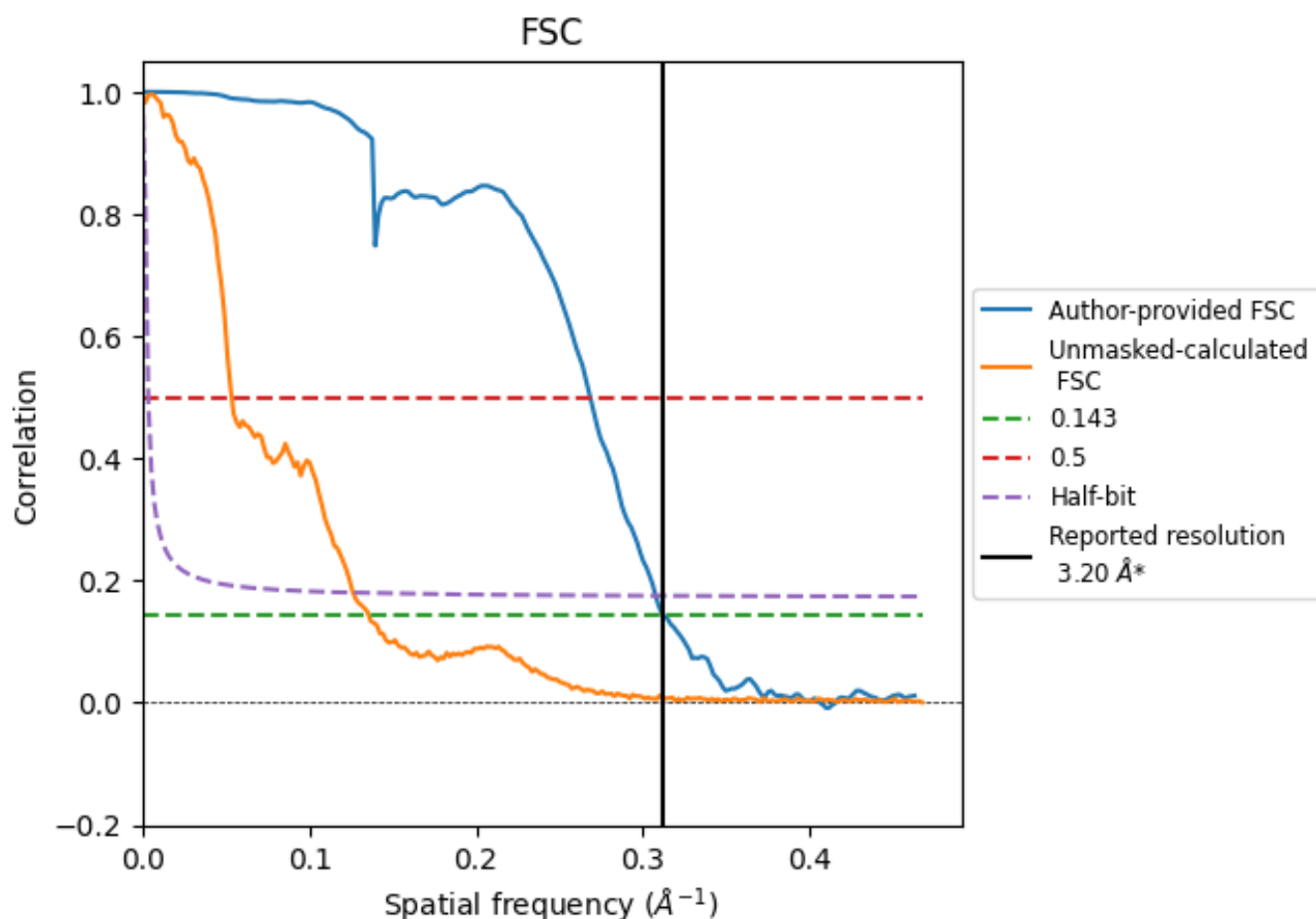


\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

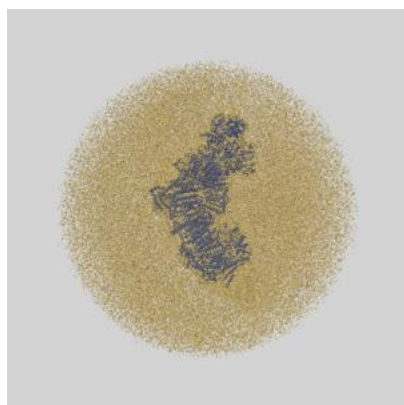
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.73	3.25
Unmasked-calculated*	7.37	18.66	7.91

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.37 differs from the reported value 3.2 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45463 and PDB model 9CD6. Per-residue inclusion information can be found in section [3](#) on page [15](#).

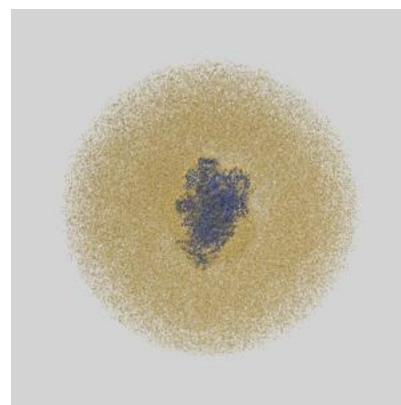
### 9.1 Map-model overlay [i](#)



X



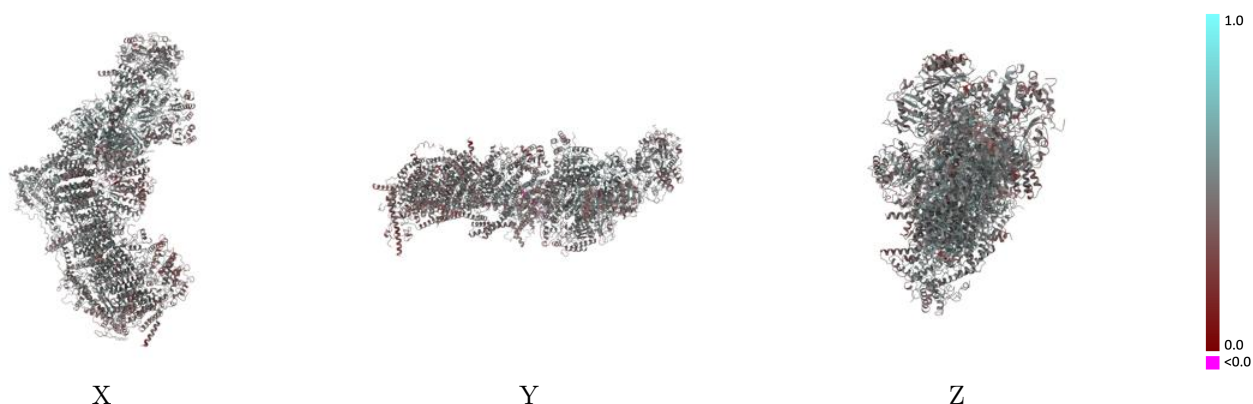
Y



Z

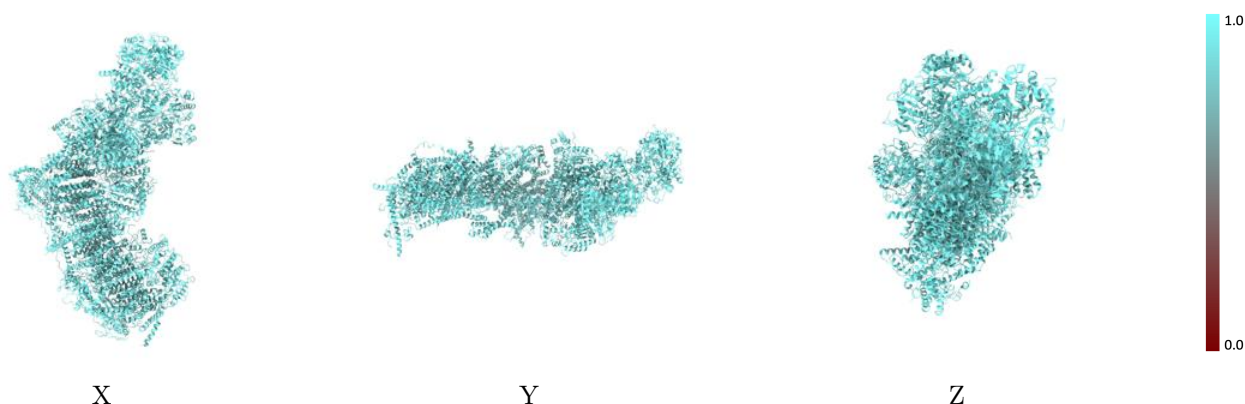
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



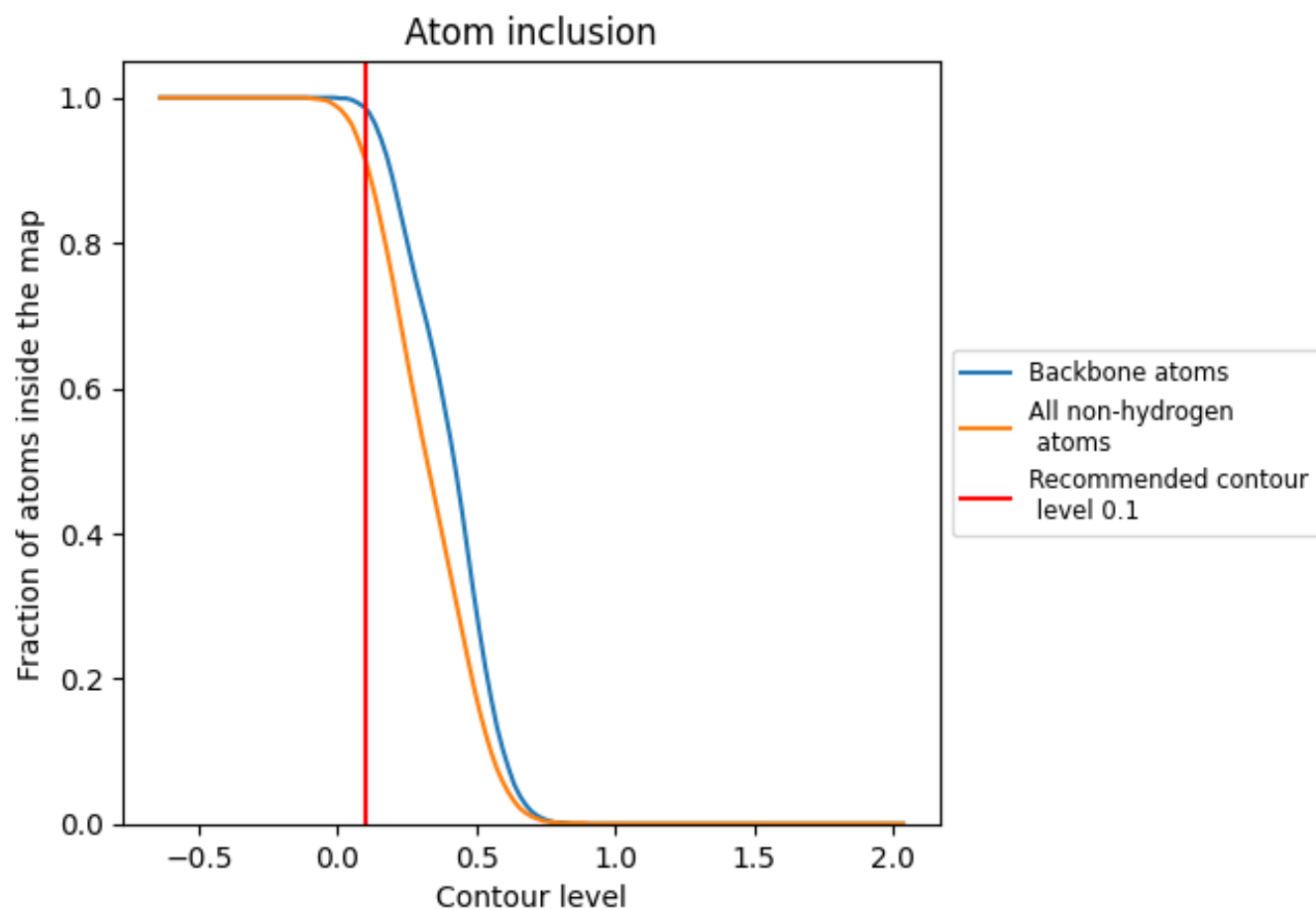
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9150	 0.4610
B	 0.9450	 0.4660
C	 0.9250	 0.5020
D	 0.9370	 0.5090
E	 0.9330	 0.4420
F	 0.9240	 0.4740
G	 0.9350	 0.4810
H	 0.9510	 0.5110
I	 0.9350	 0.4930
J	 0.9270	 0.4960
K	 0.9350	 0.4890
L	 0.9080	 0.4360
M	 0.9310	 0.4990
N	 0.9120	 0.4360
O	 0.8310	 0.3470
P	 0.9110	 0.4140
Q	 0.8970	 0.4530
R	 0.9370	 0.4320
S	 0.9560	 0.5030
T	 0.9310	 0.4610
U	 0.8900	 0.4300
V	 0.9220	 0.4420
W	 0.9430	 0.4850
X	 0.8680	 0.3850
Y	 0.8780	 0.3720
Z	 0.8790	 0.3700
a	 0.9360	 0.4770
b	 0.8720	 0.3600
c	 0.9020	 0.4440
d	 0.9170	 0.4390
e	 0.8910	 0.4220
f	 0.9000	 0.4230
g	 0.9370	 0.4800
h	 0.9280	 0.4620
i	 0.9240	 0.5010



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Chain	Atom inclusion	Q-score
j	 0.8680	 0.4440
k	 0.8980	 0.4880
l	 0.8940	 0.4560
m	 0.8800	 0.4300
n	 0.8810	 0.4060
o	 0.8940	 0.4350
p	 0.9080	 0.4170
q	 0.9160	 0.4930
r	 0.9120	 0.4900
s	 0.9250	 0.4760
t	 0.8920	 0.3650