Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 01:55 PM EDT

PDB ID	:	9BWD / pdb_00009bwd
EMDB ID	:	EMD-44967
Title	:	Cryo-EM structure of respiratory supercomplex I
Authors	:	Zhang, Z.; Maharjan, R.; Tringides, M.
Deposited on	:	2024-05-21
Resolution	:	2.88 Å(reported)

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

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

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

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

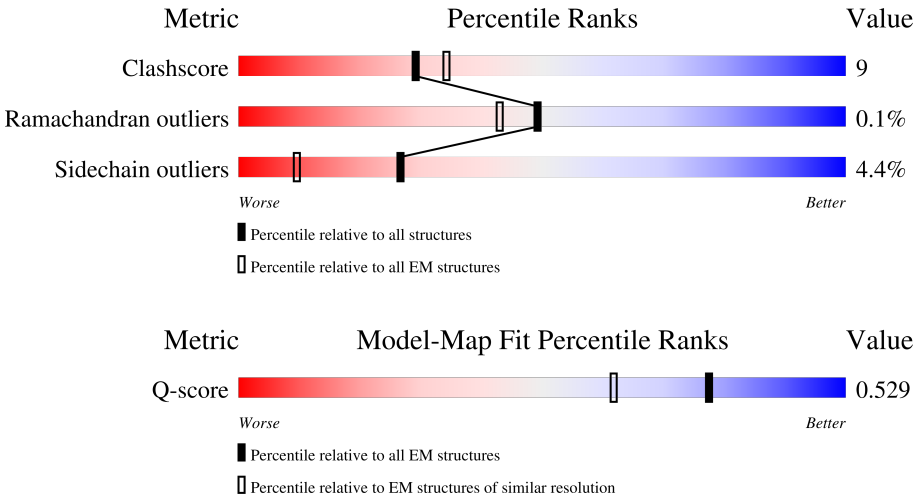
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.50

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 2.88 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12111 (2.38 - 3.38)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	72% 20% 8%
2	C	469	71% 20% 8%
3	D	264	58% 20% 21%
4	F	123	63% 10% 24%

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Mol	Chain	Length	Quality of chain
5	G	727	73% 20% 6%
6	I	258	45% 15% 40%
7	J	175	51% 15% 33%
8	K	145	84% 15%
9	M	113	73% 12% 15%
10	N	116	89% 8%
11	O	156	37% 13% 47%
11	X	156	37% 13% 46%
12	P	99	66% 16% 16%
13	Q	154	60% 11% 27%
14	U	357	72% 17% 11%
15	V	141	81% 18%
16	Y	105	48% 14% 37%
17	Z	114	60% 8% 32%
18	a	189	60% 12% 27%
19	c	186	66% 16% 18%
20	H	212	56% 25% 17%
21	S	70	71% 21% 7%
22	E	249	63% 20% 14%
23	L	372	69% 21% 9%
24	T	169	36% 12% 51%
25	W	144	76% 20%
26	b	188	39% 19% 41%
27	d	176	70% 23%
28	e	154	42% 22% 36%

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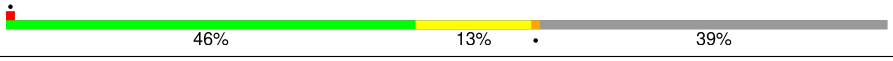
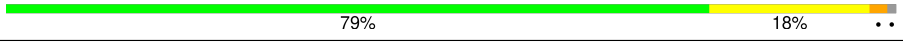
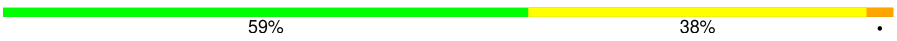
Mol	Chain	Length	Quality of chain
29	f	76	
30	g	122	
31	h	106	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	58	
38	o	129	
39	p	221	
40	q	459	
41	r	318	
42	s	249	
43	t	137	
44	R	110	

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	H	301	-	-	X	-
47	FES	E	301	-	-	X	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 65929 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
			Total	C	N	O	S		
1	B	429	3300	2084	587	609	20	0	0

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

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

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

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

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

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

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

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

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

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

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

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

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

- Molecule 11 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	O	83	Total	C	N	O	S	0	0
			668	431	99	133	5		
11	X	85	Total	C	N	O	S	0	0
			689	445	101	138	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

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

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

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

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

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

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

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

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

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

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

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

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

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

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

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

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

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

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

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

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

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

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L	340	Total	C	N	O	S	0	0
			2735	1771	479	476	9		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

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

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

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

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

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

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

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

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

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

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

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

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

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

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 2.

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

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	114	Total	C	N	O	S	0	0
			905	610	133	155	7		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

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

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 5.

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

- Molecule 36 is a protein called NADH-ubiquinone oxidoreductase chain 6.

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

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

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

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

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 4.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	318	Total	C	N	O	S	0	0
			2508	1678	385	424	21		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

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

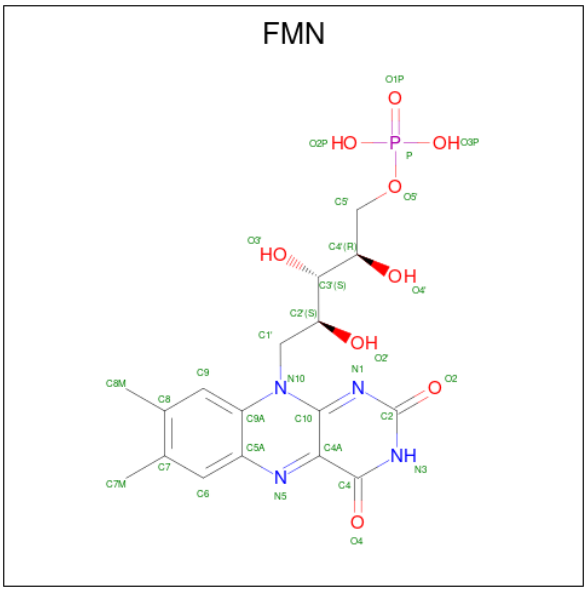
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

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

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

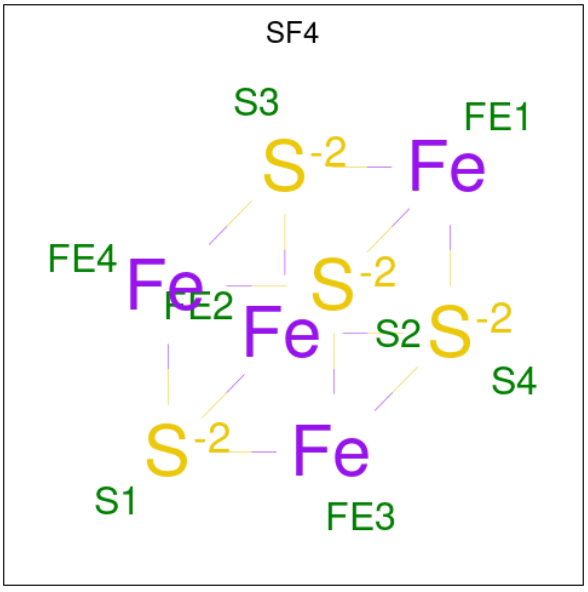
Mol	Chain	Residues	Atoms					AltConf	Trace
44	R	35	Total	C	N	O	S	0	0
			295	185	55	54	1		

- Molecule 45 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
46	B	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	

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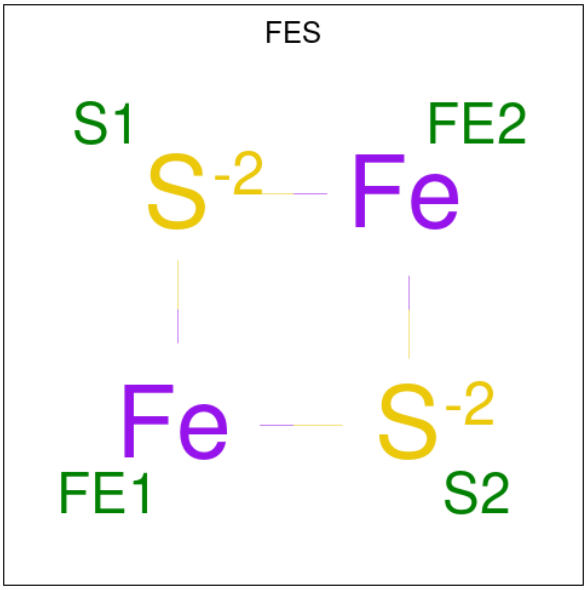
Mol	Chain	Residues	Atoms	AltConf
46	I	1	Total Fe S 8 4 4	0
46	H	1	Total Fe S 8 4 4	0
46	H	1	Total Fe S 8 4 4	0

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



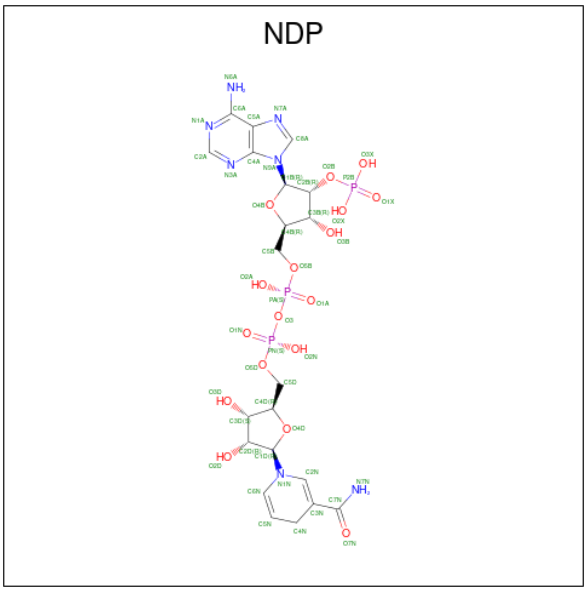
Mol	Chain	Residues	Atoms	AltConf
47	G	1	Total Fe S 4 2 2	0
47	E	1	Total Fe S 4 2 2	0

- Molecule 48 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
48	Q	1	Total	C	N	O	P	S	0
			30	18	2	8	1	1	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



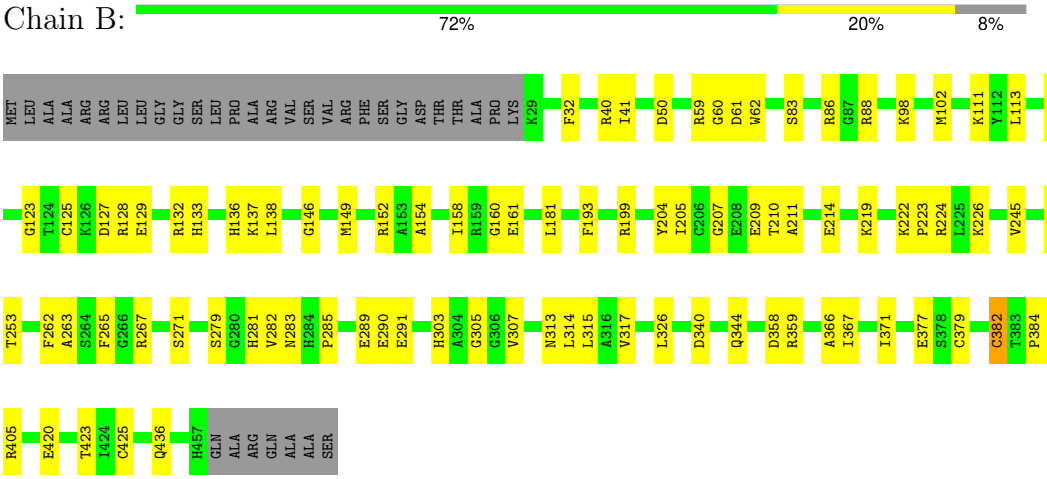
Mol	Chain	Residues	Atoms					AltConf
49	L	1	Total	C	N	O	P	0
			48	21	7	17	3	

3 Residue-property plots (i)

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

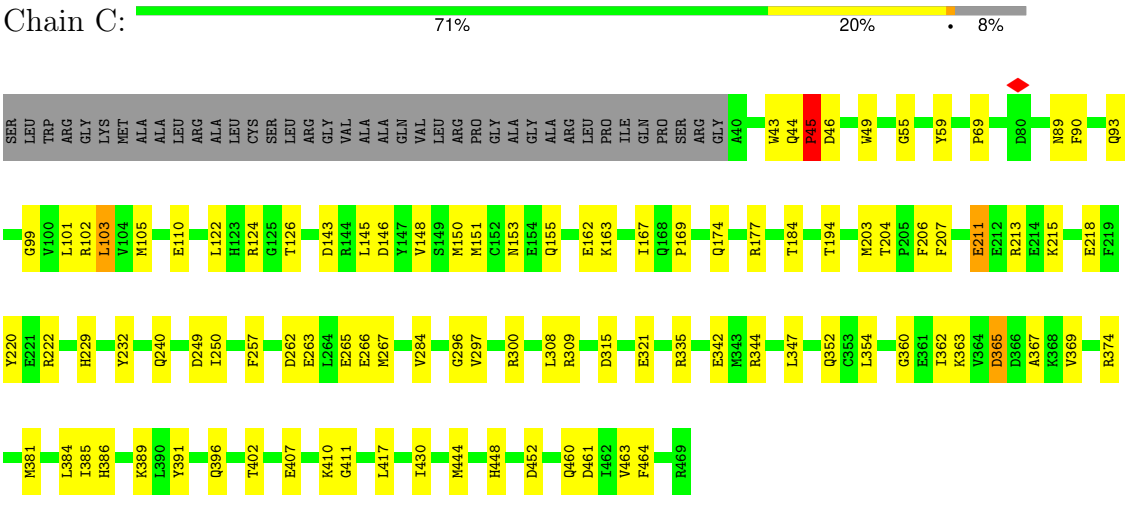
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain B:



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

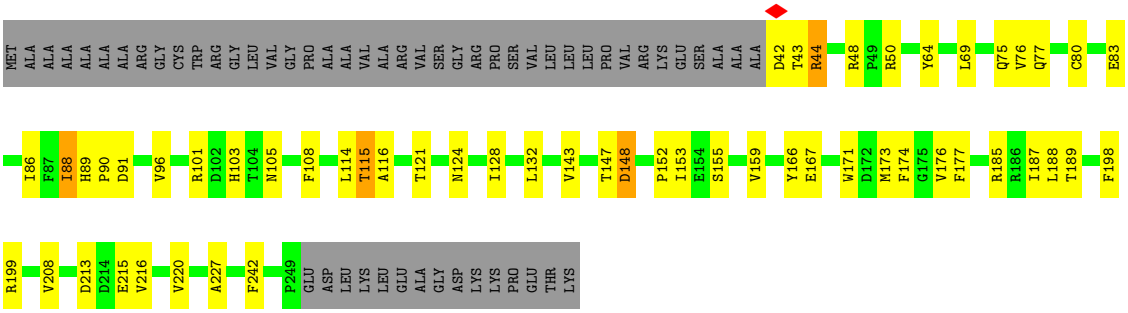
Chain C:



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

Chain D:

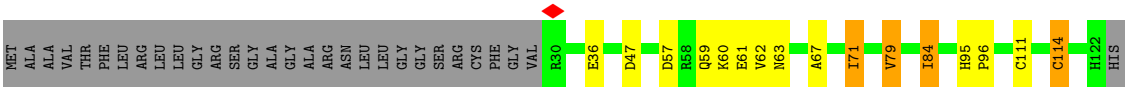




• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain F:

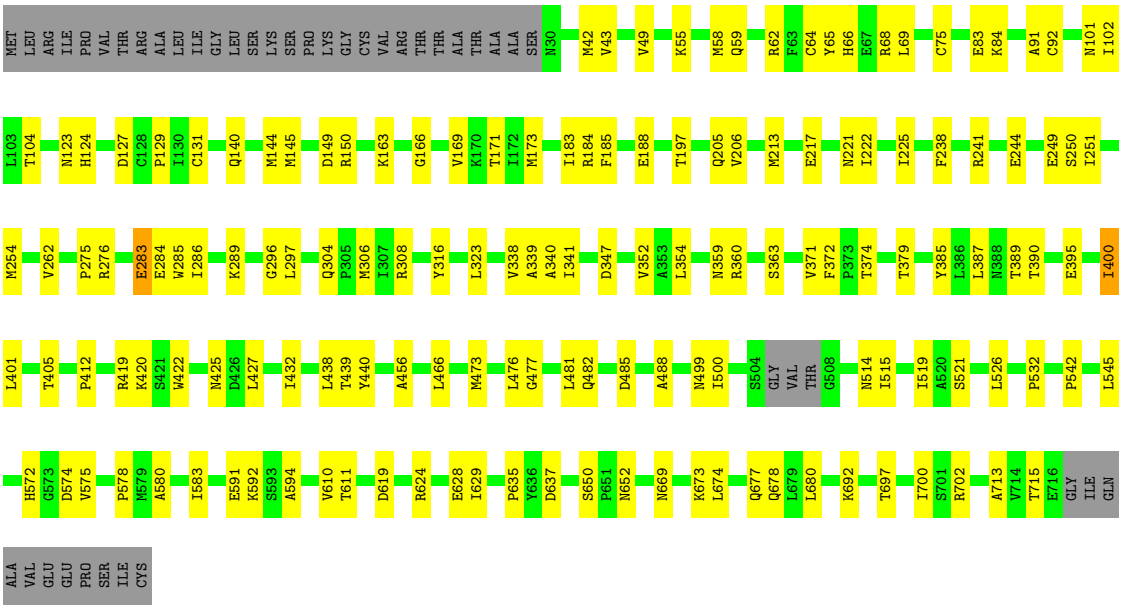




• Molecule 5: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

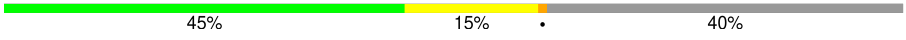
Chain G:

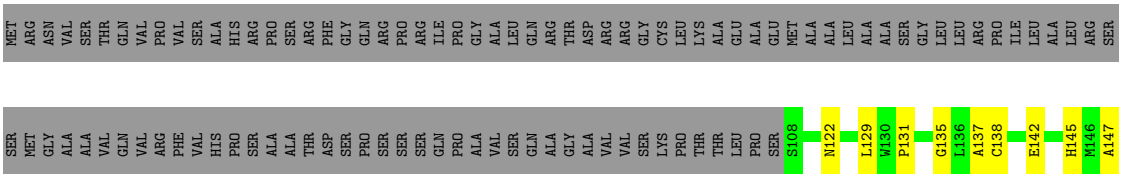




• Molecule 6: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain I:







• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain J:



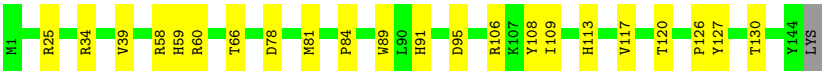




• Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain K:

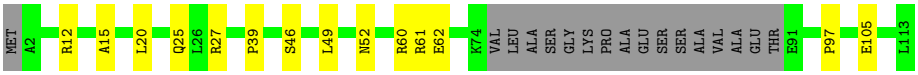




• Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain M:





• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain N:

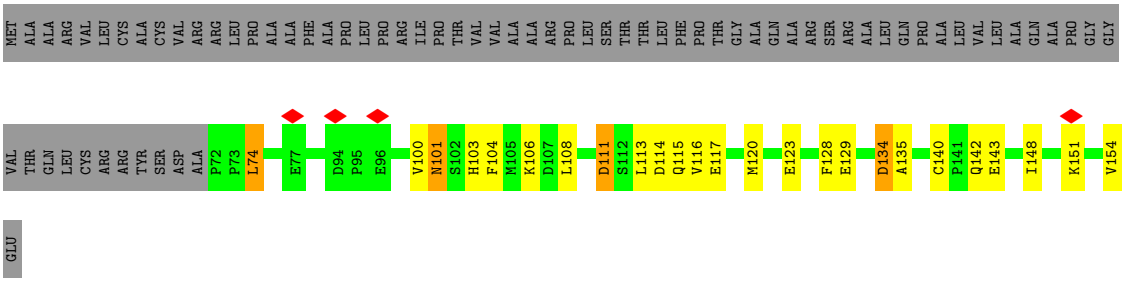




• Molecule 11: Acyl carrier protein

Chain O:

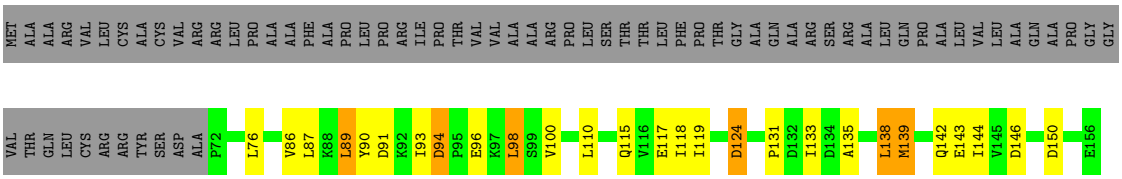




• Molecule 11: Acyl carrier protein

Chain X:

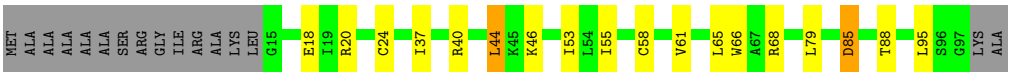




• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain P:

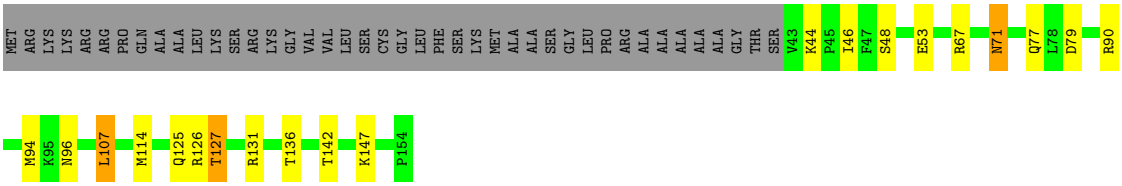




• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain Q:

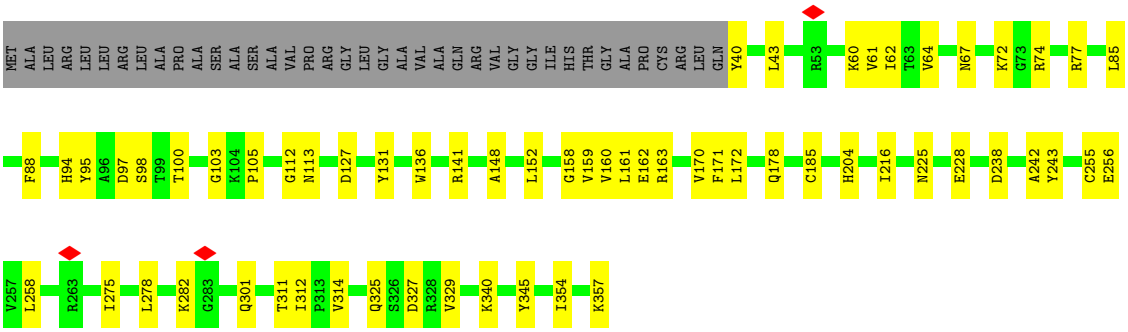




• Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain U:





• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V:

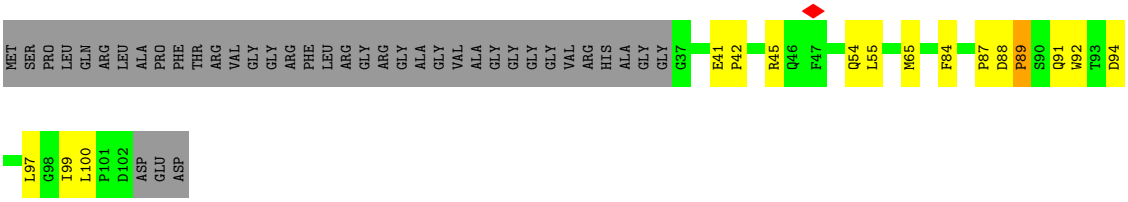




• Molecule 16: NADH:ubiquinone oxidoreductase subunit B2

Chain Y:

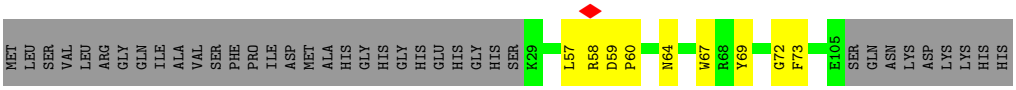




• Molecule 17: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z:



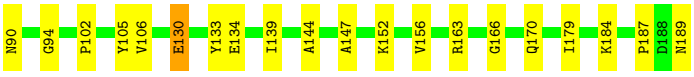


• Molecule 18: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a:





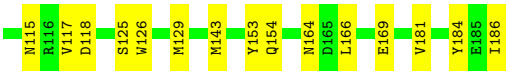


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c:





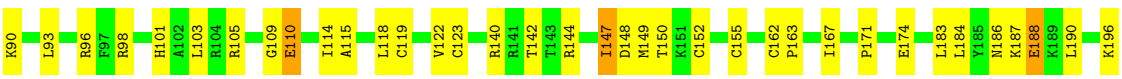


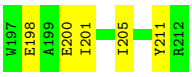
• Molecule 20: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain H:



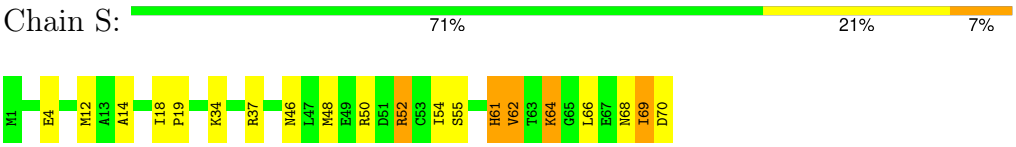






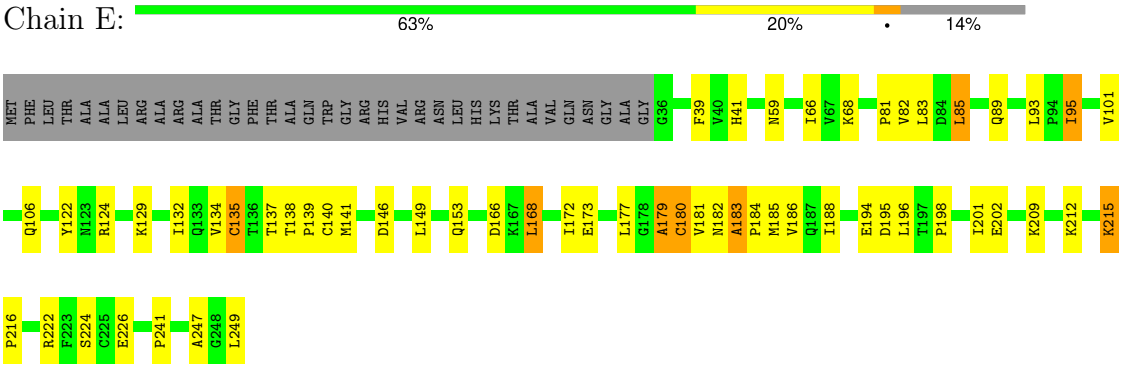
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S:



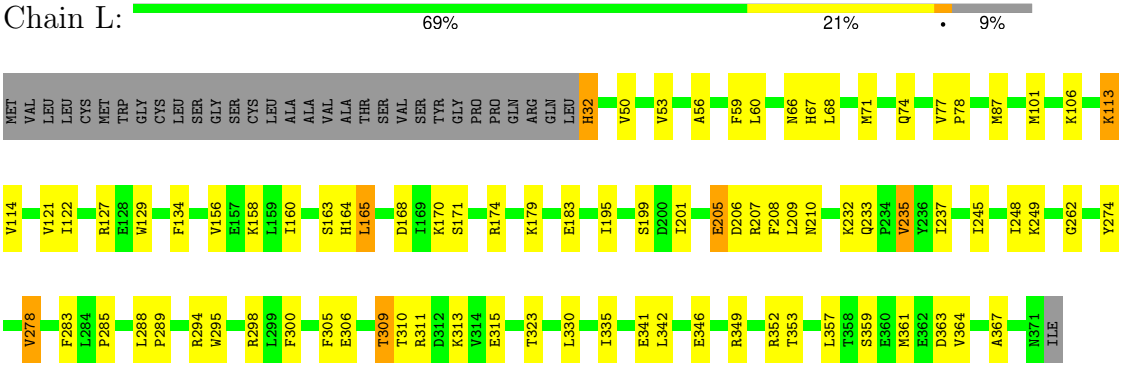
• Molecule 22: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



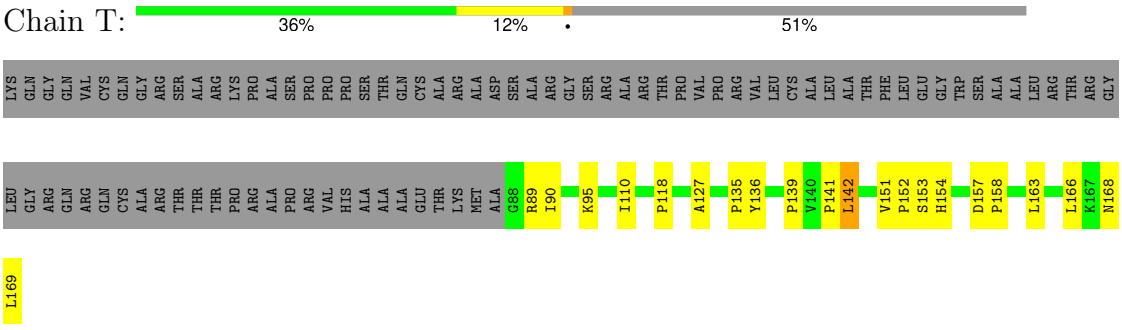
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain L:



• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain T:



• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

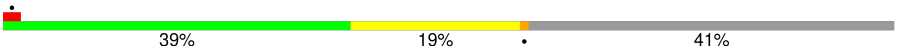
Chain W:

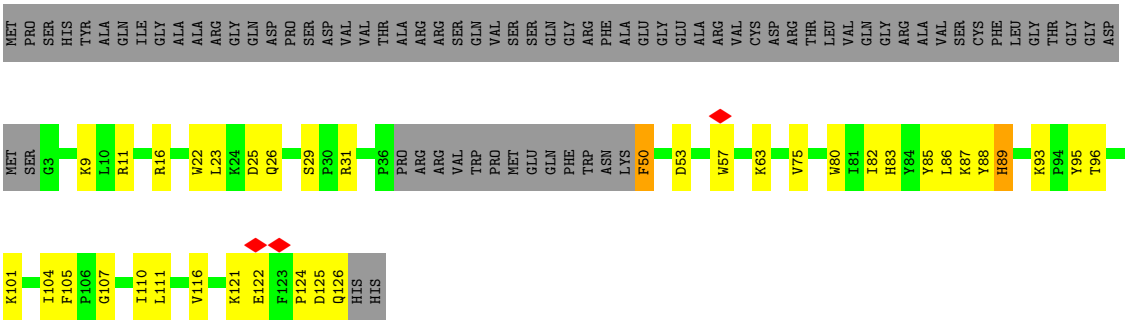




• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b:

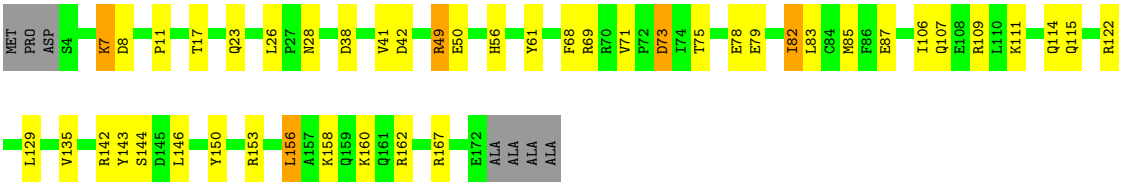




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

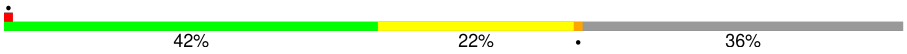
Chain d:

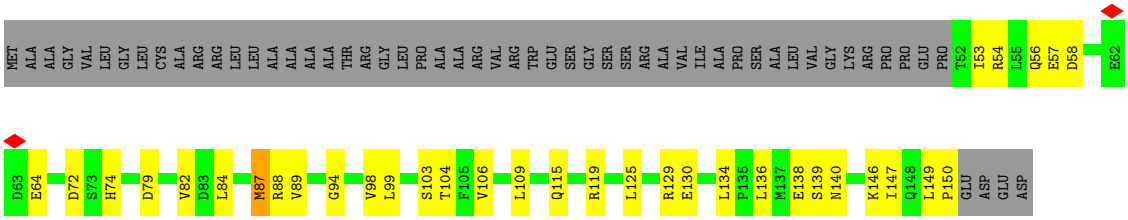




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

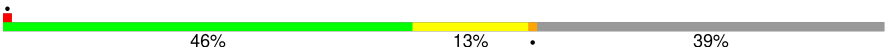
Chain e:

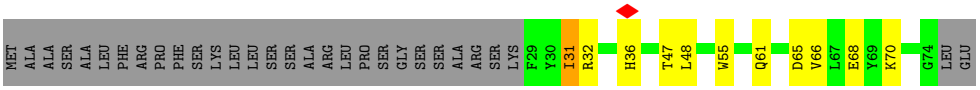




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

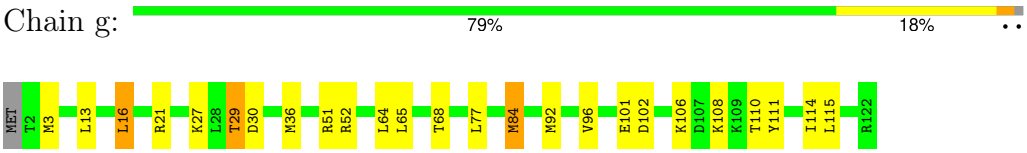
Chain f:





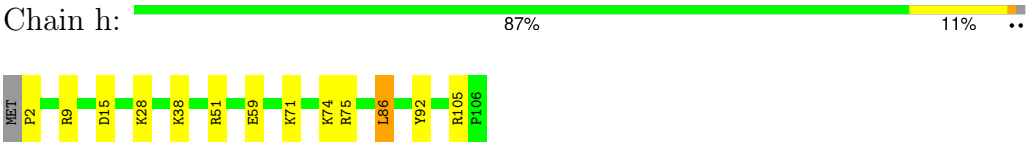
• Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g:



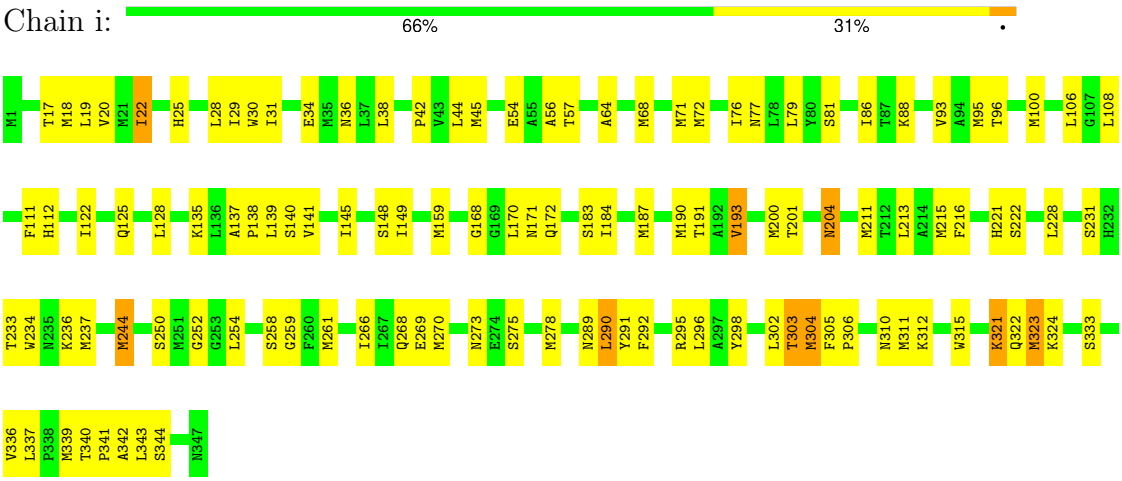
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:



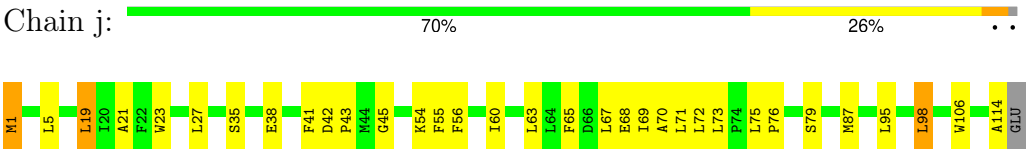
• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

Chain i:



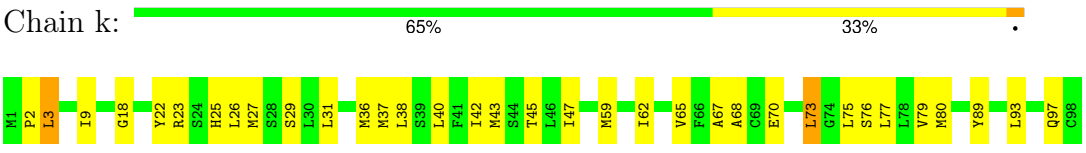
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:



• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

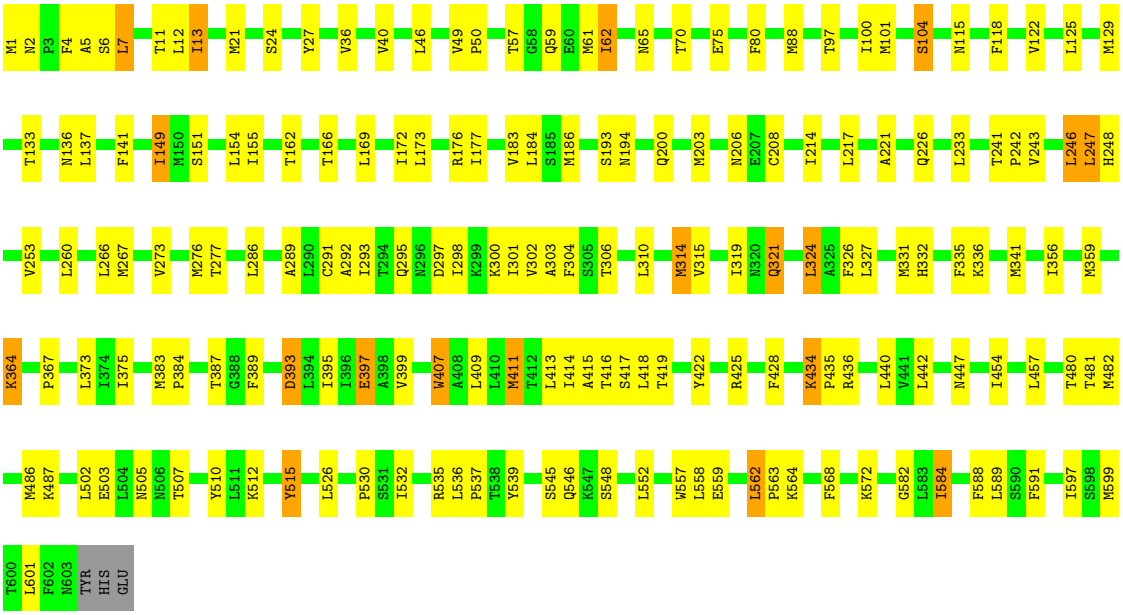
Chain k:



• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

Chain l:

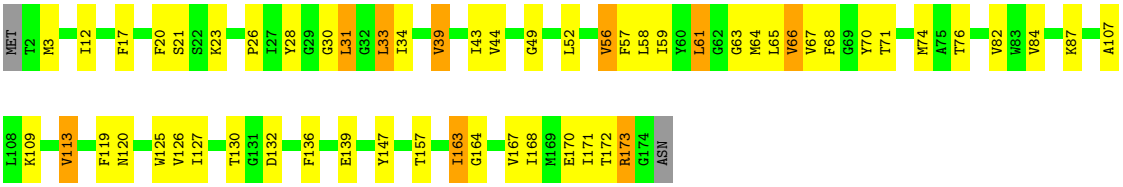




• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

Chain m:

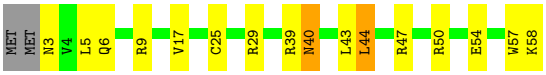




• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:

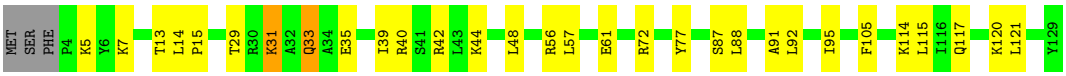




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:

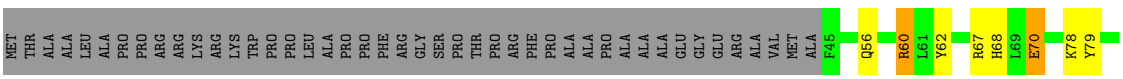


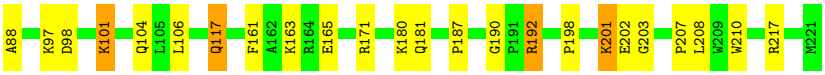


• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:



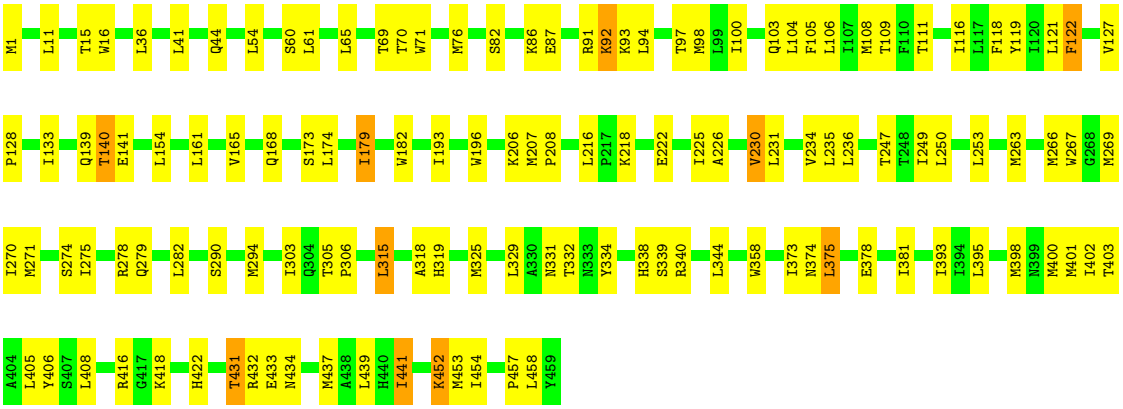




• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain q:

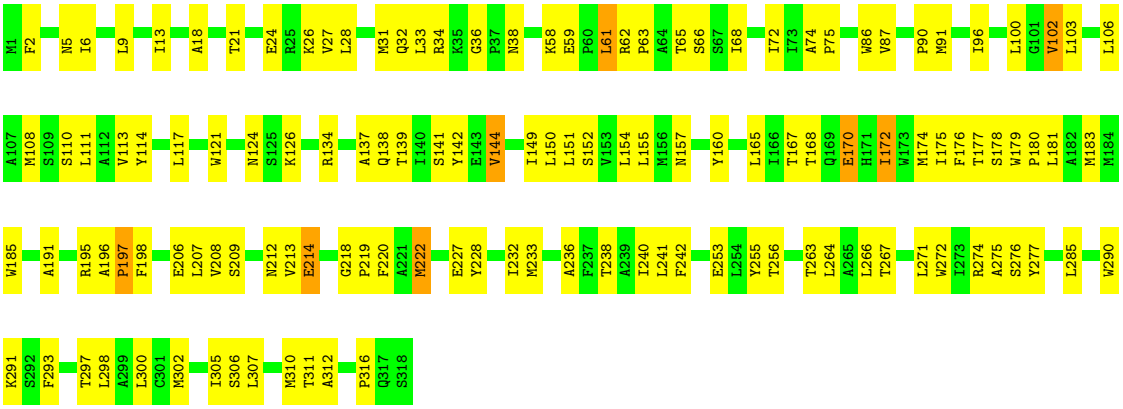




• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

Chain r:

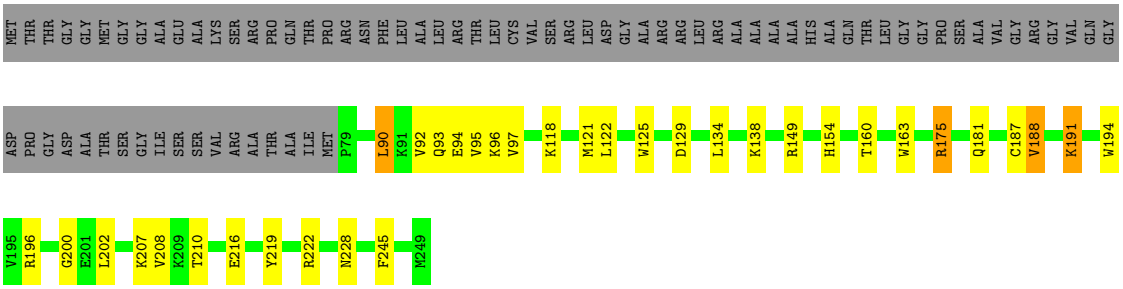




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

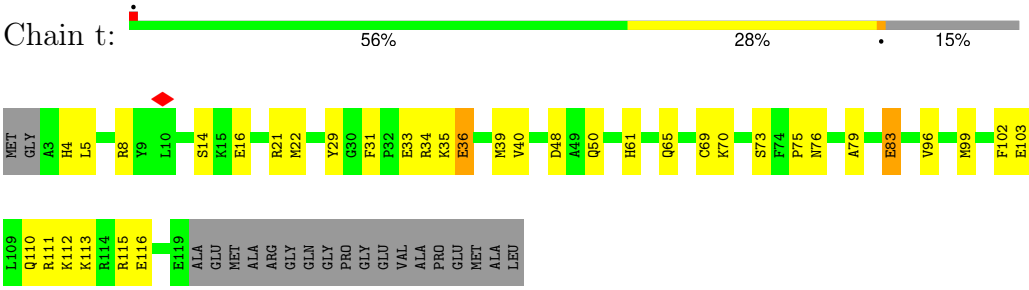
Chain s:





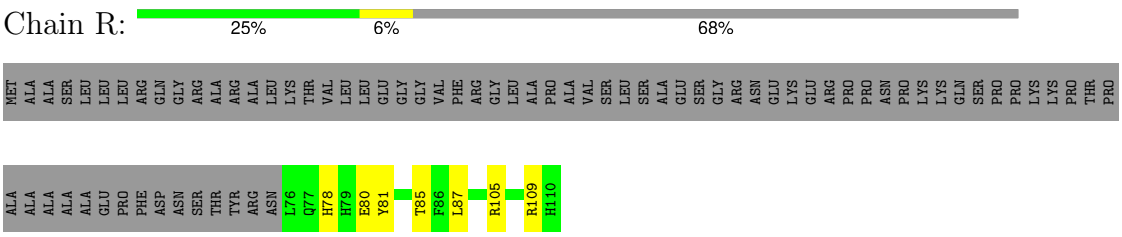
• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain t:



• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64500	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 ($e^-/Å^2$)	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	1.907	Depositor
Minimum map value	-0.559	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.15	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, FMN, FES, NDP, ZMP

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	0.13	0/3375	0.32	0/4561
2	C	0.20	0/3545	0.37	1/4805 (0.0%)
3	D	0.13	0/1788	0.31	0/2435
4	F	0.36	0/733	0.54	0/988
5	G	0.21	0/5347	0.37	0/7243
6	I	0.17	0/1280	0.34	0/1730
7	J	0.11	0/986	0.28	0/1329
8	K	0.17	0/1244	0.30	0/1693
9	M	0.12	0/792	0.34	0/1069
10	N	0.12	0/930	0.26	0/1258
11	O	0.09	0/679	0.30	0/916
11	X	0.11	0/701	0.27	0/946
12	P	0.29	0/680	0.46	0/916
13	Q	0.10	0/979	0.27	0/1317
14	U	0.35	0/2633	0.47	0/3565
15	V	0.17	0/1042	0.28	0/1411
16	Y	0.43	0/597	0.58	0/818
17	Z	0.09	0/639	0.24	0/864
18	a	0.12	0/1184	0.29	0/1603
19	c	0.29	0/1346	0.42	0/1840
20	H	0.49	0/1443	0.69	0/1952
21	S	0.38	0/577	0.55	0/777
22	E	0.24	0/1698	0.42	2/2311 (0.1%)
23	L	0.38	0/2812	0.49	0/3812
24	T	0.14	0/659	0.39	0/905
25	W	0.12	0/1193	0.28	0/1609
26	b	0.14	0/976	0.40	0/1328
27	d	0.16	0/1458	0.32	0/1965
28	e	0.24	0/849	0.38	0/1153
29	f	0.10	0/404	0.29	0/547
30	g	0.19	0/1031	0.33	0/1394
31	h	0.15	0/889	0.29	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	i	0.27	0/2773	0.43	0/3768
33	j	0.15	0/929	0.35	0/1269
34	k	0.36	0/759	0.58	0/1029
35	l	0.29	0/4914	0.50	0/6683
36	m	0.33	0/1356	0.53	0/1839
37	n	0.20	0/491	0.49	0/663
38	o	0.13	0/1070	0.36	0/1451
39	p	0.10	0/1585	0.31	0/2148
40	q	0.28	0/3721	0.47	0/5073
41	r	0.42	0/2581	0.62	0/3529
42	s	0.14	0/1436	0.31	0/1938
43	t	0.31	0/1038	0.48	0/1389
44	R	0.11	0/304	0.31	0/410
All	All	0.25	0/67446	0.42	3/91439 (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
14	U	0	1
20	H	0	3
21	S	0	2
23	L	0	1
27	d	0	1
32	i	0	1
35	l	0	1
41	r	0	1
All	All	0	11

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	E	247	ALA	CB-CA-C	-5.71	109.97	116.54
2	C	148	VAL	N-CA-C	-5.16	107.80	112.96
22	E	179	ALA	N-CA-C	-5.00	104.44	110.44

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
20	H	105	ARG	Sidechain
20	H	96	ARG	Sidechain
20	H	98	ARG	Sidechain
23	L	174	ARG	Sidechain
21	S	50	ARG	Sidechain
21	S	52	ARG	Sidechain
14	U	163	ARG	Sidechain
27	d	153	ARG	Sidechain
32	i	295	ARG	Sidechain
35	l	425	ARG	Sidechain
41	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	3263	77	0
2	C	3453	0	3389	77	0
3	D	1737	0	1691	37	0
4	F	720	0	683	16	0
5	G	5260	0	5287	99	0
6	I	1249	0	1254	34	0
7	J	963	0	962	23	0
8	K	1203	0	1161	16	0
9	M	774	0	801	13	0
10	N	911	0	950	5	0
11	O	668	0	672	17	0
11	X	689	0	687	19	0
12	P	669	0	675	12	0
13	Q	955	0	960	21	0
14	U	2573	0	2534	38	0
15	V	1021	0	1025	13	0
16	Y	571	0	522	18	0
17	Z	620	0	602	8	0
18	a	1151	0	1164	23	0
19	c	1291	0	1185	26	0
20	H	1412	0	1366	53	0
21	S	562	0	557	13	0
22	E	1658	0	1662	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	L	2735	0	2751	50	0
24	T	638	0	637	20	0
25	W	1162	0	1156	31	0
26	b	946	0	963	28	0
27	d	1426	0	1394	37	0
28	e	826	0	788	28	0
29	f	391	0	392	7	0
30	g	1000	0	994	19	0
31	h	867	0	871	14	0
32	i	2710	0	2874	84	0
33	j	905	0	945	34	0
34	k	748	0	799	39	0
35	l	4785	0	4935	121	0
36	m	1321	0	1320	58	0
37	n	479	0	486	9	0
38	o	1041	0	1053	14	0
39	p	1529	0	1465	23	0
40	q	3630	0	3837	82	0
41	r	2508	0	2607	104	0
42	s	1398	0	1374	32	0
43	t	1014	0	983	30	0
44	R	295	0	279	4	0
45	B	31	0	19	1	0
46	B	8	0	0	21	0
46	G	16	0	0	0	0
46	H	16	0	0	8	0
46	I	8	0	0	1	0
47	E	4	0	0	9	0
47	G	4	0	0	0	0
48	Q	30	0	30	1	0
49	L	48	0	26	3	0
All	All	65929	0	66030	1224	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (1224) 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:425:CYS:SG	46:B:502:SF4:FE1	1.08	1.46
1:B:379:CYS:SG	46:B:502:SF4:FE3	1.10	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:E:140:CYS:SG	47:E:301:FES:FE2	1.12	1.38
1:B:382:CYS:SG	46:B:502:SF4:FE4	1.15	1.38
22:E:135:CYS:SG	47:E:301:FES:FE2	1.40	1.13
4:F:71:ILE:HG12	20:H:110:GLU:HG3	1.45	0.98
1:B:379:CYS:HG	46:B:502:SF4:FE3	0.78	0.97
20:H:152:CYS:SG	46:H:301:SF4:FE1	1.59	0.94
1:B:385:CYS:SG	46:B:502:SF4:FE2	1.60	0.91
36:m:65:LEU:HD12	41:r:117:LEU:HD21	1.52	0.91
34:k:31:LEU:HD21	36:m:64:MET:HE1	1.52	0.91
20:H:155:CYS:SG	46:H:301:SF4:FE3	1.61	0.91
1:B:425:CYS:HG	46:B:502:SF4:FE1	0.83	0.91
1:B:425:CYS:SG	46:B:502:SF4:S3	2.70	0.90
20:H:123:CYS:HG	46:H:301:SF4:FE2	0.58	0.88
14:U:256:GLU:HG2	14:U:282:LYS:HG3	1.54	0.87
16:Y:87:PRO:HG3	43:t:96:VAL:HG22	1.56	0.86
4:F:67:ALA:HB1	20:H:110:GLU:HG2	1.57	0.85
22:E:180:CYS:SG	47:E:301:FES:S1	2.74	0.85
35:l:562:LEU:HB2	35:l:563:PRO:HD3	1.57	0.84
18:a:130:GLU:HB2	37:n:58:LYS:HD2	1.60	0.81
22:E:135:CYS:SG	47:E:301:FES:S1	2.78	0.81
1:B:379:CYS:SG	46:B:502:SF4:S1	2.82	0.78
1:B:382:CYS:SG	46:B:502:SF4:S1	2.82	0.78
4:F:111:CYS:SG	4:F:114:CYS:N	2.57	0.78
35:l:253:VAL:HB	35:l:310:LEU:HD11	1.67	0.76
22:E:183:ALA:HB3	22:E:195:ASP:HA	1.68	0.76
32:i:18:MET:O	32:i:22:ILE:HB	1.85	0.76
1:B:382:CYS:SG	46:B:502:SF4:S3	2.83	0.76
32:i:258:SER:HB2	32:i:336:VAL:HG12	1.67	0.75
1:B:385:CYS:HB2	46:B:502:SF4:S3	2.26	0.75
2:C:213:ARG:HH11	6:I:145:HIS:HE1	1.35	0.74
40:q:208:PRO:HG3	40:q:216:LEU:HD22	1.68	0.74
17:Z:60:PRO:HB2	11:X:90:TYR:HE1	1.53	0.73
27:d:162:ARG:NH1	28:e:139:SER:O	2.21	0.73
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.71	0.73
36:m:65:LEU:HD21	41:r:139:THR:OG1	1.89	0.72
32:i:42:PRO:HG3	36:m:167:VAL:HG22	1.72	0.72
41:r:28:LEU:HD22	41:r:275:ALA:HB2	1.71	0.72
8:K:106:ARG:HB2	8:K:109:ILE:HG13	1.72	0.72
20:H:123:CYS:SG	46:H:301:SF4:FE2	1.76	0.72
36:m:65:LEU:CD1	41:r:117:LEU:HD21	2.18	0.71
4:F:95:HIS:NE2	4:F:114:CYS:SG	2.64	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:69:ILE:HG13	15:V:100:THR:HG21	1.72	0.71
1:B:379:CYS:SG	46:B:502:SF4:S2	2.88	0.71
41:r:196:ALA:HB1	41:r:197:PRO:HD2	1.72	0.70
33:j:70:ALA:HB2	36:m:59:ILE:HD11	1.72	0.70
6:I:225:PRO:HB2	23:L:87:MET:HG3	1.72	0.70
32:i:236:LYS:HG2	32:i:237:MET:HG3	1.73	0.70
10:N:38:ILE:O	10:N:45:ARG:NH1	2.24	0.69
32:i:252:GLY:HA3	32:i:290:LEU:HD23	1.74	0.69
34:k:18:GLY:O	36:m:23:LYS:NZ	2.21	0.69
35:l:319:ILE:HG13	35:l:399:VAL:HG22	1.75	0.69
2:C:367:ALA:HB3	5:G:149:ASP:HB2	1.75	0.69
26:b:11:ARG:NH2	39:p:207:PRO:O	2.26	0.68
32:i:268:GLN:HA	40:q:165:VAL:HG11	1.73	0.68
25:W:122:GLY:HA3	36:m:126:VAL:HG13	1.74	0.68
24:T:142:LEU:HD11	24:T:151:VAL:HG11	1.76	0.68
4:F:71:ILE:HG23	20:H:110:GLU:HB2	1.75	0.68
2:C:360:GLY:O	25:W:8:GLN:NE2	2.26	0.67
39:p:187:PRO:HB2	39:p:192:ARG:HH21	1.60	0.67
6:I:166:GLN:HE22	41:r:212:ASN:HD22	1.42	0.67
34:k:75:LEU:HD22	36:m:70:TYR:HD2	1.59	0.67
35:l:397:GLU:HG3	35:l:482:MET:HE1	1.76	0.67
33:j:67:LEU:HD22	34:k:65:VAL:HA	1.76	0.67
2:C:146:ASP:HB3	2:C:153:ASN:HD21	1.59	0.66
20:H:77:LEU:HB2	41:r:31:MET:HG2	1.77	0.66
2:C:203:MET:HE2	41:r:32:GLN:HE22	1.60	0.66
22:E:177:LEU:HB2	22:E:185:MET:HE3	1.75	0.66
6:I:165:ARG:NH2	33:j:35:SER:O	2.29	0.66
17:Z:64:ASN:HA	11:X:89:LEU:HD23	1.78	0.66
3:D:148:ASP:N	3:D:148:ASP:OD1	2.28	0.66
15:V:2:ALA:HB2	35:l:601:LEU:HD22	1.77	0.66
1:B:113:LEU:HD13	1:B:149:MET:HE1	1.77	0.66
5:G:387:LEU:HD12	5:G:514:ASN:HB3	1.77	0.66
34:k:31:LEU:CD2	36:m:64:MET:HE1	2.24	0.66
5:G:456:ALA:O	5:G:499:ASN:ND2	2.29	0.66
43:t:22:MET:HG3	43:t:105:GLU:HG3	1.76	0.66
35:l:100:ILE:HG21	35:l:246:LEU:HB2	1.78	0.65
11:O:116:VAL:HG12	11:O:120:MET:HE2	1.78	0.65
42:s:181:GLN:OE1	42:s:196:ARG:NH1	2.28	0.65
3:D:88:ILE:HD13	3:D:143:VAL:HG13	1.79	0.65
4:F:71:ILE:CG1	20:H:110:GLU:HG3	2.25	0.65
29:f:31:ILE:HD12	29:f:32:ARG:HG3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:g:84:MET:HB3	32:i:344:SER:HB3	1.79	0.65
36:m:64:MET:HE2	36:m:67:VAL:HG21	1.79	0.65
37:n:25:CYS:SG	37:n:29:ARG:NH1	2.70	0.65
18:a:82:VAL:HG11	28:e:104:THR:HG21	1.77	0.64
22:E:215:LYS:HE2	22:E:216:PRO:HD2	1.78	0.64
23:L:352:ARG:NH2	23:L:359:SER:OG	2.30	0.64
28:e:150:PRO:HG2	30:g:115:LEU:HD22	1.78	0.64
41:r:134:ARG:NH2	41:r:206:GLU:OE2	2.29	0.64
17:Z:57:LEU:HD21	39:p:88:ALA:HB2	1.78	0.64
34:k:75:LEU:HD22	36:m:70:TYR:CD2	2.33	0.64
14:U:72:LYS:HE2	14:U:162:GLU:HB3	1.79	0.64
1:B:385:CYS:HB3	46:B:502:SF4:S1	2.39	0.63
22:E:39:PHE:HA	22:E:124:ARG:HH12	1.63	0.63
33:j:67:LEU:HD11	34:k:68:ALA:HB3	1.79	0.63
40:q:15:THR:O	40:q:93:LYS:NZ	2.31	0.63
14:U:148:ALA:HB1	14:U:159:VAL:HG11	1.81	0.63
1:B:86:ARG:O	1:B:88:ARG:NH1	2.29	0.63
1:B:425:CYS:SG	46:B:502:SF4:S4	2.97	0.63
12:P:20:ARG:HB2	12:P:66:TRP:HB2	1.81	0.63
1:B:425:CYS:SG	46:B:502:SF4:S2	2.97	0.63
3:D:215:GLU:HG3	23:L:66:ASN:HD22	1.63	0.63
5:G:83:GLU:OE1	5:G:101:ASN:ND2	2.31	0.63
24:T:154:HIS:CD2	24:T:157:ASP:HB2	2.33	0.63
11:X:124:ASP:HB3	39:p:67:ARG:HH22	1.64	0.63
1:B:265:PHE:HB3	1:B:291:GLU:HG3	1.81	0.63
1:B:279:SER:HB3	22:E:181:VAL:HG12	1.79	0.63
5:G:400:ILE:HG13	5:G:427:LEU:HD11	1.81	0.63
12:P:24:CYS:N	12:P:58:CYS:SG	2.72	0.62
39:p:190:GLY:O	39:p:192:ARG:NH2	2.32	0.62
41:r:236:ALA:HA	41:r:263:THR:HG22	1.81	0.62
20:H:142:THR:O	20:H:187:LYS:NZ	2.32	0.62
35:l:214:ILE:HG12	35:l:276:MET:HE1	1.82	0.62
5:G:83:GLU:HG2	5:G:84:LYS:HG3	1.82	0.62
35:l:356:ILE:HA	35:l:359:MET:HE2	1.82	0.62
43:t:112:LYS:NZ	43:t:116:GLU:OE2	2.29	0.62
5:G:69:LEU:O	7:J:158:LYS:NZ	2.33	0.62
25:W:120:MET:HE2	36:m:126:VAL:HG12	1.82	0.62
34:k:80:MET:HE3	36:m:172:THR:HA	1.81	0.62
14:U:258:LEU:HD21	14:U:278:LEU:HD21	1.80	0.62
40:q:266:MET:HE2	40:q:395:LEU:HD12	1.80	0.62
27:d:68:PHE:HB3	37:n:44:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:101:LYS:O	43:t:50:GLN:NE2	2.31	0.61
28:e:98:VAL:HG12	40:q:36:LEU:HB2	1.82	0.61
41:r:24:GLU:HA	41:r:271:LEU:HD13	1.82	0.61
5:G:145:MET:O	9:M:61:ARG:NH1	2.32	0.61
22:E:140:CYS:SG	47:E:301:FES:S1	2.99	0.61
9:M:46:SER:O	9:M:52:ASN:ND2	2.33	0.61
14:U:170:VAL:HG13	14:U:242:ALA:HB3	1.83	0.61
14:U:178:GLN:NE2	14:U:238:ASP:OD2	2.34	0.61
30:g:27:LYS:HG2	30:g:29:THR:H	1.65	0.61
2:C:444:MET:SD	2:C:460:GLN:NE2	2.74	0.61
14:U:88:PHE:HB2	14:U:161:LEU:HD23	1.82	0.61
18:a:179:ILE:HG21	31:h:38:LYS:HG3	1.81	0.61
32:i:128:LEU:HD11	32:i:213:LEU:HD23	1.81	0.61
8:K:127:TYR:O	20:H:186:ASN:ND2	2.31	0.61
18:a:166:GLY:O	18:a:170:GLN:NE2	2.33	0.61
5:G:64:CYS:HB3	5:G:75:CYS:HB3	1.83	0.61
35:l:5:ALA:HB2	35:l:61:MET:HE1	1.82	0.61
32:i:170:LEU:HD22	32:i:291:TYR:HD2	1.65	0.60
35:l:341:MET:HE2	35:l:457:LEU:HD12	1.83	0.60
19:c:118:ASP:O	35:l:535:ARG:NH1	2.33	0.60
22:E:140:CYS:SG	47:E:301:FES:S2	2.99	0.60
2:C:155:GLN:NE2	2:C:315:ASP:OD2	2.32	0.60
9:M:105:GLU:O	20:H:37:THR:N	2.33	0.60
33:j:73:LEU:HD23	41:r:151:LEU:HD12	1.82	0.60
1:B:50:ASP:O	1:B:59:ARG:NH1	2.34	0.60
12:P:18:GLU:HG2	12:P:68:ARG:HB3	1.82	0.60
23:L:60:LEU:HA	23:L:237:ILE:HD11	1.82	0.60
26:b:53:ASP:HA	26:b:57:TRP:HB2	1.83	0.60
25:W:137:THR:HG21	36:m:125:TRP:HB2	1.82	0.60
1:B:40:ARG:NH1	1:B:289:GLU:O	2.35	0.60
23:L:349:ARG:HA	23:L:352:ARG:HD3	1.83	0.60
35:l:141:PHE:HE2	40:q:375:LEU:HD11	1.67	0.60
2:C:386:HIS:ND1	5:G:144:MET:SD	2.72	0.60
22:E:137:THR:HB	47:E:301:FES:S1	2.41	0.60
27:d:109:ARG:NH1	28:e:130:GLU:OE2	2.31	0.60
32:i:96:THR:O	32:i:100:MET:HG2	2.01	0.60
40:q:403:THR:HA	40:q:406:TYR:CE2	2.36	0.60
18:a:189:ASN:ND2	42:s:219:TYR:OH	2.35	0.60
32:i:68:MET:HE2	34:k:36:MET:HB3	1.84	0.60
1:B:248:VAL:O	1:B:251:SER:OG	2.20	0.60
34:k:37:MET:HE3	34:k:67:ALA:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:222:ILE:HA	5:G:225:ILE:HG12	1.84	0.59
11:X:94:ASP:OD1	11:X:94:ASP:N	2.32	0.59
2:C:229:HIS:CD2	6:I:234:PRO:HD3	2.37	0.59
32:i:193:VAL:HG23	32:i:201:THR:HG22	1.84	0.59
1:B:379:CYS:SG	46:B:502:SF4:S4	3.01	0.59
5:G:275:PRO:HG3	5:G:286:ILE:HG12	1.84	0.59
5:G:400:ILE:HD12	5:G:427:LEU:HD21	1.84	0.59
2:C:211:GLU:HG2	6:I:149:PRO:HG2	1.84	0.59
21:S:34:LYS:NZ	21:S:61:HIS:O	2.35	0.59
32:i:44:LEU:HD22	32:i:122:ILE:HG21	1.85	0.59
33:j:71:LEU:O	36:m:147:TYR:OH	2.21	0.59
35:l:184:LEU:HD12	40:q:393:ILE:HG21	1.85	0.59
35:l:88:MET:HE2	35:l:326:PHE:HE2	1.67	0.59
5:G:374:THR:HG22	5:G:532:PRO:HG2	1.85	0.59
36:m:67:VAL:O	36:m:71:THR:HG23	2.03	0.59
1:B:385:CYS:SG	46:B:502:SF4:S1	3.01	0.59
14:U:327:ASP:OD1	40:q:91:ARG:NH2	2.32	0.59
34:k:31:LEU:HD22	36:m:33:LEU:HD12	1.85	0.59
41:r:100:LEU:HD23	41:r:103:LEU:HD12	1.85	0.59
23:L:59:PHE:HD1	23:L:205:GLU:HG2	1.68	0.58
32:i:30:TRP:HZ2	34:k:37:MET:HE1	1.67	0.58
20:H:101:HIS:H	20:H:149:MET:HE1	1.68	0.58
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.38	0.58
5:G:283:GLU:OE2	5:G:420:LYS:NZ	2.30	0.58
23:L:168:ASP:HB3	23:L:171:SER:HB3	1.85	0.58
22:E:66:ILE:HD13	22:E:81:PRO:HB2	1.85	0.58
41:r:185:TRP:HE1	41:r:238:THR:HG22	1.68	0.58
5:G:43:VAL:HG12	5:G:55:LYS:HD2	1.86	0.58
11:X:87:LEU:HB3	11:X:98:LEU:HD11	1.85	0.58
21:S:4:GLU:OE2	41:r:38:ASN:ND2	2.36	0.58
4:F:63:ASN:H	20:H:188:GLU:HG3	1.67	0.58
19:c:153:TYR:H	43:t:5:LEU:HD21	1.67	0.58
32:i:45:MET:HE1	36:m:171:ILE:HG23	1.84	0.58
33:j:54:LYS:HB3	33:j:114:ALA:H	1.69	0.58
18:a:53:ARG:NH2	26:b:29:SER:O	2.37	0.58
27:d:71:VAL:HG11	27:d:87:GLU:HB3	1.86	0.58
33:j:27:LEU:HD23	41:r:59:GLU:HG3	1.86	0.58
35:l:1:MET:SD	35:l:2:ASN:N	2.77	0.58
14:U:40:TYR:HB3	14:U:301:GLN:HE22	1.69	0.58
32:i:72:MET:HE3	32:i:76:ILE:HD11	1.86	0.58
33:j:65:PHE:HB3	41:r:144:VAL:HG11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLY:HA2	22:E:241:PRO:HA	1.86	0.58
2:C:410:LYS:NZ	2:C:461:ASP:OD1	2.37	0.58
11:O:129:GLU:O	11:O:151:LYS:NZ	2.36	0.58
20:H:70:LEU:HG	41:r:272:TRP:CE2	2.39	0.58
32:i:88:LYS:HD2	32:i:148:SER:HB3	1.84	0.58
6:I:192:PRO:HG2	41:r:58:LYS:HE2	1.84	0.57
6:I:193:GLU:HG2	6:I:195:ARG:HD3	1.85	0.57
23:L:122:ILE:HG23	23:L:160:ILE:HB	1.86	0.57
8:K:108:TYR:HE1	20:H:198:GLU:HG2	1.69	0.57
20:H:152:CYS:HG	46:H:301:SF4:FE1	1.18	0.57
41:r:31:MET:HE1	41:r:272:TRP:HA	1.86	0.57
35:l:510:TYR:O	39:p:78:LYS:NZ	2.38	0.57
5:G:163:LYS:NZ	5:G:205:GLN:OE1	2.36	0.57
35:l:183:VAL:HG21	40:q:400:MET:HE1	1.86	0.57
35:l:286:LEU:HD22	35:l:411:MET:HG3	1.85	0.57
7:J:75:ARG:NH2	7:J:119:ASP:OD1	2.38	0.57
18:a:163:ARG:NH1	30:g:102:ASP:OD2	2.34	0.57
33:j:56:PHE:HB2	36:m:70:TYR:OH	2.03	0.57
41:r:138:GLN:NE2	41:r:191:ALA:O	2.28	0.57
24:T:89:ARG:HG3	24:T:90:ILE:HD12	1.86	0.57
11:X:143:GLU:OE2	26:b:9:LYS:NZ	2.37	0.57
19:c:164:ASN:HA	19:c:181:VAL:HB	1.87	0.57
26:b:50:PHE:HB3	26:b:53:ASP:HB2	1.87	0.57
27:d:156:LEU:HD22	27:d:160:LYS:HE2	1.85	0.57
25:W:88:ARG:NH1	25:W:92:GLU:OE2	2.37	0.57
5:G:163:LYS:HG2	5:G:173:MET:HG3	1.86	0.57
6:I:122:ASN:ND2	6:I:254:GLU:O	2.33	0.57
18:a:94:GLY:O	27:d:61:TYR:OH	2.22	0.57
26:b:104:ILE:HB	43:t:48:ASP:HB3	1.87	0.56
32:i:106:LEU:HD22	32:i:187:MET:HE2	1.87	0.56
35:l:341:MET:HE3	35:l:454:ILE:HG12	1.86	0.56
11:O:128:PHE:HZ	11:O:148:ILE:HG12	1.70	0.56
23:L:163:SER:O	49:L:401:NDP:H6N	2.05	0.56
20:H:118:LEU:HD11	20:H:163:PRO:HD3	1.86	0.56
25:W:63:GLU:OE2	42:s:196:ARG:NH2	2.37	0.56
41:r:90:PRO:HD2	41:r:240:ILE:HD13	1.87	0.56
5:G:592:LYS:NZ	5:G:619:ASP:OD2	2.38	0.56
7:J:68:PRO:HG2	7:J:71:HIS:HD2	1.70	0.56
25:W:60:LEU:HD13	42:s:175:ARG:HG2	1.87	0.56
38:o:29:THR:O	38:o:33:GLN:NE2	2.38	0.56
19:c:110:ASP:OD1	19:c:110:ASP:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:71:MET:SD	23:L:249:LYS:NZ	2.79	0.56
33:j:73:LEU:O	41:r:160:TYR:OH	2.21	0.56
5:G:49:VAL:HG13	5:G:102:ILE:HD13	1.86	0.56
32:i:112:HIS:HB2	32:i:184:ILE:HD13	1.88	0.56
2:C:308:LEU:HB2	2:C:407:GLU:HB2	1.86	0.56
11:X:93:ILE:HD11	11:X:110:LEU:HD11	1.88	0.56
3:D:173:MET:HB3	3:D:198:PHE:HB2	1.87	0.56
5:G:68:ARG:HE	5:G:284:GLU:HB2	1.71	0.56
35:l:176:ARG:HG2	40:q:401:MET:HA	1.88	0.56
35:l:419:THR:HA	35:l:422:TYR:CE2	2.40	0.56
36:m:113:VAL:HG13	36:m:119:PHE:HB2	1.87	0.56
2:C:391:TYR:HD1	20:H:122:VAL:HG21	1.71	0.55
14:U:113:ASN:HB2	32:i:312:LYS:HE2	1.88	0.55
23:L:158:LYS:NZ	23:L:248:ILE:O	2.39	0.55
23:L:274:TYR:HB2	23:L:367:ALA:HB2	1.88	0.55
38:o:56:ARG:NH2	40:q:422:HIS:O	2.38	0.55
40:q:122:PHE:HE1	40:q:206:LYS:HG3	1.72	0.55
5:G:323:LEU:HB3	5:G:629:ILE:HD12	1.87	0.55
11:O:123:GLU:OE1	13:Q:67:ARG:NH2	2.40	0.55
22:E:132:ILE:HG13	22:E:188:ILE:HG12	1.87	0.55
11:X:138:LEU:HG	11:X:144:ILE:HG12	1.88	0.55
20:H:73:THR:HG21	41:r:276:SER:HB3	1.88	0.55
35:l:154:LEU:HD12	35:l:247:LEU:HD11	1.88	0.55
2:C:265:GLU:OE2	25:W:23:ARG:NH2	2.40	0.55
2:C:321:GLU:O	2:C:352:GLN:NE2	2.39	0.55
23:L:50:VAL:HG22	23:L:74:GLN:HB3	1.89	0.55
23:L:342:LEU:HA	23:L:361:MET:HE1	1.88	0.55
25:W:108:GLU:O	31:h:75:ARG:NH1	2.40	0.55
20:H:155:CYS:HG	46:H:301:SF4:FE3	1.20	0.55
19:c:184:TYR:HA	43:t:36:GLU:HA	1.88	0.55
22:E:59:ASN:ND2	22:E:89:GLN:OE1	2.38	0.55
28:e:129:ARG:NE	28:e:136:LEU:O	2.40	0.55
1:B:61:ASP:OD1	1:B:137:LYS:NZ	2.40	0.55
16:Y:41:GLU:HG2	16:Y:42:PRO:HD2	1.88	0.55
40:q:193:ILE:HA	40:q:253:LEU:HD21	1.87	0.55
6:I:149:PRO:HA	41:r:34:ARG:HG2	1.88	0.55
20:H:73:THR:HG23	41:r:272:TRP:HE1	1.71	0.55
40:q:306:PRO:HA	40:q:458:LEU:HD22	1.89	0.55
2:C:218:GLU:OE2	9:M:27:ARG:NH1	2.34	0.54
4:F:62:VAL:HA	20:H:188:GLU:HG2	1.89	0.54
15:V:15:GLY:O	15:V:79:GLN:NE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:68:ARG:NH2	25:W:26:PRO:O	2.40	0.54
22:E:180:CYS:SG	47:E:301:FES:S2	3.05	0.54
31:h:105:ARG:NH1	42:s:90:LEU:O	2.34	0.54
34:k:97:GLN:HA	35:l:582:GLY:HA3	1.89	0.54
2:C:222:ARG:NH1	2:C:249:ASP:OD2	2.33	0.54
8:K:34:ARG:NH2	8:K:58:ARG:O	2.41	0.54
9:M:12:ARG:HG2	9:M:20:LEU:HD12	1.90	0.54
23:L:183:GLU:HG3	23:L:195:ILE:HD13	1.89	0.54
18:a:106:VAL:HB	37:n:50:ARG:HH12	1.71	0.54
28:e:79:ASP:HB3	28:e:82:VAL:HG12	1.88	0.54
31:h:86:LEU:HD23	31:h:92:TYR:HB2	1.88	0.54
34:k:27:MET:HE2	36:m:67:VAL:HG13	1.90	0.54
11:O:120:MET:HG2	13:Q:67:ARG:HH21	1.72	0.54
20:H:76:TYR:HA	20:H:79:ARG:HD2	1.89	0.54
29:f:61:GLN:NE2	29:f:65:ASP:OD1	2.41	0.54
40:q:119:TYR:CZ	40:q:161:LEU:HB2	2.42	0.54
42:s:95:VAL:HG12	42:s:97:VAL:HG22	1.89	0.54
20:H:115:ALA:O	20:H:140:ARG:NH2	2.31	0.54
35:l:88:MET:HE2	35:l:326:PHE:CE2	2.43	0.54
35:l:172:ILE:HG21	40:q:408:LEU:HD12	1.90	0.54
35:l:177:ILE:HG12	40:q:401:MET:HE2	1.88	0.54
40:q:104:LEU:HG	40:q:108:MET:HE2	1.89	0.54
1:B:314:LEU:HD11	1:B:317:VAL:HG23	1.89	0.54
5:G:254:MET:HB3	5:G:289:LYS:HD2	1.90	0.54
7:J:84:ARG:HD3	7:J:91:VAL:HG12	1.90	0.54
40:q:339:SER:HB3	40:q:344:LEU:HD22	1.90	0.54
2:C:90:PHE:HB3	2:C:103:LEU:HB3	1.90	0.54
5:G:400:ILE:HG12	5:G:473:MET:HB3	1.90	0.54
13:Q:77:GLN:O	23:L:349:ARG:NH1	2.41	0.54
18:a:147:ALA:HB2	40:q:173:SER:HB2	1.88	0.54
41:r:157:ASN:HA	41:r:168:THR:HG21	1.89	0.54
1:B:160:GLY:O	1:B:199:ARG:NH2	2.41	0.53
5:G:64:CYS:O	5:G:184:ARG:NH2	2.40	0.53
28:e:53:ILE:HG13	28:e:54:ARG:HG2	1.89	0.53
2:C:90:PHE:HB2	2:C:105:MET:HE2	1.90	0.53
27:d:111:LYS:NZ	35:l:200:GLN:OE1	2.41	0.53
40:q:226:ALA:O	40:q:230:VAL:HG22	2.09	0.53
16:Y:65:MET:HE2	35:l:375:ILE:HG12	1.90	0.53
24:T:135:PRO:HB2	25:W:69:ILE:HD11	1.91	0.53
37:n:40:ASN:HD21	37:n:47:ARG:H	1.54	0.53
42:s:208:VAL:HG12	42:s:210:THR:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:U:85:LEU:HD22	14:U:158:GLY:HA3	1.91	0.53
24:T:157:ASP:HB3	24:T:158:PRO:HD2	1.91	0.53
31:h:2:PRO:HD2	32:i:140:SER:HA	1.90	0.53
33:j:75:LEU:HD13	41:r:305:ILE:HD11	1.89	0.53
33:j:19:LEU:HD13	33:j:23:TRP:CD1	2.43	0.53
33:j:106:TRP:CE2	41:r:291:LYS:HD2	2.44	0.53
40:q:315:LEU:HD12	40:q:381:ILE:HD12	1.90	0.53
7:J:84:ARG:NH1	7:J:88:GLN:O	2.41	0.53
16:Y:94:ASP:HB3	16:Y:99:ILE:HB	1.90	0.53
31:h:51:ARG:NH1	42:s:228:ASN:OD1	2.34	0.53
41:r:152:SER:HA	41:r:155:LEU:HD12	1.90	0.53
2:C:43:TRP:CD2	40:q:140:THR:HB	2.44	0.53
3:D:76:VAL:HG22	3:D:86:ILE:HG23	1.90	0.53
32:i:64:ALA:O	32:i:68:MET:HG2	2.08	0.53
32:i:79:LEU:HD23	34:k:47:ILE:HG12	1.91	0.53
32:i:95:MET:HE2	32:i:149:ILE:HA	1.90	0.53
41:r:102:VAL:HG21	41:r:154:LEU:HD11	1.91	0.53
3:D:101:ARG:NH1	3:D:159:VAL:O	2.42	0.53
19:c:166:LEU:HB3	19:c:169:GLU:HB2	1.89	0.53
23:L:59:PHE:CD1	23:L:205:GLU:HG2	2.43	0.53
5:G:284:GLU:OE2	7:J:84:ARG:NH2	2.42	0.53
18:a:139:ILE:HG23	40:q:54:LEU:HD23	1.90	0.53
24:T:136:TYR:HB3	36:m:136:PHE:CZ	2.44	0.53
33:j:42:ASP:N	33:j:42:ASP:OD1	2.40	0.53
41:r:26:LYS:HG2	41:r:36:GLY:HA3	1.90	0.53
41:r:219:PRO:HA	41:r:222:MET:HE3	1.91	0.53
5:G:66:HIS:O	7:J:158:LYS:NZ	2.42	0.53
23:L:278:VAL:O	23:L:352:ARG:NH1	2.33	0.53
28:e:125:LEU:O	28:e:129:ARG:HG2	2.08	0.53
3:D:69:LEU:HD13	3:D:96:VAL:HG22	1.91	0.52
6:I:166:GLN:NE2	41:r:212:ASN:O	2.42	0.52
16:Y:94:ASP:HA	16:Y:99:ILE:HD12	1.91	0.52
18:a:152:LYS:HE2	30:g:96:VAL:HG21	1.90	0.52
20:H:147:ILE:HG22	20:H:190:LEU:HD11	1.91	0.52
22:E:135:CYS:SG	47:E:301:FES:S2	3.07	0.52
30:g:111:TYR:HA	30:g:114:ILE:HG12	1.91	0.52
35:l:97:THR:HG21	35:l:125:LEU:HD22	1.91	0.52
36:m:52:LEU:O	36:m:56:VAL:HG22	2.09	0.52
26:b:80:TRP:HD1	27:d:41:VAL:HG13	1.72	0.52
38:o:14:LEU:HD12	38:o:15:PRO:HD2	1.91	0.52
2:C:300:ARG:NH2	2:C:342:GLU:OE2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:78:ASP:HB3	8:K:81:MET:HG3	1.90	0.52
16:Y:45:ARG:HB3	17:Z:67:TRP:CG	2.44	0.52
32:i:57:THR:HG22	34:k:77:LEU:HB3	1.91	0.52
36:m:170:GLU:OE1	36:m:173:ARG:NH1	2.42	0.52
1:B:385:CYS:CB	46:B:502:SF4:S3	2.96	0.52
5:G:304:GLN:HB2	5:G:316:TYR:HD1	1.74	0.52
6:I:255:LYS:HB3	6:I:258:ARG:HB2	1.90	0.52
27:d:122:ARG:HH21	35:l:206:ASN:HD21	1.57	0.52
33:j:67:LEU:HD21	34:k:68:ALA:HB3	1.90	0.52
11:X:150:ASP:OD2	26:b:16:ARG:NH1	2.40	0.52
32:i:71:MET:HG3	34:k:40:LEU:HD13	1.91	0.52
41:r:18:ALA:O	41:r:21:THR:OG1	2.22	0.52
5:G:341:ILE:HG13	5:G:545:LEU:HD11	1.92	0.52
5:G:519:ILE:HG22	5:G:521:SER:H	1.75	0.52
30:g:106:LYS:O	30:g:108:LYS:NZ	2.40	0.52
35:l:303:ALA:O	35:l:306:THR:OG1	2.21	0.52
7:J:111:LEU:HD11	8:K:126:PRO:HG2	1.92	0.52
1:B:326:LEU:HD23	1:B:367:ILE:HD11	1.92	0.52
7:J:81:VAL:HG21	7:J:150:ARG:HD2	1.92	0.52
12:P:37:ILE:HD13	12:P:55:ILE:HD13	1.92	0.52
19:c:96:ASP:OD1	19:c:96:ASP:N	2.43	0.52
36:m:30:GLY:HA2	36:m:64:MET:SD	2.50	0.52
36:m:64:MET:CE	36:m:67:VAL:HG21	2.39	0.52
12:P:85:ASP:N	12:P:85:ASP:OD1	2.41	0.52
20:H:51:LYS:HG2	25:W:33:TYR:HE2	1.75	0.52
27:d:160:LYS:HZ3	28:e:147:ILE:HG23	1.74	0.52
43:t:106:ARG:HG3	43:t:110:GLN:HE22	1.75	0.52
1:B:315:LEU:HB2	1:B:359:ARG:HA	1.91	0.52
3:D:220:VAL:HG21	13:Q:136:THR:HG21	1.92	0.52
32:i:159:MET:HB2	32:i:278:MET:HE1	1.90	0.52
40:q:94:LEU:O	40:q:98:MET:HG2	2.10	0.52
1:B:111:LYS:O	1:B:152:ARG:N	2.36	0.51
2:C:45:PRO:HG2	32:i:303:THR:HG23	1.91	0.51
15:V:44:LYS:O	15:V:55:ARG:NH1	2.38	0.51
38:o:31:LYS:O	38:o:35:GLU:HG2	2.10	0.51
40:q:116:ILE:HG21	42:s:245:PHE:HB3	1.91	0.51
41:r:26:LYS:HA	41:r:36:GLY:HA3	1.90	0.51
2:C:89:ASN:HB3	33:j:38:GLU:HG3	1.91	0.51
2:C:124:ARG:HG2	6:I:175:THR:HG21	1.91	0.51
3:D:50:ARG:HH21	3:D:80:CYS:HB2	1.73	0.51
41:r:74:ALA:HB3	41:r:75:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:308:ARG:NE	5:G:580:ALA:O	2.32	0.51
7:J:131:LYS:HE3	7:J:147:VAL:HG11	1.91	0.51
26:b:82:ILE:HD11	35:l:13:ILE:HG13	1.93	0.51
2:C:150:MET:SD	2:C:150:MET:N	2.84	0.51
22:E:224:SER:OG	22:E:226:GLU:OE1	2.25	0.51
23:L:68:LEU:HA	23:L:71:MET:HE2	1.92	0.51
27:d:162:ARG:NH1	28:e:140:ASN:OD1	2.44	0.51
31:h:59:GLU:OE2	42:s:222:ARG:NH1	2.42	0.51
35:l:4:PHE:HD2	35:l:61:MET:HE2	1.76	0.51
1:B:263:ALA:HA	1:B:271:SER:HB3	1.91	0.51
5:G:296:GLY:O	5:G:572:HIS:NE2	2.36	0.51
6:I:165:ARG:HD2	41:r:214:GLU:HA	1.93	0.51
22:E:146:ASP:OD1	22:E:146:ASP:N	2.44	0.51
27:d:122:ARG:HH22	35:l:203:MET:HA	1.76	0.51
6:I:259:ILE:O	6:I:263:ARG:HG3	2.11	0.51
14:U:62:ILE:HD13	14:U:275:ILE:HD13	1.93	0.51
26:b:89:HIS:HE2	26:b:96:THR:HB	1.75	0.51
40:q:139:GLN:HG3	40:q:340:ARG:HH22	1.76	0.51
1:B:102:MET:HE1	1:B:111:LYS:HB3	1.93	0.51
1:B:366:ALA:HA	22:E:141:MET:HE1	1.92	0.51
13:Q:48:SER:HB2	13:Q:53:GLU:HB2	1.92	0.51
15:V:22:ALA:O	15:V:26:THR:OG1	2.25	0.51
21:S:19:PRO:HB3	41:r:9:LEU:HD12	1.92	0.51
24:T:151:VAL:HB	42:s:207:LYS:HD3	1.93	0.51
35:l:306:THR:HG22	35:l:336:LYS:HG2	1.91	0.51
1:B:119:GLU:OE2	1:B:127:ASP:N	2.43	0.51
14:U:225:ASN:HD22	14:U:228:GLU:HG3	1.76	0.51
20:H:119:CYS:HB3	46:H:302:SF4:S3	2.50	0.51
28:e:74:HIS:HA	40:q:431:THR:HB	1.93	0.51
34:k:31:LEU:HD21	36:m:64:MET:CE	2.34	0.51
1:B:210:THR:HB	1:B:224:ARG:H	1.76	0.51
3:D:171:TRP:HE1	13:Q:114:MET:HE1	1.76	0.51
19:c:117:VAL:HG11	35:l:539:TYR:HB2	1.93	0.51
26:b:89:HIS:NE2	26:b:96:THR:HB	2.26	0.51
41:r:27:VAL:HG12	41:r:31:MET:HE2	1.93	0.51
41:r:185:TRP:NE1	41:r:238:THR:HG22	2.26	0.51
4:F:36:GLU:OE2	4:F:60:LYS:NZ	2.35	0.51
17:Z:72:GLY:O	35:l:364:LYS:NZ	2.37	0.51
22:E:179:ALA:HB3	22:E:185:MET:SD	2.51	0.51
23:L:278:VAL:HG12	23:L:364:VAL:HG21	1.93	0.51
36:m:17:PHE:HA	36:m:20:PHE:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASN:ND2	1:B:207:GLY:O	2.34	0.50
9:M:39:PRO:HG3	20:H:211:TYR:CZ	2.45	0.50
23:L:283:PHE:CE2	23:L:285:PRO:HG3	2.46	0.50
26:b:83:HIS:NE2	27:d:42:ASP:OD1	2.44	0.50
35:l:129:MET:O	35:l:133:THR:OG1	2.29	0.50
36:m:64:MET:HE2	36:m:64:MET:HA	1.93	0.50
7:J:94:THR:O	7:J:150:ARG:NH2	2.44	0.50
13:Q:142:THR:HA	13:Q:147:LYS:HE3	1.93	0.50
17:Z:58:ARG:NH1	11:X:91:ASP:OD1	2.44	0.50
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.93	0.50
40:q:133:ILE:HD11	40:q:231:LEU:HD11	1.91	0.50
2:C:59:TYR:H	32:i:171:ASN:ND2	2.09	0.50
2:C:362:ILE:HD12	2:C:363:LYS:HG3	1.92	0.50
11:O:113:LEU:HD12	13:Q:94:MET:HE2	1.93	0.50
25:W:43:LEU:HG	41:r:179:TRP:HE1	1.76	0.50
33:j:45:GLY:O	41:r:126:LYS:NZ	2.43	0.50
13:Q:46:ILE:HD13	13:Q:107:LEU:HD13	1.93	0.50
22:E:85:LEU:HG	44:R:87:LEU:HD13	1.92	0.50
26:b:29:SER:OG	26:b:31:ARG:O	2.29	0.50
35:l:100:ILE:O	35:l:104:SER:OG	2.28	0.50
40:q:118:PHE:O	40:q:122:PHE:HB3	2.11	0.50
1:B:211:ALA:HB2	1:B:223:PRO:HG3	1.93	0.50
2:C:374:ARG:NH2	20:H:162:CYS:O	2.29	0.50
5:G:49:VAL:HB	5:G:91:ALA:HA	1.93	0.50
11:O:117:GLU:HA	11:O:120:MET:HE3	1.94	0.50
18:a:55:PHE:O	39:p:217:ARG:NH2	2.45	0.50
28:e:106:VAL:HG22	40:q:453:MET:HE3	1.93	0.50
32:i:111:PHE:HA	35:l:591:PHE:CE1	2.47	0.50
41:r:198:PHE:CD1	41:r:285:LEU:HD13	2.47	0.50
30:g:36:MET:HE2	32:i:339:MET:HE2	1.94	0.50
40:q:70:THR:HA	40:q:103:GLN:HE21	1.75	0.50
41:r:195:ARG:HH12	41:r:274:ARG:HB2	1.77	0.50
42:s:187:CYS:SG	42:s:188:VAL:N	2.84	0.50
42:s:188:VAL:HG13	42:s:194:TRP:HB2	1.93	0.50
43:t:103:GLU:OE2	43:t:106:ARG:NH1	2.44	0.50
2:C:386:HIS:NE2	5:G:149:ASP:HA	2.27	0.50
21:S:68:ASN:HD22	42:s:96:LYS:HB3	1.77	0.50
22:E:149:LEU:HG	22:E:153:GLN:HE21	1.76	0.50
32:i:30:TRP:CZ2	34:k:37:MET:HE1	2.47	0.50
41:r:197:PRO:HG3	41:r:277:TYR:HB2	1.94	0.50
1:B:385:CYS:HG	46:B:502:SF4:FE2	1.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:64:TYR:OH	3:D:103:HIS:NE2	2.34	0.50
5:G:249:GLU:HB2	7:J:78:ARG:HH12	1.77	0.50
1:B:161:GLU:OE1	1:B:161:GLU:N	2.44	0.49
11:O:114:ASP:OD1	13:Q:90:ARG:NH1	2.44	0.49
14:U:98:SER:HA	14:U:103:GLY:HA2	1.92	0.49
16:Y:54:GLN:NE2	35:l:367:PRO:HD2	2.27	0.49
10:N:40:LYS:HA	10:N:45:ARG:HD3	1.94	0.49
30:g:51:ARG:HD3	32:i:322:GLN:HE21	1.77	0.49
35:l:324:LEU:HD22	35:l:395:ILE:HG13	1.94	0.49
2:C:263:GLU:OE2	20:H:79:ARG:NH2	2.45	0.49
2:C:381:MET:HE2	5:G:124:HIS:HD2	1.78	0.49
12:P:65:LEU:HB2	12:P:79:LEU:HD11	1.94	0.49
27:d:142:ARG:NH2	27:d:143:TYR:OH	2.45	0.49
35:l:315:VAL:O	35:l:319:ILE:HG12	2.12	0.49
38:o:115:LEU:HB3	38:o:121:LEU:HB2	1.93	0.49
24:T:154:HIS:NE2	24:T:157:ASP:O	2.45	0.49
11:X:119:ILE:HG21	11:X:135:ALA:HB1	1.94	0.49
34:k:79:VAL:HG12	36:m:74:MET:HE3	1.95	0.49
35:l:12:LEU:HD22	35:l:129:MET:HB3	1.94	0.49
1:B:384:PRO:HB2	1:B:423:THR:HG22	1.95	0.49
2:C:46:ASP:HA	28:e:54:ARG:NH2	2.27	0.49
22:E:134:VAL:HG22	22:E:186:VAL:HG12	1.95	0.49
32:i:337:LEU:O	32:i:340:THR:HG23	2.11	0.49
1:B:223:PRO:HG2	1:B:425:CYS:HB3	1.94	0.49
3:D:242:PHE:HE1	9:M:60:ARG:HG2	1.77	0.49
5:G:183:ILE:HD11	5:G:206:VAL:HG13	1.95	0.49
21:S:12:MET:HE3	41:r:264:LEU:HD22	1.95	0.49
22:E:177:LEU:HB2	22:E:185:MET:CE	2.41	0.49
23:L:294:ARG:HH21	23:L:311:ARG:HH21	1.60	0.49
25:W:57:ARG:NH1	41:r:168:THR:HG22	2.28	0.49
25:W:70:ALA:HB2	42:s:202:LEU:HD13	1.94	0.49
27:d:85:MET:HE1	40:q:182:TRP:CD1	2.47	0.49
32:i:200:MET:HG3	32:i:269:GLU:HG3	1.95	0.49
36:m:64:MET:HE2	36:m:67:VAL:CG2	2.43	0.49
40:q:71:TRP:HH2	40:q:439:LEU:HD22	1.78	0.49
5:G:340:ALA:HB1	5:G:354:LEU:HD21	1.95	0.49
6:I:165:ARG:HD3	41:r:61:LEU:HD11	1.94	0.49
24:T:163:LEU:HD23	42:s:200:GLY:HA3	1.95	0.49
43:t:33:GLU:OE1	43:t:35:LYS:NZ	2.46	0.49
5:G:379:THR:HG21	5:G:526:LEU:HD22	1.94	0.49
26:b:22:TRP:O	26:b:26:GLN:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:173:LEU:HD13	40:q:405:LEU:HD11	1.95	0.49
35:l:193:SER:O	35:l:200:GLN:NE2	2.45	0.49
16:Y:84:PHE:HE1	26:b:126:GLN:HE21	1.61	0.49
21:S:54:ILE:HD12	42:s:96:LYS:HA	1.95	0.49
27:d:107:GLN:OE1	35:l:194:ASN:ND2	2.41	0.49
33:j:38:GLU:HB3	33:j:41:PHE:O	2.13	0.49
1:B:62:TRP:HE1	1:B:136:HIS:HB3	1.78	0.48
2:C:163:LYS:HG3	3:D:48:ARG:NH1	2.28	0.48
2:C:381:MET:HE3	2:C:385:ILE:HG13	1.95	0.48
3:D:91:ASP:OD2	13:Q:44:LYS:NZ	2.46	0.48
5:G:624:ARG:NH2	5:G:637:ASP:OD1	2.45	0.48
17:Z:73:PHE:CG	35:l:435:PRO:HG3	2.48	0.48
11:X:115:GLN:O	11:X:118:ILE:HG13	2.13	0.48
32:i:106:LEU:O	32:i:135:LYS:NZ	2.44	0.48
41:r:307:LEU:HA	41:r:310:MET:HG2	1.95	0.48
2:C:232:TYR:OH	2:C:240:GLN:O	2.30	0.48
41:r:86:TRP:NE1	41:r:233:MET:HB2	2.29	0.48
4:F:59:GLN:NE2	4:F:61:GLU:OE1	2.45	0.48
41:r:87:VAL:HG12	41:r:96:ILE:HB	1.95	0.48
5:G:422:TRP:HA	5:G:427:LEU:H	1.77	0.48
22:E:222:ARG:NH2	22:E:226:GLU:O	2.46	0.48
24:T:153:SER:HB3	42:s:207:LYS:HB2	1.95	0.48
24:T:154:HIS:CG	24:T:157:ASP:HB2	2.47	0.48
25:W:84:LEU:HD12	42:s:134:LEU:HD21	1.96	0.48
25:W:124:LEU:HD12	36:m:130:THR:HG21	1.94	0.48
26:b:85:TYR:HE2	35:l:65:ASN:HB2	1.77	0.48
26:b:93:LYS:HB3	26:b:96:THR:HG21	1.96	0.48
32:i:231:SER:O	32:i:234:TRP:HD1	1.97	0.48
41:r:196:ALA:C	41:r:198:PHE:H	2.21	0.48
3:D:115:THR:OG1	3:D:116:ALA:N	2.46	0.48
5:G:488:ALA:HB2	5:G:677:GLN:HB3	1.95	0.48
6:I:147:ALA:HA	6:I:153:MET:HG2	1.95	0.48
8:K:113:HIS:CE1	20:H:196:LYS:HD3	2.48	0.48
11:O:103:HIS:HB3	11:O:106:LYS:HB2	1.95	0.48
32:i:222:SER:HB2	32:i:233:THR:HG21	1.95	0.48
38:o:39:ILE:HG23	38:o:42:ARG:HH21	1.78	0.48
39:p:98:ASP:HB3	39:p:101:LYS:HB2	1.95	0.48
40:q:106:LEU:HD13	40:q:234:VAL:HG11	1.96	0.48
40:q:358:TRP:CE3	40:q:441:ILE:HD12	2.49	0.48
1:B:205:ILE:HG12	1:B:379:CYS:HB3	1.96	0.48
25:W:110:VAL:HG22	31:h:71:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:23:GLN:HE21	43:t:73:SER:HB3	1.79	0.48
32:i:183:SER:O	32:i:187:MET:HG2	2.14	0.48
41:r:207:LEU:O	41:r:209:SER:N	2.46	0.48
41:r:267:THR:O	41:r:271:LEU:HG	2.13	0.48
3:D:124:ASN:HD21	10:N:108:PRO:HG2	1.79	0.48
32:i:128:LEU:HD13	32:i:216:PHE:HB2	1.95	0.48
32:i:211:MET:HG2	32:i:333:SER:HB2	1.95	0.48
42:s:175:ARG:H	42:s:175:ARG:HG3	1.43	0.48
2:C:44:GLN:OE1	32:i:304:MET:HB2	2.14	0.48
4:F:71:ILE:H	4:F:71:ILE:HG13	1.55	0.48
22:E:198:PRO:O	22:E:202:GLU:HG2	2.14	0.48
23:L:233:GLN:NE2	23:L:262:GLY:O	2.39	0.48
32:i:31:ILE:HD11	34:k:62:ILE:HG21	1.95	0.48
18:a:130:GLU:O	18:a:134:GLU:HG2	2.14	0.48
21:S:55:SER:HB2	21:S:62:VAL:HG13	1.96	0.48
31:h:15:ASP:OD1	31:h:15:ASP:N	2.45	0.48
5:G:42:MET:O	5:G:55:LYS:NZ	2.46	0.48
32:i:193:VAL:HG13	32:i:266:ILE:HG23	1.96	0.48
32:i:228:LEU:O	32:i:231:SER:OG	2.29	0.48
35:l:118:PHE:O	35:l:122:VAL:HG23	2.13	0.48
36:m:26:PRO:HB2	36:m:71:THR:CG2	2.44	0.48
40:q:41:LEU:O	40:q:44:GLN:NE2	2.46	0.48
41:r:139:THR:HA	41:r:142:TYR:CE2	2.49	0.48
2:C:194:THR:HB	2:C:206:PHE:HA	1.96	0.47
5:G:169:VAL:HG21	5:G:222:ILE:HD11	1.96	0.47
11:O:100:VAL:HG12	11:O:142:GLN:HB2	1.96	0.47
35:l:154:LEU:HD13	35:l:243:VAL:HG22	1.96	0.47
35:l:321:GLN:HG2	35:l:324:LEU:HD12	1.96	0.47
37:n:39:ARG:HH11	37:n:57:TRP:HA	1.80	0.47
2:C:257:PHE:HD2	2:C:347:LEU:HD11	1.78	0.47
12:P:58:CYS:HB2	12:P:61:VAL:HG12	1.96	0.47
14:U:357:LYS:HE3	29:f:36:HIS:HB2	1.95	0.47
23:L:129:TRP:CZ2	23:L:306:GLU:HG2	2.49	0.47
31:h:15:ASP:HB2	32:i:25:HIS:HB2	1.96	0.47
3:D:88:ILE:HG12	3:D:96:VAL:HG21	1.96	0.47
5:G:405:THR:HB	5:G:477:GLY:HA3	1.94	0.47
16:Y:97:LEU:O	43:t:104:ARG:NH1	2.43	0.47
22:E:186:VAL:HG22	22:E:196:LEU:HD11	1.96	0.47
28:e:54:ARG:HH21	32:i:306:PRO:HB3	1.78	0.47
32:i:93:VAL:HG13	35:l:599:MET:HE1	1.95	0.47
42:s:122:LEU:HD22	42:s:208:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:s:160:THR:HA	42:s:163:TRP:NE1	2.29	0.47
2:C:284:VAL:HG22	2:C:444:MET:HG2	1.95	0.47
3:D:43:THR:O	3:D:44:ARG:HB2	2.14	0.47
16:Y:55:LEU:HD23	35:l:367:PRO:HG3	1.96	0.47
21:S:37:ARG:HD2	21:S:48:MET:HG2	1.95	0.47
22:E:183:ALA:HB1	22:E:184:PRO:HD2	1.95	0.47
23:L:106:LYS:HE3	23:L:134:PHE:CE1	2.48	0.47
27:d:82:ILE:HD12	27:d:83:LEU:HG	1.96	0.47
33:j:21:ALA:HB1	41:r:218:GLY:HA3	1.96	0.47
40:q:1:MET:HE2	40:q:111:THR:HG21	1.96	0.47
40:q:105:PHE:O	40:q:109:THR:HG23	2.15	0.47
41:r:228:TYR:O	41:r:232:ILE:HG13	2.14	0.47
1:B:117:ALA:HB3	1:B:158:ILE:HA	1.96	0.47
1:B:209:GLU:OE2	1:B:226:LYS:NZ	2.38	0.47
1:B:283:ASN:ND2	1:B:305:GLY:O	2.47	0.47
2:C:309:ARG:HG3	2:C:407:GLU:HB3	1.96	0.47
5:G:58:MET:HE2	5:G:104:THR:HB	1.97	0.47
13:Q:96:ASN:HB2	48:Q:201:ZMP:H14	1.97	0.47
17:Z:69:TYR:CD2	35:l:434:LYS:HG2	2.50	0.47
23:L:121:VAL:HG23	23:L:156:VAL:HG11	1.96	0.47
19:c:58:ARG:NH2	19:c:60:GLU:OE1	2.47	0.47
33:j:1:MET:SD	33:j:1:MET:N	2.79	0.47
41:r:196:ALA:O	41:r:198:PHE:N	2.47	0.47
18:a:90:ASN:O	27:d:56:HIS:NE2	2.41	0.47
20:H:155:CYS:SG	46:H:301:SF4:S1	3.13	0.47
26:b:110:ILE:HG22	26:b:111:LEU:HD13	1.97	0.47
32:i:57:THR:HA	34:k:77:LEU:HD13	1.95	0.47
35:l:289:ALA:HB1	35:l:418:LEU:HB2	1.96	0.47
35:l:293:ILE:HD11	35:l:418:LEU:HD22	1.96	0.47
41:r:65:THR:O	41:r:124:ASN:ND2	2.42	0.47
41:r:175:ILE:HB	41:r:242:PHE:HB3	1.97	0.47
43:t:22:MET:HE1	43:t:102:PHE:CD2	2.50	0.47
15:V:62:THR:HG22	15:V:104:ARG:HE	1.80	0.47
22:E:66:ILE:HD11	44:R:87:LEU:HD22	1.97	0.47
27:d:115:GLN:HG2	35:l:62:ILE:HG22	1.97	0.47
32:i:221:HIS:HA	32:i:321:LYS:HZ2	1.80	0.47
39:p:68:HIS:CE1	39:p:117:GLN:HG3	2.50	0.47
42:s:160:THR:HA	42:s:163:TRP:CD1	2.50	0.47
1:B:129:GLU:OE1	1:B:132:ARG:NH2	2.43	0.47
5:G:166:GLY:HA2	5:G:213:MET:HG3	1.95	0.47
6:I:258:ARG:HB3	6:I:262:ARG:HH21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:168:GLY:O	32:i:172:GLN:HG2	2.15	0.47
32:i:215:MET:HE1	32:i:244:MET:HE3	1.97	0.47
32:i:298:TYR:HA	32:i:302:LEU:HB2	1.97	0.47
36:m:164:GLY:O	36:m:168:ILE:HG12	2.15	0.47
42:s:154:HIS:HB3	42:s:191:LYS:HB3	1.97	0.47
43:t:61:HIS:O	43:t:65:GLN:NE2	2.47	0.47
2:C:267:MET:HE1	41:r:276:SER:HA	1.97	0.47
3:D:152:PRO:HB3	3:D:177:PHE:HD2	1.79	0.47
27:d:38:ASP:HA	27:d:42:ASP:HB2	1.97	0.47
2:C:265:GLU:OE1	25:W:23:ARG:NE	2.47	0.46
5:G:697:THR:O	5:G:702:ARG:NH1	2.47	0.46
18:a:102:PRO:HG2	18:a:105:TYR:HB3	1.96	0.46
19:c:78:LEU:HB2	19:c:106:HIS:CD2	2.50	0.46
20:H:201:ILE:O	20:H:205:ILE:HG12	2.15	0.46
30:g:16:LEU:HD13	30:g:16:LEU:HA	1.82	0.46
34:k:2:PRO:HG3	36:m:127:ILE:HD13	1.97	0.46
2:C:167:ILE:HD13	2:C:369:VAL:HG11	1.97	0.46
6:I:165:ARG:HA	6:I:192:PRO:HD3	1.98	0.46
7:J:64:LEU:HD13	13:Q:107:LEU:HD23	1.97	0.46
33:j:79:SER:HA	33:j:87:MET:HE2	1.97	0.46
34:k:75:LEU:O	34:k:79:VAL:HG13	2.15	0.46
35:l:208:CYS:SG	35:l:266:LEU:HB3	2.55	0.46
36:m:28:TYR:HA	36:m:31:LEU:HD21	1.97	0.46
40:q:231:LEU:HA	40:q:235:LEU:HB2	1.98	0.46
2:C:215:LYS:NZ	9:M:25:GLN:O	2.35	0.46
2:C:365:ASP:OD2	5:G:150:ARG:NH1	2.36	0.46
5:G:59:GLN:NE2	7:J:89:SER:O	2.49	0.46
9:M:15:ALA:HB3	20:H:75:SER:HB2	1.98	0.46
11:O:111:ASP:N	11:O:111:ASP:OD1	2.47	0.46
20:H:171:PRO:HG3	20:H:200:GLU:CD	2.40	0.46
23:L:298:ARG:HB2	23:L:311:ARG:HD2	1.98	0.46
35:l:298:ILE:O	35:l:302:VAL:HG23	2.15	0.46
6:I:129:LEU:O	6:I:158:VAL:HA	2.16	0.46
27:d:167:ARG:HD3	28:e:149:LEU:HD23	1.98	0.46
36:m:26:PRO:HB2	36:m:71:THR:HG22	1.97	0.46
40:q:108:MET:HB3	40:q:121:LEU:HD13	1.96	0.46
40:q:334:TYR:CD1	40:q:340:ARG:HG3	2.51	0.46
41:r:113:VAL:CG1	41:r:139:THR:HG21	2.44	0.46
5:G:338:VAL:O	5:G:363:SER:OG	2.33	0.46
11:O:134:ASP:N	11:O:134:ASP:OD1	2.46	0.46
32:i:270:MET:HE1	32:i:278:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:3:LEU:HD11	36:m:107:ALA:HB1	1.98	0.46
40:q:11:LEU:HB3	40:q:100:ILE:HD13	1.96	0.46
40:q:16:TRP:NE1	40:q:97:THR:HG21	2.31	0.46
40:q:267:TRP:O	40:q:271:MET:HG2	2.15	0.46
40:q:325:MET:SD	40:q:441:ILE:HG13	2.55	0.46
1:B:290:GLU:OE1	1:B:303:HIS:NE2	2.48	0.46
37:n:54:GLU:OE1	37:n:54:GLU:N	2.47	0.46
40:q:179:ILE:HG12	40:q:249:ILE:HG21	1.98	0.46
6:I:182:PRO:HB3	13:Q:127:THR:HG21	1.97	0.46
7:J:109:ASN:HD22	7:J:112:MET:H	1.64	0.46
13:Q:127:THR:O	13:Q:131:ARG:HG3	2.16	0.46
32:i:28:LEU:HD23	32:i:31:ILE:HD12	1.98	0.46
34:k:25:HIS:CE1	34:k:89:TYR:HE1	2.33	0.46
34:k:76:SER:O	34:k:79:VAL:HG22	2.14	0.46
35:l:155:ILE:HD11	35:l:248:HIS:CE1	2.51	0.46
35:l:399:VAL:HG12	35:l:409:LEU:HG	1.98	0.46
35:l:414:ILE:O	35:l:418:LEU:HG	2.16	0.46
36:m:68:PHE:HZ	41:r:121:TRP:HB2	1.81	0.46
12:P:44:LEU:HD21	12:P:95:LEU:HD11	1.96	0.46
16:Y:88:ASP:HB2	16:Y:91:GLN:HB3	1.97	0.46
19:c:58:ARG:NE	19:c:61:ASP:OD2	2.48	0.46
11:X:117:GLU:OE2	39:p:62:TYR:OH	2.33	0.46
35:l:248:HIS:HA	35:l:253:VAL:HG13	1.98	0.46
5:G:58:MET:HG2	5:G:104:THR:HG21	1.96	0.46
6:I:142:GLU:HG2	6:I:235:PRO:O	2.16	0.46
8:K:91:HIS:CE1	20:H:90:LYS:HD2	2.50	0.46
14:U:311:THR:HG22	32:i:310:ASN:HB2	1.98	0.46
14:U:311:THR:HG21	32:i:311:MET:HG2	1.97	0.46
19:c:126:TRP:HZ3	35:l:535:ARG:HD2	1.80	0.46
23:L:310:THR:H	23:L:313:LYS:HB3	1.81	0.46
27:d:75:THR:O	30:g:110:THR:OG1	2.30	0.46
3:D:185:ARG:HA	13:Q:114:MET:HE3	1.98	0.46
3:D:187:ILE:HG23	3:D:188:LEU:HG	1.98	0.46
11:O:74:LEU:HB3	11:O:154:VAL:HG21	1.98	0.46
14:U:64:VAL:HG12	14:U:72:LYS:HB2	1.98	0.46
27:d:73:ASP:OD1	27:d:73:ASP:N	2.48	0.46
34:k:62:ILE:HG13	36:m:157:THR:HG21	1.97	0.46
35:l:415:ALA:O	35:l:419:THR:HG23	2.16	0.46
40:q:196:TRP:CD1	40:q:250:LEU:HB3	2.51	0.46
40:q:231:LEU:O	40:q:236:LEU:HG	2.16	0.46
2:C:126:THR:HG22	6:I:210:TYR:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:266:GLU:OE2	20:H:68:ARG:NE	2.49	0.45
5:G:422:TRP:CE3	5:G:440:TYR:HB2	2.51	0.45
14:U:67:ASN:HB3	14:U:216:ILE:HD13	1.99	0.45
18:a:156:VAL:HG21	30:g:92:MET:HG3	1.99	0.45
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.98	0.45
39:p:202:GLU:OE1	39:p:203:GLY:N	2.49	0.45
40:q:290:SER:HA	40:q:319:HIS:HE2	1.81	0.45
43:t:111:ARG:HH22	43:t:115:ARG:NH2	2.13	0.45
1:B:128:ARG:NH2	22:E:194:GLU:OE2	2.49	0.45
4:F:47:ASP:OD1	4:F:47:ASP:N	2.48	0.45
16:Y:45:ARG:HH22	11:X:86:VAL:HG22	1.80	0.45
22:E:129:LYS:HB3	22:E:168:LEU:HD23	1.98	0.45
23:L:67:HIS:HB3	23:L:245:ILE:HG13	1.99	0.45
24:T:110:ILE:HG21	41:r:300:LEU:HD23	1.99	0.45
25:W:23:ARG:HG3	25:W:25:LEU:HD13	1.97	0.45
25:W:53:TRP:NE1	25:W:57:ARG:HD2	2.31	0.45
33:j:38:GLU:HB2	33:j:43:PRO:HG3	1.97	0.45
40:q:127:VAL:HB	40:q:128:PRO:HD3	1.99	0.45
40:q:303:ILE:HG22	40:q:305:THR:HG23	1.98	0.45
5:G:185:PHE:CZ	5:G:221:ASN:HB2	2.51	0.45
5:G:574:ASP:OD2	5:G:702:ARG:NE	2.38	0.45
6:I:194:PRO:HB3	6:I:256:ARG:HH12	1.81	0.45
14:U:131:TYR:CD1	14:U:185:CYS:HB3	2.52	0.45
14:U:325:GLN:HB2	28:e:57:GLU:HG2	1.99	0.45
20:H:85:ASN:O	20:H:89:GLU:N	2.46	0.45
27:d:106:ILE:HG13	27:d:135:VAL:HG21	1.98	0.45
1:B:382:CYS:SG	46:B:502:SF4:S2	3.14	0.45
2:C:124:ARG:HD2	6:I:210:TYR:CE2	2.51	0.45
2:C:448:HIS:HB3	2:C:452:ASP:HB2	1.97	0.45
15:V:9:TYR:CZ	15:V:21:LYS:HE3	2.51	0.45
5:G:611:THR:HG21	7:J:105:GLU:HA	1.99	0.45
14:U:255:CYS:HA	14:U:282:LYS:HB3	1.98	0.45
27:d:26:LEU:HD12	43:t:76:ASN:HB2	1.99	0.45
30:g:13:LEU:O	31:h:9:ARG:NH1	2.49	0.45
35:l:562:LEU:HB2	35:l:563:PRO:CD	2.38	0.45
40:q:334:TYR:O	40:q:338:HIS:N	2.47	0.45
5:G:306:MET:HB2	5:G:583:ILE:HB	1.98	0.45
32:i:77:ASN:O	32:i:81:SER:OG	2.27	0.45
41:r:179:TRP:CG	41:r:180:PRO:HD3	2.52	0.45
5:G:360:ARG:NH2	5:G:635:PRO:HD3	2.32	0.45
21:S:70:ASP:OD2	42:s:149:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:201:ILE:HA	23:L:235:VAL:O	2.17	0.45
35:l:545:SER:OG	40:q:274:SER:O	2.22	0.45
39:p:68:HIS:HE1	39:p:117:GLN:HG3	1.82	0.45
39:p:187:PRO:HG2	39:p:192:ARG:HE	1.81	0.45
41:r:209:SER:HB3	41:r:213:VAL:HA	1.98	0.45
5:G:485:ASP:HB3	5:G:680:LEU:HG	1.98	0.45
15:V:3:LYS:HG2	15:V:7:HIS:CD2	2.51	0.45
25:W:95:ALA:HA	25:W:106:VAL:HG11	1.98	0.45
29:f:66:VAL:HG12	29:f:70:LYS:HE3	1.99	0.45
33:j:72:LEU:O	41:r:151:LEU:HD11	2.16	0.45
41:r:178:SER:HB2	41:r:181:LEU:HB2	1.98	0.45
5:G:221:ASN:ND2	5:G:285:TRP:HB3	2.32	0.45
5:G:677:GLN:HG2	5:G:678:GLN:H	1.82	0.45
20:H:148:ASP:HB2	20:H:150:THR:HG22	1.99	0.45
28:e:54:ARG:HD3	28:e:56:GLN:HB2	1.97	0.45
39:p:56:GLN:HB3	39:p:60:ARG:HH21	1.82	0.45
40:q:208:PRO:HD3	40:q:236:LEU:HD22	1.99	0.45
7:J:169:ARG:CZ	7:J:169:ARG:HB3	2.46	0.45
14:U:329:VAL:HG12	32:i:315:TRP:HZ3	1.82	0.45
16:Y:54:GLN:HG2	35:l:367:PRO:HG2	1.99	0.45
31:h:105:ARG:NH2	42:s:94:GLU:OE2	2.46	0.45
41:r:149:ILE:HG21	41:r:185:TRP:HB2	1.99	0.45
2:C:262:ASP:OD1	2:C:344:ARG:NH2	2.41	0.44
3:D:75:GLN:NE2	3:D:77:GLN:HE21	2.15	0.44
11:O:115:GLN:NE2	11:O:135:ALA:O	2.49	0.44
20:H:74:LEU:HB2	41:r:272:TRP:CZ2	2.52	0.44
22:E:182:ASN:HB3	22:E:194:GLU:HB3	1.99	0.44
25:W:108:GLU:HB3	31:h:75:ARG:HH22	1.82	0.44
35:l:149:ILE:HD13	35:l:149:ILE:HA	1.76	0.44
18:a:133:TYR:OH	27:d:87:GLU:OE1	2.33	0.44
22:E:68:LYS:HE2	22:E:68:LYS:HB3	1.84	0.44
24:T:152:PRO:HB2	24:T:154:HIS:NE2	2.32	0.44
35:l:568:PHE:O	35:l:572:LYS:HG2	2.17	0.44
41:r:293:PHE:O	41:r:297:THR:HG23	2.16	0.44
43:t:108:LEU:HA	43:t:111:ARG:HG2	1.99	0.44
1:B:204:TYR:HB3	1:B:377:GLU:HB3	1.99	0.44
2:C:143:ASP:HB3	2:C:229:HIS:ND1	2.32	0.44
10:N:72:LEU:HD13	10:N:80:VAL:HG11	1.99	0.44
23:L:56:ALA:HB3	23:L:77:VAL:HG13	1.99	0.44
39:p:181:GLN:NE2	39:p:198:PRO:O	2.49	0.44
40:q:65:LEU:O	40:q:69:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:s:92:VAL:HG22	42:s:138:LYS:HG2	1.99	0.44
5:G:127:ASP:O	5:G:131:CYS:N	2.49	0.44
5:G:197:THR:HG22	5:G:206:VAL:HG22	1.98	0.44
6:I:174:GLY:HA2	46:I:301:SF4:S3	2.57	0.44
20:H:50:MET:HE2	24:T:95:LYS:HE2	1.99	0.44
26:b:83:HIS:ND1	35:l:6:SER:OG	2.44	0.44
32:i:137:ALA:HB3	32:i:138:PRO:HD3	2.00	0.44
32:i:340:THR:N	32:i:341:PRO:HD2	2.32	0.44
3:D:213:ASP:HB3	3:D:216:VAL:HG22	1.99	0.44
13:Q:107:LEU:HD12	13:Q:107:LEU:HA	1.83	0.44
14:U:95:TYR:O	14:U:98:SER:OG	2.29	0.44
24:T:141:PRO:HG3	42:s:118:LYS:HD2	2.00	0.44
27:d:28:ASN:HA	43:t:75:PRO:HG3	2.00	0.44
32:i:45:MET:HG3	32:i:56:ALA:HB2	2.00	0.44
35:l:21:MET:O	35:l:24:SER:OG	2.32	0.44
2:C:204:THR:OG1	41:r:275:ALA:O	2.33	0.44
2:C:250:ILE:HG22	2:C:354:LEU:HD11	2.00	0.44
2:C:402:THR:OG1	3:D:83:GLU:OE2	2.35	0.44
3:D:173:MET:HE3	3:D:188:LEU:HB2	1.99	0.44
5:G:692:LYS:HD3	5:G:715:THR:HG22	1.99	0.44
8:K:39:VAL:HG21	8:K:89:TRP:CZ2	2.53	0.44
16:Y:100:LEU:H	16:Y:100:LEU:HD23	1.82	0.44
18:a:187:PRO:HA	42:s:125:TRP:CE2	2.52	0.44
19:c:115:ASN:HA	35:l:166:THR:HG22	2.00	0.44
21:S:14:ALA:O	21:S:18:ILE:HG13	2.17	0.44
21:S:54:ILE:HG22	21:S:64:LYS:HG3	1.98	0.44
23:L:59:PHE:CZ	23:L:237:ILE:HB	2.52	0.44
28:e:115:GLN:HE22	40:q:452:LYS:HE2	1.83	0.44
37:n:3:ASN:HB2	37:n:6:GLN:HG3	2.00	0.44
40:q:318:ALA:HB1	40:q:374:ASN:CG	2.41	0.44
40:q:398:MET:O	40:q:402:ILE:HG13	2.17	0.44
43:t:29:TYR:O	43:t:104:ARG:NH2	2.50	0.44
1:B:98:LYS:NZ	45:B:501:FMN:O3P	2.44	0.44
5:G:213:MET:HE1	5:G:713:ALA:HB1	2.00	0.44
14:U:61:VAL:HG23	14:U:152:LEU:HD22	1.99	0.44
19:c:110:ASP:OD2	40:q:278:ARG:NE	2.41	0.44
19:c:125:SER:O	19:c:129:MET:HG3	2.18	0.44
32:i:298:TYR:O	32:i:303:THR:HG22	2.18	0.44
33:j:54:LYS:HD2	33:j:114:ALA:HA	1.99	0.44
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.98	0.44
40:q:457:PRO:HG2	40:q:458:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:r:113:VAL:HG11	41:r:139:THR:HG21	2.00	0.44
41:r:310:MET:HG3	41:r:311:THR:HG23	2.00	0.44
7:J:112:MET:SD	8:K:126:PRO:HB2	2.57	0.44
14:U:345:TYR:HD1	14:U:354:ILE:HG23	1.83	0.44
15:V:114:ALA:O	15:V:118:MET:HB2	2.17	0.44
20:H:63:TRP:CH2	41:r:183:MET:HB3	2.52	0.44
24:T:127:ALA:HB2	41:r:312:ALA:HA	2.00	0.44
32:i:139:LEU:HD11	32:i:187:MET:HE1	2.00	0.44
33:j:21:ALA:CB	41:r:218:GLY:HA3	2.48	0.44
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.99	0.44
35:l:557:TRP:CZ2	38:o:87:SER:HA	2.53	0.44
39:p:67:ARG:HA	39:p:67:ARG:HD3	1.84	0.44
41:r:114:TYR:HA	41:r:117:LEU:HB2	1.99	0.44
41:r:172:ILE:HD11	41:r:176:PHE:HB2	2.00	0.44
1:B:385:CYS:CB	46:B:502:SF4:S1	3.06	0.44
5:G:347:ASP:HB3	5:G:594:ALA:HB1	2.00	0.44
8:K:60:ARG:HH22	8:K:95:ASP:HA	1.82	0.44
28:e:54:ARG:NH1	28:e:56:GLN:OE1	2.51	0.44
28:e:129:ARG:NH2	28:e:138:GLU:OE2	2.50	0.44
3:D:108:PHE:HB3	3:D:132:LEU:HB3	1.98	0.43
8:K:84:PRO:HG2	20:H:196:LYS:O	2.17	0.43
14:U:141:ARG:HH12	14:U:171:PHE:HE2	1.66	0.43
16:Y:42:PRO:HB3	35:l:442:LEU:HD23	2.00	0.43
32:i:54:GLU:HG3	34:k:93:LEU:HB3	2.00	0.43
35:l:297:ASP:HB3	35:l:300:LYS:HB2	2.00	0.43
35:l:297:ASP:O	35:l:301:ILE:HG13	2.18	0.43
43:t:4:HIS:HB2	43:t:106:ARG:HH22	1.82	0.43
1:B:41:ILE:HG12	1:B:253:THR:HG21	2.00	0.43
1:B:146:GLY:HA3	1:B:193:PHE:CE1	2.52	0.43
2:C:43:TRP:HH2	2:C:49:TRP:CD2	2.36	0.43
4:F:57:ASP:OD2	23:L:113:LYS:NZ	2.49	0.43
5:G:262:VAL:HG23	5:G:276:ARG:HB2	2.00	0.43
14:U:312:ILE:HG22	14:U:314:VAL:HG23	1.99	0.43
16:Y:92:TRP:HH2	43:t:99:MET:HG2	1.83	0.43
19:c:108:ASP:HB3	19:c:111:MET:HE2	1.98	0.43
25:W:57:ARG:HB3	41:r:316:PRO:HG3	1.99	0.43
11:X:139:MET:SD	11:X:139:MET:N	2.92	0.43
35:l:65:ASN:HD21	35:l:80:PHE:HE2	1.65	0.43
36:m:63:GLY:O	36:m:66:VAL:HG22	2.18	0.43
1:B:282:VAL:HG23	1:B:285:PRO:HG3	2.00	0.43
1:B:290:GLU:HG3	1:B:291:GLU:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:93:GLN:NE2	6:I:162:ALA:O	2.50	0.43
3:D:174:PHE:O	3:D:199:ARG:NE	2.44	0.43
4:F:79:VAL:HG21	4:F:84:ILE:HG12	2.01	0.43
5:G:575:VAL:O	5:G:578:PRO:HD2	2.18	0.43
16:Y:89:PRO:HB3	43:t:103:GLU:HG3	1.99	0.43
23:L:300:PHE:HD2	23:L:309:THR:HG22	1.83	0.43
27:d:69:ARG:HG2	37:n:44:LEU:HA	1.99	0.43
28:e:119:ARG:NH2	35:l:75:GLU:OE2	2.50	0.43
35:l:413:LEU:O	35:l:416:THR:OG1	2.29	0.43
40:q:168:GLN:HB2	40:q:174:LEU:HG	2.00	0.43
41:r:233:MET:HB3	41:r:233:MET:HE3	1.71	0.43
2:C:162:GLU:OE2	2:C:177:ARG:NH2	2.44	0.43
2:C:265:GLU:CD	2:C:344:ARG:HH12	2.26	0.43
5:G:188:GLU:O	5:G:419:ARG:NE	2.47	0.43
25:W:116:TRP:HB2	42:s:129:ASP:OD1	2.18	0.43
32:i:270:MET:O	32:i:275:SER:OG	2.25	0.43
35:l:302:VAL:O	35:l:306:THR:HG23	2.18	0.43
35:l:597:ILE:O	35:l:601:LEU:HG	2.18	0.43
39:p:171:ARG:HD2	39:p:210:TRP:CD2	2.53	0.43
19:c:81:ARG:HG2	38:o:13:THR:HG21	2.00	0.43
23:L:201:ILE:HG13	49:L:401:NDP:H42N	2.01	0.43
23:L:206:ASP:CG	23:L:208:PHE:H	2.27	0.43
25:W:121:MET:SD	36:m:130:THR:HG22	2.59	0.43
28:e:109:LEU:HD12	28:e:109:LEU:HA	1.90	0.43
33:j:63:LEU:HD12	33:j:63:LEU:HA	1.78	0.43
34:k:22:TYR:HA	36:m:23:LYS:HE2	1.99	0.43
35:l:548:SER:O	35:l:552:LEU:HB3	2.17	0.43
35:l:557:TRP:O	35:l:558:LEU:C	2.62	0.43
14:U:74:ARG:HA	14:U:77:ARG:HE	1.83	0.43
35:l:40:VAL:HG21	35:l:101:MET:SD	2.59	0.43
36:m:17:PHE:O	36:m:21:SER:OG	2.35	0.43
3:D:147:THR:HB	3:D:153:ILE:HD11	1.99	0.43
24:T:154:HIS:CG	24:T:157:ASP:H	2.37	0.43
25:W:68:ARG:O	25:W:72:MET:HG3	2.19	0.43
32:i:250:SER:O	32:i:259:GLY:HA3	2.18	0.43
35:l:7:LEU:O	35:l:11:THR:HG23	2.18	0.43
35:l:414:ILE:O	35:l:417:SER:OG	2.28	0.43
41:r:174:MET:HE2	41:r:241:LEU:O	2.19	0.43
1:B:138:LEU:HD13	1:B:245:VAL:HG13	2.01	0.43
3:D:42:ASP:N	9:M:62:GLU:OE1	2.52	0.43
22:E:82:VAL:HG12	22:E:101:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.99	0.43
35:l:503:GLU:O	35:l:507:THR:HG23	2.19	0.43
40:q:275:ILE:O	40:q:279:GLN:HG2	2.19	0.43
41:r:222:MET:HE3	41:r:222:MET:HB2	1.84	0.43
41:r:238:THR:OG1	41:r:266:LEU:HD13	2.19	0.43
20:H:74:LEU:O	20:H:77:LEU:HB3	2.19	0.43
23:L:311:ARG:O	23:L:315:GLU:HG2	2.19	0.43
35:l:137:LEU:HD13	35:l:186:MET:HG2	2.01	0.43
35:l:291:CYS:O	35:l:295:GLN:HG2	2.18	0.43
43:t:14:SER:OG	43:t:113:LYS:NZ	2.49	0.43
44:R:81:TYR:CD1	44:R:85:THR:HG21	2.54	0.43
1:B:313:ASN:ND2	1:B:358:ASP:HB2	2.33	0.43
5:G:674:LEU:HD21	12:P:46:LYS:HE2	2.00	0.43
18:a:184:LYS:HA	31:h:28:LYS:HB3	2.01	0.43
22:E:41:HIS:CD2	22:E:95:ILE:HD12	2.54	0.43
26:b:105:PHE:O	26:b:107:GLY:N	2.50	0.43
32:i:141:VAL:O	32:i:145:ILE:HG12	2.19	0.43
35:l:247:LEU:HD12	35:l:248:HIS:CE1	2.54	0.43
35:l:515:TYR:HD1	35:l:515:TYR:HA	1.74	0.43
43:t:69:CYS:SG	43:t:70:LYS:N	2.91	0.43
2:C:89:ASN:HD21	2:C:102:ARG:HE	1.66	0.42
5:G:466:LEU:HD13	5:G:500:ILE:HD11	2.01	0.42
5:G:476:LEU:HD21	5:G:481:LEU:HD21	2.01	0.42
22:E:138:THR:HB	22:E:139:PRO:HD3	2.01	0.42
39:p:161:PHE:O	39:p:165:GLU:HG2	2.19	0.42
1:B:420:GLU:OE1	1:B:436:GLN:NE2	2.44	0.42
2:C:145:LEU:HD13	2:C:430:ILE:HG21	2.00	0.42
5:G:238:PHE:CG	20:H:140:ARG:HG2	2.54	0.42
5:G:591:GLU:HG2	5:G:610:VAL:HG23	2.02	0.42
10:N:44:TYR:O	10:N:48:THR:OG1	2.22	0.42
22:E:83:LEU:HD23	22:E:101:VAL:HG21	2.01	0.42
26:b:95:TYR:OH	27:d:11:PRO:O	2.32	0.42
35:l:428:PHE:CD2	35:l:505:ASN:HB3	2.53	0.42
38:o:48:LEU:HB3	39:p:208:LEU:HD13	2.00	0.42
40:q:60:SER:HB2	40:q:457:PRO:HA	2.01	0.42
42:s:216:GLU:H	42:s:216:GLU:HG3	1.70	0.42
1:B:154:ALA:HB2	1:B:193:PHE:CZ	2.55	0.42
2:C:169:PRO:HG2	2:C:174:GLN:HE21	1.84	0.42
15:V:73:THR:HB	15:V:93:GLY:HA2	2.01	0.42
18:a:52:LYS:HB2	18:a:52:LYS:HE3	1.80	0.42
23:L:127:ARG:NH1	23:L:207:ARG:HH22	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:L:165:LEU:HD23	23:L:165:LEU:HA	1.83	0.42
34:k:76:SER:OG	36:m:168:ILE:HD12	2.20	0.42
35:l:546:GLN:OE1	38:o:72:ARG:NH2	2.52	0.42
40:q:76:MET:SD	40:q:230:VAL:HG13	2.59	0.42
1:B:32:PHE:CE1	1:B:267:ARG:HG2	2.54	0.42
2:C:45:PRO:HG2	32:i:303:THR:CG2	2.48	0.42
2:C:389:LYS:HG3	5:G:144:MET:HG3	2.01	0.42
5:G:385:TYR:HA	5:G:515:ILE:HD12	2.01	0.42
19:c:186:ILE:HD11	43:t:34:ARG:CZ	2.49	0.42
23:L:32:HIS:HD1	23:L:32:HIS:N	2.17	0.42
26:b:122:GLU:OE1	26:b:124:PRO:HD3	2.20	0.42
27:d:160:LYS:NZ	28:e:147:ILE:HG23	2.34	0.42
29:f:47:THR:HG23	30:g:65:LEU:HD22	2.01	0.42
35:l:162:THR:O	35:l:166:THR:HG23	2.19	0.42
35:l:327:LEU:O	35:l:331:MET:HG2	2.20	0.42
35:l:389:PHE:O	35:l:393:ASP:HB3	2.20	0.42
39:p:70:GLU:HG3	39:p:79:TYR:CE1	2.55	0.42
40:q:433:GLU:O	40:q:437:MET:HG2	2.19	0.42
2:C:384:LEU:HD21	5:G:129:PRO:HD3	2.02	0.42
2:C:385:ILE:HG23	5:G:140:GLN:HG2	2.01	0.42
3:D:227:ALA:O	7:J:116:SER:OG	2.31	0.42
5:G:371:VAL:O	5:G:482:GLN:NE2	2.53	0.42
6:I:151:TYR:CE1	6:I:238:GLU:HG2	2.55	0.42
13:Q:79:ASP:OD2	13:Q:126:ARG:NH2	2.39	0.42
14:U:225:ASN:ND2	14:U:228:GLU:HG3	2.34	0.42
20:H:76:TYR:HA	20:H:79:ARG:HH11	1.84	0.42
33:j:98:LEU:HD13	41:r:298:LEU:HD21	2.00	0.42
40:q:358:TRP:HE3	40:q:441:ILE:HD12	1.84	0.42
5:G:359:ASN:OD1	12:P:68:ARG:NH2	2.53	0.42
6:I:152:ASP:OD2	41:r:34:ARG:HB3	2.20	0.42
8:K:117:VAL:O	8:K:120:THR:OG1	2.33	0.42
14:U:94:HIS:CG	14:U:105:PRO:HB3	2.54	0.42
19:c:143:MET:HE2	19:c:143:MET:HA	2.02	0.42
20:H:101:HIS:HB3	20:H:167:ILE:HD11	2.02	0.42
22:E:183:ALA:HB1	22:E:184:PRO:CD	2.50	0.42
40:q:329:LEU:HD23	40:q:437:MET:HE3	2.02	0.42
1:B:367:ILE:O	1:B:371:ILE:HG12	2.20	0.42
3:D:155:SER:OG	3:D:167:GLU:OE1	2.33	0.42
5:G:297:LEU:HD21	5:G:700:ILE:HD13	2.01	0.42
5:G:669:ASN:HD21	5:G:673:LYS:HE3	1.85	0.42
23:L:206:ASP:O	23:L:210:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:7:LYS:H	27:d:7:LYS:HG2	1.65	0.42
27:d:146:LEU:HD23	27:d:150:TYR:HB2	2.01	0.42
33:j:56:PHE:O	33:j:60:ILE:HG13	2.20	0.42
35:l:267:MET:HE1	35:l:277:THR:HG21	2.00	0.42
40:q:225:ILE:HD13	40:q:331:ASN:HB2	2.01	0.42
1:B:123:GLY:HA2	22:E:180:CYS:HB3	2.02	0.42
2:C:184:THR:OG1	2:C:220:TYR:OH	2.32	0.42
13:Q:125:GLN:HE21	33:j:42:ASP:H	1.68	0.42
14:U:67:ASN:HB3	14:U:216:ILE:CD1	2.50	0.42
19:c:89:TRP:CE3	11:X:131:PRO:HG3	2.55	0.42
29:f:55:TRP:NE1	30:g:68:THR:HG22	2.35	0.42
32:i:190:MET:HG2	32:i:204:ASN:HB3	2.02	0.42
35:l:267:MET:HE3	35:l:273:VAL:HG12	2.01	0.42
35:l:584:ILE:H	35:l:584:ILE:HG12	1.52	0.42
36:m:61:LEU:HD23	41:r:110:SER:HB2	2.02	0.42
39:p:201:LYS:HE2	39:p:201:LYS:HB3	1.89	0.42
41:r:255:TYR:O	41:r:256:THR:C	2.62	0.42
6:I:155:ARG:NH2	20:H:84:ILE:O	2.53	0.42
7:J:112:MET:HG3	20:H:184:LEU:HD23	2.02	0.42
8:K:130:THR:HG23	20:H:144:ARG:HB2	2.00	0.42
11:O:140:CYS:HB2	11:O:143:GLU:HG3	2.01	0.42
14:U:354:ILE:HA	14:U:357:LYS:HB3	2.02	0.42
19:c:154:GLN:HE22	35:l:486:MET:HE1	1.85	0.42
25:W:88:ARG:O	25:W:92:GLU:HG2	2.19	0.42
32:i:254:LEU:HD21	40:q:154:LEU:HD11	2.01	0.42
35:l:46:LEU:HD23	35:l:46:LEU:HA	1.91	0.42
35:l:151:SER:O	35:l:155:ILE:HG12	2.20	0.42
35:l:241:THR:OG1	35:l:242:PRO:HD3	2.19	0.42
42:s:121:MET:HE2	42:s:121:MET:HA	2.01	0.42
1:B:62:TRP:CD2	1:B:181:LEU:HD13	2.55	0.42
2:C:296:GLY:HA3	2:C:411:GLY:HA2	2.02	0.42
5:G:59:GLN:HE21	5:G:62:ARG:NH2	2.17	0.42
5:G:372:PHE:HB3	5:G:532:PRO:HB2	2.00	0.42
5:G:692:LYS:HE2	5:G:692:LYS:HB3	1.85	0.42
19:c:82:SER:HA	19:c:112:TYR:HB3	2.02	0.42
19:c:153:TYR:OH	43:t:8:ARG:NE	2.35	0.42
21:S:46:ASN:ND2	36:m:132:ASP:OD1	2.53	0.42
32:i:125:GLN:H	32:i:125:GLN:HG2	1.57	0.42
35:l:137:LEU:HD23	35:l:137:LEU:HA	1.89	0.42
41:r:141:SER:HA	41:r:290:TRP:HE1	1.85	0.42
43:t:76:ASN:ND2	43:t:79:ALA:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:99:GLY:HA3	6:I:135:GLY:O	2.19	0.41
6:I:131:PRO:HA	6:I:169:VAL:O	2.20	0.41
26:b:87:LYS:HG2	27:d:49:ARG:HG3	2.02	0.41
26:b:121:LYS:HD3	43:t:40:VAL:HG22	2.02	0.41
29:f:68:GLU:HG2	30:g:21:ARG:HE	1.85	0.41
41:r:298:LEU:O	41:r:302:MET:HG3	2.20	0.41
2:C:297:VAL:HG12	2:C:335:ARG:HG2	2.01	0.41
5:G:217:GLU:HG3	5:G:412:PRO:HB3	2.01	0.41
5:G:241:ARG:O	5:G:244:GLU:HG2	2.20	0.41
5:G:389:THR:OG1	5:G:514:ASN:ND2	2.39	0.41
25:W:134:LEU:HD21	36:m:3:MET:HA	2.02	0.41
33:j:95:LEU:HB3	41:r:302:MET:HE2	2.02	0.41
35:l:564:LYS:HG3	38:o:77:TYR:CZ	2.55	0.41
43:t:69:CYS:SG	43:t:83:GLU:HG3	2.60	0.41
1:B:340:ASP:O	1:B:344:GLN:HG2	2.21	0.41
12:P:40:ARG:NH1	12:P:88:THR:OG1	2.51	0.41
15:V:95:CYS:HA	15:V:115:CYS:HA	2.03	0.41
23:L:164:HIS:O	23:L:165:LEU:C	2.62	0.41
28:e:129:ARG:HA	28:e:134:LEU:HB2	2.02	0.41
32:i:34:GLU:O	32:i:38:LEU:HG	2.20	0.41
34:k:26:LEU:O	34:k:29:SER:OG	2.37	0.41
35:l:100:ILE:HG13	35:l:246:LEU:HD23	2.02	0.41
36:m:12:ILE:HB	36:m:39:VAL:HG21	2.03	0.41
36:m:57:PHE:O	36:m:61:LEU:HB2	2.20	0.41
36:m:163:ILE:HD12	36:m:163:ILE:HA	1.89	0.41
38:o:105:PHE:CD2	40:q:263:MET:HE2	2.56	0.41
1:B:214:GLU:OE1	1:B:219:LYS:HD2	2.19	0.41
5:G:250:SER:OG	5:G:251:ILE:N	2.54	0.41
5:G:438:LEU:O	5:G:439:THR:OG1	2.32	0.41
5:G:650:SER:HB2	5:G:652:ASN:OD1	2.19	0.41
11:O:104:PHE:HD1	11:O:108:LEU:HD12	1.84	0.41
13:Q:71:ASN:OD1	13:Q:71:ASN:N	2.53	0.41
18:a:67:PHE:CE2	40:q:434:ASN:HB3	2.55	0.41
21:S:66:LEU:O	21:S:69:ILE:HG23	2.20	0.41
26:b:125:ASP:OD1	26:b:125:ASP:N	2.49	0.41
30:g:77:LEU:HD11	32:i:342:ALA:HB1	2.03	0.41
34:k:31:LEU:HD23	34:k:31:LEU:HA	1.82	0.41
34:k:38:LEU:O	34:k:42:ILE:HG12	2.20	0.41
34:k:45:THR:HG23	36:m:52:LEU:HD13	2.01	0.41
43:t:73:SER:HB2	43:t:79:ALA:HB3	2.01	0.41
1:B:132:ARG:HG2	1:B:133:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:LYS:O	7:J:175:LYS:NZ	2.50	0.41
1:B:307:VAL:HG21	1:B:314:LEU:HB2	2.03	0.41
2:C:101:LEU:HB2	2:C:464:PHE:CZ	2.55	0.41
4:F:95:HIS:ND1	4:F:96:PRO:O	2.52	0.41
23:L:53:VAL:HG22	23:L:122:ILE:HD12	2.01	0.41
23:L:78:PRO:HB3	23:L:114:VAL:HG21	2.01	0.41
11:X:146:ASP:OD1	26:b:16:ARG:NH1	2.49	0.41
30:g:27:LYS:O	30:g:30:ASP:HB2	2.20	0.41
32:i:337:LEU:C	32:i:339:MET:H	2.28	0.41
40:q:269:MET:HG3	40:q:270:ILE:HD12	2.02	0.41
40:q:318:ALA:HB2	40:q:373:ILE:HG13	2.03	0.41
41:r:113:VAL:HG12	41:r:117:LEU:HD13	2.02	0.41
1:B:281:HIS:ND1	1:B:358:ASP:OD1	2.54	0.41
1:B:387:GLU:OE1	5:G:123:ASN:ND2	2.49	0.41
5:G:401:LEU:HD11	5:G:432:ILE:HG13	2.02	0.41
16:Y:92:TRP:HB2	16:Y:97:LEU:HD21	2.03	0.41
25:W:86:MET:HE3	25:W:124:LEU:HD22	2.03	0.41
11:X:100:VAL:HG12	11:X:142:GLN:HB2	2.03	0.41
11:X:150:ASP:OD2	26:b:16:ARG:HD2	2.21	0.41
35:l:260:LEU:HD12	35:l:314:MET:HE2	2.01	0.41
35:l:584:ILE:HG22	35:l:588:PHE:CE1	2.55	0.41
40:q:87:GLU:HB3	40:q:92:LYS:HD2	2.01	0.41
40:q:218:LYS:O	40:q:222:GLU:HG2	2.20	0.41
41:r:167:THR:O	41:r:170:GLU:HB2	2.20	0.41
2:C:103:LEU:HD23	2:C:103:LEU:HA	1.81	0.41
2:C:151:MET:HG3	2:C:220:TYR:CE2	2.56	0.41
3:D:105:ASN:O	9:M:97:PRO:HD3	2.20	0.41
19:c:78:LEU:HB2	19:c:106:HIS:HD2	1.86	0.41
24:T:118:PRO:HG3	41:r:306:SER:HB2	2.02	0.41
28:e:87:MET:HG3	28:e:88:ARG:N	2.36	0.41
35:l:27:TYR:O	35:l:115:ASN:ND2	2.46	0.41
38:o:91:ALA:O	38:o:95:ILE:HG13	2.20	0.41
39:p:180:LYS:HE3	39:p:180:LYS:HB3	1.90	0.41
2:C:410:LYS:HE3	2:C:463:VAL:HB	2.01	0.41
3:D:89:HIS:CG	3:D:90:PRO:HD2	2.55	0.41
5:G:65:TYR:HB2	5:G:92:CYS:HB2	2.03	0.41
19:c:40:PRO:O	19:c:74:ASP:HB3	2.20	0.41
23:L:288:LEU:HD12	23:L:289:PRO:HD2	2.03	0.41
36:m:28:TYR:O	36:m:31:LEU:HG	2.21	0.41
40:q:294:MET:HE3	40:q:319:HIS:ND1	2.36	0.41
41:r:209:SER:OG	41:r:212:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:55:GLY:HA2	2:C:69:PRO:HG3	2.02	0.41
2:C:122:LEU:HD11	6:I:137:ALA:HB2	2.02	0.41
2:C:207:PHE:CD1	41:r:34:ARG:HD3	2.56	0.41
3:D:128:ILE:HD11	3:D:176:VAL:HG11	2.03	0.41
5:G:163:LYS:O	5:G:171:THR:OG1	2.21	0.41
5:G:339:ALA:HB3	5:G:542:PRO:HG3	2.02	0.41
5:G:395:GLU:O	5:G:425:ASN:ND2	2.54	0.41
12:P:44:LEU:HD22	12:P:53:ILE:HD11	2.02	0.41
14:U:85:LEU:HB2	14:U:160:VAL:HG23	2.01	0.41
14:U:112:GLY:HA2	14:U:136:TRP:CD2	2.55	0.41
14:U:127:ASP:N	14:U:127:ASP:OD1	2.53	0.41
15:V:66:ILE:HD11	15:V:101:LEU:HB2	2.01	0.41
15:V:141:VAL:N	32:i:273:ASN:OD1	2.44	0.41
23:L:78:PRO:HA	23:L:101:MET:O	2.21	0.41
49:L:401:NDP:H2N	49:L:401:NDP:H2D	1.77	0.41
24:T:139:PRO:HD3	25:W:69:ILE:HD13	2.02	0.41
27:d:122:ARG:HA	27:d:122:ARG:NH1	2.36	0.41
27:d:144:SER:O	27:d:158:LYS:NZ	2.46	0.41
34:k:73:LEU:HD23	34:k:73:LEU:HA	1.83	0.41
35:l:559:GLU:O	35:l:563:PRO:HD2	2.21	0.41
41:r:196:ALA:C	41:r:198:PHE:N	2.79	0.41
1:B:405:ARG:HH21	9:M:49:LEU:HD11	1.86	0.41
5:G:389:THR:O	5:G:390:THR:OG1	2.28	0.41
22:E:106:GLN:O	44:R:109:ARG:NH2	2.54	0.41
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.02	0.41
40:q:82:SER:HB3	40:q:432:ARG:NH2	2.36	0.41
1:B:251:SER:OG	1:B:252:PRO:HD3	2.21	0.40
8:K:25:ARG:HH21	8:K:66:THR:HG21	1.86	0.40
28:e:103:SER:HA	28:e:106:VAL:HG12	2.02	0.40
32:i:323:MET:HE2	32:i:323:MET:HB3	2.01	0.40
33:j:73:LEU:O	33:j:76:PRO:HD2	2.21	0.40
33:j:95:LEU:HD13	41:r:302:MET:HG2	2.03	0.40
38:o:114:LYS:HB3	38:o:114:LYS:HE2	1.86	0.40
41:r:72:ILE:O	41:r:75:PRO:HD2	2.21	0.40
8:K:108:TYR:CD2	20:H:109:GLY:HA2	2.56	0.40
14:U:60:LYS:HA	14:U:204:HIS:CE1	2.57	0.40
22:E:212:LYS:HE3	22:E:212:LYS:HB2	1.82	0.40
23:L:278:VAL:HA	23:L:364:VAL:HG11	2.03	0.40
24:T:154:HIS:ND1	24:T:154:HIS:C	2.79	0.40
35:l:526:LEU:HD12	35:l:530:PRO:HG3	2.03	0.40
40:q:329:LEU:O	40:q:332:THR:OG1	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:396:GLN:O	9:M:60:ARG:HD2	2.21	0.40
3:D:213:ASP:OD1	23:L:66:ASN:ND2	2.36	0.40
13:Q:79:ASP:OD2	23:L:346:GLU:HG2	2.22	0.40
18:a:144:ALA:CB	27:d:82:ILE:HG12	2.51	0.40
22:E:93:LEU:HD12	22:E:122:TYR:HB3	2.02	0.40
28:e:94:GLY:O	28:e:99:LEU:HB2	2.22	0.40
32:i:231:SER:HB2	32:i:305:PHE:HB2	2.04	0.40
32:i:261:MET:HE2	32:i:261:MET:HB3	1.93	0.40
33:j:55:PHE:CZ	41:r:137:ALA:HB2	2.56	0.40
35:l:221:ALA:HA	35:l:226:GLN:HG2	2.03	0.40
35:l:295:GLN:HB2	35:l:301:ILE:HG12	2.04	0.40
36:m:44:VAL:HG12	36:m:49:GLY:O	2.21	0.40
3:D:114:LEU:HB3	3:D:166:TYR:HB3	2.04	0.40
4:F:67:ALA:O	4:F:71:ILE:HG13	2.21	0.40
5:G:624:ARG:NH1	5:G:628:GLU:HB2	2.36	0.40
6:I:161:ARG:HH21	41:r:220:PHE:HZ	1.68	0.40
7:J:77:VAL:HG13	7:J:99:MET:HG3	2.03	0.40
23:L:353:THR:O	23:L:357:LEU:HG	2.22	0.40
35:l:332:HIS:HA	35:l:335:PHE:CE2	2.57	0.40
36:m:34:ILE:CD1	36:m:61:LEU:HD12	2.51	0.40
36:m:39:VAL:O	36:m:43:ILE:HG13	2.20	0.40
41:r:2:PHE:CE2	41:r:6:ILE:HD11	2.57	0.40
1:B:83:SER:HB2	1:B:262:PHE:CD2	2.57	0.40
3:D:173:MET:HE1	3:D:189:THR:HG23	2.03	0.40
7:J:108:GLU:HG3	7:J:113:GLY:HA2	2.04	0.40
11:O:101:ASN:N	11:O:101:ASN:OD1	2.53	0.40
14:U:340:LYS:O	30:g:52:ARG:NH2	2.55	0.40
19:c:143:MET:HB3	35:l:407:TRP:CD2	2.56	0.40
32:i:72:MET:HE1	34:k:9:ILE:HG12	2.02	0.40
35:l:384:PRO:HA	35:l:389:PHE:CD1	2.56	0.40
39:p:192:ARG:HB3	39:p:192:ARG:HH11	1.86	0.40
40:q:44:GLN:HG3	40:q:60:SER:HA	2.04	0.40
41:r:63:PRO:HB2	41:r:66:SER:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	427/464 (92%)	423 (99%)	4 (1%)	0	100	100
2	C	428/469 (91%)	414 (97%)	13 (3%)	1 (0%)	43	70
3	D	206/264 (78%)	199 (97%)	7 (3%)	0	100	100
4	F	91/123 (74%)	89 (98%)	2 (2%)	0	100	100
5	G	680/727 (94%)	668 (98%)	11 (2%)	1 (0%)	48	74
6	I	154/258 (60%)	149 (97%)	5 (3%)	0	100	100
7	J	116/175 (66%)	113 (97%)	3 (3%)	0	100	100
8	K	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
9	M	92/113 (81%)	88 (96%)	4 (4%)	0	100	100
10	N	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
11	O	81/156 (52%)	80 (99%)	1 (1%)	0	100	100
11	X	83/156 (53%)	79 (95%)	3 (4%)	1 (1%)	10	31
12	P	81/99 (82%)	79 (98%)	2 (2%)	0	100	100
13	Q	110/154 (71%)	106 (96%)	4 (4%)	0	100	100
14	U	316/357 (88%)	309 (98%)	7 (2%)	0	100	100
15	V	138/141 (98%)	137 (99%)	1 (1%)	0	100	100
16	Y	64/105 (61%)	59 (92%)	4 (6%)	1 (2%)	7	24
17	Z	75/114 (66%)	75 (100%)	0	0	100	100
18	a	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
19	c	151/186 (81%)	147 (97%)	4 (3%)	0	100	100
20	H	174/212 (82%)	171 (98%)	3 (2%)	0	100	100
21	S	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
22	E	212/249 (85%)	201 (95%)	10 (5%)	1 (0%)	24	51
23	L	338/372 (91%)	326 (96%)	11 (3%)	1 (0%)	36	62
24	T	80/169 (47%)	74 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	W	138/144 (96%)	135 (98%)	3 (2%)	0	100	100
26	b	107/188 (57%)	93 (87%)	13 (12%)	1 (1%)	14	38
27	d	167/176 (95%)	163 (98%)	4 (2%)	0	100	100
28	e	97/154 (63%)	90 (93%)	7 (7%)	0	100	100
29	f	44/76 (58%)	44 (100%)	0	0	100	100
30	g	119/122 (98%)	118 (99%)	1 (1%)	0	100	100
31	h	103/106 (97%)	102 (99%)	1 (1%)	0	100	100
32	i	345/347 (99%)	336 (97%)	9 (3%)	0	100	100
33	j	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
34	k	96/98 (98%)	94 (98%)	2 (2%)	0	100	100
35	l	601/606 (99%)	571 (95%)	29 (5%)	1 (0%)	43	70
36	m	171/175 (98%)	166 (97%)	5 (3%)	0	100	100
37	n	54/58 (93%)	52 (96%)	1 (2%)	1 (2%)	6	21
38	o	124/129 (96%)	122 (98%)	2 (2%)	0	100	100
39	p	175/221 (79%)	173 (99%)	2 (1%)	0	100	100
40	q	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
41	r	316/318 (99%)	304 (96%)	10 (3%)	2 (1%)	21	48
42	s	169/249 (68%)	161 (95%)	8 (5%)	0	100	100
43	t	115/137 (84%)	113 (98%)	2 (2%)	0	100	100
44	R	33/110 (30%)	33 (100%)	0	0	100	100
All	All	8096/9571 (85%)	7860 (97%)	225 (3%)	11 (0%)	49	74

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
37	n	44	LEU
41	r	197	PRO
2	C	45	PRO
22	E	183	ALA
23	L	199	SER
11	X	139	MET
35	l	562	LEU
5	G	283	GLU
16	Y	89	PRO
26	b	63	LYS

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Mol	Chain	Res	Type
41	r	208	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	343/368 (93%)	341 (99%)	2 (1%)	78 92
2	C	370/398 (93%)	364 (98%)	6 (2%)	55 81
3	D	190/228 (83%)	184 (97%)	6 (3%)	34 65
4	F	77/97 (79%)	73 (95%)	4 (5%)	21 50
5	G	576/610 (94%)	574 (100%)	2 (0%)	86 95
6	I	132/212 (62%)	127 (96%)	5 (4%)	29 61
7	J	107/152 (70%)	104 (97%)	3 (3%)	38 70
8	K	130/131 (99%)	129 (99%)	1 (1%)	73 89
9	M	86/98 (88%)	86 (100%)	0	100 100
10	N	99/101 (98%)	98 (99%)	1 (1%)	68 87
11	O	77/132 (58%)	73 (95%)	4 (5%)	21 50
11	X	79/132 (60%)	71 (90%)	8 (10%)	7 22
12	P	74/82 (90%)	72 (97%)	2 (3%)	39 70
13	Q	105/134 (78%)	102 (97%)	3 (3%)	37 68
14	U	281/307 (92%)	276 (98%)	5 (2%)	51 78
15	V	101/102 (99%)	98 (97%)	3 (3%)	36 67
16	Y	60/84 (71%)	60 (100%)	0	100 100
17	Z	59/90 (66%)	58 (98%)	1 (2%)	53 80
18	a	121/158 (77%)	119 (98%)	2 (2%)	53 80
19	c	138/160 (86%)	138 (100%)	0	100 100
20	H	151/176 (86%)	141 (93%)	10 (7%)	15 40
21	S	58/58 (100%)	53 (91%)	5 (9%)	10 28
22	E	183/207 (88%)	171 (93%)	12 (7%)	15 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	L	294/320 (92%)	276 (94%)	18 (6%)	17 43
24	T	69/134 (52%)	65 (94%)	4 (6%)	18 46
25	W	122/124 (98%)	120 (98%)	2 (2%)	55 81
26	b	104/166 (63%)	96 (92%)	8 (8%)	12 33
27	d	153/156 (98%)	141 (92%)	12 (8%)	11 32
28	e	91/129 (70%)	84 (92%)	7 (8%)	12 33
29	f	42/66 (64%)	40 (95%)	2 (5%)	23 53
30	g	108/109 (99%)	102 (94%)	6 (6%)	19 47
31	h	93/94 (99%)	91 (98%)	2 (2%)	45 75
32	i	311/311 (100%)	294 (94%)	17 (6%)	19 48
33	j	99/100 (99%)	93 (94%)	6 (6%)	17 43
34	k	85/85 (100%)	80 (94%)	5 (6%)	18 45
35	l	537/540 (99%)	498 (93%)	39 (7%)	13 35
36	m	139/141 (99%)	122 (88%)	17 (12%)	5 14
37	n	53/55 (96%)	48 (91%)	5 (9%)	8 24
38	o	110/114 (96%)	98 (89%)	12 (11%)	6 18
39	p	159/190 (84%)	149 (94%)	10 (6%)	16 42
40	q	409/409 (100%)	389 (95%)	20 (5%)	22 51
41	r	275/275 (100%)	255 (93%)	20 (7%)	13 35
42	s	153/206 (74%)	148 (97%)	5 (3%)	33 65
43	t	108/120 (90%)	102 (94%)	6 (6%)	19 47
44	R	34/92 (37%)	31 (91%)	3 (9%)	9 27
All	All	7145/8153 (88%)	6834 (96%)	311 (4%)	27 56

All (311) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	125	CYS
1	B	382	CYS
2	C	45	PRO
2	C	103	LEU
2	C	110	GLU
2	C	211	GLU
2	C	365	ASP

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Mol	Chain	Res	Type
2	C	417	LEU
3	D	44	ARG
3	D	88	ILE
3	D	115	THR
3	D	121	THR
3	D	148	ASP
3	D	208	VAL
4	F	71	ILE
4	F	79	VAL
4	F	84	ILE
4	F	114	CYS
5	G	352	VAL
5	G	400	ILE
6	I	138	CYS
6	I	158	VAL
6	I	160	PHE
6	I	187	VAL
6	I	195	ARG
7	J	61	ILE
7	J	77	VAL
7	J	169	ARG
8	K	59	HIS
10	N	5	LEU
11	O	74	LEU
11	O	101	ASN
11	O	111	ASP
11	O	134	ASP
12	P	44	LEU
12	P	85	ASP
13	Q	71	ASN
13	Q	107	LEU
13	Q	127	THR
14	U	43	LEU
14	U	97	ASP
14	U	100	THR
14	U	172	LEU
14	U	243	TYR
15	V	88	LEU
15	V	115	CYS
15	V	138	GLU
17	Z	59	ASP
18	a	52	LYS

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Mol	Chain	Res	Type
18	a	130	GLU
20	H	70	LEU
20	H	83	THR
20	H	93	LEU
20	H	103	LEU
20	H	110	GLU
20	H	114	ILE
20	H	147	ILE
20	H	174	GLU
20	H	183	LEU
20	H	188	GLU
21	S	52	ARG
21	S	61	HIS
21	S	62	VAL
21	S	64	LYS
21	S	69	ILE
22	E	85	LEU
22	E	95	ILE
22	E	135	CYS
22	E	166	ASP
22	E	168	LEU
22	E	172	ILE
22	E	173	GLU
22	E	180	CYS
22	E	201	ILE
22	E	209	LYS
22	E	215	LYS
22	E	249	LEU
23	L	32	HIS
23	L	113	LYS
23	L	165	LEU
23	L	170	LYS
23	L	179	LYS
23	L	205	GLU
23	L	209	LEU
23	L	232	LYS
23	L	235	VAL
23	L	278	VAL
23	L	295	TRP
23	L	305	PHE
23	L	309	THR
23	L	323	THR

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Mol	Chain	Res	Type
23	L	330	LEU
23	L	335	ILE
23	L	341	GLU
23	L	363	ASP
24	T	142	LEU
24	T	166	LEU
24	T	168	ASN
24	T	169	LEU
25	W	99	LYS
25	W	110	VAL
11	X	76	LEU
11	X	89	LEU
11	X	94	ASP
11	X	96	GLU
11	X	98	LEU
11	X	124	ASP
11	X	133	ILE
11	X	138	LEU
26	b	23	LEU
26	b	25	ASP
26	b	50	PHE
26	b	75	VAL
26	b	86	LEU
26	b	88	TYR
26	b	89	HIS
26	b	116	VAL
27	d	7	LYS
27	d	8	ASP
27	d	17	THR
27	d	49	ARG
27	d	50	GLU
27	d	73	ASP
27	d	78	GLU
27	d	79	GLU
27	d	82	ILE
27	d	114	GLN
27	d	129	LEU
27	d	156	LEU
28	e	58	ASP
28	e	64	GLU
28	e	72	ASP
28	e	84	LEU

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Mol	Chain	Res	Type
28	e	87	MET
28	e	89	VAL
28	e	146	LYS
29	f	31	ILE
29	f	48	LEU
30	g	3	MET
30	g	16	LEU
30	g	29	THR
30	g	64	LEU
30	g	84	MET
30	g	101	GLU
31	h	74	LYS
31	h	86	LEU
32	i	17	THR
32	i	19	LEU
32	i	22	ILE
32	i	29	ILE
32	i	36	ASN
32	i	86	ILE
32	i	193	VAL
32	i	204	ASN
32	i	244	MET
32	i	290	LEU
32	i	296	LEU
32	i	303	THR
32	i	304	MET
32	i	321	LYS
32	i	323	MET
32	i	324	LYS
32	i	343	LEU
33	j	1	MET
33	j	5	LEU
33	j	19	LEU
33	j	68	GLU
33	j	69	ILE
33	j	98	LEU
34	k	3	LEU
34	k	43	MET
34	k	59	MET
34	k	70	GLU
34	k	73	LEU
35	l	7	LEU

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Mol	Chain	Res	Type
35	l	13	ILE
35	l	36	VAL
35	l	57	THR
35	l	59	GLN
35	l	62	ILE
35	l	70	THR
35	l	104	SER
35	l	136	ASN
35	l	149	ILE
35	l	169	LEU
35	l	217	LEU
35	l	233	LEU
35	l	246	LEU
35	l	247	LEU
35	l	314	MET
35	l	321	GLN
35	l	324	LEU
35	l	364	LYS
35	l	373	LEU
35	l	383	MET
35	l	387	THR
35	l	393	ASP
35	l	397	GLU
35	l	407	TRP
35	l	411	MET
35	l	434	LYS
35	l	436	ARG
35	l	440	LEU
35	l	447	ASN
35	l	480	THR
35	l	481	THR
35	l	487	LYS
35	l	502	LEU
35	l	512	LYS
35	l	515	TYR
35	l	532	ILE
35	l	584	ILE
35	l	589	LEU
36	m	31	LEU
36	m	33	LEU
36	m	39	VAL
36	m	56	VAL

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Mol	Chain	Res	Type
36	m	58	LEU
36	m	61	LEU
36	m	66	VAL
36	m	76	THR
36	m	82	VAL
36	m	84	VAL
36	m	87	LYS
36	m	109	LYS
36	m	113	VAL
36	m	120	ASN
36	m	139	GLU
36	m	163	ILE
36	m	173	ARG
37	n	5	LEU
37	n	9	ARG
37	n	17	VAL
37	n	40	ASN
37	n	43	LEU
38	o	5	LYS
38	o	7	LYS
38	o	31	LYS
38	o	33	GLN
38	o	40	ARG
38	o	44	LYS
38	o	57	LEU
38	o	61	GLU
38	o	88	LEU
38	o	92	LEU
38	o	117	GLN
38	o	120	LYS
39	p	60	ARG
39	p	70	GLU
39	p	97	LYS
39	p	101	LYS
39	p	104	GLN
39	p	106	LEU
39	p	117	GLN
39	p	163	LYS
39	p	192	ARG
39	p	201	LYS
40	q	61	LEU
40	q	86	LYS

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Mol	Chain	Res	Type
40	q	92	LYS
40	q	122	PHE
40	q	140	THR
40	q	141	GLU
40	q	179	ILE
40	q	207	MET
40	q	230	VAL
40	q	247	THR
40	q	282	LEU
40	q	315	LEU
40	q	375	LEU
40	q	378	GLU
40	q	416	ARG
40	q	418	LYS
40	q	431	THR
40	q	441	ILE
40	q	452	LYS
40	q	454	ILE
41	r	5	ASN
41	r	13	ILE
41	r	33	LEU
41	r	61	LEU
41	r	62	ARG
41	r	68	ILE
41	r	102	VAL
41	r	106	LEU
41	r	108	MET
41	r	111	LEU
41	r	144	VAL
41	r	150	LEU
41	r	165	LEU
41	r	170	GLU
41	r	172	ILE
41	r	177	THR
41	r	214	GLU
41	r	222	MET
41	r	227	GLU
41	r	253	GLU
42	s	90	LEU
42	s	93	GLN
42	s	175	ARG
42	s	188	VAL

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Mol	Chain	Res	Type
42	s	191	LYS
43	t	16	GLU
43	t	21	ARG
43	t	31	PHE
43	t	36	GLU
43	t	39	MET
43	t	83	GLU
44	R	78	HIS
44	R	80	GLU
44	R	105	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	244	ASN
1	B	277	ASN
1	B	313	ASN
2	C	42	GLN
2	C	118	HIS
2	C	153	ASN
2	C	174	GLN
2	C	387	HIS
3	D	55	HIS
3	D	77	GLN
3	D	107	GLN
3	D	181	HIS
3	D	196	HIS
4	F	63	ASN
5	G	142	GLN
5	G	282	ASN
5	G	304	GLN
5	G	425	ASN
5	G	688	GLN
6	I	145	HIS
7	J	71	HIS
7	J	88	GLN
7	J	92	ASN
7	J	109	ASN
8	K	31	ASN
10	N	50	GLN
10	N	83	GLN
12	P	22	HIS

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Mol	Chain	Res	Type
12	P	81	ASN
13	Q	125	GLN
14	U	87	HIS
14	U	188	HIS
14	U	301	GLN
14	U	324	HIS
16	Y	39	HIS
16	Y	46	GLN
17	Z	64	ASN
17	Z	76	ASN
18	a	181	HIS
18	a	189	ASN
19	c	94	HIS
19	c	127	ASN
19	c	132	HIS
19	c	154	GLN
19	c	183	HIS
20	H	159	GLN
21	S	58	ASN
21	S	68	ASN
22	E	153	GLN
23	L	145	HIS
23	L	318	HIS
25	W	76	GLN
26	b	126	GLN
27	d	23	GLN
30	g	81	GLN
31	h	21	GLN
31	h	34	HIS
31	h	97	HIS
32	i	36	ASN
32	i	134	GLN
32	i	171	ASN
32	i	289	ASN
32	i	322	GLN
33	j	28	ASN
34	k	25	HIS
34	k	52	HIS
35	l	56	HIS
35	l	67	HIS
35	l	170	GLN
35	l	206	ASN

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Mol	Chain	Res	Type
35	l	309	GLN
35	l	447	ASN
35	l	505	ASN
36	m	120	ASN
37	n	14	HIS
37	n	40	ASN
38	o	50	GLN
38	o	79	ASN
38	o	117	GLN
40	q	30	HIS
41	r	38	ASN
41	r	47	GLN
41	r	212	ASN
42	s	108	HIS
42	s	141	ASN
43	t	44	GLN
43	t	47	ASN
43	t	65	GLN
43	t	92	HIS

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	$\#\|Z\| > 2$
49	NDP	L	401	-	51,52,52	0.50	0	71,80,80	0.75	1 (1%)
45	FMN	B	501	-	33,33,33	1.05	2 (6%)	48,50,50	1.20	7 (14%)
47	FES	G	803	5	0,4,4	-	-	-		
46	SF4	H	302	20	0,12,12	-	-	-		
46	SF4	H	301	20	0,12,12	-	-	-		
46	SF4	I	301	6	0,12,12	-	-	-		
48	ZMP	Q	201	-	27,29,36	1.77	6 (22%)	34,38,45	1.66	5 (14%)
46	SF4	G	801	5	0,12,12	-	-	-		
46	SF4	G	802	5	0,12,12	-	-	-		
47	FES	E	301	-	0,4,4	-	-	-		
46	SF4	B	502	-	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
49	NDP	L	401	-	-	7/34/77/77	0/5/5/5
45	FMN	B	501	-	-	7/18/18/18	0/3/3/3
47	FES	G	803	5	-	-	0/1/1/1
46	SF4	H	302	20	-	-	0/6/5/5
46	SF4	H	301	20	-	-	0/6/5/5
46	SF4	I	301	6	-	-	0/6/5/5
48	ZMP	Q	201	-	-	9/36/36/43	-
46	SF4	G	801	5	-	-	0/6/5/5
46	SF4	G	802	5	-	-	0/6/5/5
47	FES	E	301	-	-	-	0/1/1/1
46	SF4	B	502	-	-	-	0/6/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Q	201	ZMP	C13-N1	5.17	1.45	1.33
48	Q	201	ZMP	C16-N2	5.09	1.45	1.33
45	B	501	FMN	C4A-N5	3.39	1.38	1.30
48	Q	201	ZMP	C10-S1	2.50	1.82	1.76
45	B	501	FMN	C10-N1	2.43	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Q	201	ZMP	C9-C10	2.36	1.53	1.50
48	Q	201	ZMP	O3-C16	-2.27	1.19	1.23
48	Q	201	ZMP	O2-C13	-2.22	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Q	201	ZMP	C9-C10-S1	5.56	120.03	113.40
49	L	401	NDP	P2B-O2B-C2B	-5.04	109.97	123.43
48	Q	201	ZMP	O1-C10-C9	-3.35	120.11	123.98
45	B	501	FMN	C4-N3-C2	-3.17	120.02	125.64
45	B	501	FMN	C4A-C10-N10	2.69	120.33	116.48
45	B	501	FMN	C4A-C4-N3	2.58	119.83	113.25
48	Q	201	ZMP	C11-S1-C10	2.56	109.40	101.84
45	B	501	FMN	O4-C4-C4A	-2.40	120.21	126.53
45	B	501	FMN	C10-C4A-N5	-2.31	120.09	124.81
48	Q	201	ZMP	O3-C16-N2	-2.23	118.27	122.98
48	Q	201	ZMP	O1-C10-S1	-2.22	119.86	122.68
45	B	501	FMN	C5A-C9A-N10	2.20	119.96	117.97
45	B	501	FMN	C4A-C10-N1	-2.01	119.66	124.59

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	N10-C1'-C2'-C3'
45	B	501	FMN	C3'-C4'-C5'-O5'
45	B	501	FMN	O4'-C4'-C5'-O5'
45	B	501	FMN	C5'-O5'-P-O1P
45	B	501	FMN	C5'-O5'-P-O2P
45	B	501	FMN	C5'-O5'-P-O3P
48	Q	201	ZMP	O3-C16-C17-O4
48	Q	201	ZMP	C17-C16-N2-C15
48	Q	201	ZMP	S1-C11-C12-N1
48	Q	201	ZMP	C12-C11-S1-C10
49	L	401	NDP	C5D-O5D-PN-O1N
48	Q	201	ZMP	O3-C16-N2-C15
49	L	401	NDP	C2D-C1D-N1N-C6N
49	L	401	NDP	C2D-C1D-N1N-C2N
48	Q	201	ZMP	C6-C7-C8-C9
49	L	401	NDP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
48	Q	201	ZMP	N2-C16-C17-O4
49	L	401	NDP	O4D-C1D-N1N-C2N
49	L	401	NDP	O4D-C1D-N1N-C6N
48	Q	201	ZMP	O3-C16-C17-C18
48	Q	201	ZMP	N2-C16-C17-C18
49	L	401	NDP	O4B-C4B-C5B-O5B

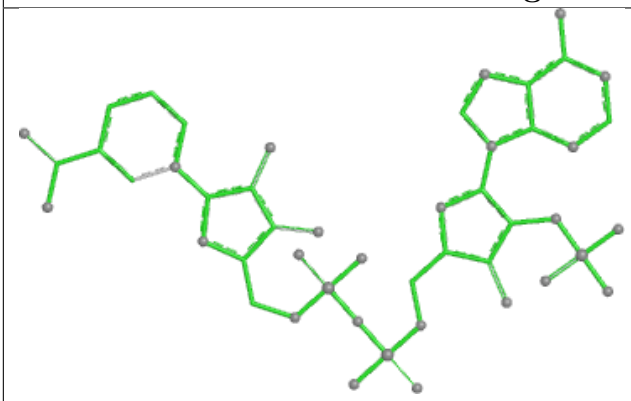
There are no ring outliers.

8 monomers are involved in 44 short contacts:

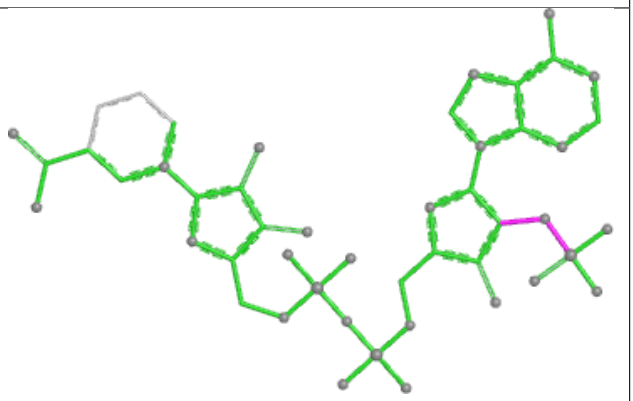
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	L	401	NDP	3	0
45	B	501	FMN	1	0
46	H	302	SF4	1	0
46	H	301	SF4	7	0
46	I	301	SF4	1	0
48	Q	201	ZMP	1	0
47	E	301	FES	9	0
46	B	502	SF4	21	0

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

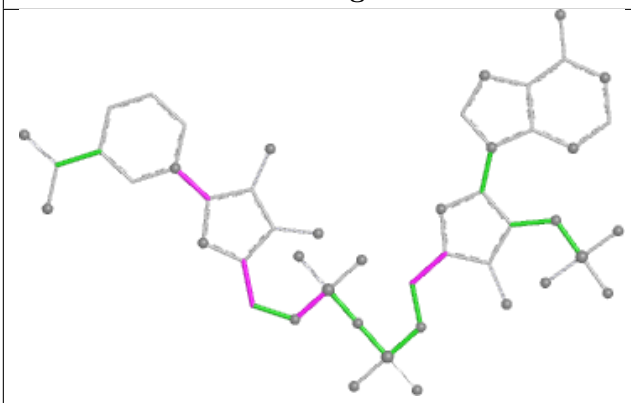
Ligand NDP L 401



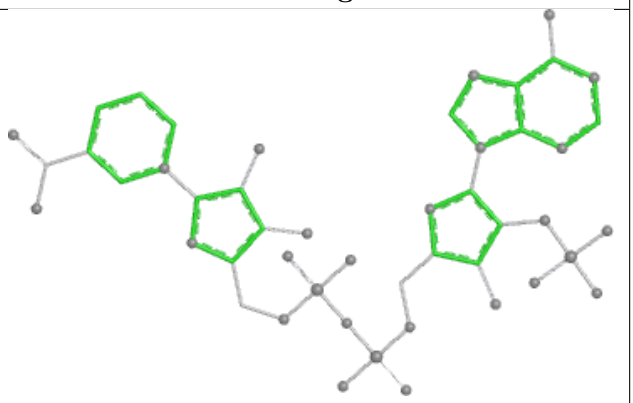
Bond lengths



Bond angles

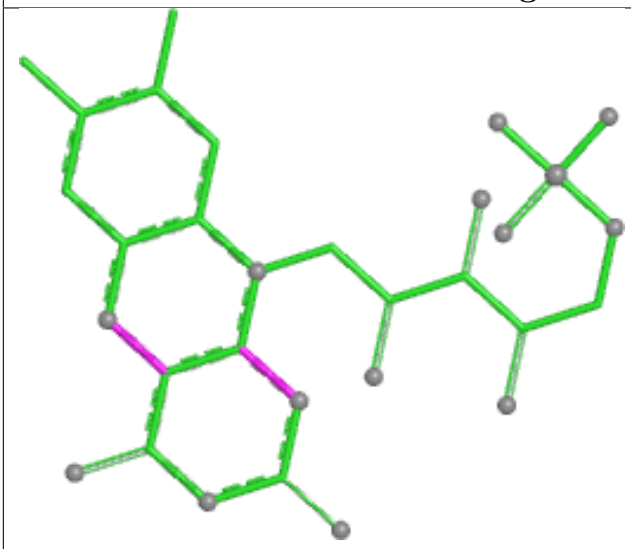


Torsions

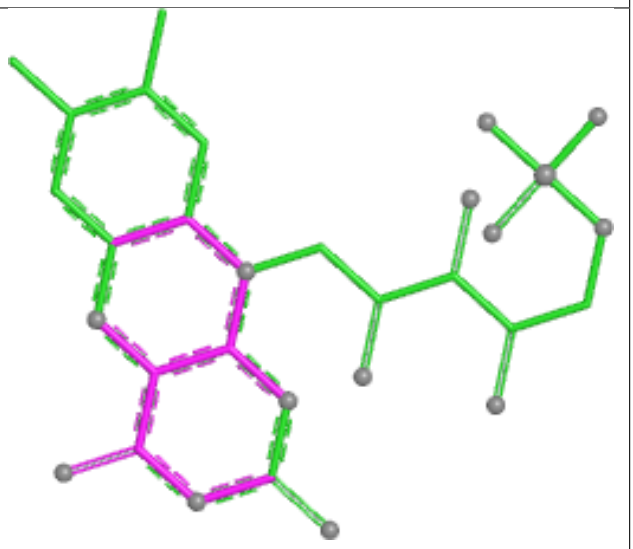


Rings

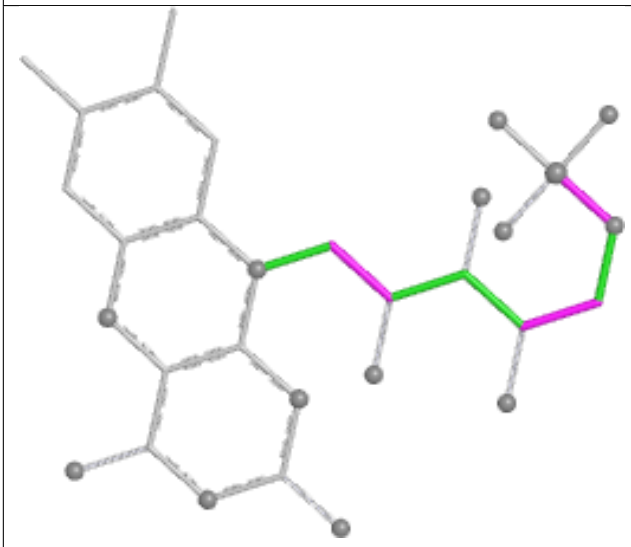
Ligand FMN B 501



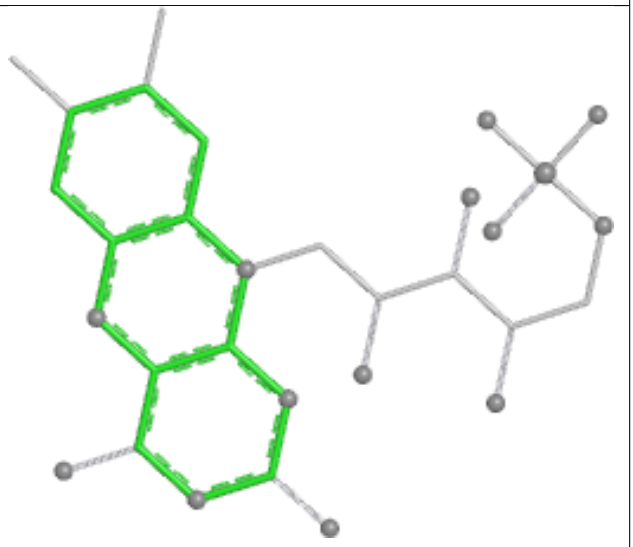
Bond lengths



Bond angles

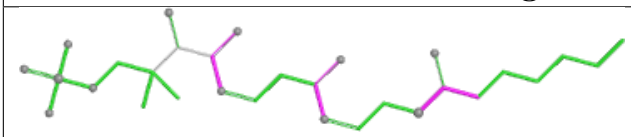


Torsions

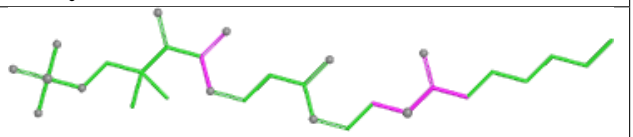


Rings

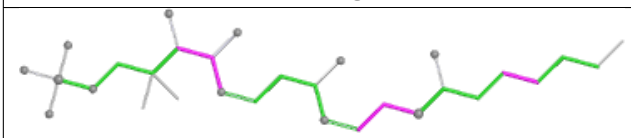
Ligand ZMP Q 201



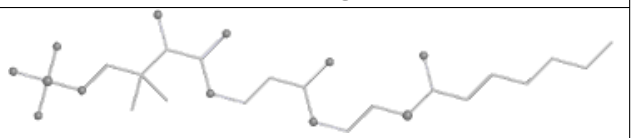
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

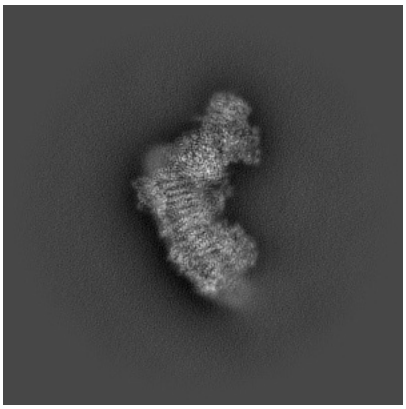
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44967. These allow visual inspection of the internal detail of the map and identification of artifacts.

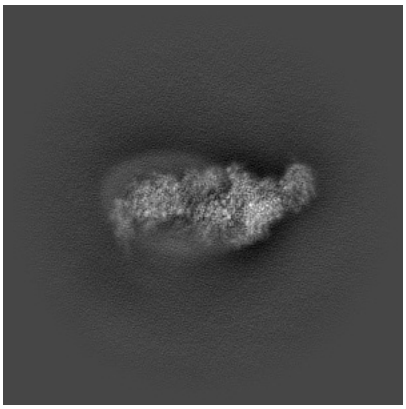
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

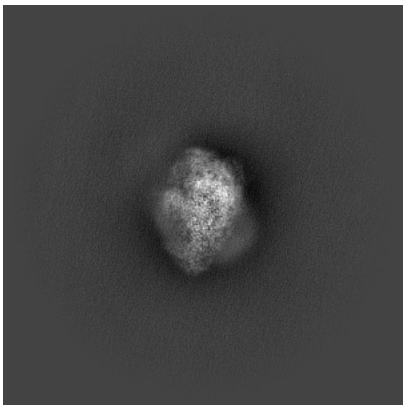
6.1.1 Primary map



X

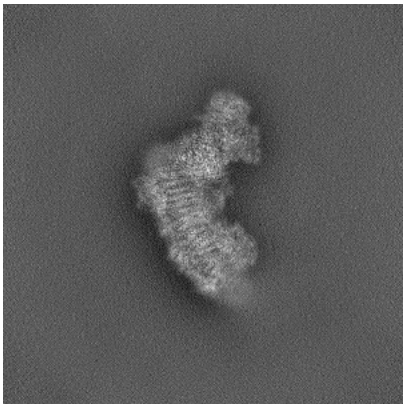


Y

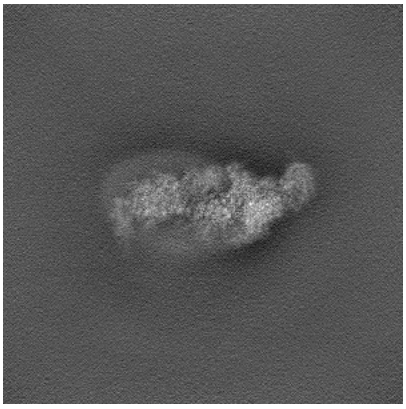


Z

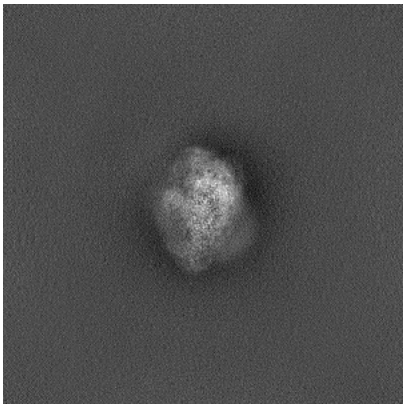
6.1.2 Raw map



X



Y

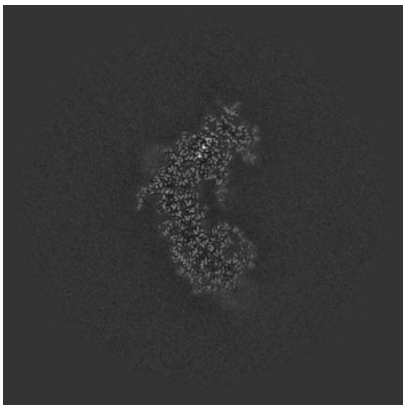


Z

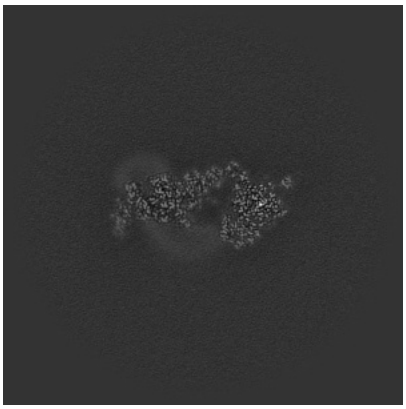
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

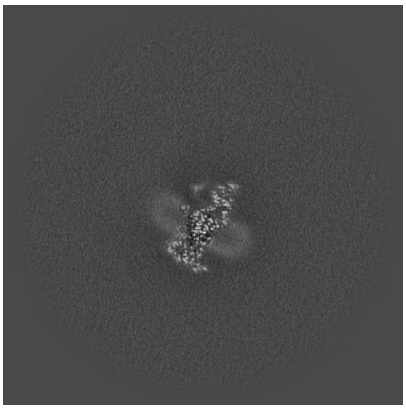
6.2.1 Primary map



X Index: 256

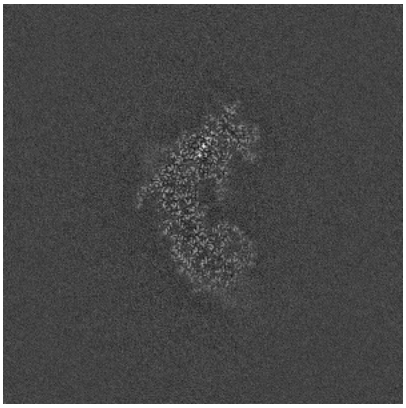


Y Index: 256

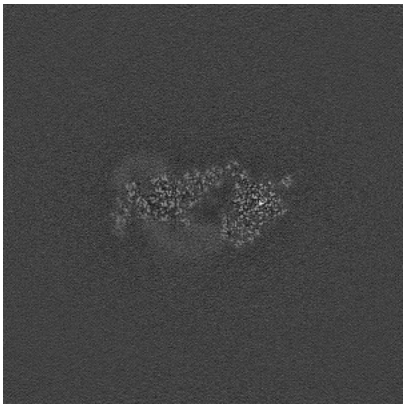


Z Index: 256

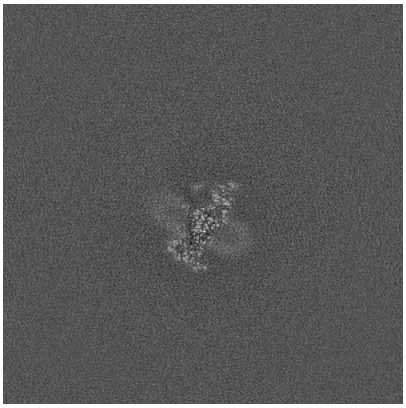
6.2.2 Raw map



X Index: 256



Y Index: 256

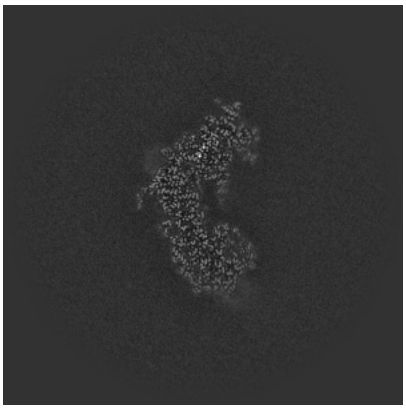


Z Index: 256

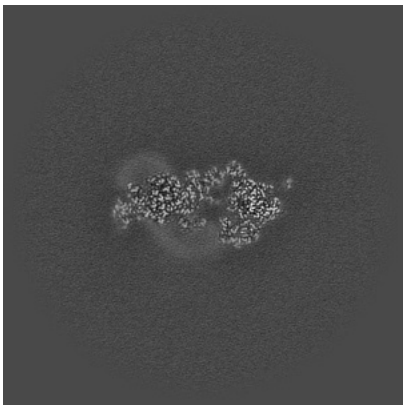
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

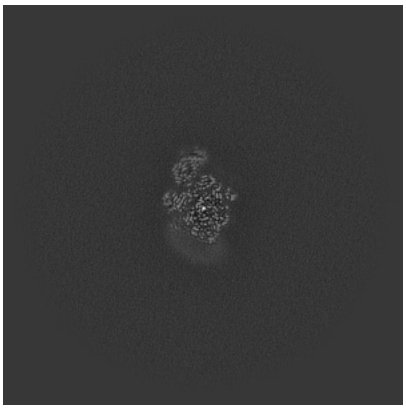
6.3.1 Primary map



X Index: 257

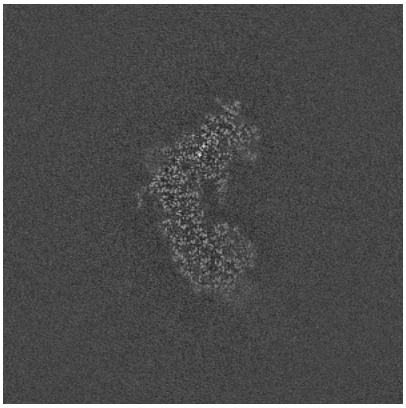


Y Index: 253

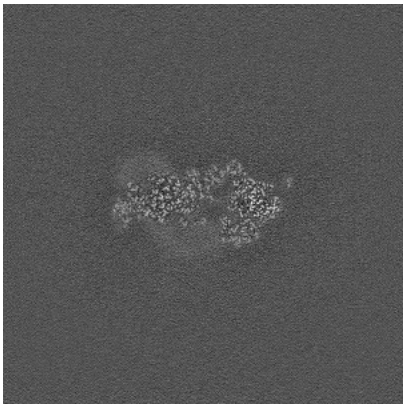


Z Index: 318

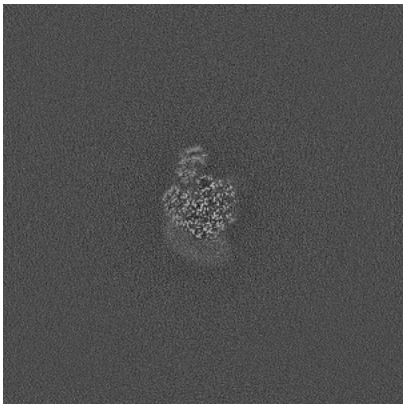
6.3.2 Raw map



X Index: 257



Y Index: 253

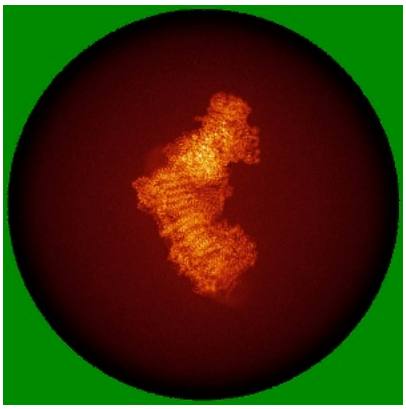


Z Index: 313

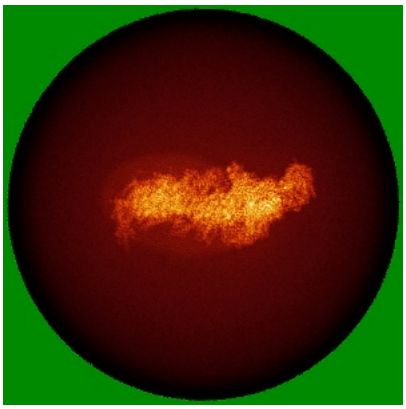
The images above show the largest variance slices of the map in three orthogonal directions.

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

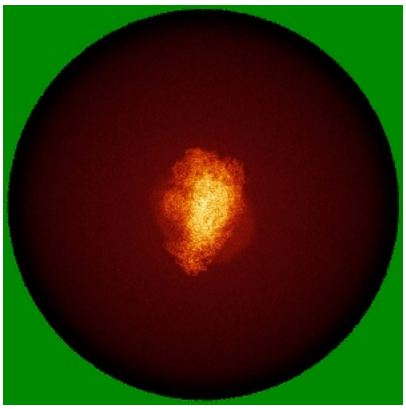
6.4.1 Primary map



X

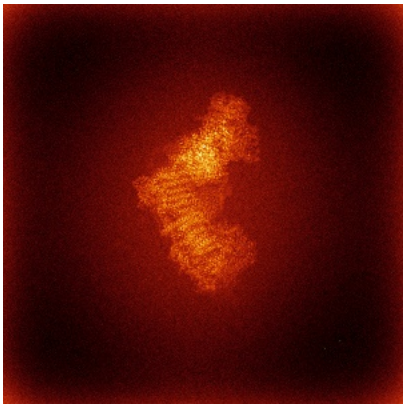


Y

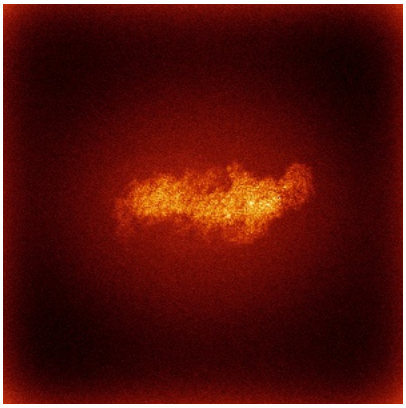


Z

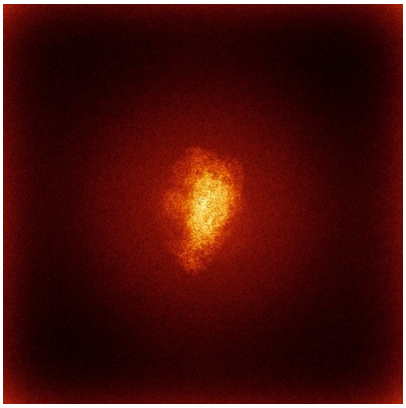
6.4.2 Raw map



X



Y

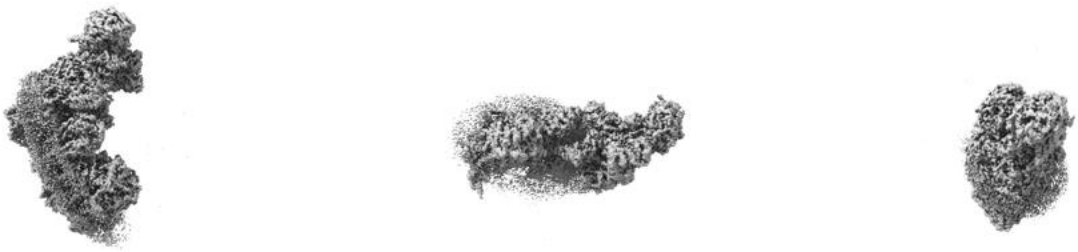


Z

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 0.15. 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.

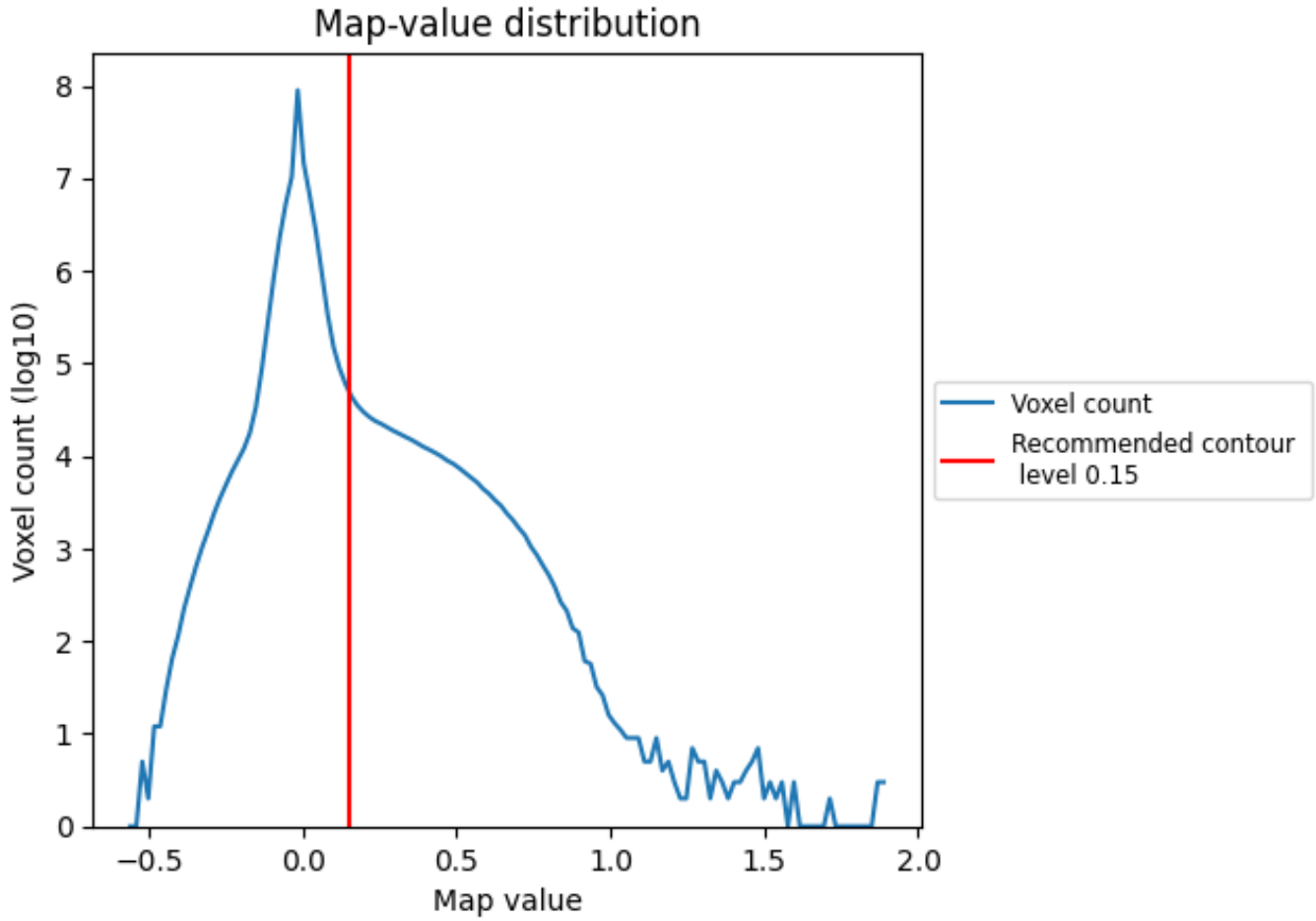
6.6 Mask visualisation (i)

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

7 Map analysis

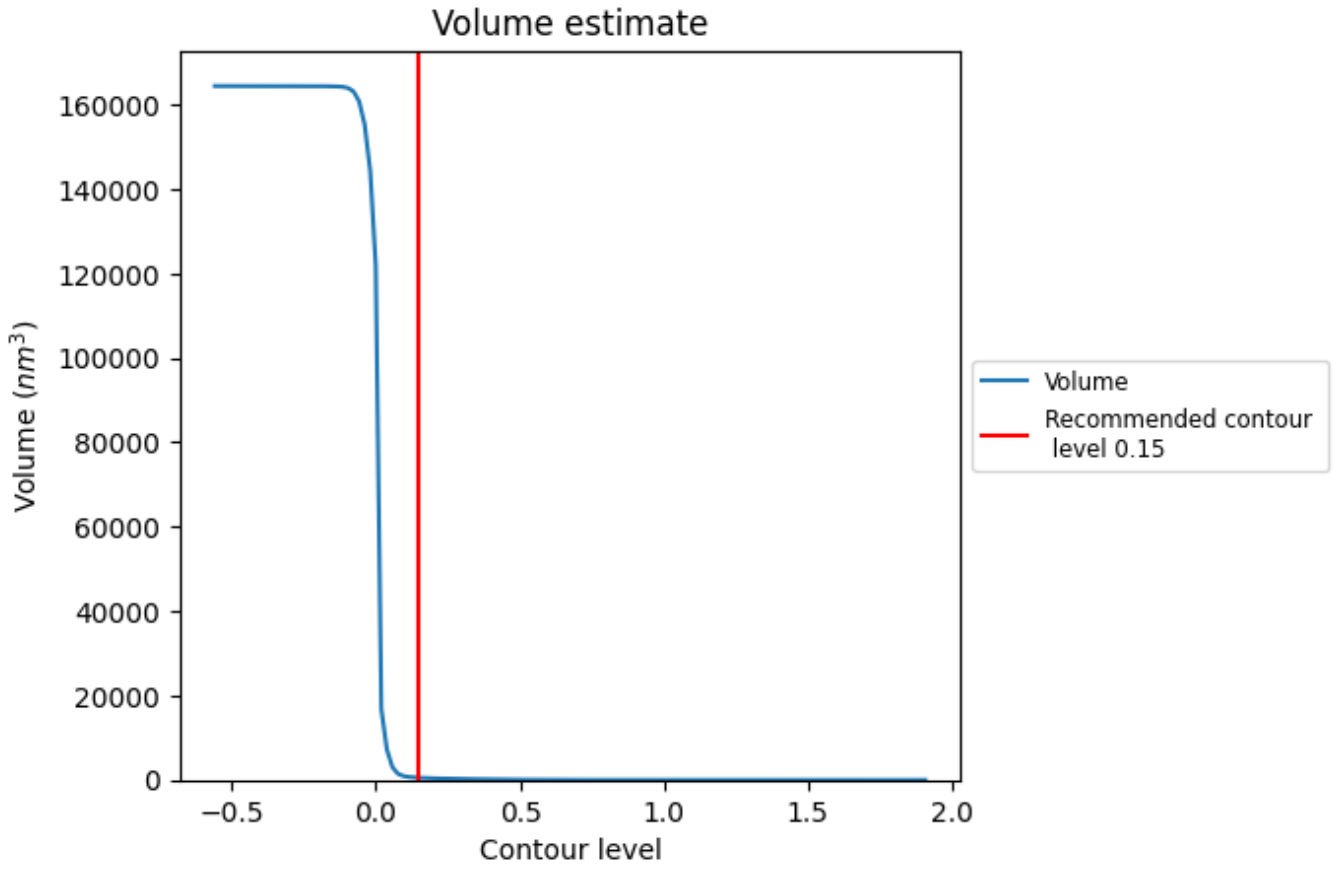
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

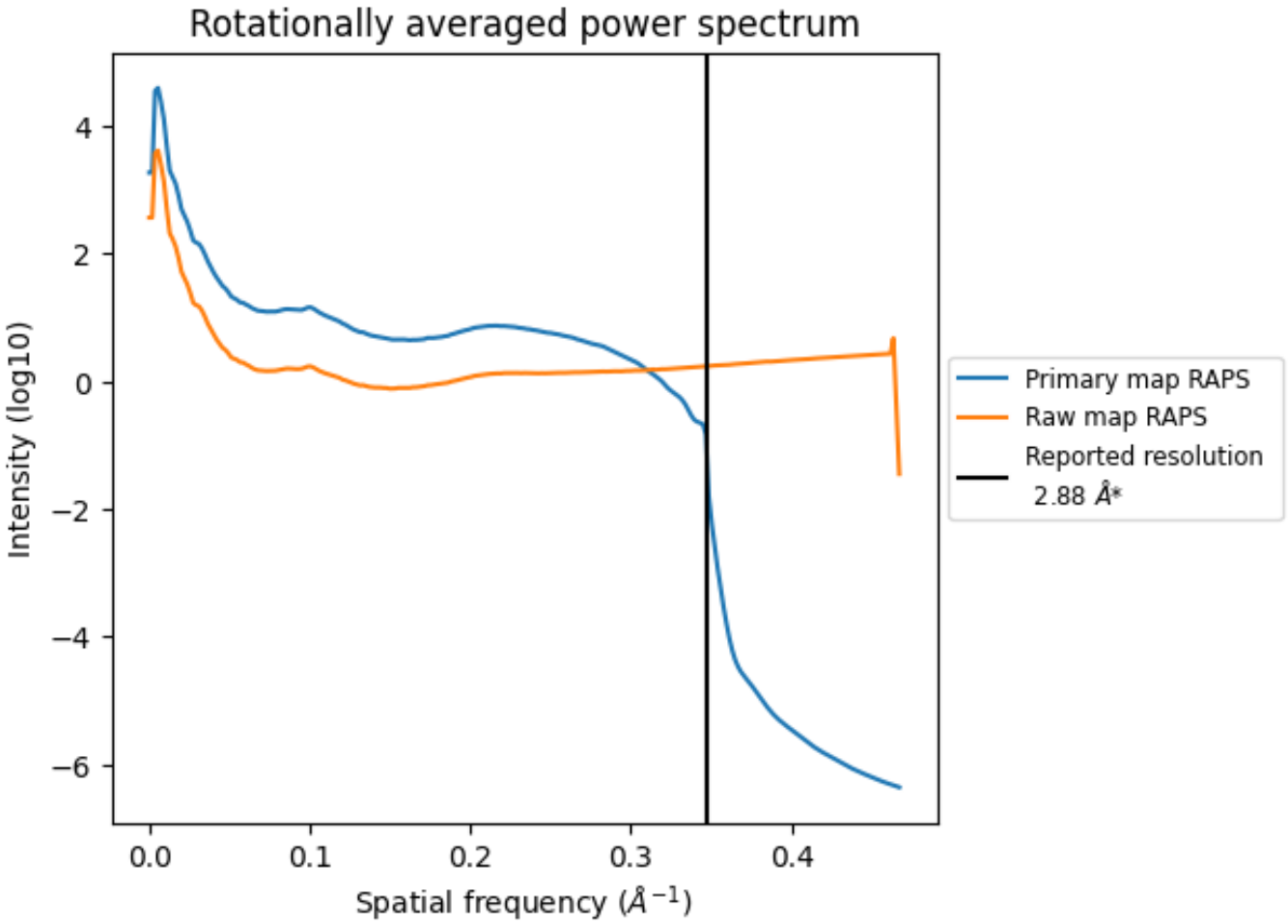
7.2 Volume estimate



The volume at the recommended contour level is 518 nm^3; this corresponds to an approximate mass of 468 kDa.

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

7.3 Rotationally averaged power spectrum (i)

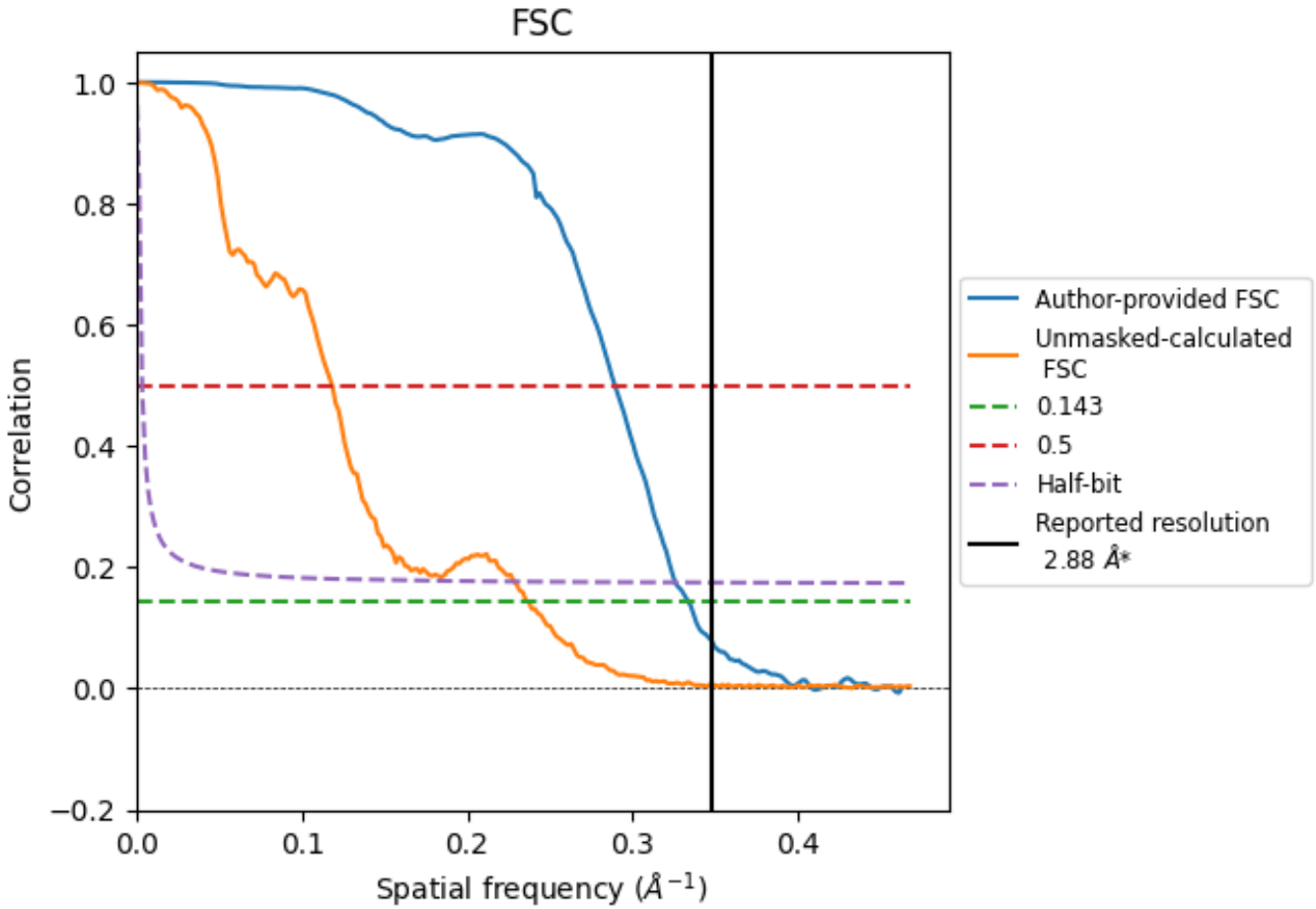


*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

8.2 Resolution estimates (i)

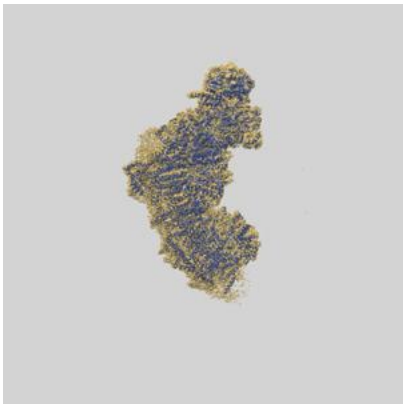
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	3.00	3.46	3.07
Unmasked-calculated*	4.22	8.45	4.38

*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 4.22 differs from the reported value 2.88 by more than 10 %

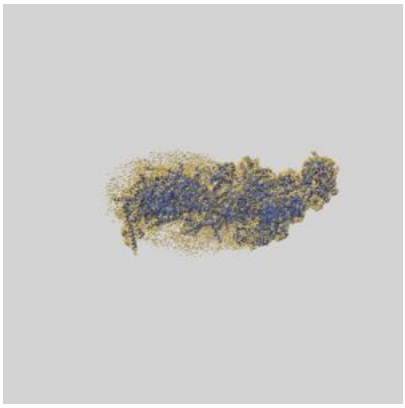
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44967 and PDB model 9BWD. Per-residue inclusion information can be found in section 3 on page 15.

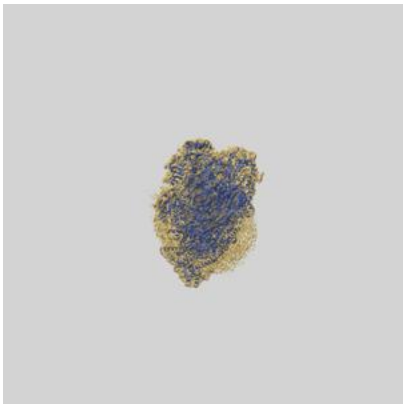
9.1 Map-model overlay



X



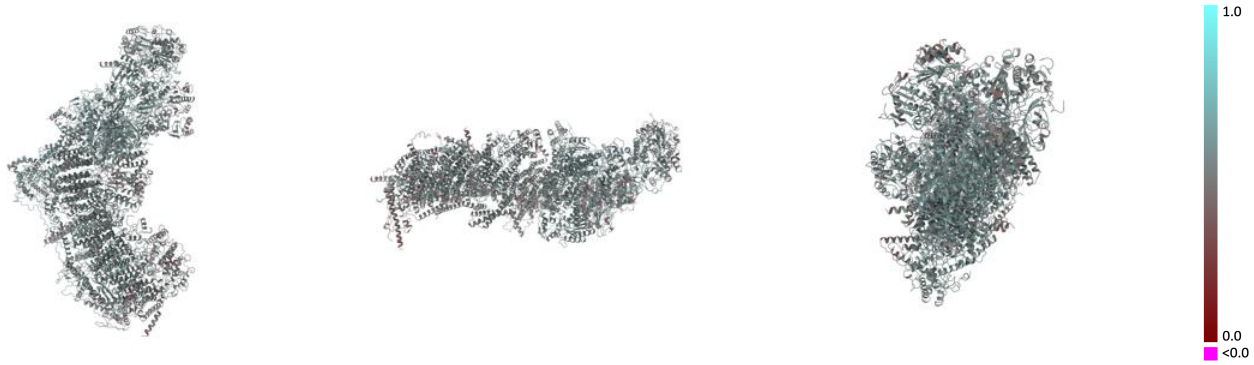
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

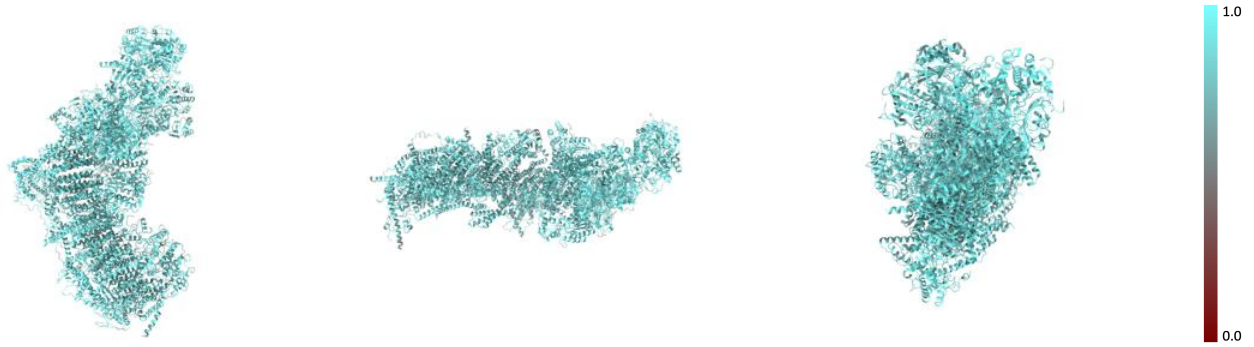
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

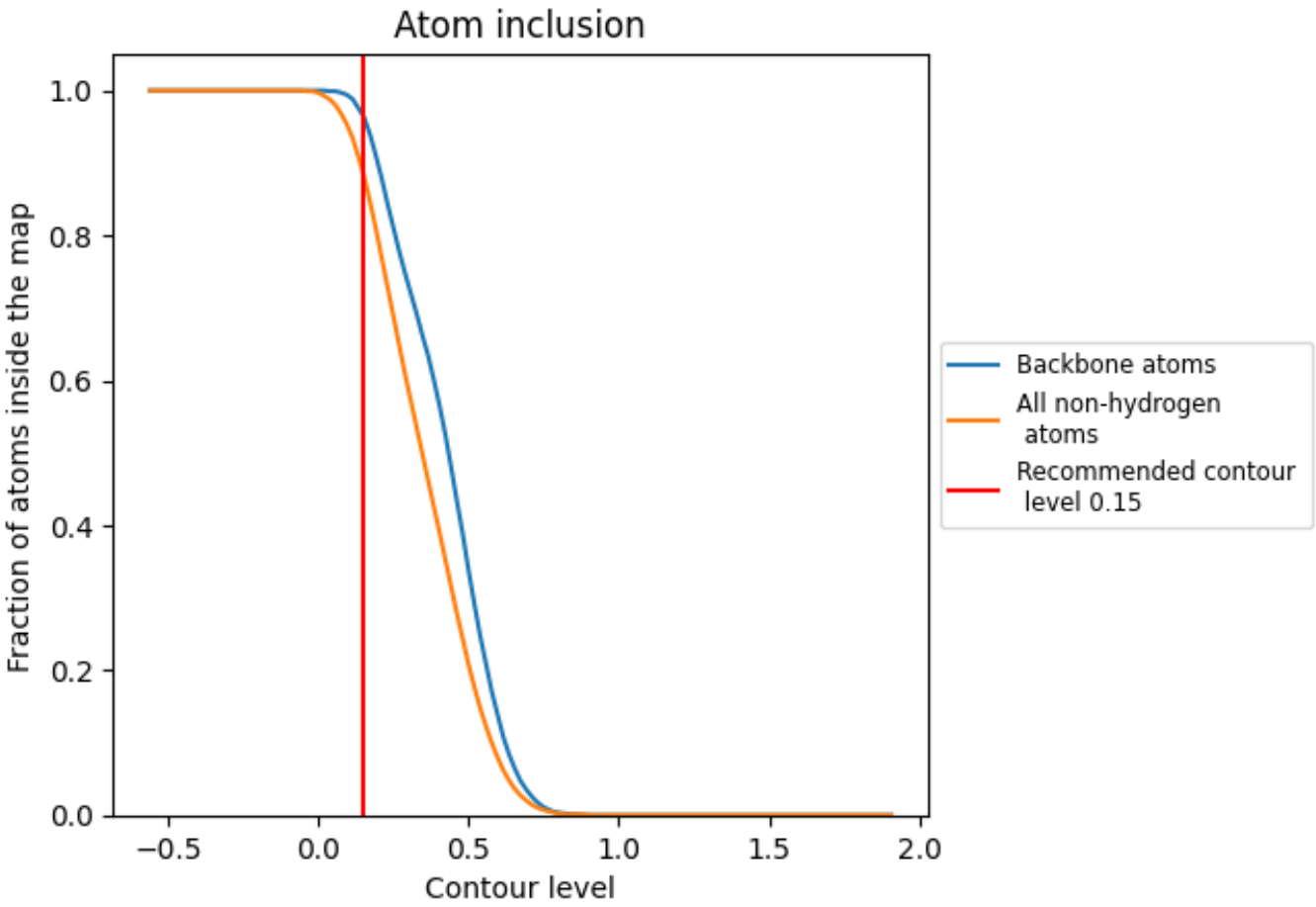
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 89% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8860	0.5290
B	0.9110	0.5270
C	0.9330	0.5710
D	0.9370	0.5680
E	0.8920	0.5130
F	0.8730	0.5450
G	0.8990	0.5390
H	0.9350	0.5630
I	0.9510	0.5690
J	0.9060	0.5470
K	0.8810	0.5500
L	0.9040	0.5420
M	0.8890	0.5510
N	0.8880	0.5320
O	0.7800	0.4520
P	0.8400	0.4740
Q	0.8870	0.5320
R	0.8400	0.4950
S	0.9310	0.5540
T	0.8770	0.5090
U	0.8480	0.4990
V	0.8590	0.5010
W	0.8950	0.5360
X	0.8050	0.4700
Y	0.8330	0.4540
Z	0.8060	0.4720
a	0.9130	0.5490
b	0.8140	0.4530
c	0.8610	0.5150
d	0.8830	0.5010
e	0.8410	0.5030
f	0.7950	0.4750
g	0.9150	0.5400
h	0.8860	0.5240
i	0.9040	0.5510



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Chain	Atom inclusion	Q-score
j	0.8810	0.5460
k	0.8710	0.5410
l	0.8620	0.5260
m	0.8540	0.5220
n	0.8380	0.4830
o	0.8540	0.5060
p	0.8570	0.4990
q	0.9010	0.5510
r	0.9050	0.5540
s	0.9020	0.5360
t	0.8180	0.4430