Full wwPDB EM Validation Report ⓘ

Sep 8, 2026 – 01:22 am BST

PDB ID	:	6QC8 / pdb_00006qc8
EMDB ID	:	EMD-4500
Title	:	Ovine respiratory complex I FRC open class 2
Authors	:	Letts, J.A.; Sazanov, L.A.
Deposited on	:	2018-12-27
Resolution	:	4.20 Å(reported)
Based on initial model	:	5LNK

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:

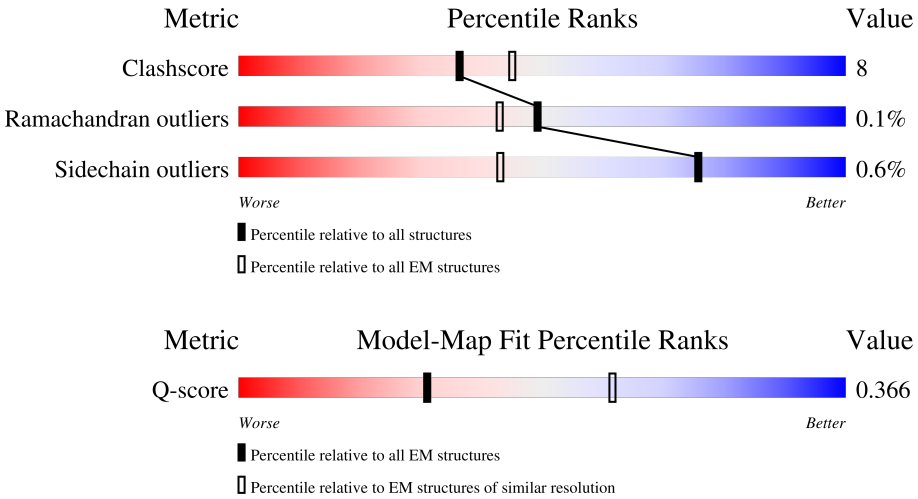
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	V1	445	14% 76% 20%
2	V2	217	16% 77% 19%
3	S1	704	14% 74% 23%
4	S2	430	20% 80% 20%

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Mol	Chain	Length	Quality of chain
5	S3	228	11% 75% 16% 9%
6	S7	179	13% 66% 21% 13%
7	S8	176	10% 80% 19%
8	V3	75	9% 43% 11% 45%
9	S6	96	25% 85% 14%
10	S4	133	17% 70% 25% 5%
11	A9	338	23% 64% 21% 15%
12	A2	98	18% 59% 24% 16%
13	A5	115	25% 81% 15%
14	A6	127	20% 77% 13% 10%
15	A7	112	35% 67% 17% 14%
16	AL	145	42% 86% 13%
17	AA	88	36% 75% 16% 9%
17	AB	88	34% 82% 16%
18	D3	115	33% 67% 11% 22%
19	D1	318	27% 75% 19% 5%
20	D6	175	47% 78% 19%
21	4L	98	44% 80% 20%
22	D5	606	37% 75% 25%
23	D4	459	28% 74% 25%
24	D2	347	24% 71% 29%
25	AK	140	55% 85% 13%
26	B5	143	23% 77% 20%
27	A8	171	25% 85% 14%
28	BJ	175	25% 81% 15%

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Mol	Chain	Length	Quality of chain
29	AJ	320	33% 75% 25%
30	S5	105	30% 79% 14% 6%
31	A3	83	25% 75% 14% 11%
32	B3	97	34% 58% 15% 25%
33	C2	120	32% 88% 11%
34	B4	128	41% 83% 17%
35	AM	143	22% 78% 20%
36	B6	127	31% 57% 17% 24%
37	B7	136	34% 66% 21% 12%
38	B9	178	24% 76% 21%
39	B2	72	40% 82% 8% 10%
40	B8	158	36% 75% 22%
41	BK	125	33% 74% 8% 18%
42	C1	49	31% 86% 8% 6%
43	B1	57	46% 75% 16% 9%
44	A1	70	23% 90% 10%

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
45	SF4	S1	801	-	-	X	-

2 Entry composition (i)

There are 53 unique types of molecules in this entry. The entry contains 65394 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	V1	430	3312	2086	593	613	20	0	0

- Molecule 2 is a protein called NDUFV2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V2	212	1647	1052	277	308	10	0	0

- Molecule 3 is a protein called NADH:ubiquinone oxidoreductase core subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	S1	688	5275	3301	922	1011	41	0	0

- Molecule 4 is a protein called NADH:ubiquinone oxidoreductase core subunit S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S2	430	3455	2205	594	631	25	0	0

- Molecule 5 is a protein called NADH:ubiquinone oxidoreductase core subunit S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S3	208	1726	1112	296	315	3	0	0

- Molecule 6 is a protein called NADH:ubiquinone oxidoreductase core subunit S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	S7	156	1247	795	225	213	14	0	0

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S8	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 8 is a protein called NADH:ubiquinone oxidoreductase subunit V3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	V3	41	Total	C	N	O	S	0	0
			345	215	63	66	1		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	S6	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 10 is a protein called NADH:ubiquinone oxidoreductase subunit S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	S4	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 11 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	A9	287	Total	C	N	O	S	0	0
			2293	1464	419	405	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A2	82	Total	C	N	O	S	0	0
			665	419	124	120	2		

- Molecule 13 is a protein called NDUFA5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A5	111	Total	C	N	O	S	0	0
			901	583	151	165	2		

- Molecule 14 is a protein called NADH:ubiquinone oxidoreductase subunit A6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A6	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

- Molecule 15 is a protein called NDUFA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A7	96	Total	C	N	O	S	0	0
			766	478	146	139	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AL	144	Total	C	N	O	S	0	0
			1201	773	215	209	4		

- Molecule 17 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AA	80	Total	C	N	O	S	0	0
			645	416	96	128	5		
17	AB	87	Total	C	N	O	S	0	0
			702	451	103	143	5		

- Molecule 18 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	D3	90	Total	C	N	O	S	0	0
			728	500	103	120	5		

- Molecule 19 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	D1	303	Total	C	N	O	S	0	0
			2415	1633	368	395	19		

- Molecule 20 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	D6	171	Total	C	N	O	S	0	0
			1308	878	187	230	13		

- Molecule 21 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4L	98	Total	C	N	O	S	0	0
			748	489	112	132	15		

- Molecule 22 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D5	606	Total	C	N	O	S	0	0
			4805	3187	746	828	44		

- Molecule 23 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D4	459	Total	C	N	O	S	0	0
			3646	2428	571	607	40		

- Molecule 24 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D2	347	Total	C	N	O	S	0	0
			2724	1808	416	460	40		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AK	140	Total	C	N	O	S	0	0
			1025	654	175	190	6		

- Molecule 26 is a protein called NADH:ubiquinone oxidoreductase subunit B5.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B5	139	Total	C	N	O	S	0	0
			1156	761	194	199	2		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A8	171	Total	C	N	O	S	0	0
			1404	889	253	252	10		

- Molecule 28 is a protein called NADH:ubiquinone oxidoreductase subunit B10.

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

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	AJ	319	Total	C	N	O	S	0	0
			2583	1653	430	490	10		

- Molecule 30 is a protein called NADH:ubiquinone oxidoreductase subunit S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	S5	99	Total	C	N	O	S	0	0
			822	520	154	142	6		

- Molecule 31 is a protein called NADH:ubiquinone oxidoreductase subunit A3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A3	74	Total	C	N	O	S	0	0
			582	379	96	105	2		

- Molecule 32 is a protein called NADH:ubiquinone oxidoreductase subunit B3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	B3	73	Total	C	N	O	S	0	0
			578	378	100	98	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	C2	119	Total	C	N	O	S	0	0
			997	647	174	172	4		

- Molecule 34 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B4	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AM	139	Total	C	N	O	S	0	0
			1143	733	200	201	9		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	B6	96	Total	C	N	O	S	0	0
			815	536	139	139	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B7	119	Total	C	N	O	S	0	0
			1026	641	196	181	8		

- Molecule 38 is a protein called NADH:ubiquinone oxidoreductase subunit B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	B9	176	Total	C	N	O	S	0	0
			1515	970	278	261	6		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	B2	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	B8	157	Total	C	N	O	S	0	0
			1324	855	217	243	9		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BK	102	Total	C	N	O	S	0	0
			853	547	141	161	4		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	C1	46	Total	C	N	O	0	0
			391	258	67	66		

- Molecule 43 is a protein called NADH dehydrogenase (Ubiquinone) 1 beta subcomplex, 1, 7kDa.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	B1	52	Total	C	N	O	0	0
			449	296	79	74		

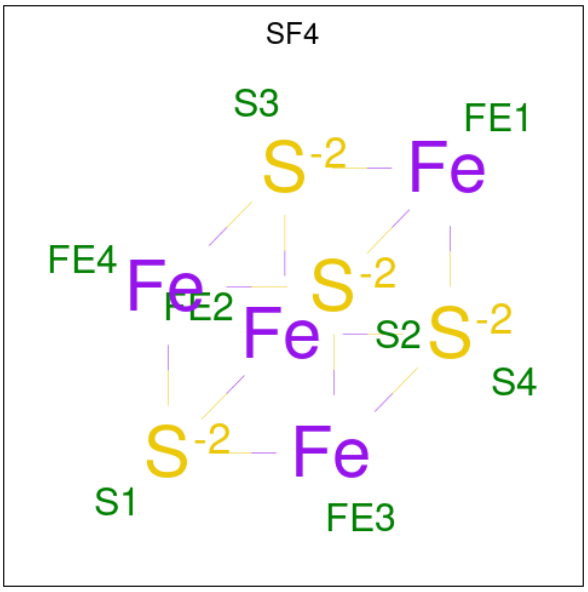
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	16	VAL	GLY	conflict	UNP W5QG39
B1	35	ALA	THR	conflict	UNP W5QG39
B1	38	ARG	TRP	conflict	UNP W5QG39

- Molecule 44 is a protein called NADH dehydrogenase 1 alpha subcomplex.

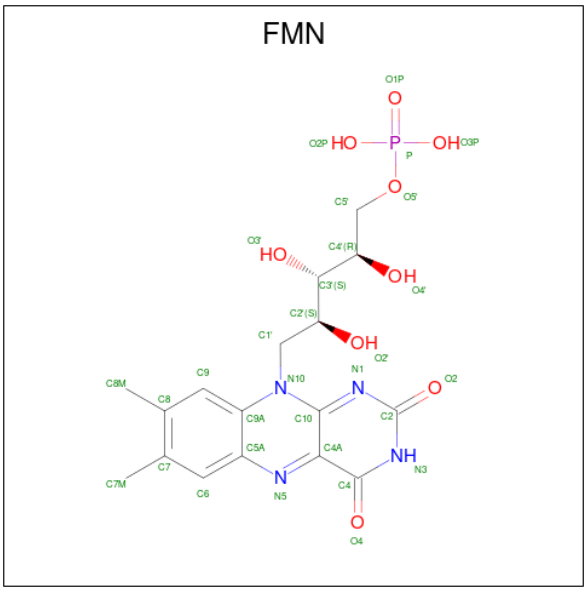
Mol	Chain	Residues	Atoms					AltConf	Trace
44	A1	70	Total	C	N	O	S	0	0
			577	369	106	97	5		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



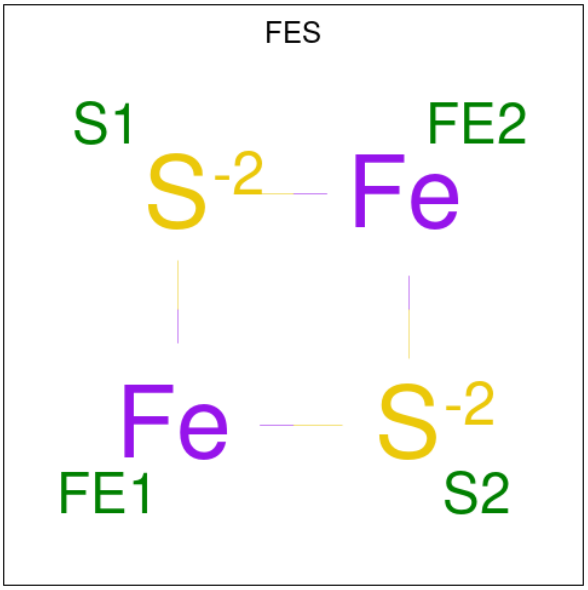
Mol	Chain	Residues	Atoms	AltConf
45	V1	1	Total Fe S 8 4 4	0
45	S1	1	Total Fe S 8 4 4	0
45	S1	1	Total Fe S 8 4 4	0
45	S7	1	Total Fe S 8 4 4	0
45	S8	1	Total Fe S 8 4 4	0
45	S8	1	Total Fe S 8 4 4	0

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
46	V1	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

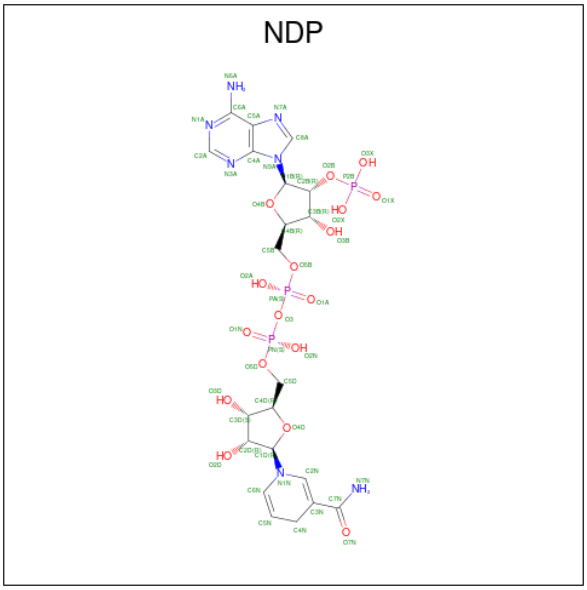


Mol	Chain	Residues	Atoms			AltConf
47	V2	1	Total	Fe	S	0
			4	2	2	
47	S1	1	Total	Fe	S	0
			4	2	2	

- Molecule 48 is ZINC ION (CCD ID: ZN) (formula: Zn).

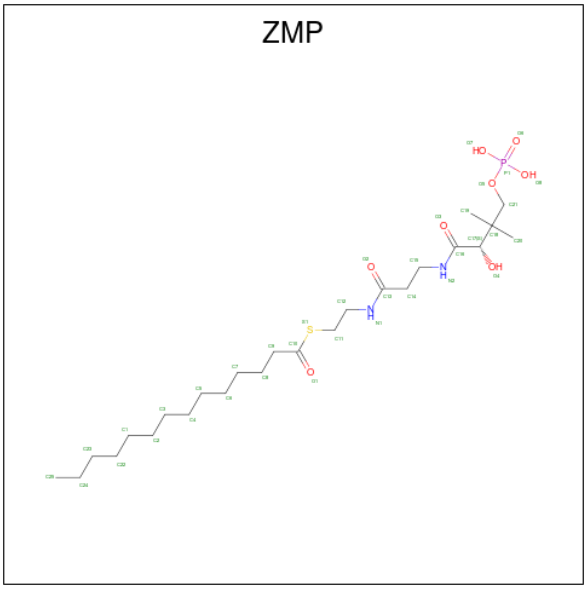
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
48	S6	1	1	1	0

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



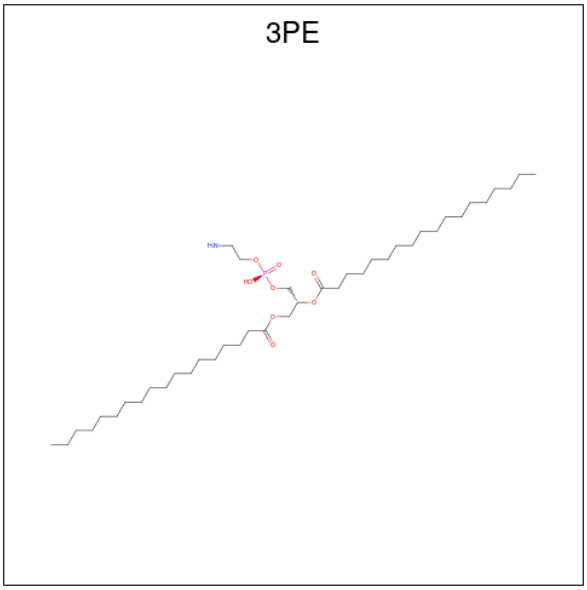
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
49	A9	1	48	21	7	17	3	0

- Molecule 50 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



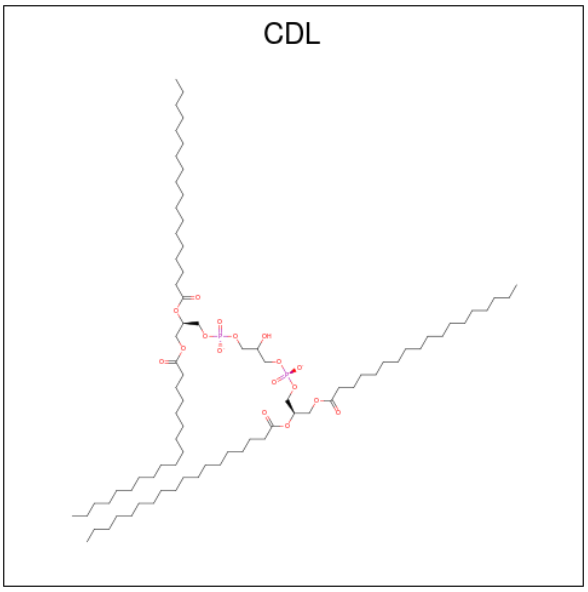
Mol	Chain	Residues	Atoms						AltConf
50	AA	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	
50	AB	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	

- Molecule 51 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



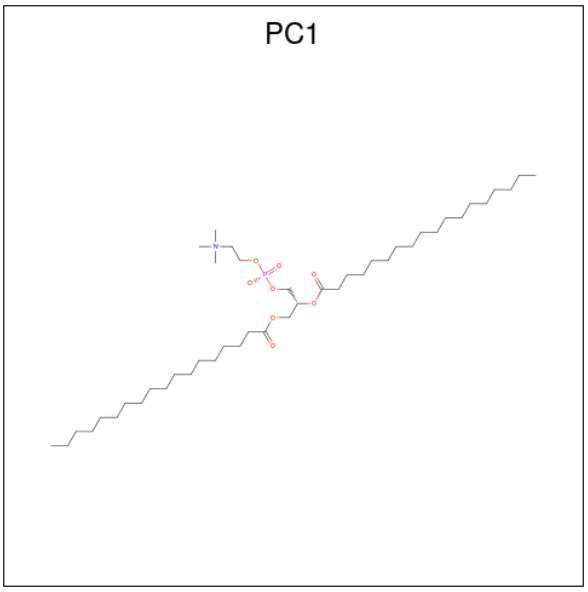
Mol	Chain	Residues	Atoms					AltConf
51	D1	1	Total	C	N	O	P	0
			26	16	1	8	1	
51	D5	1	Total	C	N	O	P	0
			38	28	1	8	1	
51	D4	1	Total	C	N	O	P	0
			40	30	1	8	1	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
52	D5	1	Total	C	O	P	0
			60	41	17	2	

- Molecule 53 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



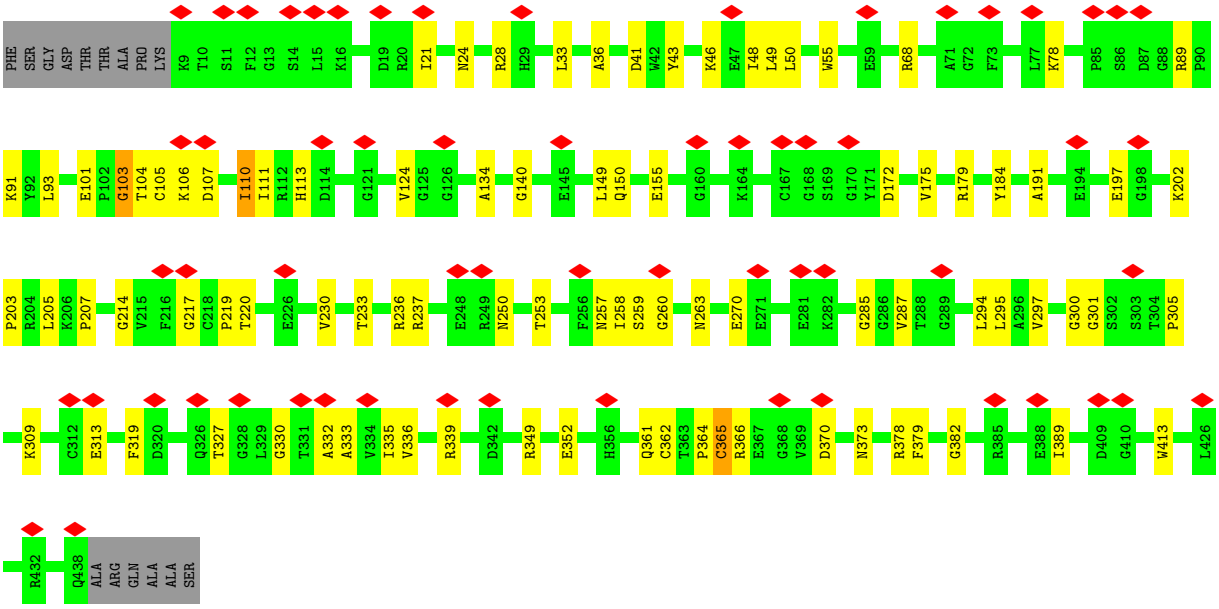
Mol	Chain	Residues	Atoms					AltConf
53	AK	1	Total	C	N	O	P	0
			28	18	1	8	1	

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.

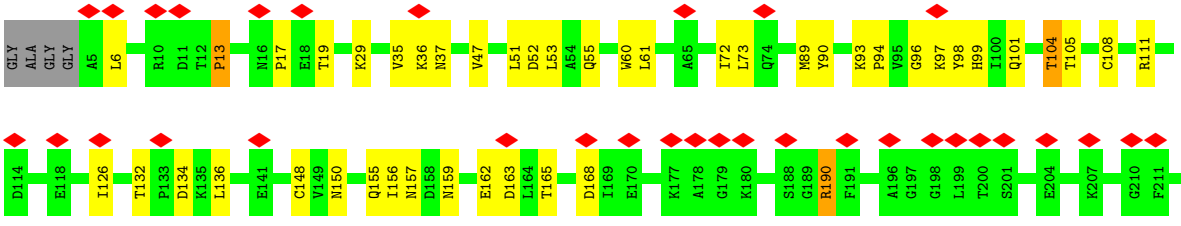
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain V1:



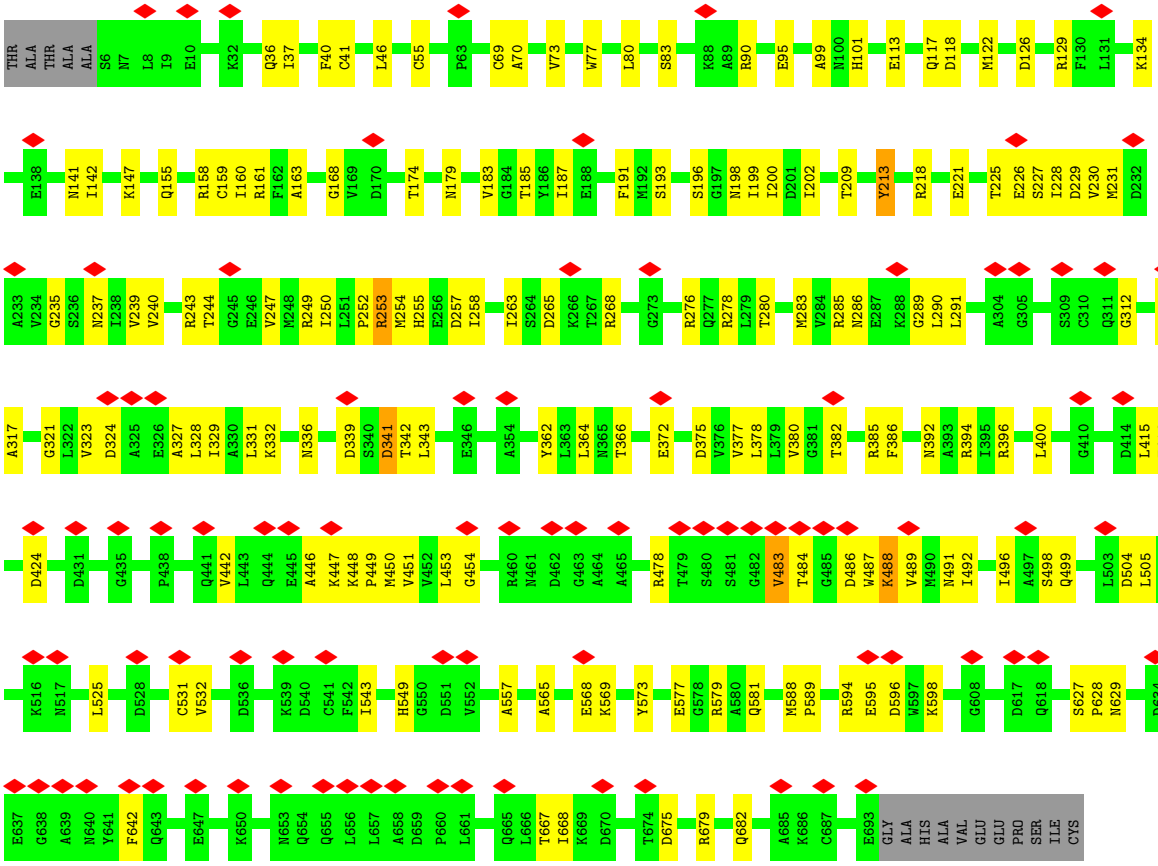
• Molecule 2: NDUFV2

Chain V2:



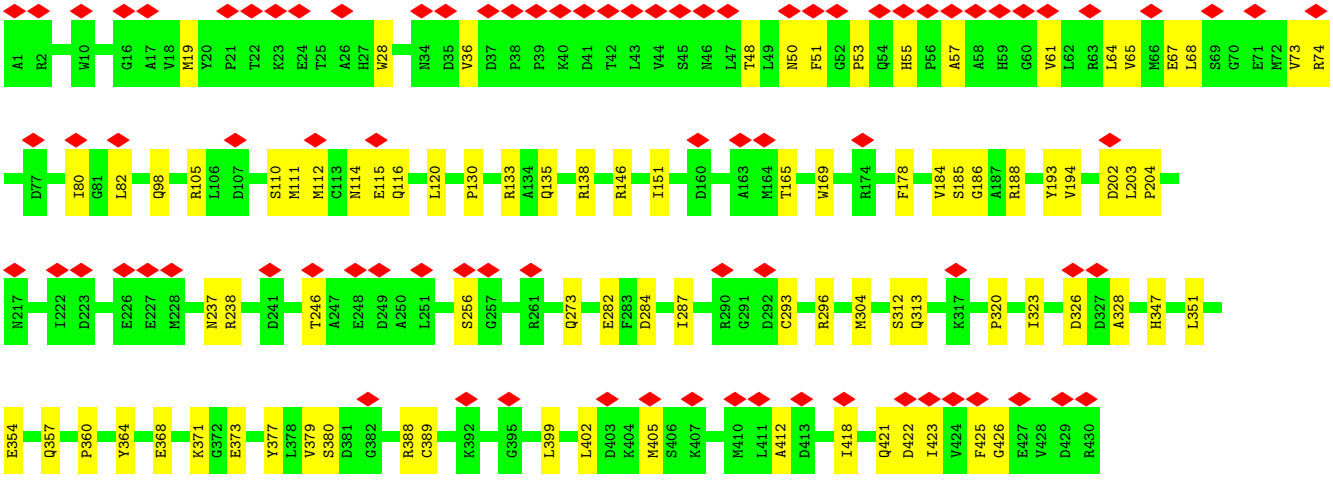
• Molecule 3: NADH:ubiquinone oxidoreductase core subunit S1

Chain S1:



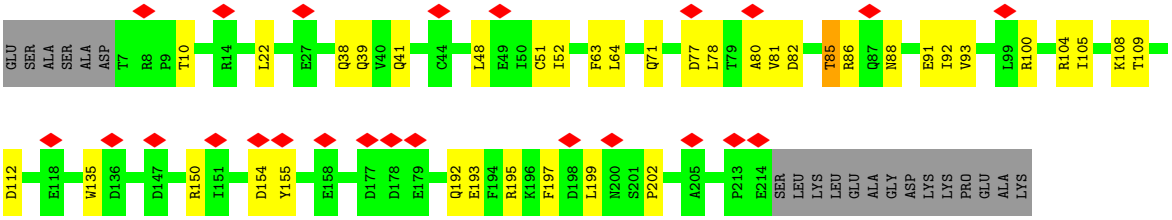
• Molecule 4: NADH:ubiquinone oxidoreductase core subunit S2

Chain S2:

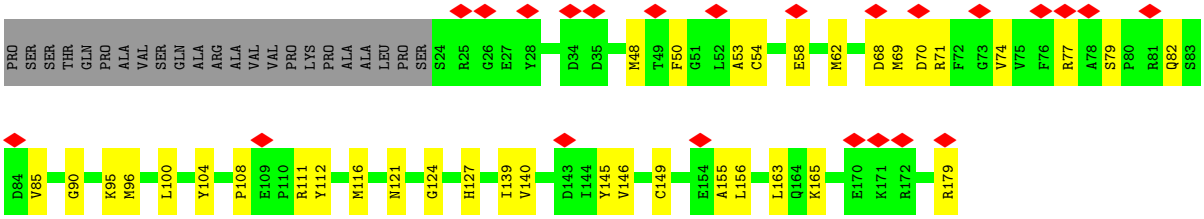


• Molecule 5: NADH:ubiquinone oxidoreductase core subunit S3

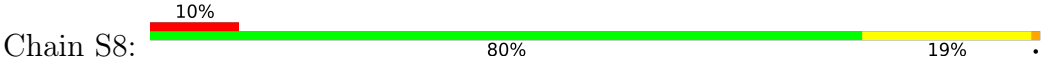
Chain S3:

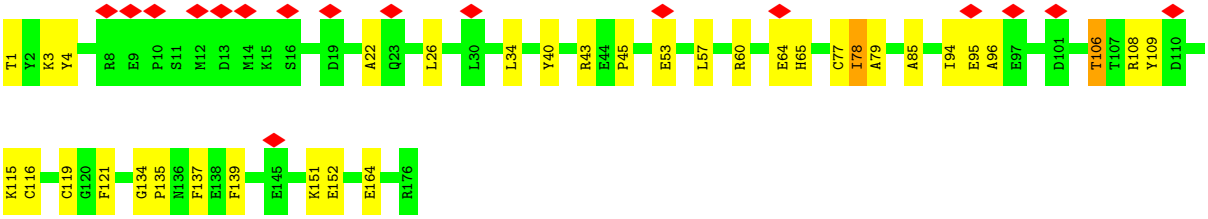


• Molecule 6: NADH:ubiquinone oxidoreductase core subunit S7

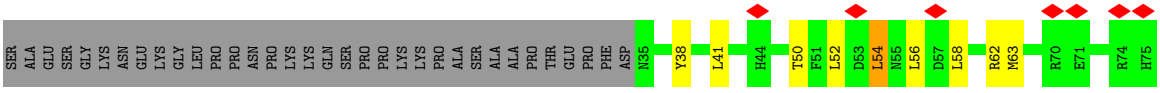


• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

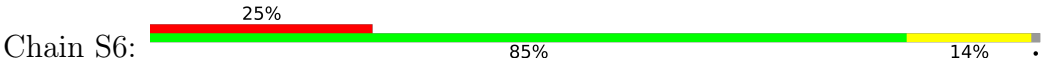


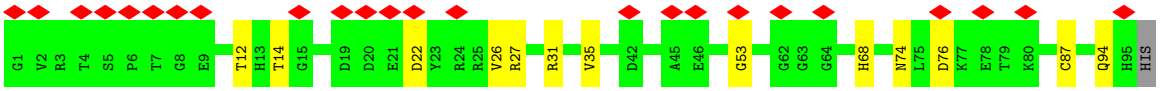


• Molecule 8: NADH:ubiquinone oxidoreductase subunit V3

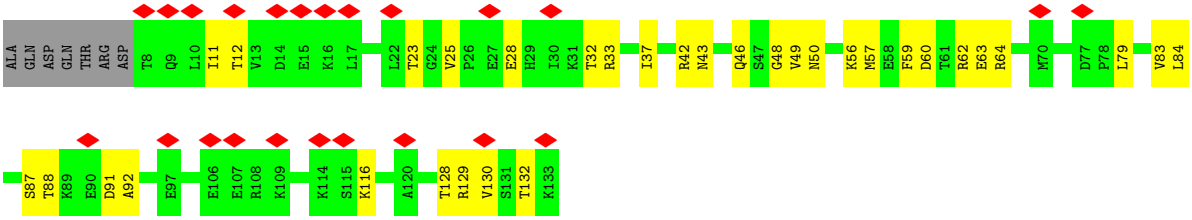


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



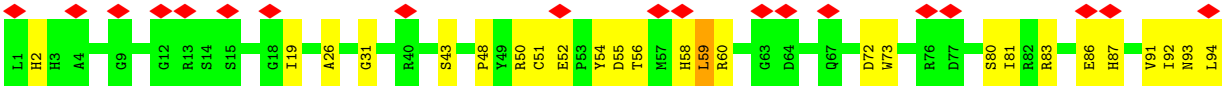


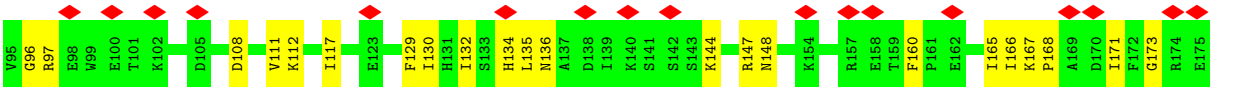
• Molecule 10: NADH:ubiquinone oxidoreductase subunit S4

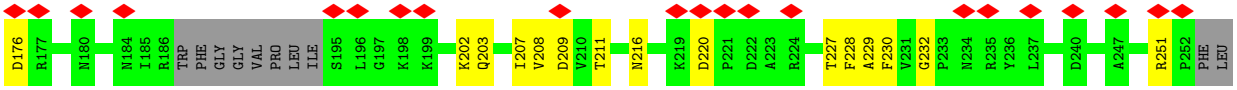


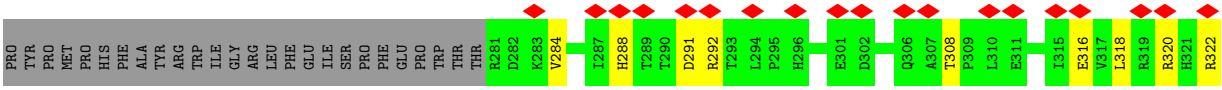
• Molecule 11: NADH:ubiquinone oxidoreductase subunit A9

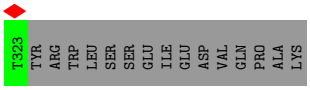
Chain A9:





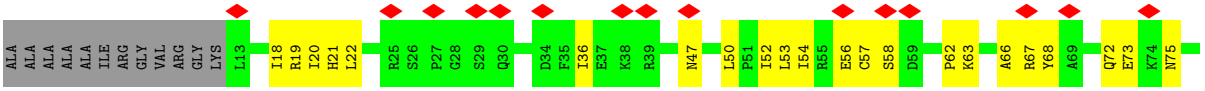


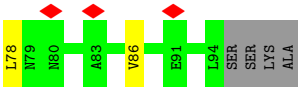




• Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

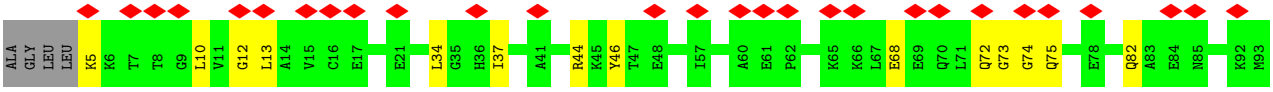
Chain A2:

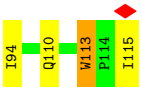




• Molecule 13: NDUFA5

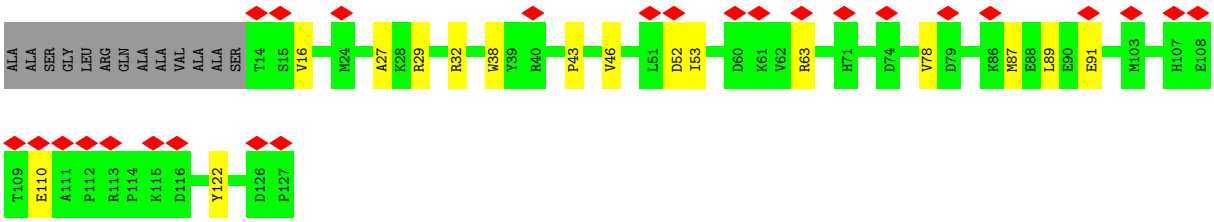
Chain A5:





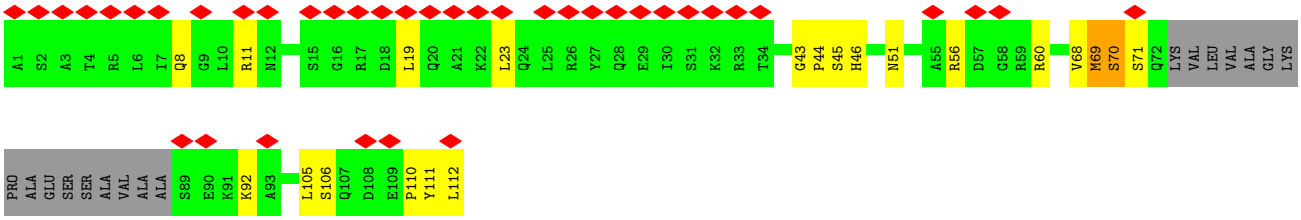
• Molecule 14: NADH:ubiquinone oxidoreductase subunit A6

Chain A6:



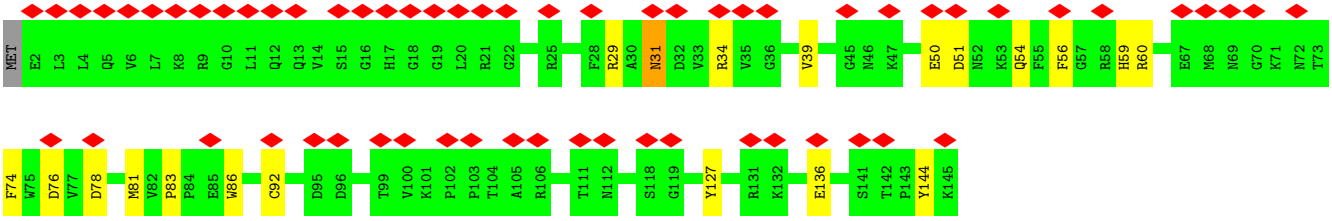
• Molecule 15: NDUFA7

Chain A7:



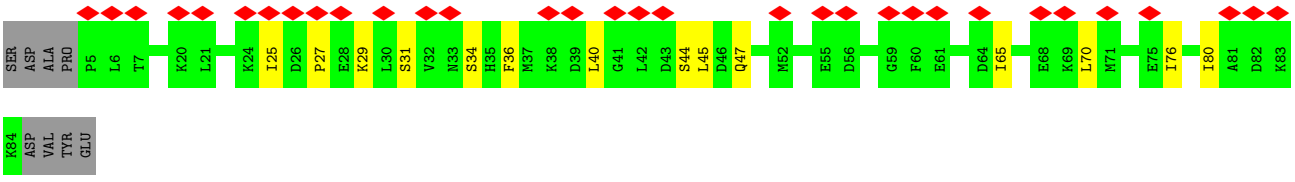
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain AL:



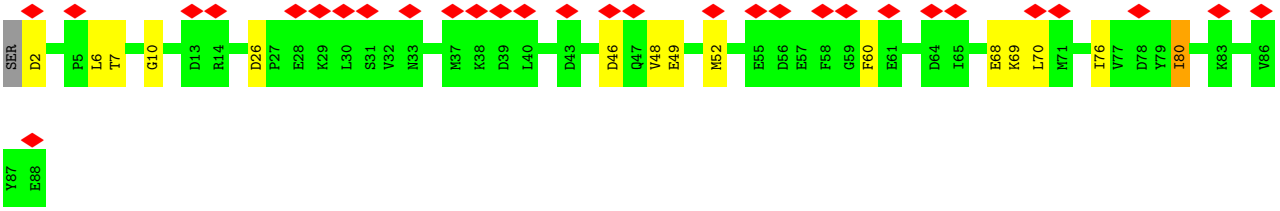
• Molecule 17: Acyl carrier protein

Chain AA:



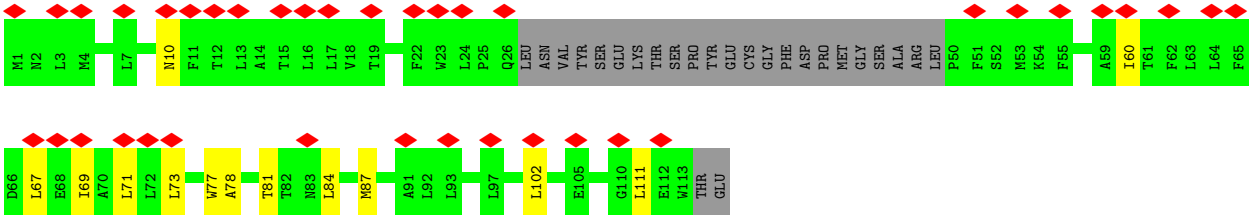
• Molecule 17: Acyl carrier protein

Chain AB:



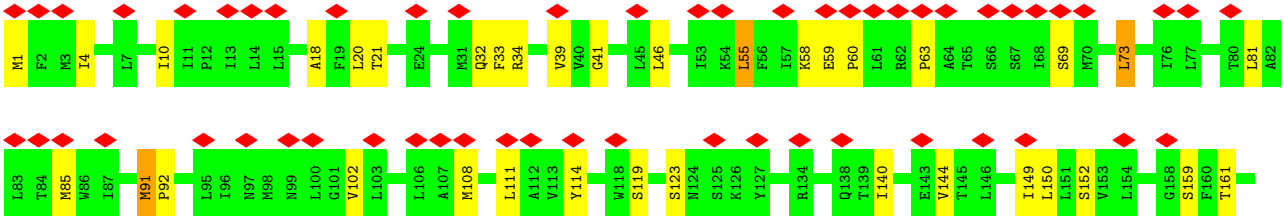
• Molecule 18: NADH-ubiquinone oxidoreductase chain 3

Chain D3:



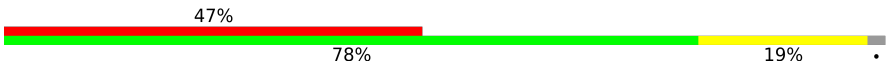
• Molecule 19: NADH-ubiquinone oxidoreductase chain 1

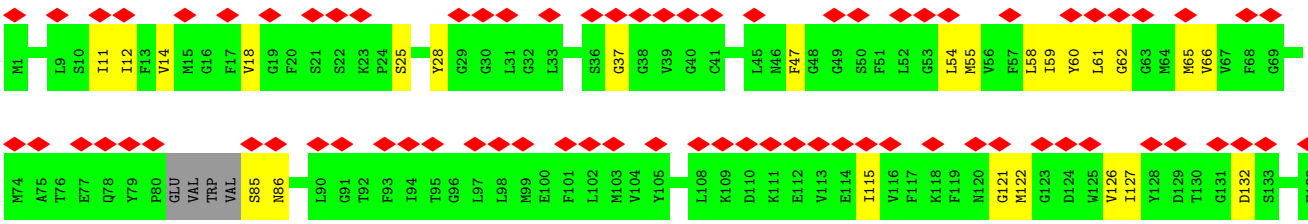
Chain D1:

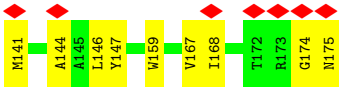


• Molecule 20: NADH-ubiquinone oxidoreductase chain 6

Chain D6:

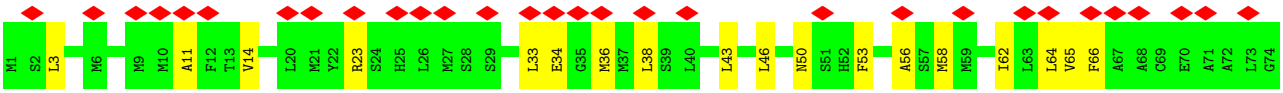


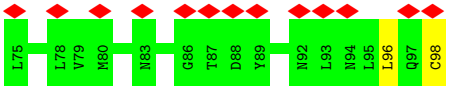




• Molecule 21: NADH-ubiquinone oxidoreductase chain 4L

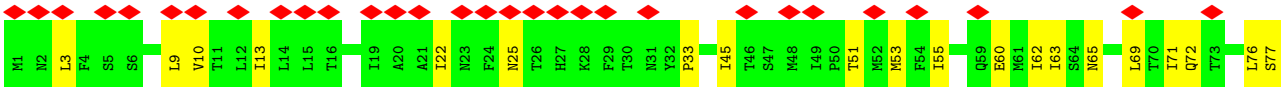
Chain 4L:

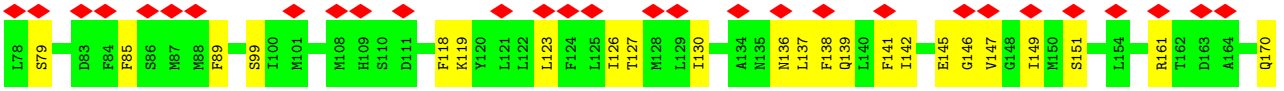


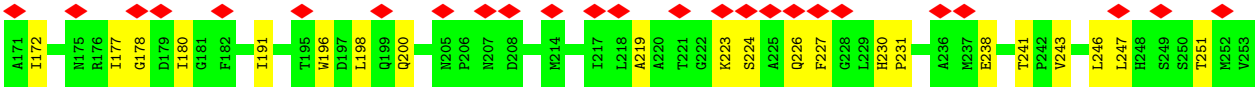


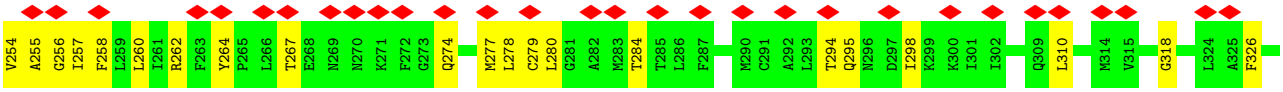
• Molecule 22: NADH-ubiquinone oxidoreductase chain 5

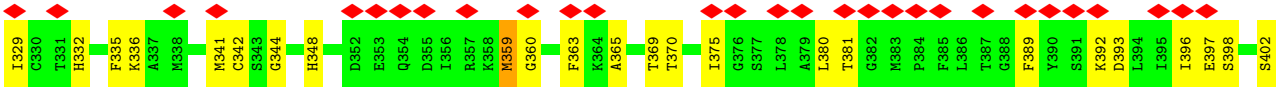
Chain D5:

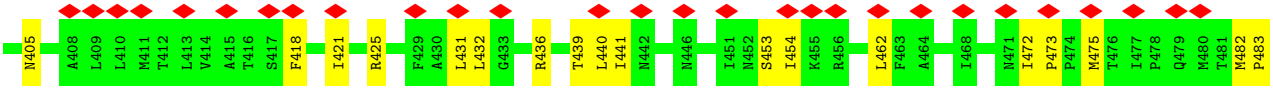


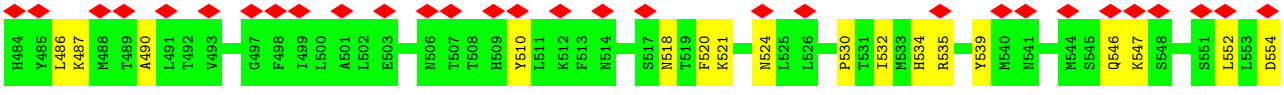


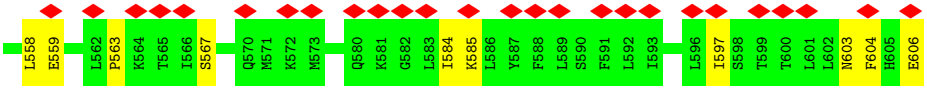






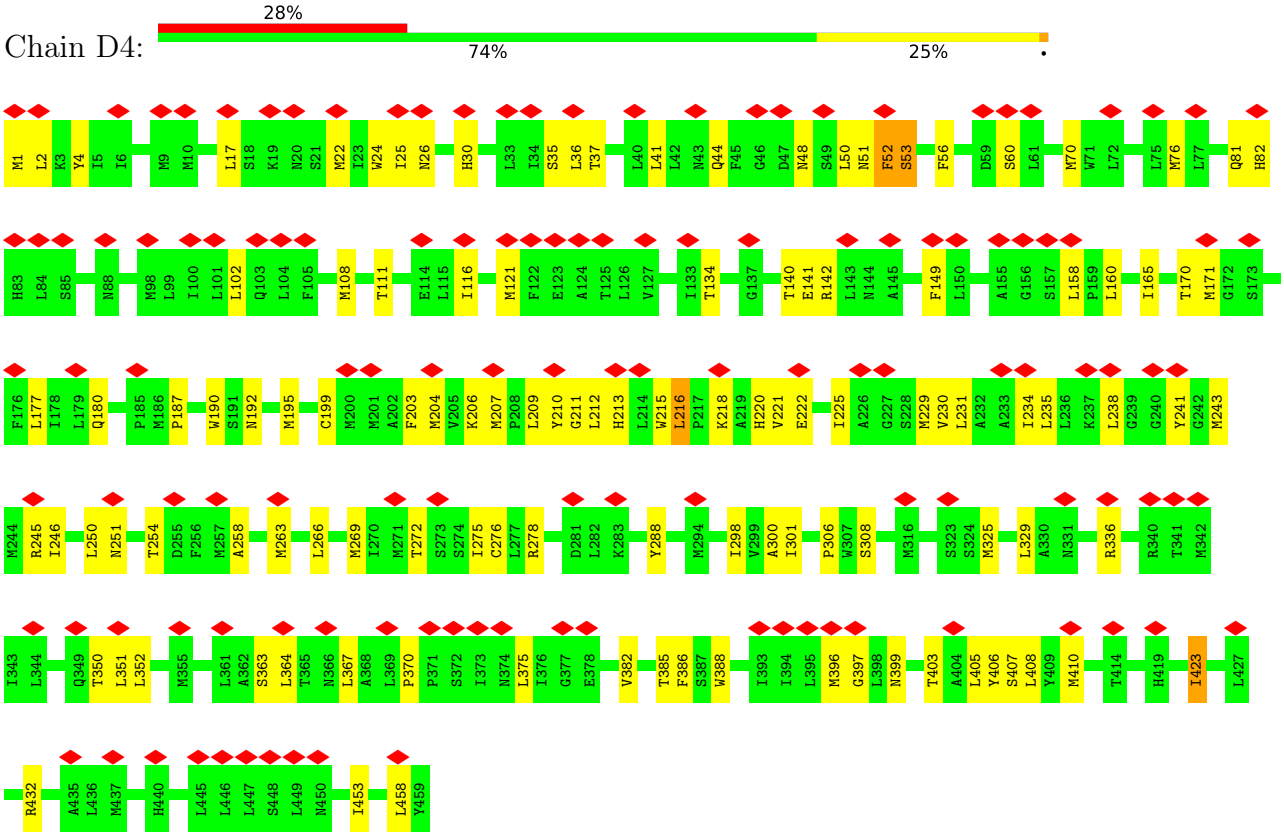






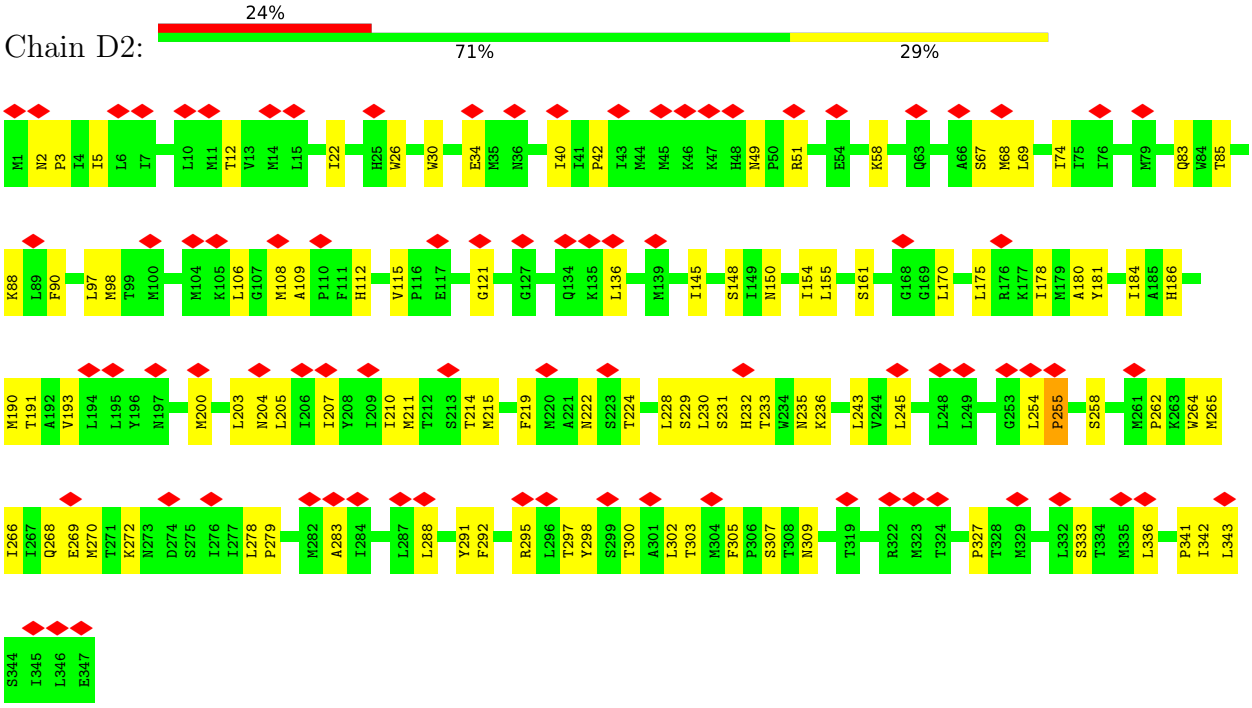
• Molecule 23: NADH-ubiquinone oxidoreductase chain 4

Chain D4:



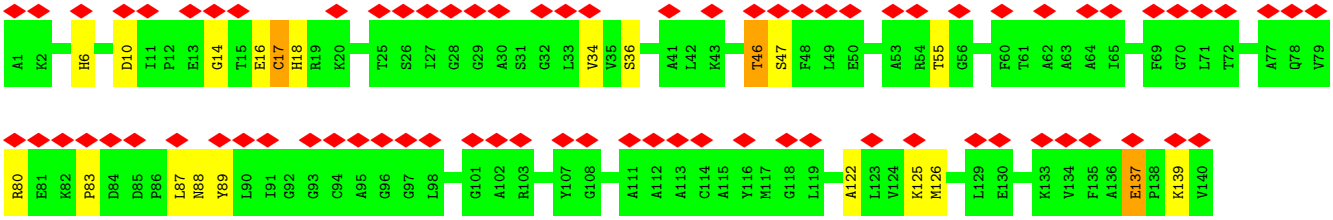
• Molecule 24: NADH-ubiquinone oxidoreductase chain 2

Chain D2:

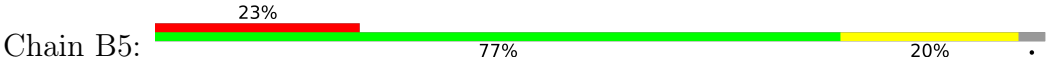


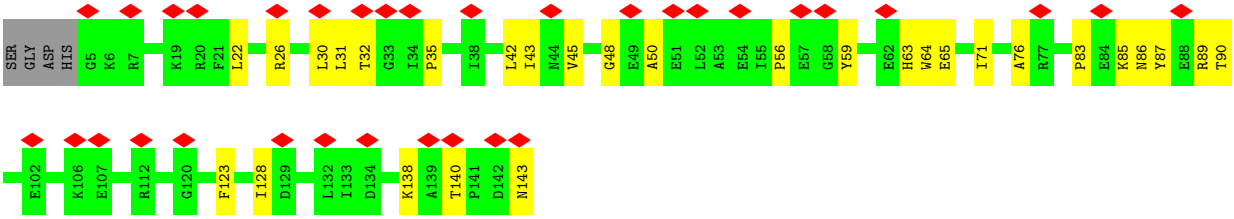
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain AK:

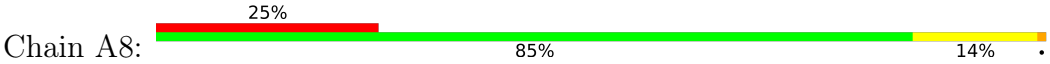


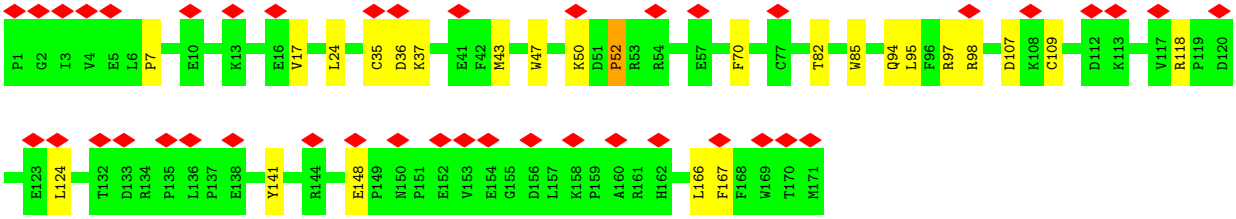
• Molecule 26: NADH:ubiquinone oxidoreductase subunit B5



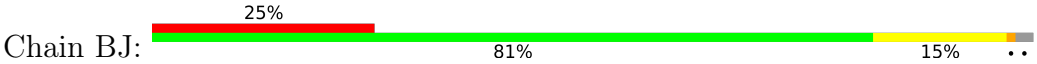


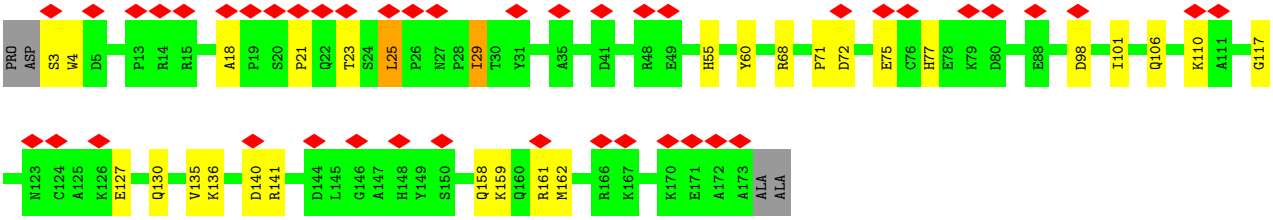
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



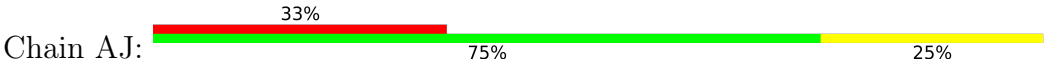


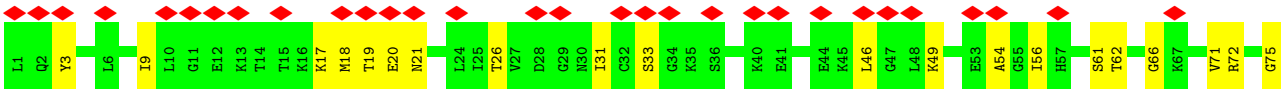
• Molecule 28: NADH:ubiquinone oxidoreductase subunit B10

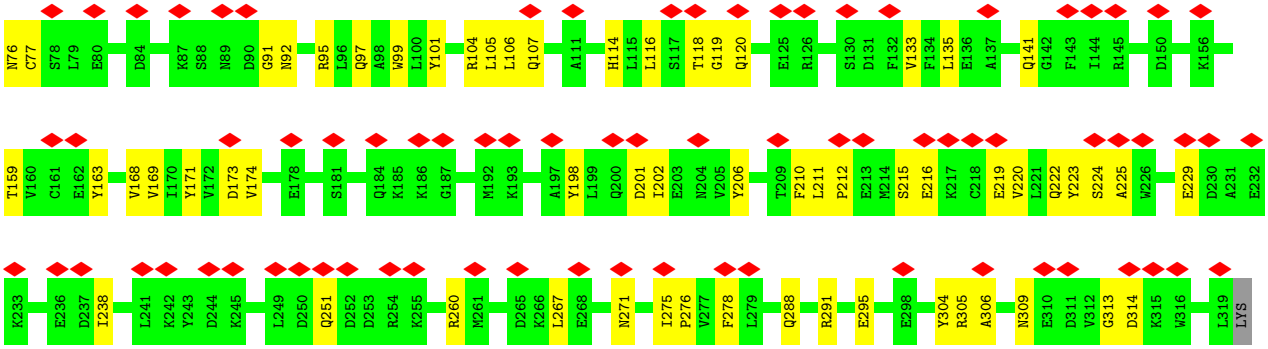




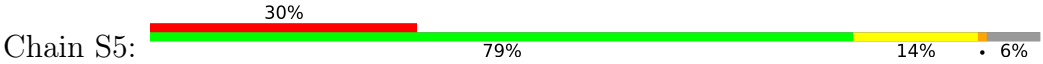
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

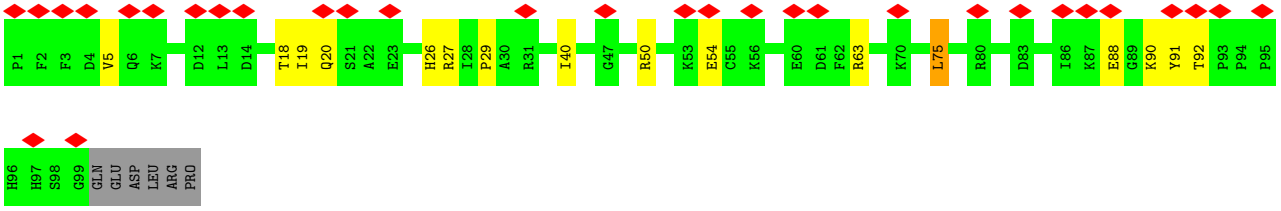




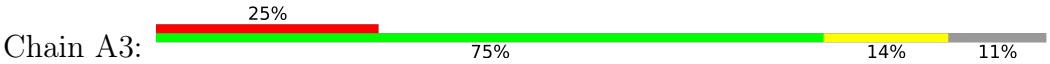


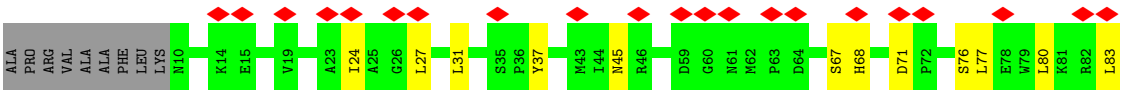
• Molecule 30: NADH:ubiquinone oxidoreductase subunit S5



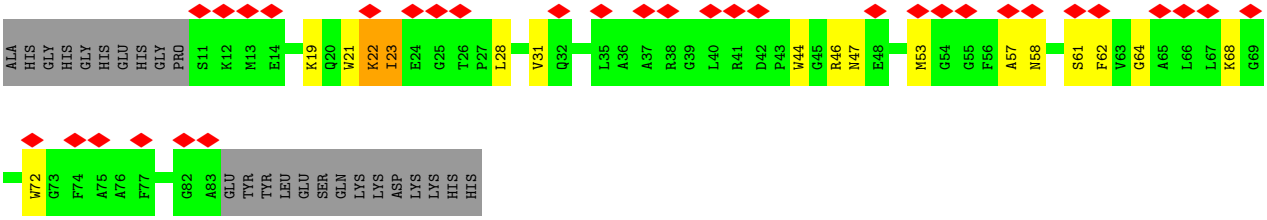


• Molecule 31: NADH:ubiquinone oxidoreductase subunit A3

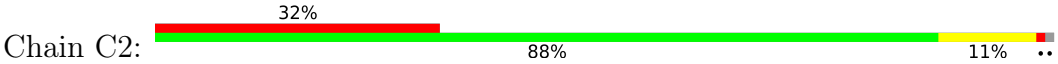


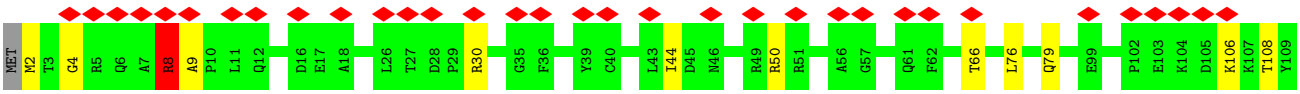


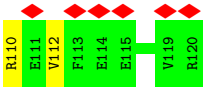
• Molecule 32: NADH:ubiquinone oxidoreductase subunit B3



• Molecule 33: NADH dehydrogenase [ubiquinone] 1 subunit C2

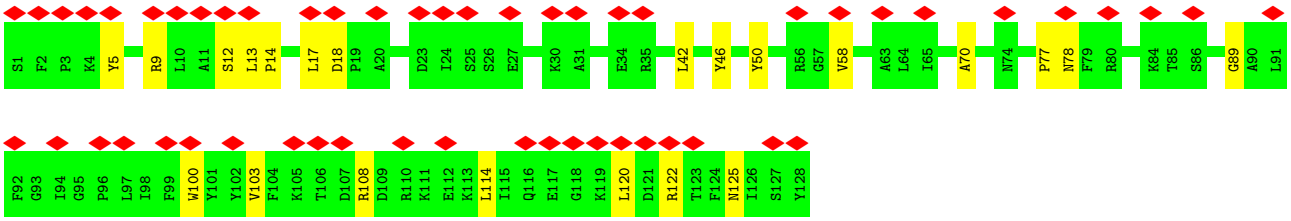






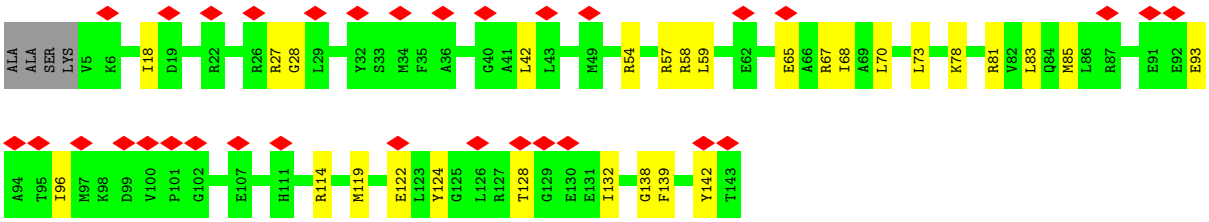
• Molecule 34: NADH:ubiquinone oxidoreductase subunit B4

Chain B4:



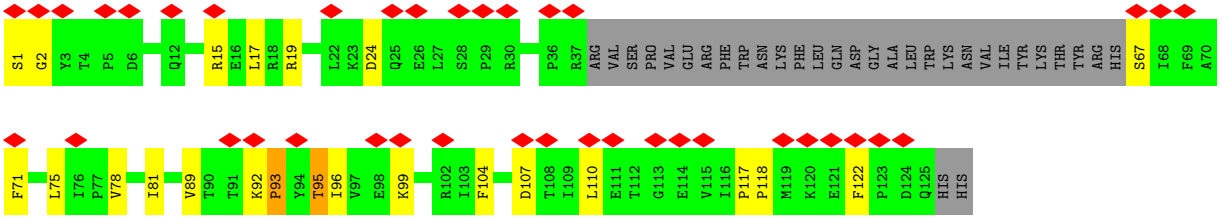
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain AM:



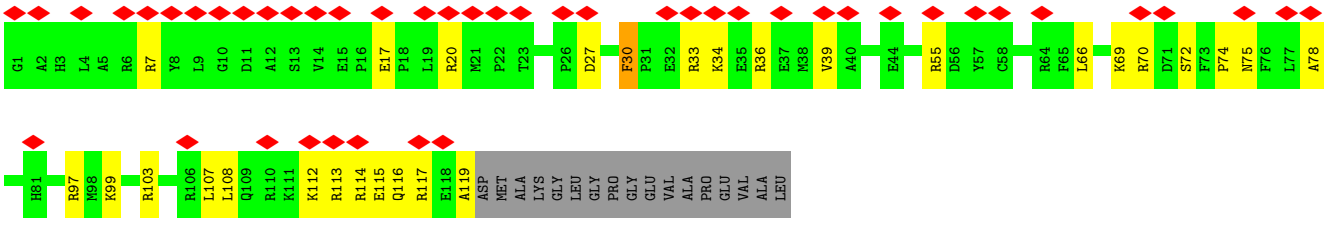
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain B6:



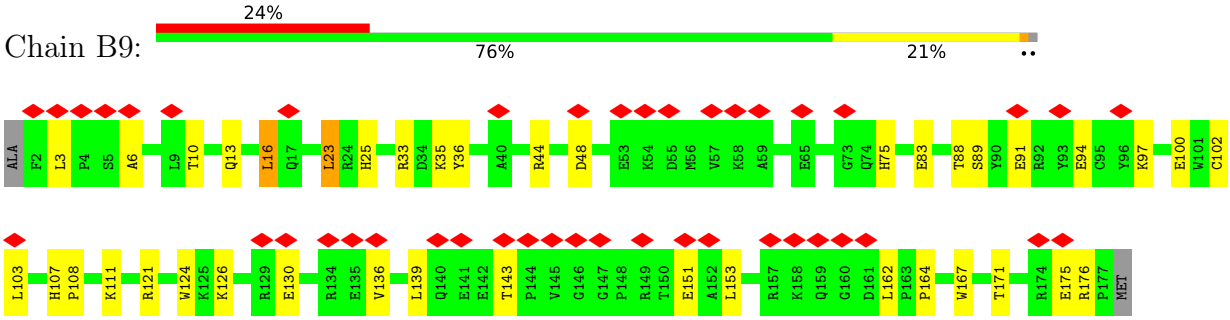
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain B7:



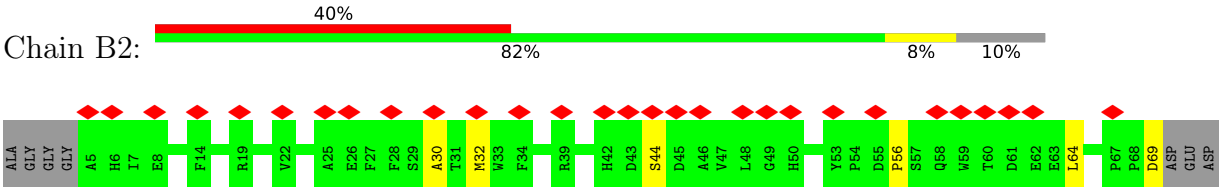
• Molecule 38: NADH:ubiquinone oxidoreductase subunit B9

Chain B9:



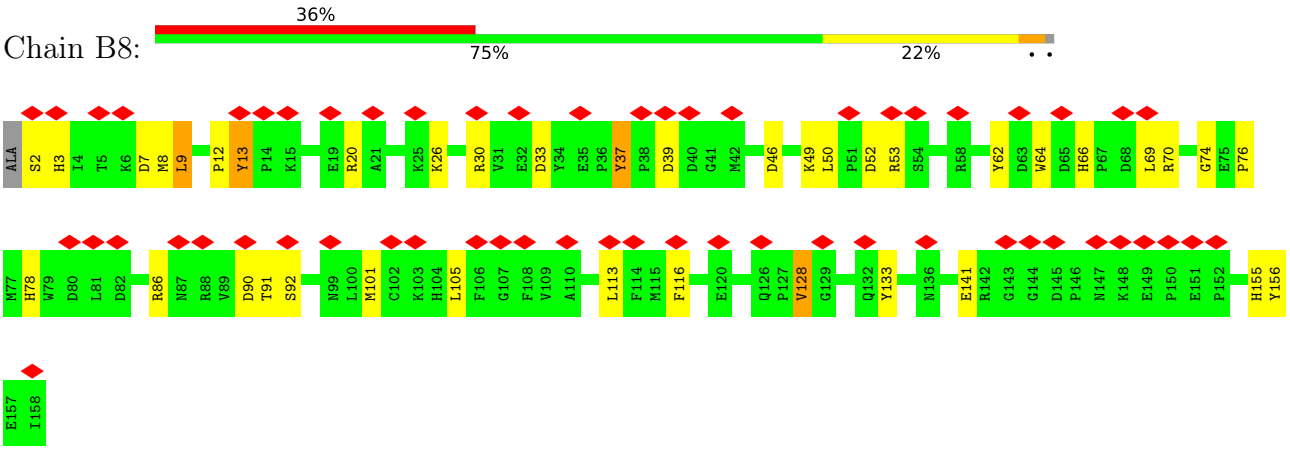
• Molecule 39: NADH:ubiquinone oxidoreductase subunit B2

Chain B2:



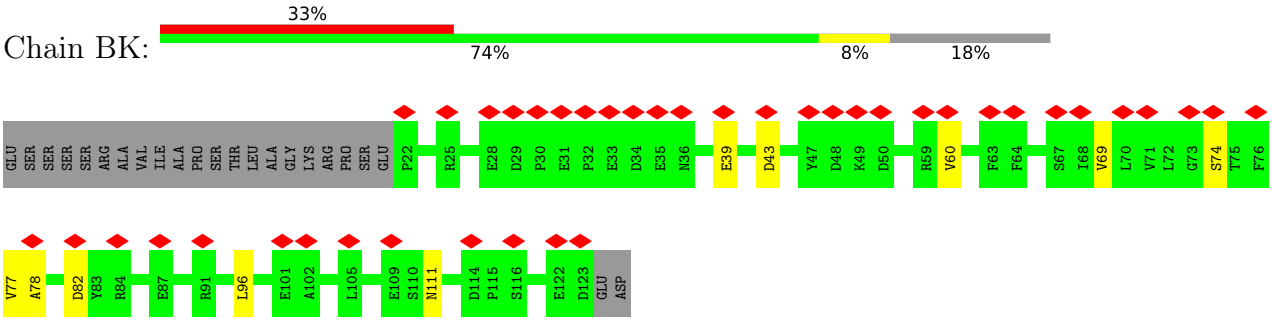
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain B8:



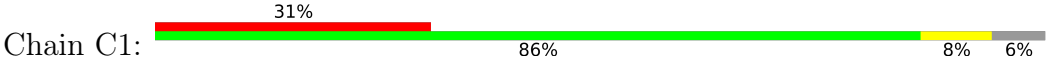
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

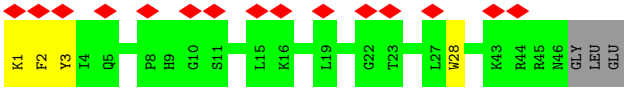
Chain BK:



• Molecule 42: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

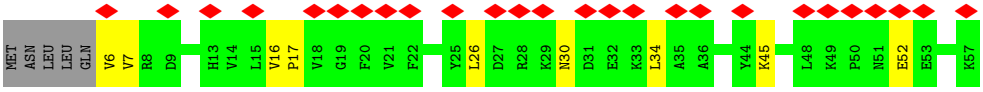
Chain C1:





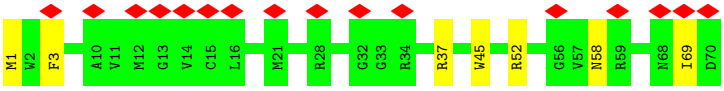
• Molecule 43: NADH dehydrogenase (Ubiquinone) 1 beta subcomplex, 1, 7kDa

Chain B1:



• Molecule 44: NADH dehydrogenase 1 alpha subcomplex

Chain A1:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25404	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 ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	100000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.367	Depositor
Minimum map value	-0.381	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	716.8, 716.8, 716.8	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	V1	0.37	0/3386	0.68	0/4575
2	V2	0.36	0/1687	0.81	4/2295 (0.2%)
3	S1	0.37	0/5362	0.66	0/7266
4	S2	0.40	0/3547	0.68	2/4808 (0.0%)
5	S3	0.39	0/1776	0.74	0/2417
6	S7	0.41	0/1278	0.70	0/1728
7	S8	0.45	0/1445	0.70	0/1956
8	V3	0.29	0/355	0.71	0/480
9	S6	0.31	0/749	0.58	0/1009
10	S4	0.34	0/1047	0.60	0/1415
11	A9	0.32	0/2343	0.71	3/3164 (0.1%)
12	A2	0.30	0/676	0.65	0/911
13	A5	0.33	0/921	0.69	0/1249
14	A6	0.31	0/993	0.68	2/1336 (0.1%)
15	A7	0.28	0/784	0.68	0/1060
16	AL	0.30	0/1242	0.68	0/1688
17	AA	0.28	0/655	0.74	0/881
17	AB	0.29	0/714	0.59	0/963
18	D3	0.33	0/747	0.67	0/1022
19	D1	0.39	0/2487	0.76	3/3401 (0.1%)
20	D6	0.31	0/1339	0.68	0/1810
21	4L	0.37	0/758	0.70	0/1024
22	D5	0.36	0/4933	0.73	1/6710 (0.0%)
23	D4	0.40	0/3740	0.77	2/5095 (0.0%)
24	D2	0.39	0/2788	0.70	2/3795 (0.1%)
25	AK	0.29	0/1046	0.72	4/1419 (0.3%)
26	B5	0.30	0/1189	0.59	0/1607
27	A8	0.32	0/1441	0.69	2/1942 (0.1%)
28	BJ	0.32	0/1475	0.70	3/1989 (0.2%)
29	AJ	0.31	0/2644	0.69	8/3579 (0.2%)
30	S5	0.34	0/843	0.69	0/1128
31	A3	0.30	0/602	0.70	0/828

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	B3	0.32	0/595	0.80	0/803
33	C2	0.32	0/1028	0.71	4/1388 (0.3%)
34	B4	0.30	0/1085	0.65	0/1467
35	AM	0.33	0/1172	0.69	0/1579
36	B6	0.32	0/841	0.77	1/1144 (0.1%)
37	B7	0.33	0/1051	0.71	1/1408 (0.1%)
38	B9	0.31	0/1568	0.68	0/2123
39	B2	0.31	0/590	0.75	2/810 (0.2%)
40	B8	0.32	0/1379	0.82	6/1884 (0.3%)
41	BK	0.31	0/880	0.67	0/1196
42	C1	0.25	0/404	0.58	0/548
43	B1	0.27	0/462	0.64	0/624
44	A1	0.29	0/592	0.68	0/795
All	All	0.35	0/66639	0.70	50/90319 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	V1	0	2
2	V2	0	2
3	S1	0	7
4	S2	0	3
7	S8	0	1
8	V3	0	1
10	S4	0	1
13	A5	0	1
15	A7	0	3
16	AL	0	1
17	AB	0	1
19	D1	0	1
20	D6	0	1
22	D5	0	2
23	D4	0	3
24	D2	0	1
25	AK	0	2
27	A8	0	1
29	AJ	0	2
30	S5	0	1
32	B3	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
33	C2	0	1
35	AM	0	1
37	B7	0	1
39	B2	0	1
40	B8	0	1
41	BK	0	1
43	B1	0	1
All	All	0	46

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	V2	36	LYS	N-CA-C	-7.66	104.83	114.56
29	AJ	229	GLU	CA-C-N	7.57	135.32	121.70
29	AJ	229	GLU	C-N-CA	7.57	135.32	121.70
28	BJ	21	PRO	CA-C-N	7.47	135.15	121.70
28	BJ	21	PRO	C-N-CA	7.47	135.15	121.70
14	A6	110	GLU	CA-C-N	7.28	134.79	121.70
14	A6	110	GLU	C-N-CA	7.28	134.79	121.70
39	B2	44	SER	CA-C-N	7.22	134.70	121.70
39	B2	44	SER	C-N-CA	7.22	134.70	121.70
4	S2	426	GLY	N-CA-C	-6.96	106.03	114.66
19	D1	63	PRO	CA-C-N	6.78	133.90	121.70
19	D1	63	PRO	C-N-CA	6.78	133.90	121.70
33	C2	8	ARG	CA-C-N	6.64	133.65	121.70
33	C2	8	ARG	C-N-CA	6.64	133.65	121.70
24	D2	342	ILE	N-CA-C	-6.58	106.05	111.91
29	AJ	275	ILE	C-N-CD	-6.50	106.30	120.60
25	AK	17	CYS	CA-C-N	6.12	133.24	121.54
25	AK	17	CYS	C-N-CA	6.12	133.24	121.54
11	A9	59	LEU	CA-C-N	6.04	126.53	119.83
11	A9	59	LEU	C-N-CA	6.04	126.53	119.83
2	V2	13	PRO	CA-C-N	5.84	132.69	121.54
2	V2	13	PRO	C-N-CA	5.84	132.69	121.54
28	BJ	25	LEU	C-N-CD	-5.81	107.83	120.60
33	C2	4	GLY	CA-C-N	5.77	132.09	121.70
33	C2	4	GLY	C-N-CA	5.77	132.09	121.70
4	S2	165	THR	N-CA-C	5.58	122.14	109.81
2	V2	190	ARG	CA-CB-CG	5.48	125.06	114.10
37	B7	39	VAL	N-CA-C	-5.46	107.05	111.91
24	D2	255	PRO	N-CA-C	5.41	117.30	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	B8	13	TYR	N-CA-C	5.35	121.63	109.81
40	B8	86	ARG	CA-C-N	5.27	135.49	126.32
40	B8	86	ARG	C-N-CA	5.27	135.49	126.32
29	AJ	275	ILE	CA-C-N	5.27	139.64	127.00
29	AJ	275	ILE	C-N-CA	5.27	139.64	127.00
19	D1	32	GLN	CA-CB-CG	5.22	124.54	114.10
27	A8	52	PRO	CA-C-N	5.20	131.46	121.54
27	A8	52	PRO	C-N-CA	5.20	131.46	121.54
40	B8	37	TYR	CA-C-N	5.19	139.45	127.00
40	B8	37	TYR	C-N-CA	5.19	139.45	127.00
23	D4	423	ILE	CA-C-N	5.17	131.42	121.54
23	D4	423	ILE	C-N-CA	5.17	131.42	121.54
25	AK	137	GLU	CA-C-N	5.14	139.33	127.00
25	AK	137	GLU	C-N-CA	5.14	139.33	127.00
36	B6	122	PHE	N-CA-C	5.13	121.16	109.81
29	AJ	304	TYR	CA-CB-CG	5.11	123.10	113.90
40	B8	37	TYR	C-N-CD	-5.11	109.36	120.60
29	AJ	251	GLN	CA-C-N	5.04	130.78	121.70
29	AJ	251	GLN	C-N-CA	5.04	130.78	121.70
22	D5	69	LEU	CA-CB-CG	5.01	133.85	116.30
11	A9	320	ARG	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A5	113	TRP	Peptide
15	A7	68	VAL	Peptide
15	A7	69	MET	Peptide
15	A7	70	SER	Peptide
27	A8	52	PRO	Peptide
17	AB	68	GLU	Peptide
29	AJ	216	GLU	Peptide
29	AJ	278	PHE	Peptide
25	AK	16	GLU	Peptide
25	AK	46	THR	Peptide
16	AL	31	ASN	Peptide
35	AM	128	THR	Peptide
43	B1	52	GLU	Peptide
39	B2	56	PRO	Peptide
32	B3	22	LYS	Peptide
32	B3	58	ASN	Peptide

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Mol	Chain	Res	Type	Group
37	B7	30	PHE	Peptide
40	B8	53	ARG	Peptide
41	BK	39	GLU	Peptide
33	C2	8	ARG	Peptide
19	D1	91	MET	Peptide
24	D2	309	ASN	Peptide
23	D4	216	LEU	Peptide
23	D4	52	PHE	Peptide
23	D4	53	SER	Peptide
22	D5	359	MET	Peptide
22	D5	365	ALA	Peptide
20	D6	115	ILE	Peptide
3	S1	213	TYR	Peptide
3	S1	218	ARG	Peptide
3	S1	247	VAL	Peptide
3	S1	253	ARG	Peptide
3	S1	254	MET	Peptide
3	S1	341	ASP	Peptide
3	S1	380	VAL	Peptide
4	S2	55	HIS	Peptide
4	S2	68	LEU	Peptide
4	S2	73	VAL	Peptide
10	S4	11	ILE	Peptide
30	S5	92	THR	Peptide
7	S8	106	THR	Peptide
1	V1	103	GLY	Peptide
1	V1	207	PRO	Peptide
2	V2	13	PRO	Peptide
2	V2	35	VAL	Peptide
8	V3	63	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	V1	3312	0	3266	62	0
2	V2	1647	0	1657	30	0
3	S1	5275	0	5300	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	S2	3455	0	3395	59	0
5	S3	1726	0	1676	39	0
6	S7	1247	0	1256	26	0
7	S8	1414	0	1371	29	0
8	V3	345	0	323	7	0
9	S6	737	0	710	8	0
10	S4	1024	0	1023	24	0
11	A9	2293	0	2326	49	0
12	A2	665	0	678	14	0
13	A5	901	0	936	13	0
14	A6	969	0	980	12	0
15	A7	766	0	779	17	0
16	AL	1201	0	1170	15	0
17	AA	645	0	649	8	0
17	AB	702	0	692	11	0
18	D3	728	0	773	14	0
19	D1	2415	0	2542	41	0
20	D6	1308	0	1329	30	0
21	4L	748	0	794	22	0
22	D5	4805	0	4950	107	0
23	D4	3646	0	3850	83	0
24	D2	2724	0	2930	70	0
25	AK	1025	0	1033	12	0
26	B5	1156	0	1177	25	0
27	A8	1404	0	1384	18	0
28	BJ	1441	0	1417	21	0
29	AJ	2583	0	2547	44	0
30	S5	822	0	820	14	0
31	A3	582	0	583	13	0
32	B3	578	0	570	11	0
33	C2	997	0	983	11	0
34	B4	1059	0	1062	16	0
35	AM	1143	0	1137	22	0
36	B6	815	0	837	20	0
37	B7	1026	0	995	22	0
38	B9	1515	0	1469	30	0
39	B2	563	0	509	7	0
40	B8	1324	0	1219	29	0
41	BK	853	0	800	9	0
42	C1	391	0	391	3	0
43	B1	449	0	453	6	0
44	A1	577	0	570	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	S1	16	0	0	2	0
45	S7	8	0	0	1	0
45	S8	16	0	0	0	0
45	V1	8	0	0	1	0
46	V1	31	0	19	3	0
47	S1	4	0	0	0	0
47	V2	4	0	0	0	0
48	S6	1	0	0	0	0
49	A9	48	0	26	7	0
50	AA	34	0	40	1	0
50	AB	31	0	34	0	0
51	D1	26	0	26	0	0
51	D4	40	0	54	4	0
51	D5	38	0	50	3	0
52	D5	60	0	64	2	0
53	AK	28	0	30	0	0
All	All	65394	0	65654	1013	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 8.

All (1013) 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)
5:S3:80:ALA:HA	5:S3:91:GLU:O	1.17	1.32
5:S3:38:GLN:O	15:A7:70:SER:HA	1.44	1.14
5:S3:80:ALA:CA	5:S3:91:GLU:O	2.07	1.01
3:S1:449:PRO:O	3:S1:489:VAL:HA	1.60	1.01
5:S3:38:GLN:O	15:A7:70:SER:CA	2.21	0.88
5:S3:78:LEU:HA	5:S3:93:VAL:O	1.79	0.82
1:V1:202:LYS:HB3	1:V1:361:GLN:HE21	1.48	0.77
5:S3:80:ALA:HA	5:S3:91:GLU:C	2.09	0.77
32:B3:64:GLY:O	32:B3:68:LYS:HB2	1.86	0.75
11:A9:108:ASP:O	11:A9:112:LYS:HB3	1.84	0.75
35:AM:138:GLY:O	35:AM:142:TYR:HB2	1.87	0.74
23:D4:363:SER:O	23:D4:367:LEU:HB2	1.87	0.73
22:D5:389:PHE:O	22:D5:393:ASP:HB2	1.88	0.73
3:S1:227:SER:H	3:S1:253:ARG:HH22	1.37	0.72
36:B6:15:ARG:HD3	36:B6:19:ARG:HH21	1.56	0.71
36:B6:67:SER:O	36:B6:71:PHE:HB2	1.91	0.70
23:D4:52:PHE:O	23:D4:56:PHE:HB2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:192:GLN:HE21	5:S3:195:ARG:HH12	1.38	0.70
4:S2:282:GLU:HB2	4:S2:313:GLN:HE22	1.57	0.69
11:A9:135:LEU:HA	11:A9:167:LYS:HD3	1.76	0.68
22:D5:547:LYS:O	22:D5:552:LEU:HB2	1.95	0.67
33:C2:30:ARG:HE	33:C2:76:LEU:HD11	1.58	0.67
12:A2:66:ALA:O	12:A2:73:GLU:HA	1.95	0.67
4:S2:238:ARG:HH22	4:S2:412:ALA:HB1	1.58	0.66
11:A9:52:GLU:HG2	11:A9:54:TYR:H	1.61	0.66
11:A9:92:ILE:HG22	11:A9:130:ILE:HB	1.77	0.66
3:S1:243:ARG:HG2	3:S1:244:THR:HG23	1.77	0.66
32:B3:22:LYS:H	32:B3:46:ARG:HH11	1.43	0.66
1:V1:101:GLU:H	1:V1:184:TYR:HE1	1.41	0.66
19:D1:69:SER:O	19:D1:73:LEU:HB2	1.95	0.65
24:D2:22:ILE:HD11	30:S5:5:VAL:H	1.62	0.65
3:S1:117:GLN:NE2	45:S1:801:SF4:S3	2.70	0.65
18:D3:10:ASN:HD21	19:D1:10:ILE:HG21	1.62	0.65
38:B9:44:ARG:NH1	38:B9:48:ASP:OD2	2.30	0.65
11:A9:51:CYS:SG	11:A9:52:GLU:N	2.70	0.64
22:D5:279:CYS:SG	22:D5:405:ASN:ND2	2.70	0.64
10:S4:56:LYS:HA	10:S4:84:LEU:O	1.98	0.64
12:A2:22:LEU:HB2	12:A2:56:GLU:HG2	1.78	0.64
22:D5:149:ILE:HG12	23:D4:364:LEU:HD21	1.80	0.64
23:D4:177:LEU:O	23:D4:180:GLN:C	2.41	0.64
1:V1:233:THR:O	1:V1:237:ARG:HB2	1.99	0.63
11:A9:132:ILE:HD13	49:A9:401:NDP:H1D	1.80	0.63
5:S3:71:GLN:HE21	13:A5:82:GLN:HE22	1.46	0.63
12:A2:20:ILE:HD12	12:A2:54:ILE:HG12	1.81	0.63
4:S2:405:MET:SD	4:S2:421:GLN:NE2	2.71	0.63
22:D5:597:ILE:HD11	25:AK:34:VAL:HG22	1.80	0.63
26:B5:138:LYS:HG3	30:S5:27:ARG:HG2	1.81	0.63
1:V1:179:ARG:NH1	2:V2:52:ASP:OD2	2.32	0.63
11:A9:136:ASN:HD22	11:A9:292:ARG:HD2	1.64	0.63
4:S2:246:THR:HG23	13:A5:12:GLY:HA3	1.79	0.62
22:D5:267:THR:O	22:D5:274:GLN:NE2	2.31	0.62
3:S1:442:VAL:O	3:S1:446:ALA:HB2	2.00	0.62
22:D5:76:LEU:HB2	22:D5:136:ASN:HD21	1.63	0.62
4:S2:53:PRO:HB3	4:S2:61:VAL:HG13	1.82	0.62
11:A9:50:ARG:HG2	49:A9:401:NDP:H2A	1.82	0.62
24:D2:203:LEU:HD13	24:D2:343:LEU:HD12	1.80	0.62
24:D2:235:ASN:ND2	24:D2:307:SER:OG	2.32	0.62
38:B9:126:LYS:O	38:B9:130:GLU:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:229:ASP:HB3	3:S1:235:GLY:HA2	1.82	0.61
22:D5:535:ARG:HH21	40:B8:92:SER:HB2	1.64	0.61
29:AJ:54:ALA:HB2	29:AJ:107:GLN:HG2	1.81	0.61
20:D6:159:TRP:HE1	24:D2:12:THR:HG22	1.65	0.61
4:S2:371:LYS:NZ	4:S2:422:ASP:O	2.34	0.61
26:B5:56:PRO:HG2	26:B5:59:TYR:HB3	1.82	0.61
4:S2:204:PRO:HD3	7:S8:60:ARG:HH22	1.65	0.61
11:A9:166:ILE:HG13	11:A9:228:PHE:HB2	1.81	0.61
23:D4:207:MET:HG3	23:D4:298:ILE:HD11	1.82	0.61
28:BJ:23:THR:HG21	37:B7:74:PRO:HD2	1.82	0.61
3:S1:377:VAL:HG22	3:S1:450:MET:HB3	1.83	0.61
4:S2:256:SER:HB3	4:S2:373:GLU:H	1.66	0.60
4:S2:105:ARG:NH1	6:S7:149:CYS:SG	2.67	0.60
9:S6:12:THR:OG1	9:S6:14:THR:O	2.19	0.60
28:BJ:117:GLY:HA2	36:B6:99:LYS:HE2	1.83	0.60
38:B9:25:HIS:HD2	38:B9:75:HIS:H	1.49	0.60
20:D6:14:VAL:HG22	21:4L:11:ALA:HB2	1.82	0.60
22:D5:161:ARG:NH2	22:D5:238:GLU:OE1	2.34	0.60
25:AK:17:CYS:SG	25:AK:18:HIS:N	2.74	0.60
3:S1:594:ARG:NH2	14:A6:122:TYR:O	2.32	0.60
7:S8:53:GLU:OE2	16:AL:34:ARG:NH2	2.35	0.60
17:AA:27:PRO:HG2	17:AA:29:LYS:HB2	1.83	0.60
22:D5:138:PHE:HB2	22:D5:196:TRP:HE1	1.67	0.60
23:D4:225:ILE:HG13	23:D4:229:MET:HE2	1.83	0.60
10:S4:37:ILE:HD13	10:S4:92:ALA:HB1	1.84	0.60
15:A7:45:SER:O	15:A7:46:HIS:ND1	2.35	0.60
24:D2:170:LEU:HD22	24:D2:291:TYR:HD2	1.67	0.60
3:S1:40:PHE:O	3:S1:158:ARG:NH2	2.34	0.60
17:AA:25:ILE:HD11	17:AA:40:LEU:HD23	1.82	0.60
22:D5:200:GLN:OE1	28:BJ:110:LYS:NZ	2.35	0.60
23:D4:134:THR:O	23:D4:142:ARG:NH1	2.34	0.60
1:V1:91:LYS:HG2	1:V1:219:PRO:HG2	1.83	0.59
22:D5:198:LEU:HD21	22:D5:262:ARG:HD2	1.83	0.59
22:D5:547:LYS:O	22:D5:552:LEU:CB	2.50	0.59
2:V2:53:LEU:HD12	8:V3:52:LEU:HD13	1.84	0.59
11:A9:56:THR:HA	11:A9:59:LEU:HG	1.84	0.59
19:D1:102:VAL:HB	19:D1:150:LEU:HD21	1.83	0.59
23:D4:4:TYR:HE2	23:D4:41:LEU:HD12	1.67	0.59
4:S2:130:PRO:HG2	4:S2:135:GLN:HE21	1.67	0.59
11:A9:202:LYS:NZ	11:A9:291:ASP:OD2	2.34	0.59
19:D1:288:LEU:O	19:D1:292:ASN:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AK:122:ALA:O	25:AK:126:MET:HB2	2.02	0.59
17:AB:70:LEU:HD23	17:AB:76:ILE:HG12	1.84	0.59
32:B3:21:TRP:HB2	32:B3:46:ARG:HD2	1.84	0.59
3:S1:198:ASN:HD21	3:S1:263:ILE:H	1.50	0.59
4:S2:237:ASN:O	19:D1:284:GLN:NE2	2.34	0.59
23:D4:269:MET:SD	23:D4:399:ASN:ND2	2.76	0.59
1:V1:297:VAL:HG22	1:V1:336:VAL:HG12	1.84	0.59
3:S1:240:VAL:HG12	3:S1:250:ILE:HG22	1.84	0.59
1:V1:89:ARG:NH1	1:V1:217:GLY:O	2.36	0.59
12:A2:57:CYS:SG	12:A2:58:SER:N	2.74	0.59
1:V1:36:ALA:HB1	1:V1:41:ASP:HB2	1.84	0.59
1:V1:140:GLY:O	1:V1:179:ARG:NH2	2.34	0.59
23:D4:48:ASN:HD21	26:B5:90:THR:HG21	1.67	0.59
17:AB:49:GLU:HB3	32:B3:44:TRP:HZ3	1.68	0.59
5:S3:48:LEU:HB3	5:S3:105:ILE:HG22	1.84	0.58
27:A8:148:GLU:OE1	30:S5:50:ARG:NH1	2.36	0.58
5:S3:202:PRO:HA	10:S4:50:ASN:HB3	1.85	0.58
1:V1:365:CYS:SG	1:V1:366:ARG:N	2.76	0.58
18:D3:73:LEU:HD21	20:D6:55:MET:HE1	1.86	0.58
23:D4:102:LEU:HD21	23:D4:230:VAL:HG11	1.85	0.58
29:AJ:141:GLN:NE2	29:AJ:201:ASP:OD2	2.36	0.58
19:D1:149:ILE:HG21	19:D1:185:TRP:HB2	1.85	0.58
35:AM:93:GLU:HA	35:AM:96:ILE:HG22	1.85	0.58
3:S1:101:HIS:CD2	45:S1:801:SF4:S4	2.73	0.58
12:A2:78:LEU:HD22	12:A2:86:VAL:HG22	1.85	0.57
21:4L:58:MET:HB3	21:4L:62:ILE:HD12	1.86	0.57
6:S7:85:VAL:HG12	6:S7:112:TYR:HB2	1.86	0.57
40:B8:8:MET:O	40:B8:26:LYS:NZ	2.36	0.57
9:S6:53:GLY:HA2	9:S6:94:GLN:H	1.69	0.57
4:S2:82:LEU:HG	6:S7:95:LYS:HG2	1.86	0.57
6:S7:179:ARG:HG3	11:A9:50:ARG:HH22	1.69	0.57
22:D5:397:GLU:HB3	22:D5:482:MET:HE2	1.85	0.57
27:A8:37:LYS:NZ	31:A3:67:SER:O	2.37	0.57
4:S2:354:GLU:OE2	4:S2:357:GLN:NE2	2.37	0.57
24:D2:69:LEU:HD11	24:D2:97:LEU:HD22	1.86	0.57
1:V1:257:ASN:HD22	1:V1:332:ALA:HB2	1.69	0.57
3:S1:449:PRO:HG2	3:S1:489:VAL:HG22	1.87	0.57
22:D5:554:ASP:O	22:D5:558:LEU:HB3	2.04	0.57
22:D5:278:LEU:HB3	22:D5:318:GLY:HA3	1.87	0.57
23:D4:204:MET:HB3	23:D4:209:LEU:HD22	1.86	0.57
24:D2:327:PRO:HB3	33:C2:44:ILE:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:85:THR:HG21	10:S4:87:SER:H	1.69	0.57
7:S8:22:ALA:O	7:S8:26:LEU:HB2	2.05	0.57
31:A3:27:LEU:O	31:A3:31:LEU:HB3	2.05	0.57
6:S7:165:LYS:NZ	16:AL:78:ASP:OD1	2.37	0.57
3:S1:118:ASP:OD2	10:S4:46:GLN:NE2	2.38	0.56
28:BJ:161:ARG:NH2	41:BK:111:ASN:OD1	2.38	0.56
5:S3:86:ARG:NH1	5:S3:91:GLU:OE2	2.38	0.56
11:A9:56:THR:O	11:A9:60:ARG:HB2	2.05	0.56
22:D5:559:GLU:OE2	23:D4:218:LYS:NZ	2.34	0.56
3:S1:257:ASP:O	3:S1:394:ARG:NH2	2.38	0.56
16:AL:60:ARG:NH1	16:AL:92:CYS:SG	2.79	0.56
19:D1:20:LEU:HD22	19:D1:232:ILE:HD11	1.86	0.56
1:V1:253:THR:HA	1:V1:270:GLU:O	2.05	0.56
5:S3:77:ASP:O	5:S3:93:VAL:O	2.24	0.56
5:S3:193:GLU:OE2	10:S4:64:ARG:NH2	2.38	0.56
23:D4:22:MET:O	23:D4:26:ASN:ND2	2.38	0.56
23:D4:170:THR:HG23	23:D4:171:MET:HG3	1.86	0.56
24:D2:233:THR:HA	24:D2:236:LYS:HG2	1.86	0.56
27:A8:166:LEU:HD23	27:A8:167:PHE:H	1.71	0.56
18:D3:84:LEU:HD11	31:A3:45:ASN:HD22	1.70	0.56
1:V1:33:LEU:HD23	1:V1:155:GLU:HB3	1.87	0.56
3:S1:588:MET:HG3	10:S4:63:GLU:HA	1.88	0.56
20:D6:121:GLY:HA2	21:4L:3:LEU:HD11	1.87	0.56
3:S1:37:ILE:HG23	3:S1:90:ARG:HH21	1.71	0.56
3:S1:364:LEU:HG	3:S1:491:ASN:HB2	1.87	0.56
11:A9:208:VAL:HA	11:A9:211:THR:HG22	1.88	0.56
22:D5:546:GLN:OE1	23:D4:278:ARG:NH1	2.39	0.56
28:BJ:18:ALA:HA	36:B6:110:LEU:HD12	1.87	0.56
35:AM:124:TYR:HB3	35:AM:132:ILE:HG22	1.87	0.56
38:B9:100:GLU:O	38:B9:121:ARG:NH2	2.39	0.56
29:AJ:26:THR:HB	29:AJ:169:VAL:HG22	1.88	0.56
5:S3:38:GLN:HA	15:A7:70:SER:O	2.05	0.55
29:AJ:77:CYS:O	29:AJ:92:ASN:ND2	2.39	0.55
36:B6:92:LYS:O	36:B6:95:THR:OG1	2.23	0.55
7:S8:135:PRO:HG3	7:S8:164:GLU:HG2	1.88	0.55
23:D4:187:PRO:O	23:D4:192:ASN:ND2	2.38	0.55
3:S1:255:HIS:HD2	3:S1:258:ILE:H	1.54	0.55
22:D5:191:ILE:HD12	23:D4:386:PHE:HD2	1.69	0.55
40:B8:13:TYR:HE1	40:B8:39:ASP:H	1.54	0.55
43:B1:16:VAL:HG23	43:B1:17:PRO:HD3	1.89	0.55
22:D5:462:LEU:HD11	39:B2:32:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D4:251:ASN:OD1	23:D4:251:ASN:N	2.40	0.55
37:B7:113:ARG:NH2	37:B7:116:GLN:OE1	2.40	0.55
23:D4:140:THR:HG23	23:D4:141:GLU:HG3	1.89	0.55
26:B5:143:ASN:HD22	30:S5:29:PRO:HG3	1.70	0.55
1:V1:295:LEU:HB2	1:V1:339:ARG:HA	1.88	0.55
22:D5:241:THR:HG21	22:D5:344:GLY:HA3	1.88	0.55
29:AJ:17:LYS:HE3	29:AJ:118:THR:HG23	1.89	0.55
4:S2:116:GLN:HG3	4:S2:138:ARG:HD3	1.89	0.55
5:S3:78:LEU:CA	5:S3:93:VAL:O	2.54	0.55
19:D1:41:GLY:HA3	19:D1:46:LEU:HD21	1.88	0.55
22:D5:9:LEU:HB3	36:B6:81:ILE:HD13	1.88	0.55
22:D5:161:ARG:NH1	38:B9:88:THR:O	2.39	0.55
23:D4:221:VAL:HG23	23:D4:222:GLU:HG3	1.88	0.55
24:D2:292:PHE:HA	24:D2:295:ARG:HG2	1.88	0.55
24:D2:341:PRO:O	33:C2:79:GLN:NE2	2.40	0.55
17:AB:48:VAL:HG21	38:B9:16:LEU:HD21	1.88	0.55
1:V1:150:GLN:HB3	8:V3:54:LEU:HD12	1.89	0.55
7:S8:95:GLU:OE1	7:S8:108:ARG:NH1	2.38	0.55
20:D6:146:LEU:HB2	21:4L:58:MET:HE2	1.89	0.55
22:D5:137:LEU:HB3	22:D5:196:TRP:HD1	1.72	0.55
26:B5:43:ILE:HG13	26:B5:71:ILE:HD11	1.88	0.55
1:V1:21:ILE:HG21	1:V1:230:VAL:HG23	1.89	0.55
11:A9:134:HIS:ND1	11:A9:135:LEU:O	2.35	0.55
22:D5:539:TYR:OH	34:B4:9:ARG:NH2	2.40	0.55
4:S2:388:ARG:NH1	4:S2:389:CYS:O	2.41	0.54
29:AJ:72:ARG:NH1	29:AJ:295:GLU:OE1	2.40	0.54
19:D1:303:TRP:HH2	35:AM:42:LEU:HD11	1.71	0.54
27:A8:95:LEU:HB2	27:A8:98:ARG:HG2	1.89	0.54
40:B8:13:TYR:HB2	40:B8:20:ARG:HE	1.72	0.54
3:S1:250:ILE:HD11	3:S1:268:ARG:HA	1.89	0.54
3:S1:382:THR:HB	3:S1:454:GLY:HA3	1.89	0.54
20:D6:167:VAL:HG22	24:D2:42:PRO:HG2	1.89	0.54
22:D5:396:ILE:HD11	22:D5:490:ALA:HB2	1.88	0.54
25:AK:137:GLU:HB3	25:AK:139:LYS:HG3	1.90	0.54
38:B9:83:GLU:OE2	38:B9:176:ARG:NH1	2.40	0.54
11:A9:19:ILE:O	11:A9:43:SER:OG	2.24	0.54
19:D1:1:MET:HA	19:D1:4:ILE:HD12	1.88	0.54
3:S1:317:ALA:HB1	3:S1:331:LEU:HD21	1.90	0.54
5:S3:38:GLN:O	15:A7:70:SER:C	2.49	0.54
23:D4:209:LEU:HG	23:D4:211:GLY:H	1.71	0.54
25:AK:6:HIS:O	25:AK:10:ASP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V1:49:LEU:HD21	1:V1:124:VAL:HG22	1.90	0.54
3:S1:158:ARG:HA	3:S1:161:ARG:HH21	1.72	0.54
3:S1:424:ASP:OD1	3:S1:424:ASP:N	2.40	0.54
4:S2:284:ASP:OD1	4:S2:284:ASP:N	2.40	0.54
1:V1:258:ILE:HG23	1:V1:335:ILE:HG22	1.89	0.54
1:V1:362:CYS:HB3	1:V1:364:PRO:HD2	1.88	0.54
20:D6:65:MET:HE1	21:4L:34:GLU:HG2	1.89	0.54
23:D4:231:LEU:O	23:D4:235:LEU:HB2	2.08	0.54
23:D4:423:ILE:HA	34:B4:58:VAL:HG12	1.88	0.54
24:D2:106:LEU:HD11	24:D2:108:MET:HE2	1.90	0.54
25:AK:14:GLY:H	25:AK:83:PRO:HB3	1.73	0.54
31:A3:80:LEU:O	35:AM:58:ARG:NH2	2.40	0.54
22:D5:123:LEU:HA	22:D5:126:ILE:HD12	1.89	0.54
33:C2:66:THR:OG1	42:C1:28:TRP:NE1	2.40	0.54
40:B8:50:LEU:H	40:B8:78:HIS:HD2	1.54	0.54
9:S6:27:ARG:O	9:S6:31:ARG:NH2	2.41	0.54
30:S5:88:GLU:HG2	30:S5:90:LYS:HE3	1.90	0.54
1:V1:24:ASN:HA	1:V1:28:ARG:HG3	1.90	0.54
3:S1:163:ALA:O	3:S1:168:GLY:N	2.38	0.54
4:S2:347:HIS:O	4:S2:351:LEU:HB2	2.07	0.54
22:D5:227:PHE:H	22:D5:284:THR:HG22	1.72	0.54
4:S2:287:ILE:HB	7:S8:4:TYR:HB3	1.90	0.53
22:D5:62:ILE:O	36:B6:96:ILE:HA	2.09	0.53
27:A8:35:CYS:SG	27:A8:36:ASP:N	2.79	0.53
1:V1:233:THR:HA	1:V1:236:ARG:HG2	1.90	0.53
3:S1:196:SER:OG	3:S1:265:ASP:OD2	2.25	0.53
12:A2:18:ILE:O	12:A2:52:ILE:HA	2.08	0.53
3:S1:126:ASP:HB2	4:S2:328:ALA:HB3	1.89	0.53
3:S1:675:ASP:O	3:S1:679:ARG:HB2	2.09	0.53
14:A6:32:ARG:NH2	50:AA:101:ZMP:O7	2.42	0.53
22:D5:224:SER:HB3	22:D5:256:GLY:HA3	1.91	0.53
37:B7:72:SER:HB2	37:B7:75:ASN:HD22	1.73	0.53
37:B7:113:ARG:O	37:B7:117:ARG:HB2	2.08	0.53
2:V2:97:LYS:O	2:V2:157:ASN:ND2	2.38	0.53
22:D5:603:ASN:ND2	22:D5:606:GLU:OE1	2.42	0.53
24:D2:297:THR:HG22	24:D2:302:LEU:HD13	1.90	0.53
5:S3:80:ALA:HB2	5:S3:92:ILE:HD13	1.89	0.53
29:AJ:202:ILE:O	29:AJ:206:TYR:HB2	2.07	0.53
30:S5:18:THR:HG22	30:S5:19:ILE:HG13	1.91	0.53
1:V1:370:ASP:OD1	3:S1:179:ASN:ND2	2.41	0.53
22:D5:224:SER:HB2	22:D5:310:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:D2:266:ILE:O	24:D2:270:MET:HB2	2.09	0.53
37:B7:103:ARG:NH1	39:B2:64:LEU:O	2.42	0.53
1:V1:305:PRO:HG3	1:V1:413:TRP:HB3	1.90	0.53
13:A5:34:LEU:HD11	13:A5:44:ARG:HA	1.91	0.53
27:A8:82:THR:HA	27:A8:85:TRP:CD1	2.44	0.53
29:AJ:21:ASN:ND2	29:AJ:120:GLN:OE1	2.42	0.53
3:S1:159:CYS:HB2	3:S1:199:ILE:HD11	1.91	0.52
22:D5:510:TYR:O	38:B9:35:LYS:NZ	2.34	0.52
23:D4:210:TYR:O	23:D4:213:HIS:ND1	2.37	0.52
29:AJ:171:TYR:HD2	29:AJ:222:GLN:HG3	1.74	0.52
1:V1:236:ARG:HG3	1:V1:237:ARG:HG3	1.91	0.52
11:A9:91:VAL:HG13	11:A9:129:PHE:HD1	1.75	0.52
11:A9:168:PRO:HA	11:A9:230:PHE:HB2	1.90	0.52
23:D4:35:SER:OG	23:D4:70:MET:O	2.26	0.52
40:B8:52:ASP:OD1	40:B8:78:HIS:NE2	2.42	0.52
6:S7:121:ASN:HB2	6:S7:145:TYR:HD1	1.73	0.52
15:A7:8:GLN:HA	15:A7:11:ARG:HE	1.75	0.52
20:D6:47:PHE:HD2	21:4L:46:LEU:HD22	1.75	0.52
22:D5:483:PRO:HD2	22:D5:486:LEU:HD22	1.91	0.52
4:S2:105:ARG:NH1	45:S7:300:SF4:S3	2.76	0.52
7:S8:57:LEU:HD11	7:S8:137:PHE:HE1	1.75	0.52
23:D4:364:LEU:HD23	23:D4:367:LEU:HD23	1.92	0.52
29:AJ:306:ALA:HB1	42:C1:3:TYR:HE1	1.74	0.52
1:V1:301:GLY:HA2	1:V1:333:ALA:HB3	1.92	0.52
24:D2:154:ILE:HG23	24:D2:191:THR:HG22	1.92	0.52
37:B7:17:GLU:OE1	37:B7:20:ARG:NH2	2.43	0.52
3:S1:317:ALA:HB3	3:S1:343:LEU:HA	1.92	0.52
24:D2:30:TRP:NE1	24:D2:67:SER:OG	2.37	0.52
17:AB:7:THR:HG23	17:AB:10:GLY:H	1.73	0.52
29:AJ:97:GLN:HG2	29:AJ:135:LEU:HD13	1.91	0.52
40:B8:7:ASP:HA	40:B8:26:LYS:HD2	1.92	0.52
3:S1:569:LYS:NZ	3:S1:596:ASP:OD2	2.43	0.52
3:S1:595:GLU:OE1	3:S1:598:LYS:NZ	2.42	0.52
11:A9:72:ASP:O	11:A9:80:SER:OG	2.28	0.52
23:D4:300:ALA:O	23:D4:308:SER:OG	2.26	0.52
3:S1:627:SER:OG	3:S1:629:ASN:OD1	2.28	0.51
6:S7:108:PRO:HG2	19:D1:58:LYS:HE2	1.92	0.51
24:D2:115:VAL:HG12	24:D2:180:ALA:HB1	1.92	0.51
3:S1:122:MET:O	15:A7:60:ARG:NH2	2.43	0.51
3:S1:449:PRO:HD2	3:S1:483:VAL:HG21	1.91	0.51
9:S6:68:HIS:HE1	9:S6:87:CYS:SG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:AL:51:ASP:OD2	16:AL:54:GLN:NE2	2.43	0.51
28:BJ:3:SER:OG	28:BJ:4:TRP:N	2.43	0.51
34:B4:42:LEU:HD13	40:B8:74:GLY:HA3	1.93	0.51
1:V1:68:ARG:O	46:V1:501:FMN:O3P	2.29	0.51
1:V1:263:ASN:HB2	1:V1:285:GLY:HA3	1.92	0.51
3:S1:366:THR:OG1	3:S1:491:ASN:ND2	2.39	0.51
4:S2:115:GLU:HB3	4:S2:194:VAL:HB	1.92	0.51
22:D5:294:THR:H	22:D5:425:ARG:HH12	1.57	0.51
1:V1:48:ILE:HG23	1:V1:55:TRP:HZ3	1.75	0.51
3:S1:488:LYS:HB2	3:S1:642:PHE:HE2	1.76	0.51
4:S2:98:GLN:NE2	7:S8:85:ALA:O	2.43	0.51
14:A6:52:ASP:H	14:A6:53:ILE:HD12	1.75	0.51
19:D1:312:SER:OG	31:A3:37:TYR:O	2.28	0.51
1:V1:103:GLY:N	2:V2:148:CYS:SG	2.84	0.51
3:S1:453:LEU:HB3	3:S1:492:ILE:HG22	1.93	0.51
7:S8:77:CYS:SG	7:S8:78:ILE:N	2.83	0.51
22:D5:99:SER:OG	22:D5:453:SER:OG	2.27	0.51
3:S1:193:SER:OG	3:S1:385:ARG:NH2	2.43	0.51
23:D4:385:THR:HG21	23:D4:396:MET:HE3	1.93	0.51
28:BJ:98:ASP:OD2	28:BJ:141:ARG:NH2	2.43	0.51
7:S8:79:ALA:HB2	7:S8:106:THR:HG22	1.92	0.51
11:A9:173:GLY:H	11:A9:176:ASP:HB2	1.76	0.51
24:D2:230:LEU:HB3	24:D2:300:THR:HG22	1.93	0.51
33:C2:8:ARG:H	33:C2:9:ALA:HB3	1.74	0.51
1:V1:105:CYS:HG	2:V2:148:CYS:H	1.56	0.51
1:V1:107:ASP:OD1	1:V1:107:ASP:N	2.43	0.51
5:S3:150:ARG:NH2	5:S3:155:TYR:O	2.44	0.51
3:S1:447:LYS:HG3	3:S1:448:LYS:HG3	1.93	0.51
4:S2:151:ILE:HD13	4:S2:304:MET:HE1	1.92	0.51
13:A5:10:LEU:HD22	13:A5:13:LEU:HD13	1.91	0.51
13:A5:37:ILE:O	13:A5:44:ARG:NH1	2.43	0.51
19:D1:194:ASN:HB3	19:D1:200:LEU:HD21	1.93	0.51
23:D4:241:TYR:OH	23:D4:245:ARG:NH2	2.42	0.51
34:B4:46:TYR:O	34:B4:50:TYR:HB2	2.11	0.51
13:A5:5:LYS:NZ	13:A5:68:GLU:OE2	2.42	0.51
23:D4:165:ILE:HD11	24:D2:264:TRP:HE1	1.74	0.51
2:V2:126:ILE:HG21	2:V2:132:THR:HA	1.91	0.50
3:S1:285:ARG:NH2	16:AL:144:TYR:O	2.44	0.50
3:S1:372:GLU:OE2	3:S1:394:ARG:NH1	2.43	0.50
8:V3:58:LEU:O	8:V3:62:ARG:NH2	2.43	0.50
19:D1:81:LEU:HD13	19:D1:111:LEU:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:4L:96:LEU:HD11	24:D2:121:GLY:HA3	1.92	0.50
22:D5:10:VAL:HA	22:D5:13:ILE:HG22	1.93	0.50
26:B5:87:TYR:O	26:B5:90:THR:OG1	2.28	0.50
1:V1:111:ILE:HD11	1:V1:149:LEU:HD22	1.94	0.50
1:V1:214:GLY:HA3	1:V1:220:THR:HG22	1.93	0.50
3:S1:185:THR:HG22	3:S1:187:ILE:H	1.76	0.50
6:S7:155:ALA:HB2	7:S8:137:PHE:HD2	1.76	0.50
22:D5:246:LEU:O	22:D5:251:THR:OG1	2.27	0.50
22:D5:255:ALA:HA	22:D5:258:PHE:HB3	1.94	0.50
3:S1:531:CYS:SG	3:S1:532:VAL:N	2.84	0.50
5:S3:39:GLN:NE2	5:S3:41:GLN:OE1	2.45	0.50
6:S7:68:ASP:HB2	6:S7:71:ARG:HE	1.75	0.50
15:A7:51:ASN:HB2	15:A7:56:ARG:HH12	1.76	0.50
20:D6:59:ILE:HG21	21:4L:64:LEU:HD21	1.93	0.50
26:B5:31:LEU:HD23	26:B5:32:THR:HG23	1.92	0.50
29:AJ:71:VAL:O	29:AJ:76:ASN:ND2	2.44	0.50
38:B9:126:LYS:O	38:B9:130:GLU:CB	2.60	0.50
3:S1:113:GLU:OE2	10:S4:43:ASN:ND2	2.40	0.50
3:S1:316:ALA:HA	3:S1:342:THR:HG23	1.92	0.50
14:A6:63:ARG:HB2	17:AA:45:LEU:HD21	1.92	0.50
29:AJ:101:TYR:OH	29:AJ:159:THR:OG1	2.28	0.50
37:B7:115:GLU:O	37:B7:119:ALA:HB3	2.12	0.50
40:B8:12:PRO:HA	40:B8:46:ASP:HB3	1.93	0.50
19:D1:228:TYR:HA	19:D1:231:ILE:HD12	1.93	0.50
4:S2:111:MET:HG3	4:S2:112:MET:HG2	1.92	0.50
40:B8:66:HIS:HB3	40:B8:69:LEU:HB2	1.92	0.50
4:S2:28:TRP:NE1	21:4L:98:CYS:OXT	2.44	0.50
7:S8:64:GLU:HB3	7:S8:134:GLY:HA3	1.94	0.50
17:AB:46:ASP:OD1	38:B9:44:ARG:NH2	2.45	0.50
28:BJ:77:HIS:HB3	33:C2:106:LYS:HD3	1.94	0.50
2:V2:61:LEU:HD21	2:V2:90:TYR:HB3	1.94	0.50
3:S1:442:VAL:O	3:S1:446:ALA:CB	2.59	0.50
4:S2:354:GLU:HA	5:S3:199:LEU:HD22	1.92	0.50
19:D1:119:SER:O	19:D1:123:SER:OG	2.23	0.50
31:A3:68:HIS:HB3	31:A3:71:ASP:HB2	1.94	0.50
3:S1:225:THR:HB	3:S1:240:VAL:HG23	1.94	0.50
7:S8:65:HIS:NE2	7:S8:116:CYS:SG	2.82	0.50
17:AA:31:SER:HB2	17:AA:34:SER:HB2	1.93	0.50
20:D6:127:ILE:HD11	21:4L:50:ASN:HB3	1.93	0.50
20:D6:141:MET:HA	20:D6:144:ALA:HB3	1.93	0.50
23:D4:36:LEU:HD11	41:BK:69:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:C2:108:THR:HG23	33:C2:110:ARG:H	1.77	0.50
3:S1:278:ARG:HH12	3:S1:565:ALA:HB2	1.77	0.49
24:D2:26:TRP:HB3	24:D2:74:ILE:HD13	1.94	0.49
2:V2:37:ASN:OD1	8:V3:62:ARG:NH1	2.45	0.49
2:V2:55:GLN:NE2	2:V2:89:MET:O	2.42	0.49
24:D2:200:MET:HE1	24:D2:265:MET:HB3	1.95	0.49
29:AJ:61:SER:HA	29:AJ:66:GLY:HA2	1.93	0.49
4:S2:48:THR:HG22	4:S2:67:GLU:HG2	1.94	0.49
26:B5:140:THR:O	26:B5:143:ASN:ND2	2.45	0.49
1:V1:78:LYS:NZ	46:V1:501:FMN:O1P	2.40	0.49
1:V1:197:GLU:OE1	10:S4:129:ARG:NH2	2.46	0.49
11:A9:171:ILE:HD13	11:A9:207:ILE:HD13	1.93	0.49
1:V1:257:ASN:HB2	1:V1:332:ALA:HA	1.94	0.49
16:AL:78:ASP:HB2	16:AL:81:MET:HE3	1.95	0.49
3:S1:142:ILE:HG23	3:S1:191:PHE:HB3	1.95	0.49
22:D5:119:LYS:NZ	52:D5:901:CDL:OB7	2.46	0.49
22:D5:375:ILE:HD12	39:B2:32:MET:HG3	1.95	0.49
24:D2:3:PRO:HB2	29:AJ:9:ILE:HD11	1.94	0.49
29:AJ:116:LEU:O	29:AJ:260:ARG:NH2	2.43	0.49
30:S5:50:ARG:O	30:S5:54:GLU:HB2	2.13	0.49
32:B3:28:LEU:HA	32:B3:31:VAL:HG12	1.95	0.49
2:V2:98:TYR:HD2	2:V2:136:LEU:HB2	1.77	0.49
3:S1:55:CYS:SG	3:S1:69:CYS:N	2.86	0.49
18:D3:81:THR:H	31:A3:45:ASN:HD21	1.61	0.49
32:B3:44:TRP:CD1	32:B3:47:ASN:HB2	2.47	0.49
34:B4:12:SER:OG	40:B8:91:THR:O	2.30	0.49
38:B9:107:HIS:NE2	41:BK:43:ASP:OD1	2.40	0.49
22:D5:567:SER:OG	51:D4:501:3PE:O22	2.30	0.48
37:B7:108:LEU:O	37:B7:112:LYS:HB2	2.13	0.48
3:S1:286:ASN:O	3:S1:289:GLY:N	2.38	0.48
4:S2:19:MET:SD	24:D2:295:ARG:NH2	2.78	0.48
6:S7:124:GLY:HA2	7:S8:115:LYS:HA	1.95	0.48
21:4L:33:LEU:HA	21:4L:36:MET:HE2	1.94	0.48
23:D4:350:THR:OG1	23:D4:351:LEU:N	2.46	0.48
24:D2:231:SER:HB2	24:D2:305:PHE:HB2	1.95	0.48
26:B5:83:PRO:O	26:B5:87:TYR:HB2	2.13	0.48
28:BJ:68:ARG:NH2	43:B1:45:LYS:O	2.47	0.48
36:B6:107:ASP:OD2	37:B7:70:ARG:NH2	2.46	0.48
40:B8:2:SER:OG	40:B8:3:HIS:N	2.45	0.48
10:S4:12:THR:HB	14:A6:16:VAL:H	1.78	0.48
12:A2:63:LYS:HD2	12:A2:75:ASN:HD21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:D4:254:THR:O	23:D4:258:ALA:CB	2.61	0.48
17:AB:69:LYS:HA	36:B6:2:GLY:HA2	1.94	0.48
3:S1:396:ARG:NH1	3:S1:416:THR:O	2.46	0.48
23:D4:25:ILE:HG23	41:BK:60:VAL:HG11	1.95	0.48
24:D2:83:GLN:HB2	30:S5:19:ILE:HG12	1.96	0.48
29:AJ:19:THR:OG1	29:AJ:20:GLU:N	2.45	0.48
44:A1:1:MET:HG3	44:A1:3:PHE:H	1.78	0.48
11:A9:55:ASP:O	11:A9:58:HIS:ND1	2.46	0.48
36:B6:71:PHE:O	36:B6:75:LEU:HB2	2.13	0.48
4:S2:61:VAL:HG11	6:S7:96:MET:HE1	1.95	0.48
4:S2:67:GLU:OE1	4:S2:74:ARG:NH2	2.46	0.48
4:S2:110:SER:OG	4:S2:114:ASN:OD1	2.28	0.48
17:AA:70:LEU:HD13	17:AA:76:ILE:HG12	1.96	0.48
20:D6:37:GLY:HA3	20:D6:61:LEU:HD11	1.94	0.48
22:D5:71:ILE:HG13	22:D5:72:GLN:H	1.79	0.48
22:D5:243:VAL:O	22:D5:247:LEU:HB2	2.13	0.48
24:D2:109:ALA:HB2	24:D2:161:SER:HA	1.94	0.48
31:A3:83:LEU:O	35:AM:54:ARG:NH2	2.41	0.48
2:V2:165:THR:HG23	2:V2:168:ASP:H	1.79	0.48
3:S1:496:ILE:HG22	3:S1:499:GLN:H	1.77	0.48
6:S7:70:ASP:OD2	19:D1:34:ARG:NH1	2.46	0.48
22:D5:370:THR:HG22	22:D5:431:LEU:HD22	1.96	0.48
24:D2:136:LEU:HA	24:D2:205:LEU:HD21	1.96	0.48
24:D2:175:LEU:HD23	24:D2:178:ILE:HD12	1.96	0.48
24:D2:232:HIS:HE1	29:AJ:276:PRO:HG3	1.78	0.48
29:AJ:91:GLY:O	29:AJ:95:ARG:NH2	2.46	0.48
38:B9:83:GLU:HA	38:B9:89:SER:HB2	1.95	0.48
4:S2:188:ARG:NH1	6:S7:58:GLU:OE2	2.47	0.48
22:D5:226:GLN:O	22:D5:230:HIS:N	2.47	0.48
44:A1:1:MET:HE3	44:A1:3:PHE:HB2	1.96	0.48
2:V2:150:ASN:ND2	2:V2:162:GLU:OE1	2.47	0.47
3:S1:577:GLU:OE2	3:S1:579:ARG:NH2	2.46	0.47
22:D5:180:ILE:HD12	23:D4:397:GLY:HA3	1.96	0.47
22:D5:295:GLN:H	22:D5:425:ARG:HH22	1.62	0.47
27:A8:141:TYR:HA	35:AM:114:ARG:HD3	1.96	0.47
38:B9:103:LEU:HB3	38:B9:121:ARG:HH12	1.79	0.47
43:B1:6:VAL:HG13	43:B1:7:VAL:HG23	1.96	0.47
2:V2:96:GLY:HA3	2:V2:136:LEU:H	1.77	0.47
3:S1:484:THR:OG1	3:S1:487:TRP:N	2.42	0.47
4:S2:19:MET:HG2	24:D2:295:ARG:HH12	1.78	0.47
4:S2:36:VAL:HG22	24:D2:49:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S2:312:SER:HB2	35:AM:18:ILE:HD13	1.96	0.47
10:S4:23:THR:HG23	10:S4:25:VAL:HG12	1.96	0.47
29:AJ:54:ALA:HB3	29:AJ:104:ARG:HD2	1.95	0.47
29:AJ:62:THR:HG21	29:AJ:106:LEU:HD21	1.96	0.47
32:B3:23:ILE:HB	32:B3:46:ARG:HG2	1.97	0.47
1:V1:46:LYS:O	1:V1:50:LEU:HB2	2.14	0.47
3:S1:99:ALA:O	3:S1:134:LYS:NZ	2.32	0.47
4:S2:360:PRO:HA	4:S2:380:SER:O	2.14	0.47
7:S8:119:CYS:HB2	7:S8:121:PHE:H	1.79	0.47
19:D1:92:PRO:HG3	19:D1:255:TYR:HD2	1.79	0.47
37:B7:36:ARG:NH2	40:B8:156:TYR:O	2.42	0.47
1:V1:352:GLU:HG2	1:V1:373:ASN:HD21	1.78	0.47
3:S1:324:ASP:HB2	3:S1:327:ALA:H	1.79	0.47
5:S3:86:ARG:HD3	13:A5:110:GLN:HG3	1.97	0.47
15:A7:105:LEU:HD12	15:A7:110:PRO:HB2	1.95	0.47
19:D1:111:LEU:HD13	19:D1:114:TYR:HD2	1.78	0.47
22:D5:264:TYR:HA	22:D5:267:THR:HG22	1.97	0.47
22:D5:518:ASN:HA	22:D5:521:LYS:HB2	1.96	0.47
23:D4:2:LEU:HD23	43:B1:26:LEU:HD22	1.96	0.47
23:D4:325:MET:HE2	23:D4:329:LEU:HD11	1.94	0.47
24:D2:222:ASN:OD1	24:D2:222:ASN:N	2.45	0.47
25:AK:88:ASN:OD1	25:AK:89:TYR:N	2.47	0.47
31:A3:77:LEU:HB2	31:A3:80:LEU:HD23	1.96	0.47
34:B4:13:LEU:HD11	34:B4:18:ASP:HA	1.96	0.47
37:B7:103:ARG:HE	37:B7:107:LEU:HD11	1.80	0.47
3:S1:147:LYS:HB3	3:S1:209:THR:HG23	1.96	0.47
14:A6:43:PRO:HA	14:A6:46:VAL:HG12	1.96	0.47
25:AK:80:ARG:HH12	25:AK:87:LEU:HB3	1.79	0.47
29:AJ:133:VAL:HG21	29:AJ:210:PHE:HB2	1.96	0.47
3:S1:95:GLU:OE2	3:S1:129:ARG:NE	2.39	0.47
7:S8:45:PRO:HA	19:D1:33:PHE:HD1	1.80	0.47
20:D6:58:LEU:O	20:D6:62:GLY:HA3	2.14	0.47
21:4L:36:MET:HE3	24:D2:68:MET:HG3	1.97	0.47
9:S6:22:ASP:OD1	11:A9:2:HIS:NE2	2.48	0.47
10:S4:88:THR:HG23	10:S4:91:ASP:H	1.79	0.47
11:A9:83:ARG:HA	11:A9:86:GLU:HG3	1.97	0.47
11:A9:108:ASP:O	11:A9:112:LYS:CB	2.59	0.47
19:D1:287:HIS:CE1	19:D1:291:LYS:HD2	2.49	0.47
22:D5:380:LEU:HD23	22:D5:381:THR:HG23	1.96	0.47
22:D5:559:GLU:HA	22:D5:563:PRO:HD2	1.95	0.47
26:B5:50:ALA:HA	28:BJ:60:TYR:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B5:64:TRP:CD1	26:B5:65:GLU:HG3	2.50	0.47
29:AJ:141:GLN:HG3	29:AJ:198:TYR:HD1	1.80	0.47
38:B9:151:GLU:OE2	40:B8:62:TYR:OH	2.31	0.47
1:V1:233:THR:HB	1:V1:237:ARG:HD3	1.97	0.47
11:A9:26:ALA:HA	11:A9:31:GLY:HA3	1.95	0.47
14:A6:27:ALA:HB1	14:A6:78:VAL:HG11	1.97	0.47
15:A7:70:SER:OG	15:A7:71:SER:N	2.47	0.47
20:D6:18:VAL:HG22	21:4L:14:VAL:HG11	1.97	0.47
22:D5:170:GLN:NE2	51:D5:902:3PE:O11	2.48	0.47
37:B7:114:ARG:HG2	39:B2:69:ASP:HB3	1.96	0.47
1:V1:101:GLU:O	1:V1:104:THR:OG1	2.31	0.47
22:D5:60:GLU:HB2	36:B6:99:LYS:HB3	1.96	0.47
22:D5:231:PRO:HB3	22:D5:530:PRO:HG3	1.97	0.47
23:D4:453:ILE:HD11	41:BK:77:VAL:HB	1.97	0.47
3:S1:283:MET:HE2	3:S1:291:LEU:HG	1.96	0.47
4:S2:364:TYR:HB2	4:S2:377:TYR:HD1	1.79	0.47
10:S4:33:ARG:HE	10:S4:62:ARG:HE	1.62	0.47
10:S4:130:VAL:HG22	10:S4:132:THR:HG22	1.95	0.47
11:A9:318:LEU:HD13	11:A9:318:LEU:HA	1.83	0.47
18:D3:69:ILE:HD11	19:D1:144:VAL:HG13	1.95	0.47
20:D6:126:VAL:HA	20:D6:127:ILE:HA	1.61	0.47
22:D5:341:MET:HE3	22:D5:454:ILE:HD13	1.96	0.47
23:D4:177:LEU:O	23:D4:180:GLN:O	2.32	0.47
17:AB:52:MET:HE3	38:B9:23:LEU:HD12	1.96	0.47
29:AJ:173:ASP:CB	29:AJ:223:TYR:O	2.63	0.47
40:B8:50:LEU:HD21	40:B8:76:PRO:HG2	1.97	0.47
40:B8:113:LEU:HD23	40:B8:116:PHE:HD2	1.80	0.47
2:V2:47:VAL:O	2:V2:51:LEU:HB2	2.15	0.46
22:D5:65:ASN:OD1	22:D5:65:ASN:N	2.48	0.46
26:B5:85:LYS:HZ3	26:B5:89:ARG:HH22	1.63	0.46
29:AJ:173:ASP:HB3	29:AJ:223:TYR:O	2.15	0.46
35:AM:138:GLY:O	35:AM:142:TYR:CB	2.61	0.46
2:V2:163:ASP:OD2	2:V2:190:ARG:NE	2.44	0.46
15:A7:43:GLY:HA3	15:A7:44:PRO:HD3	1.80	0.46
20:D6:25:SER:HB3	20:D6:28:TYR:HD2	1.80	0.46
22:D5:532:ILE:HD12	40:B8:105:LEU:HD13	1.97	0.46
23:D4:4:TYR:HE1	23:D4:37:THR:HG22	1.81	0.46
23:D4:403:THR:HA	23:D4:406:TYR:CE1	2.50	0.46
37:B7:99:LYS:HE2	39:B2:64:LEU:HD21	1.97	0.46
3:S1:237:ASN:HB3	3:S1:253:ARG:HG3	1.97	0.46
3:S1:483:VAL:HG23	3:S1:484:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S2:50:ASN:HD22	4:S2:65:VAL:HG22	1.79	0.46
4:S2:326:ASP:HB2	5:S3:10:THR:HG21	1.97	0.46
22:D5:342:CYS:SG	22:D5:369:THR:OG1	2.63	0.46
23:D4:158:LEU:HD21	24:D2:283:ALA:HB1	1.95	0.46
24:D2:228:LEU:O	24:D2:231:SER:OG	2.29	0.46
34:B4:70:ALA:HB2	40:B8:9:LEU:HD21	1.97	0.46
22:D5:473:PRO:HB2	22:D5:475:MET:HE2	1.96	0.46
29:AJ:49:LYS:HD2	29:AJ:114:HIS:CE1	2.51	0.46
13:A5:113:TRP:O	13:A5:115:ILE:N	2.48	0.46
24:D2:90:PHE:HB3	30:S5:63:ARG:HH22	1.81	0.46
5:S3:93:VAL:HG22	5:S3:108:LYS:HG2	1.97	0.46
22:D5:3:LEU:HD22	22:D5:53:MET:HE1	1.97	0.46
26:B5:26:ARG:O	26:B5:30:LEU:HB2	2.16	0.46
26:B5:143:ASN:H	27:A8:50:LYS:HD2	1.80	0.46
27:A8:24:LEU:HG	35:AM:70:LEU:HD11	1.97	0.46
3:S1:46:LEU:O	10:S4:116:LYS:NZ	2.35	0.46
5:S3:63:PHE:HD2	5:S3:64:LEU:HD12	1.80	0.46
5:S3:88:ASN:HD22	5:S3:112:ASP:HB3	1.81	0.46
22:D5:482:MET:SD	22:D5:487:LYS:NZ	2.88	0.46
29:AJ:168:VAL:HG12	29:AJ:219:GLU:HB2	1.96	0.46
1:V1:105:CYS:SG	2:V2:148:CYS:N	2.86	0.46
5:S3:100:ARG:NH2	13:A5:73:GLY:H	2.14	0.46
10:S4:37:ILE:HD11	10:S4:57:MET:HE2	1.97	0.46
26:B5:32:THR:HA	26:B5:35:PRO:HD2	1.97	0.46
5:S3:39:GLN:HB3	5:S3:51:CYS:HB2	1.98	0.46
6:S7:139:ILE:HG22	6:S7:140:VAL:HG13	1.98	0.46
18:D3:67:LEU:HB3	21:4L:65:VAL:HG23	1.98	0.46
19:D1:91:MET:SD	19:D1:91:MET:N	2.82	0.46
23:D4:204:MET:HE2	23:D4:243:MET:HE1	1.96	0.46
29:AJ:46:LEU:HD21	29:AJ:238:ILE:HG21	1.98	0.46
19:D1:149:ILE:HG23	19:D1:181:LEU:HG	1.98	0.46
24:D2:219:PHE:HE1	24:D2:230:LEU:HD21	1.81	0.46
2:V2:101:GLN:HB2	2:V2:155:GLN:HB3	1.98	0.45
3:S1:478:ARG:NH2	3:S1:486:ASP:OD1	2.49	0.45
21:4L:96:LEU:HD12	24:D2:51:ARG:HD2	1.97	0.45
23:D4:76:MET:HE3	23:D4:76:MET:HB2	1.72	0.45
35:AM:27:ARG:HA	35:AM:28:GLY:HA3	1.73	0.45
35:AM:119:MET:HE2	35:AM:122:GLU:HG3	1.98	0.45
1:V1:378:ARG:O	1:V1:382:GLY:N	2.50	0.45
7:S8:109:TYR:HB3	7:S8:151:LYS:HB2	1.98	0.45
12:A2:19:ARG:HG2	12:A2:53:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:D6:141:MET:HG3	30:S5:26:HIS:CE1	2.51	0.45
22:D5:381:THR:HA	22:D5:392:LYS:HD2	1.98	0.45
24:D2:258:SER:HB2	24:D2:336:LEU:H	1.81	0.45
25:AK:89:TYR:CD2	25:AK:125:LYS:HB2	2.51	0.45
26:B5:48:GLY:HA2	28:BJ:55:HIS:ND1	2.31	0.45
17:AB:26:ASP:OD1	17:AB:26:ASP:N	2.48	0.45
3:S1:378:LEU:HG	3:S1:451:VAL:HG22	1.98	0.45
16:AL:56:PHE:HA	16:AL:59:HIS:CD2	2.51	0.45
18:D3:77:TRP:HA	19:D1:317:GLN:HE22	1.81	0.45
22:D5:63:ILE:HA	36:B6:96:ILE:HG22	1.98	0.45
22:D5:260:LEU:HD22	22:D5:277:MET:HE1	1.98	0.45
29:AJ:210:PHE:HD2	29:AJ:211:LEU:HD22	1.82	0.45
4:S2:184:VAL:O	7:S8:60:ARG:NH2	2.31	0.45
10:S4:59:PHE:HD2	10:S4:79:LEU:HB3	1.82	0.45
49:A9:401:NDP:O1N	49:A9:401:NDP:O2A	2.33	0.45
17:AA:36:PHE:HA	17:AA:40:LEU:HB2	1.98	0.45
21:4L:23:ARG:HG2	22:D5:585:LYS:HD2	1.97	0.45
23:D4:370:PRO:HA	23:D4:375:LEU:HD13	1.99	0.45
24:D2:211:MET:O	24:D2:214:THR:OG1	2.32	0.45
27:A8:70:PHE:HB3	44:A1:69:ILE:HD12	1.98	0.45
40:B8:133:TYR:O	40:B8:155:HIS:NE2	2.31	0.45
3:S1:80:LEU:HB3	3:S1:83:SER:HB3	1.99	0.45
3:S1:324:ASP:HA	3:S1:573:TYR:HE1	1.82	0.45
3:S1:450:MET:HA	3:S1:489:VAL:O	2.16	0.45
20:D6:122:MET:HE1	30:S5:75:LEU:HB3	1.98	0.45
51:D5:902:3PE:N	40:B8:90:ASP:OD2	2.40	0.45
23:D4:203:PHE:HE2	23:D4:246:ILE:HG12	1.81	0.45
23:D4:382:VAL:HA	23:D4:385:THR:HG22	1.99	0.45
31:A3:27:LEU:O	31:A3:31:LEU:CB	2.63	0.45
3:S1:392:ASN:HD21	3:S1:415:LEU:HD22	1.81	0.45
7:S8:34:LEU:HD12	19:D1:272:TRP:CE2	2.51	0.45
38:B9:139:LEU:O	38:B9:143:THR:OG1	2.33	0.45
3:S1:483:VAL:HA	3:S1:484:THR:HA	1.55	0.45
10:S4:60:ASP:OD1	10:S4:60:ASP:N	2.50	0.45
28:BJ:159:LYS:NZ	33:C2:112:VAL:O	2.50	0.45
7:S8:94:ILE:HG12	7:S8:109:TYR:HD1	1.81	0.45
38:B9:136:VAL:HA	38:B9:164:PRO:HB3	1.98	0.45
40:B8:50:LEU:HB2	40:B8:78:HIS:HB2	1.99	0.45
1:V1:366:ARG:NH1	3:S1:155:GLN:OE1	2.50	0.45
3:S1:328:LEU:HD22	3:S1:507:TYR:HE2	1.81	0.45
4:S2:133:ARG:HD2	4:S2:320:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S3:100:ARG:HH21	13:A5:72:GLN:HB3	1.82	0.45
11:A9:92:ILE:HD12	11:A9:94:LEU:HD13	1.98	0.45
11:A9:136:ASN:HD21	11:A9:291:ASP:HA	1.81	0.45
23:D4:149:PHE:HD1	23:D4:215:TRP:HE1	1.64	0.45
29:AJ:313:GLY:HA3	29:AJ:314:ASP:HA	1.80	0.45
6:S7:62:MET:HG2	6:S7:156:LEU:HD23	1.98	0.45
10:S4:33:ARG:HH21	10:S4:62:ARG:HD2	1.81	0.45
19:D1:307:LEU:HD12	19:D1:310:LEU:HD12	1.99	0.45
20:D6:146:LEU:HD12	21:4L:58:MET:HG3	1.98	0.45
23:D4:1:MET:HE3	23:D4:111:THR:HG21	1.97	0.45
24:D2:2:ASN:H	24:D2:5:ILE:HD12	1.82	0.45
24:D2:269:GLU:HG2	24:D2:272:LYS:HE3	1.99	0.45
29:AJ:105:LEU:HD11	29:AJ:163:TYR:HE2	1.82	0.45
38:B9:10:THR:HG23	38:B9:13:GLN:H	1.82	0.45
1:V1:93:LEU:O	1:V1:134:ALA:HA	2.17	0.44
1:V1:349:ARG:HE	2:V2:105:THR:HA	1.82	0.44
4:S2:293:CYS:SG	4:S2:296:ARG:NH1	2.91	0.44
11:A9:209:ASP:OD2	11:A9:308:THR:N	2.43	0.44
22:D5:145:GLU:HB2	23:D4:370:PRO:HG3	1.99	0.44
22:D5:223:LYS:HG2	22:D5:255:ALA:HB3	2.00	0.44
23:D4:160:LEU:HD13	23:D4:199:CYS:HA	2.00	0.44
23:D4:190:TRP:HB3	25:AK:126:MET:HE2	1.99	0.44
28:BJ:136:LYS:NZ	28:BJ:140:ASP:OD2	2.49	0.44
32:B3:53:MET:HA	32:B3:57:ALA:HB2	1.97	0.44
14:A6:38:TRP:CD2	14:A6:89:LEU:HD12	2.52	0.44
21:4L:62:ILE:HA	21:4L:65:VAL:HG12	1.98	0.44
22:D5:472:ILE:O	37:B7:69:LYS:NZ	2.50	0.44
22:D5:584:ILE:HD11	24:D2:58:LYS:HE2	1.98	0.44
23:D4:243:MET:HG2	23:D4:301:ILE:HG21	1.98	0.44
32:B3:72:TRP:CE3	39:B2:30:ALA:HB1	2.52	0.44
49:A9:401:NDP:N3A	49:A9:401:NDP:O3X	2.50	0.44
16:AL:50:GLU:HB2	16:AL:60:ARG:HG2	2.00	0.44
20:D6:58:LEU:O	20:D6:62:GLY:CA	2.65	0.44
1:V1:43:TYR:O	1:V1:236:ARG:NH1	2.40	0.44
2:V2:99:HIS:CE1	2:V2:101:GLN:HE21	2.36	0.44
4:S2:388:ARG:HD2	5:S3:81:VAL:HG22	2.00	0.44
11:A9:316:GLU:HG2	14:A6:52:ASP:HB3	1.98	0.44
29:AJ:56:ILE:O	29:AJ:99:TRP:NE1	2.36	0.44
34:B4:77:PRO:HA	34:B4:78:ASN:HA	1.72	0.44
34:B4:122:ARG:HA	34:B4:125:ASN:HB2	1.99	0.44
1:V1:24:ASN:ND2	1:V1:113:HIS:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V1:107:ASP:HA	1:V1:110:ILE:HB	1.99	0.44
3:S1:568:GLU:HB3	3:S1:589:PRO:HG3	1.98	0.44
13:A5:74:GLY:HA2	13:A5:75:GLN:HA	1.66	0.44
19:D1:316:PRO:HB3	35:AM:57:ARG:HD2	1.98	0.44
20:D6:85:SER:OG	20:D6:86:ASN:N	2.49	0.44
22:D5:10:VAL:HG11	36:B6:78:VAL:HG22	1.98	0.44
23:D4:50:LEU:HA	26:B5:86:ASN:HD21	1.83	0.44
29:AJ:306:ALA:HA	29:AJ:309:ASN:HB2	2.00	0.44
38:B9:153:LEU:HD13	38:B9:164:PRO:HG2	2.00	0.44
22:D5:178:GLY:HA2	22:D5:219:ALA:HA	2.00	0.44
24:D2:88:LYS:HG3	24:D2:148:SER:HB3	1.99	0.44
29:AJ:305:ARG:HB2	33:C2:50:ARG:HB2	2.00	0.44
3:S1:36:GLN:NE2	10:S4:49:VAL:HG22	2.33	0.44
3:S1:226:GLU:HA	3:S1:253:ARG:HH12	1.82	0.44
5:S3:80:ALA:C	5:S3:91:GLU:O	2.60	0.44
11:A9:97:ARG:NH1	49:A9:401:NDP:O2B	2.51	0.44
22:D5:85:PHE:O	22:D5:89:PHE:HB3	2.17	0.44
22:D5:332:HIS:CE1	22:D5:336:LYS:HD2	2.52	0.44
22:D5:604:PHE:O	24:D2:150:ASN:ND2	2.37	0.44
37:B7:33:ARG:HH12	39:B2:64:LEU:HA	1.82	0.44
37:B7:34:LYS:HG3	40:B8:156:TYR:HD1	1.82	0.44
40:B8:64:TRP:CZ2	40:B8:70:ARG:HG3	2.53	0.44
1:V1:259:SER:OG	2:V2:148:CYS:O	2.30	0.44
3:S1:400:LEU:O	10:S4:128:THR:OG1	2.28	0.44
4:S2:80:ILE:HD12	4:S2:80:ILE:HA	1.90	0.44
4:S2:111:MET:HE1	4:S2:178:PHE:HE1	1.83	0.44
6:S7:48:MET:HE2	6:S7:50:PHE:HB2	2.00	0.44
7:S8:152:GLU:OE1	16:AL:127:TYR:OH	2.35	0.44
11:A9:144:LYS:O	11:A9:148:ASN:ND2	2.51	0.44
22:D5:520:PHE:O	22:D5:524:ASN:HB2	2.18	0.44
23:D4:276:CYS:HB3	23:D4:288:TYR:HB2	1.99	0.44
24:D2:98:MET:HE1	24:D2:145:ILE:HG21	1.99	0.44
36:B6:1:SER:OG	36:B6:2:GLY:N	2.51	0.44
3:S1:228:ILE:HG13	3:S1:581:GLN:HB3	1.98	0.44
4:S2:120:LEU:HD23	4:S2:120:LEU:HA	1.89	0.44
5:S3:135:TRP:HE1	14:A6:87:MET:HE1	1.83	0.44
12:A2:68:TYR:O	12:A2:72:GLN:HB2	2.17	0.44
16:AL:29:ARG:NH1	16:AL:74:PHE:O	2.51	0.44
22:D5:326:PHE:HA	22:D5:329:ILE:HD12	1.99	0.44
17:AB:60:PHE:HZ	17:AB:80:ILE:HG13	1.81	0.44
2:V2:17:PRO:HA	2:V2:19:THR:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S8:3:LYS:HG3	15:A7:110:PRO:HA	2.00	0.43
11:A9:48:PRO:HB2	11:A9:73:TRP:CD1	2.53	0.43
21:4L:66:PHE:HB3	24:D2:34:GLU:OE1	2.18	0.43
22:D5:335:PHE:HD2	22:D5:336:LYS:HG3	1.83	0.43
22:D5:440:LEU:HD21	17:AB:6:LEU:HD21	2.00	0.43
23:D4:263:MET:HE1	34:B4:100:TRP:HB2	1.99	0.43
31:A3:76:SER:OG	31:A3:77:LEU:N	2.51	0.43
46:V1:501:FMN:O5'	46:V1:501:FMN:O3'	2.32	0.43
3:S1:230:VAL:HG23	3:S1:231:MET:HG3	2.00	0.43
5:S3:150:ARG:NH2	14:A6:91:GLU:OE1	2.51	0.43
6:S7:53:ALA:H	6:S7:90:GLY:HA3	1.83	0.43
9:S6:12:THR:HG22	9:S6:35:VAL:HG23	2.00	0.43
20:D6:60:TYR:HD2	21:4L:38:LEU:HD13	1.82	0.43
22:D5:139:GLN:HA	22:D5:142:ILE:HD12	1.99	0.43
51:D4:501:3PE:H342	51:D4:501:3PE:H372	1.89	0.43
38:B9:102:CYS:SG	38:B9:103:LEU:N	2.76	0.43
1:V1:309:LYS:NZ	1:V1:313:GLU:OE2	2.46	0.43
2:V2:29:LYS:HG3	8:V3:56:LEU:HD11	1.99	0.43
3:S1:312:GLY:N	3:S1:339:ASP:OD2	2.48	0.43
3:S1:386:PHE:HE1	3:S1:668:ILE:HD13	1.83	0.43
16:AL:31:ASN:HD21	19:D1:39:VAL:HG22	1.83	0.43
22:D5:141:PHE:HE2	23:D4:375:LEU:HD11	1.83	0.43
24:D2:108:MET:O	24:D2:112:HIS:N	2.51	0.43
24:D2:254:LEU:HA	24:D2:255:PRO:HD3	1.90	0.43
24:D2:270:MET:HG2	24:D2:279:PRO:HG3	2.00	0.43
27:A8:43:MET:SD	27:A8:47:TRP:NE1	2.92	0.43
29:AJ:119:GLY:HA3	29:AJ:120:GLN:HA	1.83	0.43
32:B3:61:SER:OG	32:B3:62:PHE:N	2.50	0.43
3:S1:628:PRO:HD3	12:A2:21:HIS:CE1	2.54	0.43
4:S2:112:MET:HE1	4:S2:193:TYR:HD2	1.82	0.43
10:S4:42:ARG:HD2	10:S4:48:GLY:H	1.83	0.43
11:A9:96:GLY:H	49:A9:401:NDP:H8A	1.83	0.43
29:AJ:224:SER:OG	29:AJ:225:ALA:N	2.51	0.43
35:AM:67:ARG:HD3	35:AM:68:ILE:HG13	2.00	0.43
3:S1:198:ASN:ND2	3:S1:263:ILE:O	2.50	0.43
5:S3:22:LEU:HD23	5:S3:48:LEU:HB2	2.00	0.43
23:D4:165:ILE:HG21	24:D2:268:GLN:HA	2.00	0.43
32:B3:19:LYS:HA	32:B3:46:ARG:HH12	1.83	0.43
36:B6:117:PRO:HA	36:B6:118:PRO:HD3	1.84	0.43
40:B8:64:TRP:HZ2	40:B8:70:ARG:HG3	1.83	0.43
3:S1:126:ASP:HA	4:S2:347:HIS:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:174:THR:HG22	3:S1:183:VAL:HG22	1.99	0.43
3:S1:321:GLY:O	3:S1:498:SER:OG	2.36	0.43
6:S7:100:LEU:HD23	6:S7:139:ILE:HG21	2.00	0.43
7:S8:64:GLU:HA	7:S8:139:PHE:HZ	1.84	0.43
14:A6:29:ARG:HH21	17:AA:65:ILE:HD13	1.84	0.43
22:D5:147:VAL:O	22:D5:151:SER:OG	2.36	0.43
24:D2:26:TRP:NE1	24:D2:85:THR:O	2.45	0.43
24:D2:155:LEU:HD21	24:D2:278:LEU:HD22	1.99	0.43
24:D2:181:TYR:HD1	24:D2:184:ILE:HD12	1.83	0.43
25:AK:46:THR:HA	25:AK:47:SER:HA	1.66	0.43
29:AJ:267:LEU:HD23	29:AJ:271:ASN:HD21	1.84	0.43
30:S5:91:TYR:HE2	35:AM:96:ILE:HG13	1.82	0.43
36:B6:17:LEU:HD11	38:B9:162:LEU:HD22	2.00	0.43
37:B7:7:ARG:HH21	37:B7:17:GLU:HG2	1.83	0.43
38:B9:167:TRP:O	38:B9:171:THR:OG1	2.28	0.43
11:A9:167:LYS:O	11:A9:229:ALA:HA	2.19	0.43
15:A7:111:TYR:HA	15:A7:112:LEU:HA	1.73	0.43
51:D4:501:3PE:H291	24:D2:288:LEU:HD23	2.00	0.43
29:AJ:75:GLY:HA3	29:AJ:76:ASN:HA	1.69	0.43
1:V1:260:GLY:O	2:V2:111:ARG:NH1	2.45	0.43
1:V1:305:PRO:HD2	1:V1:327:THR:HG22	1.99	0.43
23:D4:30:HIS:HB3	43:B1:16:VAL:HG21	2.00	0.43
23:D4:266:LEU:HD23	23:D4:266:LEU:HA	1.83	0.43
26:B5:63:HIS:NE2	26:B5:76:ALA:O	2.38	0.43
26:B5:128:ILE:HG21	30:S5:40:ILE:HG12	1.99	0.43
38:B9:3:LEU:HG	38:B9:6:ALA:H	1.84	0.43
3:S1:543:ILE:HD11	3:S1:557:ALA:HA	1.99	0.43
4:S2:146:ARG:NH2	4:S2:368:GLU:OE1	2.51	0.43
4:S2:379:VAL:HB	4:S2:388:ARG:O	2.18	0.43
11:A9:108:ASP:HA	11:A9:111:VAL:HB	2.00	0.43
28:BJ:158:GLN:HG3	28:BJ:162:MET:HE3	2.00	0.43
12:A2:21:HIS:O	12:A2:62:PRO:HA	2.19	0.43
20:D6:47:PHE:HD1	20:D6:47:PHE:HA	1.73	0.43
52:D5:901:CDL:HA31	26:B5:22:LEU:HD21	2.01	0.43
27:A8:17:VAL:HG21	35:AM:73:LEU:HD21	2.01	0.43
34:B4:100:TRP:HA	34:B4:103:VAL:HG22	2.01	0.43
35:AM:139:PHE:HB2	44:A1:45:TRP:CG	2.53	0.43
3:S1:202:ILE:HD13	3:S1:202:ILE:HA	1.92	0.42
3:S1:237:ASN:CG	3:S1:253:ARG:HE	2.27	0.42
3:S1:276:ARG:HH21	3:S1:682:GLN:HE21	1.67	0.42
3:S1:323:VAL:HG11	3:S1:525:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S1:336:ASN:ND2	12:A2:67:ARG:HH11	2.16	0.42
4:S2:169:TRP:CE2	7:S8:40:TYR:HD2	2.37	0.42
10:S4:57:MET:O	10:S4:83:VAL:HA	2.19	0.42
23:D4:51:ASN:ND2	26:B5:90:THR:HG22	2.34	0.42
24:D2:40:ILE:HD12	24:D2:40:ILE:HA	1.93	0.42
34:B4:5:TYR:HB3	34:B4:17:LEU:HD11	2.01	0.42
1:V1:191:ALA:HB2	1:V1:203:PRO:HG3	2.00	0.42
2:V2:156:ILE:HG13	2:V2:159:ASN:HB2	2.01	0.42
9:S6:74:ASN:ND2	9:S6:76:ASP:OD2	2.48	0.42
23:D4:216:LEU:HD11	23:D4:220:HIS:CE1	2.54	0.42
24:D2:224:THR:HG22	24:D2:229:SER:HB3	2.00	0.42
24:D2:243:LEU:HD23	24:D2:243:LEU:HA	1.73	0.42
26:B5:64:TRP:HD1	26:B5:65:GLU:HG3	1.84	0.42
2:V2:156:ILE:HD11	2:V2:159:ASN:HD22	1.84	0.42
6:S7:104:TYR:CZ	6:S7:111:ARG:HD2	2.54	0.42
11:A9:134:HIS:HA	49:A9:401:NDP:H5N	2.01	0.42
23:D4:206:LYS:HA	23:D4:206:LYS:HD2	1.85	0.42
23:D4:212:LEU:HD11	51:D4:501:3PE:H3C2	2.02	0.42
24:D2:210:ILE:HG22	24:D2:333:SER:HB3	2.01	0.42
27:A8:107:ASP:OD2	27:A8:118:ARG:NH1	2.52	0.42
28:BJ:101:ILE:HD11	41:BK:96:LEU:HD22	2.00	0.42
34:B4:114:LEU:HD22	34:B4:120:LEU:HD23	2.01	0.42
1:V1:134:ALA:HB3	1:V1:175:VAL:HG12	2.01	0.42
3:S1:160:ILE:HD11	3:S1:183:VAL:HG13	2.01	0.42
3:S1:198:ASN:ND2	3:S1:263:ILE:H	2.13	0.42
11:A9:216:ASN:O	11:A9:220:ASP:HB2	2.19	0.42
19:D1:290:TRP:CE3	19:D1:294:LEU:HD22	2.54	0.42
22:D5:130:ILE:HG23	22:D5:139:GLN:HE21	1.85	0.42
23:D4:272:THR:HA	23:D4:275:ILE:HG22	2.02	0.42
23:D4:336:ARG:HH21	23:D4:352:LEU:HD21	1.84	0.42
23:D4:407:SER:HA	23:D4:410:MET:HE2	2.01	0.42
25:AK:36:SER:HB2	25:AK:55:THR:HG22	2.01	0.42
27:A8:97:ARG:HB3	35:AM:59:LEU:HD13	2.01	0.42
27:A8:124:LEU:HD12	35:AM:65:GLU:HB3	2.02	0.42
35:AM:81:ARG:HG2	35:AM:85:MET:HE1	2.01	0.42
37:B7:75:ASN:HB3	37:B7:78:ALA:HB2	2.01	0.42
38:B9:97:LYS:HE2	38:B9:175:GLU:HA	2.00	0.42
3:S1:329:ILE:HD11	3:S1:505:LEU:HD22	2.01	0.42
6:S7:116:MET:HA	6:S7:146:VAL:HG23	2.00	0.42
22:D5:418:PHE:HA	22:D5:421:ILE:HG12	2.02	0.42
44:A1:52:ARG:HE	44:A1:58:ASN:ND2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V1:205:LEU:HD22	3:S1:70:ALA:HB3	2.02	0.42
6:S7:77:ARG:HA	6:S7:77:ARG:HD2	1.88	0.42
6:S7:127:HIS:CG	7:S8:115:LYS:HE3	2.55	0.42
10:S4:28:GLU:O	10:S4:32:THR:OG1	2.29	0.42
18:D3:87:MET:HB2	18:D3:87:MET:HE3	1.83	0.42
19:D1:201:THR:HG1	19:D1:279:ARG:HH12	1.61	0.42
24:D2:170:LEU:HD23	24:D2:292:PHE:HD1	1.85	0.42
38:B9:33:ARG:HA	38:B9:36:TYR:HB3	2.01	0.42
2:V2:60:TRP:CG	2:V2:94:PRO:HA	2.53	0.42
3:S1:362:TYR:OH	3:S1:504:ASP:OD1	2.34	0.42
4:S2:422:ASP:OD1	4:S2:422:ASP:N	2.53	0.42
6:S7:85:VAL:HG11	6:S7:163:LEU:HD21	2.02	0.42
19:D1:285:LEU:HD12	19:D1:285:LEU:HA	1.89	0.42
23:D4:234:ILE:O	23:D4:238:LEU:HB2	2.19	0.42
24:D2:298:TYR:O	24:D2:303:THR:OG1	2.31	0.42
26:B5:42:LEU:HA	26:B5:45:VAL:HG12	2.02	0.42
3:S1:213:TYR:CD1	3:S1:249:ARG:HD3	2.54	0.42
8:V3:38:TYR:HE2	8:V3:41:LEU:HB2	1.84	0.42
22:D5:298:ILE:HD11	22:D5:359:MET:HE3	2.02	0.42
23:D4:24:TRP:CH2	23:D4:81:GLN:HB3	2.55	0.42
24:D2:190:MET:HG2	24:D2:204:ASN:HB3	2.01	0.42
28:BJ:72:ASP:HB2	28:BJ:75:GLU:HB2	2.01	0.42
41:BK:82:ASP:OD1	41:BK:82:ASP:N	2.52	0.42
3:S1:375:ASP:H	3:S1:448:LYS:HB2	1.84	0.42
3:S1:667:THR:OG1	3:S1:668:ILE:N	2.52	0.42
23:D4:298:ILE:HD13	23:D4:298:ILE:HA	1.77	0.42
29:AJ:169:VAL:O	29:AJ:220:VAL:HA	2.20	0.42
1:V1:287:VAL:HG11	1:V1:294:LEU:HB3	2.01	0.41
2:V2:6:LEU:HD12	2:V2:93:LYS:HE2	2.01	0.41
9:S6:26:VAL:HB	11:A9:87:HIS:HB2	2.02	0.41
11:A9:129:PHE:HB3	11:A9:160:PHE:CE2	2.55	0.41
11:A9:165:ILE:O	11:A9:227:THR:HA	2.19	0.41
21:4L:53:PHE:CE2	21:4L:56:ALA:HB3	2.55	0.41
22:D5:22:ILE:HA	22:D5:25:ASN:HB2	2.01	0.41
22:D5:267:THR:OG1	22:D5:274:GLN:NE2	2.43	0.41
26:B5:123:PHE:HE1	33:C2:2:MET:HA	1.85	0.41
31:A3:24:ILE:HD12	31:A3:27:LEU:HD21	2.02	0.41
34:B4:13:LEU:HD22	34:B4:14:PRO:HD2	2.02	0.41
38:B9:25:HIS:CD2	38:B9:75:HIS:H	2.35	0.41
2:V2:132:THR:OG1	2:V2:134:ASP:OD1	2.35	0.41
3:S1:278:ARG:HA	3:S1:549:HIS:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:S8:43:ARG:NH1	15:A7:23:LEU:O	2.53	0.41
19:D1:159:SER:HB3	19:D1:161:THR:HG23	2.01	0.41
51:D5:902:3PE:H332	23:D4:405:LEU:HD11	2.02	0.41
22:D5:33:PRO:HB3	22:D5:118:PHE:HE2	1.84	0.41
22:D5:127:THR:HG21	22:D5:146:GLY:HA3	2.03	0.41
24:D2:83:GLN:HG2	24:D2:85:THR:H	1.85	0.41
24:D2:229:SER:O	24:D2:233:THR:HG23	2.20	0.41
36:B6:104:PHE:CZ	37:B7:66:LEU:HB3	2.54	0.41
7:S8:96:ALA:HA	7:S8:106:THR:HA	2.03	0.41
18:D3:71:LEU:O	20:D6:147:TYR:OH	2.37	0.41
19:D1:55:LEU:HA	19:D1:55:LEU:HD22	1.87	0.41
22:D5:348:HIS:NE2	17:AB:2:ASP:OD2	2.53	0.41
24:D2:155:LEU:HD12	24:D2:155:LEU:HA	1.81	0.41
37:B7:97:ARG:HB3	40:B8:128:VAL:HG13	2.01	0.41
3:S1:341:ASP:OD1	3:S1:341:ASP:N	2.52	0.41
6:S7:165:LYS:HE2	16:AL:76:ASP:HB2	2.03	0.41
16:AL:39:VAL:HG21	16:AL:50:GLU:HB3	2.02	0.41
19:D1:140:ILE:HD12	20:D6:66:VAL:HG11	2.01	0.41
20:D6:174:GLY:HA2	20:D6:175:ASN:HA	1.56	0.41
22:D5:172:ILE:HG21	23:D4:408:LEU:HD22	2.03	0.41
22:D5:254:VAL:O	22:D5:258:PHE:N	2.51	0.41
26:B5:143:ASN:HB2	27:A8:50:LYS:HE2	2.02	0.41
38:B9:3:LEU:HD11	38:B9:6:ALA:HB3	2.03	0.41
40:B8:30:ARG:HB3	40:B8:33:ASP:HB2	2.02	0.41
40:B8:37:TYR:CE1	40:B8:49:LYS:HE3	2.55	0.41
3:S1:41:CYS:O	3:S1:161:ARG:NH2	2.40	0.41
3:S1:280:THR:HG21	16:AL:136:GLU:HG2	2.02	0.41
4:S2:423:ILE:H	4:S2:423:ILE:HG13	1.65	0.41
7:S8:94:ILE:HG12	7:S8:109:TYR:CD1	2.56	0.41
11:A9:81:ILE:HG21	11:A9:117:ILE:HG22	2.02	0.41
11:A9:94:LEU:HG	11:A9:132:ILE:HG12	2.03	0.41
19:D1:59:GLU:HA	19:D1:60:PRO:HD3	1.90	0.41
22:D5:439:THR:OG1	22:D5:440:LEU:N	2.54	0.41
23:D4:44:GLN:HE22	23:D4:60:SER:N	2.18	0.41
23:D4:82:HIS:HB2	23:D4:432:ARG:HH12	1.85	0.41
42:C1:1:LYS:HD3	42:C1:2:PHE:HB2	2.01	0.41
1:V1:294:LEU:HD22	1:V1:336:VAL:HG11	2.02	0.41
2:V2:72:ILE:HG22	2:V2:73:LEU:HD12	2.02	0.41
3:S1:141:ASN:OD1	3:S1:141:ASN:N	2.54	0.41
11:A9:144:LYS:HA	11:A9:147:ARG:HG2	2.02	0.41
16:AL:83:PRO:HG2	16:AL:86:TRP:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D3:60:ILE:HG21	20:D6:168:ILE:HG21	2.03	0.41
22:D5:85:PHE:O	22:D5:89:PHE:CB	2.69	0.41
28:BJ:158:GLN:HE22	41:BK:111:ASN:HA	1.84	0.41
38:B9:91:GLU:HB3	38:B9:94:GLU:HB2	2.03	0.41
38:B9:108:PRO:HA	38:B9:111:LYS:HB2	2.03	0.41
41:BK:74:SER:O	41:BK:78:ALA:HB2	2.21	0.41
3:S1:200:ILE:HD11	3:S1:268:ARG:HD3	2.02	0.41
3:S1:332:LYS:HA	3:S1:343:LEU:HD21	2.02	0.41
4:S2:185:SER:OG	4:S2:186:GLY:N	2.53	0.41
4:S2:399:LEU:HD22	4:S2:425:PHE:HE1	1.86	0.41
5:S3:82:ASP:OD1	5:S3:82:ASP:N	2.52	0.41
12:A2:47:ASN:HB3	12:A2:50:LEU:HD13	2.02	0.41
13:A5:34:LEU:O	13:A5:44:ARG:NH1	2.54	0.41
19:D1:299:ALA:HB1	31:A3:24:ILE:HG23	2.03	0.41
22:D5:280:LEU:O	22:D5:284:THR:HG23	2.21	0.41
24:D2:186:HIS:HB3	24:D2:190:MET:HE2	2.02	0.41
43:B1:30:ASN:O	43:B1:34:LEU:HB2	2.21	0.41
3:S1:73:VAL:HG13	3:S1:77:TRP:HD1	1.85	0.41
7:S8:1:THR:HB	15:A7:106:SER:HB2	2.03	0.41
11:A9:93:ASN:O	11:A9:132:ILE:HG13	2.21	0.41
18:D3:102:LEU:HD22	19:D1:294:LEU:HD23	2.02	0.41
18:D3:111:LEU:HD13	18:D3:111:LEU:HA	1.96	0.41
19:D1:18:ALA:O	19:D1:21:THR:OG1	2.36	0.41
19:D1:85:MET:SD	19:D1:108:MET:HG3	2.61	0.41
19:D1:152:SER:HG	19:D1:301:CYS:HG	1.58	0.41
20:D6:132:ASP:OD1	35:AM:78:LYS:NZ	2.34	0.41
22:D5:360:GLY:H	22:D5:436:ARG:HG2	1.86	0.41
23:D4:388:TRP:O	34:B4:108:ARG:NH2	2.54	0.41
29:AJ:18:MET:HA	29:AJ:19:THR:HA	1.93	0.41
37:B7:55:ARG:NH1	40:B8:141:GLU:OE2	2.54	0.41
1:V1:250:ASN:HD22	1:V1:319:PHE:HB2	1.85	0.41
12:A2:36:ILE:HD12	12:A2:36:ILE:HA	1.85	0.41
18:D3:78:ALA:HA	20:D6:144:ALA:HB1	2.04	0.41
20:D6:11:ILE:HD13	20:D6:11:ILE:HA	1.96	0.41
22:D5:363:PHE:HB2	22:D5:432:LEU:HG	2.02	0.41
28:BJ:127:GLU:HA	28:BJ:130:GLN:HG2	2.02	0.41
3:S1:221:GLU:HG2	5:S3:197:PHE:HE1	1.85	0.40
5:S3:52:ILE:O	5:S3:109:THR:HA	2.21	0.40
8:V3:50:THR:O	8:V3:54:LEU:HB2	2.21	0.40
11:A9:284:VAL:HG22	11:A9:288:HIS:HD2	1.84	0.40
15:A7:11:ARG:HB3	15:A7:19:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D5:77:SER:OG	22:D5:79:SER:OG	2.37	0.40
23:D4:212:LEU:HD23	23:D4:212:LEU:HA	1.89	0.40
23:D4:325:MET:O	23:D4:329:LEU:HD12	2.21	0.40
30:S5:19:ILE:HG22	30:S5:20:GLN:H	1.86	0.40
37:B7:27:ASP:HA	37:B7:30:PHE:HB2	2.02	0.40
1:V1:172:ASP:OD1	1:V1:172:ASP:N	2.53	0.40
2:V2:104:THR:HA	2:V2:108:CYS:HB2	2.04	0.40
3:S1:488:LYS:HE3	3:S1:488:LYS:HB3	1.97	0.40
4:S2:273:GLN:OE1	5:S3:104:ARG:NH1	2.50	0.40
18:D3:67:LEU:HD22	21:4L:65:VAL:HG23	2.02	0.40
22:D5:51:THR:O	22:D5:55:ILE:HD12	2.21	0.40
22:D5:532:ILE:HD11	40:B8:101:MET:HB3	2.04	0.40
23:D4:195:MET:HE3	23:D4:250:LEU:HD11	2.04	0.40
27:A8:7:PRO:HD2	35:AM:83:LEU:HD12	2.03	0.40
36:B6:96:ILE:H	36:B6:96:ILE:HG23	1.69	0.40
1:V1:300:GLY:HA2	1:V1:330:GLY:N	2.37	0.40
1:V1:379:PHE:CZ	1:V1:389:ILE:HG22	2.56	0.40
3:S1:237:ASN:HB3	3:S1:253:ARG:O	2.22	0.40
3:S1:252:PRO:HB3	3:S1:263:ILE:HB	2.02	0.40
5:S3:154:ASP:OD1	5:S3:155:TYR:N	2.53	0.40
6:S7:69:MET:HB3	6:S7:74:VAL:HB	2.03	0.40
22:D5:177:ILE:HA	22:D5:180:ILE:HG22	2.03	0.40
22:D5:398:SER:O	22:D5:402:SER:OG	2.38	0.40
22:D5:441:ILE:H	22:D5:441:ILE:HG13	1.66	0.40
23:D4:76:MET:HG3	23:D4:229:MET:HE3	2.02	0.40
24:D2:243:LEU:HD11	33:C2:44:ILE:HD11	2.03	0.40
28:BJ:25:LEU:HD13	28:BJ:25:LEU:HA	1.99	0.40
29:AJ:33:SER:HB3	29:AJ:174:VAL:HG21	2.03	0.40
29:AJ:212:PRO:O	29:AJ:215:SER:OG	2.36	0.40
29:AJ:288:GLN:HA	29:AJ:291:ARG:HG2	2.03	0.40
1:V1:365:CYS:HB3	45:V1:500:SF4:S4	2.62	0.40
4:S2:51:PHE:HB3	4:S2:64:LEU:HB3	2.04	0.40
4:S2:51:PHE:CZ	4:S2:57:ALA:HB3	2.56	0.40
11:A9:251:ARG:HE	11:A9:322:ARG:HG3	1.87	0.40
17:AA:44:SER:HA	17:AA:47:GLN:HB3	2.03	0.40
22:D5:200:GLN:OE1	28:BJ:106:GLN:NE2	2.47	0.40
22:D5:530:PRO:O	22:D5:534:HIS:HB2	2.22	0.40
23:D4:306:PRO:HG3	23:D4:458:LEU:HD13	2.02	0.40
27:A8:94:GLN:HE22	44:A1:37:ARG:CZ	2.34	0.40
29:AJ:3:TYR:HE1	29:AJ:260:ARG:HD3	1.87	0.40
36:B6:92:LYS:HA	36:B6:93:PRO:HD3	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S2:202:ASP:HB3	4:S2:323:ILE:HG23	2.03	0.40
6:S7:79:SER:HB3	6:S7:82:GLN:HG2	2.02	0.40
11:A9:203:GLN:HB2	11:A9:232:GLY:HA3	2.03	0.40
13:A5:46:TYR:HE1	15:A7:92:LYS:HB2	1.86	0.40
22:D5:45:ILE:HD12	22:D5:45:ILE:HA	1.98	0.40
22:D5:552:LEU:HD11	34:B4:89:GLY:HA2	2.03	0.40
23:D4:108:MET:HB3	23:D4:121:MET:HG3	2.04	0.40
23:D4:116:ILE:HD13	23:D4:116:ILE:HA	1.92	0.40
24:D2:207:ILE:HD13	24:D2:262:PRO:HD3	2.03	0.40
24:D2:215:MET:HE2	24:D2:215:MET:HB2	1.96	0.40
28:BJ:29:ILE:H	28:BJ:29:ILE:HG13	1.64	0.40
36:B6:24:ASP:OD2	38:B9:124:TRP:NE1	2.49	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	V1	428/445 (96%)	389 (91%)	39 (9%)	0	100	100
2	V2	210/217 (97%)	171 (81%)	39 (19%)	0	100	100
3	S1	686/704 (97%)	609 (89%)	77 (11%)	0	100	100
4	S2	428/430 (100%)	378 (88%)	50 (12%)	0	100	100
5	S3	206/228 (90%)	177 (86%)	29 (14%)	0	100	100
6	S7	154/179 (86%)	137 (89%)	17 (11%)	0	100	100
7	S8	174/176 (99%)	160 (92%)	14 (8%)	0	100	100
8	V3	39/75 (52%)	33 (85%)	6 (15%)	0	100	100
9	S6	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
10	S4	124/133 (93%)	112 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	A9	281/338 (83%)	244 (87%)	37 (13%)	0	100	100
12	A2	80/98 (82%)	70 (88%)	10 (12%)	0	100	100
13	A5	109/115 (95%)	93 (85%)	16 (15%)	0	100	100
14	A6	112/127 (88%)	105 (94%)	7 (6%)	0	100	100
15	A7	92/112 (82%)	76 (83%)	15 (16%)	1 (1%)	11	45
16	AL	142/145 (98%)	117 (82%)	25 (18%)	0	100	100
17	AA	78/88 (89%)	67 (86%)	11 (14%)	0	100	100
17	AB	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
18	D3	86/115 (75%)	81 (94%)	5 (6%)	0	100	100
19	D1	299/318 (94%)	269 (90%)	30 (10%)	0	100	100
20	D6	167/175 (95%)	147 (88%)	20 (12%)	0	100	100
21	4L	96/98 (98%)	89 (93%)	7 (7%)	0	100	100
22	D5	604/606 (100%)	536 (89%)	68 (11%)	0	100	100
23	D4	457/459 (100%)	417 (91%)	39 (8%)	1 (0%)	43	77
24	D2	345/347 (99%)	319 (92%)	26 (8%)	0	100	100
25	AK	138/140 (99%)	129 (94%)	9 (6%)	0	100	100
26	B5	137/143 (96%)	119 (87%)	18 (13%)	0	100	100
27	A8	169/171 (99%)	138 (82%)	31 (18%)	0	100	100
28	BJ	169/175 (97%)	150 (89%)	18 (11%)	1 (1%)	21	58
29	AJ	317/320 (99%)	275 (87%)	42 (13%)	0	100	100
30	S5	97/105 (92%)	80 (82%)	17 (18%)	0	100	100
31	A3	72/83 (87%)	59 (82%)	13 (18%)	0	100	100
32	B3	71/97 (73%)	54 (76%)	16 (22%)	1 (1%)	9	39
33	C2	117/120 (98%)	104 (89%)	13 (11%)	0	100	100
34	B4	126/128 (98%)	109 (86%)	17 (14%)	0	100	100
35	AM	137/143 (96%)	123 (90%)	14 (10%)	0	100	100
36	B6	92/127 (72%)	81 (88%)	10 (11%)	1 (1%)	11	45
37	B7	117/136 (86%)	102 (87%)	15 (13%)	0	100	100
38	B9	174/178 (98%)	147 (84%)	27 (16%)	0	100	100
39	B2	63/72 (88%)	58 (92%)	5 (8%)	0	100	100
40	B8	155/158 (98%)	115 (74%)	40 (26%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	BK	100/125 (80%)	85 (85%)	15 (15%)	0	100	100
42	C1	44/49 (90%)	40 (91%)	4 (9%)	0	100	100
43	B1	50/57 (88%)	43 (86%)	7 (14%)	0	100	100
44	A1	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
All	All	7988/8509 (94%)	7032 (88%)	951 (12%)	5 (0%)	49	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	D4	53	SER
15	A7	69	MET
28	BJ	71	PRO
32	B3	23	ILE
36	B6	93	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V1	344/354 (97%)	341 (99%)	3 (1%)	70	75
2	V2	182/183 (100%)	181 (100%)	1 (0%)	81	81
3	S1	578/588 (98%)	574 (99%)	4 (1%)	76	78
4	S2	371/371 (100%)	368 (99%)	3 (1%)	73	77
5	S3	189/204 (93%)	188 (100%)	1 (0%)	81	81
6	S7	132/150 (88%)	131 (99%)	1 (1%)	73	77
7	S8	151/151 (100%)	150 (99%)	1 (1%)	76	78
8	V3	40/68 (59%)	39 (98%)	1 (2%)	42	62
9	S6	79/80 (99%)	79 (100%)	0	100	100
10	S4	113/119 (95%)	113 (100%)	0	100	100
11	A9	246/292 (84%)	246 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	A2	73/81 (90%)	73 (100%)	0	100	100
13	A5	99/101 (98%)	98 (99%)	1 (1%)	68	75
14	A6	107/113 (95%)	107 (100%)	0	100	100
15	A7	84/94 (89%)	84 (100%)	0	100	100
16	AL	130/131 (99%)	130 (100%)	0	100	100
17	AA	74/81 (91%)	73 (99%)	1 (1%)	59	70
17	AB	80/81 (99%)	79 (99%)	1 (1%)	61	71
18	D3	81/103 (79%)	81 (100%)	0	100	100
19	D1	266/278 (96%)	262 (98%)	4 (2%)	57	70
20	D6	140/144 (97%)	138 (99%)	2 (1%)	59	70
21	4L	87/87 (100%)	86 (99%)	1 (1%)	65	73
22	D5	539/539 (100%)	538 (100%)	1 (0%)	87	85
23	D4	412/412 (100%)	411 (100%)	1 (0%)	87	85
24	D2	315/315 (100%)	313 (99%)	2 (1%)	78	80
25	AK	101/101 (100%)	101 (100%)	0	100	100
26	B5	122/125 (98%)	122 (100%)	0	100	100
27	A8	154/154 (100%)	153 (99%)	1 (1%)	78	80
28	BJ	155/157 (99%)	153 (99%)	2 (1%)	61	71
29	AJ	283/284 (100%)	282 (100%)	1 (0%)	84	82
30	S5	88/94 (94%)	87 (99%)	1 (1%)	65	73
31	A3	65/71 (92%)	65 (100%)	0	100	100
32	B3	55/75 (73%)	55 (100%)	0	100	100
33	C2	106/107 (99%)	106 (100%)	0	100	100
34	B4	114/114 (100%)	114 (100%)	0	100	100
35	AM	119/121 (98%)	119 (100%)	0	100	100
36	B6	92/121 (76%)	90 (98%)	2 (2%)	45	64
37	B7	108/119 (91%)	108 (100%)	0	100	100
38	B9	159/160 (99%)	157 (99%)	2 (1%)	61	71
39	B2	59/62 (95%)	59 (100%)	0	100	100
40	B8	142/142 (100%)	140 (99%)	2 (1%)	59	70
41	BK	93/112 (83%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
42	C1	42/44 (96%)	42 (100%)	0	100 100
43	B1	48/53 (91%)	48 (100%)	0	100 100
44	A1	59/59 (100%)	59 (100%)	0	100 100
All	All	7076/7395 (96%)	7036 (99%)	40 (1%)	76 80

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	V1	106	LYS
1	V1	110	ILE
1	V1	365	CYS
2	V2	104	THR
3	S1	239	VAL
3	S1	290	LEU
3	S1	483	VAL
3	S1	488	LYS
4	S2	203	LEU
4	S2	402	LEU
4	S2	418	ILE
5	S3	85	THR
6	S7	54	CYS
7	S8	78	ILE
8	V3	54	LEU
13	A5	94	ILE
17	AA	80	ILE
19	D1	55	LEU
19	D1	73	LEU
19	D1	243	LEU
19	D1	271	LEU
20	D6	12	ILE
20	D6	54	LEU
21	4L	43	LEU
22	D5	257	ILE
23	D4	17	LEU
24	D2	193	VAL
24	D2	245	LEU
17	AB	80	ILE
27	A8	109	CYS
28	BJ	29	ILE
28	BJ	135	VAL
29	AJ	31	ILE

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Mol	Chain	Res	Type
30	S5	75	LEU
36	B6	89	VAL
36	B6	95	THR
38	B9	16	LEU
38	B9	23	LEU
40	B8	9	LEU
40	B8	128	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	V1	24	ASN
1	V1	37	GLN
1	V1	96	ASN
1	V1	116	HIS
1	V1	257	ASN
1	V1	373	ASN
2	V2	99	HIS
2	V2	155	GLN
2	V2	159	ASN
3	S1	36	GLN
3	S1	117	GLN
3	S1	336	ASN
3	S1	361	ASN
3	S1	365	ASN
3	S1	392	ASN
3	S1	421	HIS
3	S1	548	HIS
3	S1	665	GLN
3	S1	682	GLN
4	S2	34	ASN
4	S2	50	ASN
4	S2	79	HIS
4	S2	135	GLN
4	S2	306	GLN
4	S2	347	HIS
5	S3	21	GLN
5	S3	39	GLN
5	S3	88	ASN
5	S3	102	ASN
5	S3	192	GLN
6	S7	94	ASN

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Mol	Chain	Res	Type
6	S7	127	HIS
8	V3	55	ASN
9	S6	94	GLN
10	S4	46	GLN
11	A9	3	HIS
11	A9	36	ASN
11	A9	103	ASN
11	A9	136	ASN
11	A9	288	HIS
12	A2	24	GLN
13	A5	82	GLN
14	A6	69	ASN
14	A6	94	ASN
14	A6	125	HIS
15	A7	20	GLN
16	AL	31	ASN
16	AL	59	HIS
16	AL	72	ASN
17	AA	74	GLN
18	D3	10	ASN
18	D3	108	GLN
19	D1	194	ASN
19	D1	247	HIS
19	D1	287	HIS
21	4L	83	ASN
22	D5	59	GLN
22	D5	113	ASN
22	D5	136	ASN
22	D5	139	GLN
22	D5	226	GLN
22	D5	274	GLN
22	D5	295	GLN
22	D5	354	GLN
22	D5	580	GLN
23	D4	43	ASN
23	D4	83	HIS
23	D4	138	ASN
23	D4	139	GLN
23	D4	168	GLN
23	D4	220	HIS
23	D4	293	HIS
23	D4	304	GLN

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Mol	Chain	Res	Type
23	D4	319	HIS
23	D4	399	ASN
23	D4	434	ASN
24	D2	144	GLN
24	D2	172	GLN
24	D2	204	ASN
24	D2	235	ASN
24	D2	309	ASN
24	D2	310	ASN
24	D2	316	GLN
26	B5	86	ASN
26	B5	124	GLN
26	B5	143	ASN
17	AB	33	ASN
17	AB	47	GLN
27	A8	63	ASN
28	BJ	103	ASN
28	BJ	122	GLN
28	BJ	158	GLN
29	AJ	21	ASN
29	AJ	92	ASN
29	AJ	114	HIS
29	AJ	151	HIS
29	AJ	200	GLN
29	AJ	204	ASN
29	AJ	271	ASN
29	AJ	294	GLN
31	A3	10	ASN
31	A3	45	ASN
31	A3	70	GLN
32	B3	20	GLN
32	B3	47	ASN
32	B3	58	ASN
33	C2	12	GLN
33	C2	88	HIS
34	B4	74	ASN
35	AM	53	ASN
35	AM	89	ASN
36	B6	73	HIS
37	B7	43	GLN
37	B7	75	ASN
37	B7	83	GLN

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Mol	Chain	Res	Type
37	B7	91	HIS
38	B9	25	HIS
38	B9	32	HIS
39	B2	58	GLN
40	B8	56	GLN
41	BK	45	HIS
42	C1	34	GLN
43	B1	51	ASN
44	A1	58	ASN

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

Of 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
49	NDP	A9	401	-	49,52,52	0.50	0	66,80,80	0.53	1 (1%)
45	SF4	S1	802	3	0,12,12	-	-	-		
45	SF4	V1	500	1	0,12,12	-	-	-		
52	CDL	D5	901	-	59,59,99	0.40	0	65,71,111	0.54	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	FES	S1	803	3	0,4,4	-	-	-		
50	ZMP	AB	101	17	24,30,36	0.80	1 (4%)	29,37,45	1.06	2 (6%)
45	SF4	S8	202	7	0,12,12	-	-	-		
45	SF4	S8	201	7	0,12,12	-	-	-		
51	3PE	D4	501	-	39,39,50	0.33	0	42,44,55	0.32	0
53	PC1	AK	201	-	27,27,53	0.39	0	33,35,61	0.36	0
51	3PE	D1	501	-	25,25,50	0.40	0	28,30,55	0.45	0
45	SF4	S1	801	3	0,12,12	-	-	-		
47	FES	V2	300	2	0,4,4	-	-	-		
46	FMN	V1	501	-	33,33,33	0.36	0	48,50,50	0.37	0
51	3PE	D5	902	-	37,37,50	0.35	0	40,42,55	0.33	0
45	SF4	S7	300	6	0,12,12	-	-	-		
50	ZMP	AA	101	17	27,33,36	0.65	1 (3%)	32,40,45	1.12	3 (9%)

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
45	SF4	S7	300	6	-	-	0/6/5/5
45	SF4	V1	500	1	-	-	0/6/5/5
52	CDL	D5	901	-	-	19/70/70/110	-
46	FMN	V1	501	-	-	6/18/18/18	0/3/3/3
50	ZMP	AB	101	17	-	10/35/37/43	-
47	FES	S1	803	3	-	-	0/1/1/1
45	SF4	S8	202	7	-	-	0/6/5/5
45	SF4	S8	201	7	-	-	0/6/5/5
51	3PE	D4	501	-	-	5/43/43/54	-
53	PC1	AK	201	-	-	11/31/31/57	-
45	SF4	S1	801	3	-	-	0/6/5/5
51	3PE	D1	501	-	-	11/28/28/54	-
47	FES	V2	300	2	-	-	0/1/1/1
49	NDP	A9	401	-	-	11/34/77/77	0/5/5/5
51	3PE	D5	902	-	-	8/41/41/54	-
45	SF4	S1	802	3	-	-	0/6/5/5
50	ZMP	AA	101	17	-	14/38/40/43	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	AA	101	ZMP	C9-C10	2.32	1.53	1.50
50	AB	101	ZMP	C9-C10	2.30	1.53	1.50

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	AB	101	ZMP	O1-C10-C9	-3.07	120.37	123.99
50	AA	101	ZMP	O1-C10-C9	-2.75	120.74	123.99
52	D5	901	CDL	CB4-OB6-CB5	2.21	123.24	117.79
50	AA	101	ZMP	C15-C14-C13	-2.20	108.69	112.36
52	D5	901	CDL	OB6-CB4-CB3	2.11	116.04	108.40
49	A9	401	NDP	PN-O3-PA	-2.06	125.76	132.83
50	AB	101	ZMP	C9-C10-S1	2.03	115.82	113.46
50	AA	101	ZMP	C11-C12-N1	-2.02	108.18	112.42

There are no chirality outliers.

All (95) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	V1	501	FMN	C2'-C3'-C4'-O4'
46	V1	501	FMN	C2'-C3'-C4'-C5'
46	V1	501	FMN	O3'-C3'-C4'-O4'
46	V1	501	FMN	O3'-C3'-C4'-C5'
49	A9	401	NDP	C1B-C2B-O2B-P2B
49	A9	401	NDP	C5D-O5D-PN-O1N
49	A9	401	NDP	O4D-C1D-N1N-C6N
50	AA	101	ZMP	C12-C11-S1-C10
50	AA	101	ZMP	O1-C10-S1-C11
50	AA	101	ZMP	C9-C10-S1-C11
50	AB	101	ZMP	S1-C11-C12-N1
50	AB	101	ZMP	C12-C11-S1-C10
50	AB	101	ZMP	O1-C10-S1-C11
50	AB	101	ZMP	C9-C10-S1-C11
51	D1	501	3PE	C1-O11-P-O12
51	D5	902	3PE	C11-O13-P-O12
51	D5	902	3PE	O21-C2-C3-O31
51	D4	501	3PE	O13-C11-C12-N
52	D5	901	CDL	O1-C1-CA2-OA2
52	D5	901	CDL	CA2-OA2-PA1-OA4
52	D5	901	CDL	CB3-OB5-PB2-OB3
52	D5	901	CDL	CB3-OB5-PB2-OB4
53	AK	201	PC1	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
53	AK	201	PC1	C11-O13-P-O14
50	AA	101	ZMP	C14-C13-N1-C12
50	AB	101	ZMP	C14-C13-N1-C12
50	AA	101	ZMP	O2-C13-N1-C12
50	AB	101	ZMP	O2-C13-N1-C12
52	D5	901	CDL	CB2-C1-CA2-OA2
51	D4	501	3PE	C34-C35-C36-C37
51	D1	501	3PE	C11-O13-P-O11
51	D5	902	3PE	C11-O13-P-O11
52	D5	901	CDL	CA3-OA5-PA1-OA2
52	D5	901	CDL	CB2-OB2-PB2-OB5
52	D5	901	CDL	CB3-OB5-PB2-OB2
53	AK	201	PC1	C11-O13-P-O11
50	AA	101	ZMP	C6-C7-C8-C9
51	D1	501	3PE	O13-C11-C12-N
51	D5	902	3PE	C21-C22-C23-C24
51	D4	501	3PE	C35-C36-C37-C38
50	AA	101	ZMP	C4-C5-C6-C7
52	D5	901	CDL	CA2-OA2-PA1-OA5
53	AK	201	PC1	O11-C1-C2-C3
51	D5	902	3PE	C1-C2-C3-O31
50	AB	101	ZMP	N2-C16-C17-C18
53	AK	201	PC1	O11-C1-C2-O21
46	V1	501	FMN	C5'-O5'-P-O2P
46	V1	501	FMN	C5'-O5'-P-O3P
51	D1	501	3PE	C1-C2-C3-O31
49	A9	401	NDP	C5B-O5B-PA-O3
49	A9	401	NDP	PN-O3-PA-O2A
51	D1	501	3PE	C1-O11-P-O13
49	A9	401	NDP	C5B-O5B-PA-O2A
51	D1	501	3PE	C1-O11-P-O14
51	D1	501	3PE	C11-O13-P-O12
51	D1	501	3PE	C11-O13-P-O14
52	D5	901	CDL	CA2-OA2-PA1-OA3
52	D5	901	CDL	CA3-OA5-PA1-OA3
52	D5	901	CDL	CA3-OA5-PA1-OA4
52	D5	901	CDL	CB2-OB2-PB2-OB4
51	D1	501	3PE	C12-C11-O13-P
50	AA	101	ZMP	C11-C12-N1-C13
50	AA	101	ZMP	C17-C18-C21-O5
53	AK	201	PC1	O13-C11-C12-N
50	AB	101	ZMP	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
50	AB	101	ZMP	O3-C16-C17-O4
50	AA	101	ZMP	C20-C18-C21-O5
51	D5	902	3PE	C26-C27-C28-C29
53	AK	201	PC1	C1-O11-P-O13
51	D1	501	3PE	C2-C1-O11-P
53	AK	201	PC1	C2-C1-O11-P
50	AA	101	ZMP	S1-C11-C12-N1
50	AA	101	ZMP	C19-C18-C21-O5
52	D5	901	CDL	CB6-CB4-OB6-CB5
52	D5	901	CDL	C1-CB2-OB2-PB2
51	D1	501	3PE	O21-C2-C3-O31
51	D5	902	3PE	C33-C34-C35-C36
49	A9	401	NDP	O4B-C4B-C5B-O5B
49	A9	401	NDP	C3B-C2B-O2B-P2B
53	AK	201	PC1	O31-C31-C32-C33
49	A9	401	NDP	C4B-C5B-O5B-PA
52	D5	901	CDL	OB6-CB4-CB6-OB8
52	D5	901	CDL	C12-C11-CA5-OA6
50	AA	101	ZMP	C1-C2-C3-C4
49	A9	401	NDP	C2B-O2B-P2B-O3X
49	A9	401	NDP	C5D-O5D-PN-O3
51	D4	501	3PE	C25-C26-C27-C28
52	D5	901	CDL	C12-C11-CA5-OA7
53	AK	201	PC1	O32-C31-C32-C33
51	D5	902	3PE	C1-O11-P-O14
51	D4	501	3PE	C1-O11-P-O14
50	AB	101	ZMP	O3-C16-C17-C18
53	AK	201	PC1	C12-C11-O13-P
52	D5	901	CDL	C32-C31-CA7-OA8
50	AA	101	ZMP	C22-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	A9	401	NDP	7	0
45	V1	500	SF4	1	0
52	D5	901	CDL	2	0
51	D4	501	3PE	4	0
45	S1	801	SF4	2	0
46	V1	501	FMN	3	0
51	D5	902	3PE	3	0

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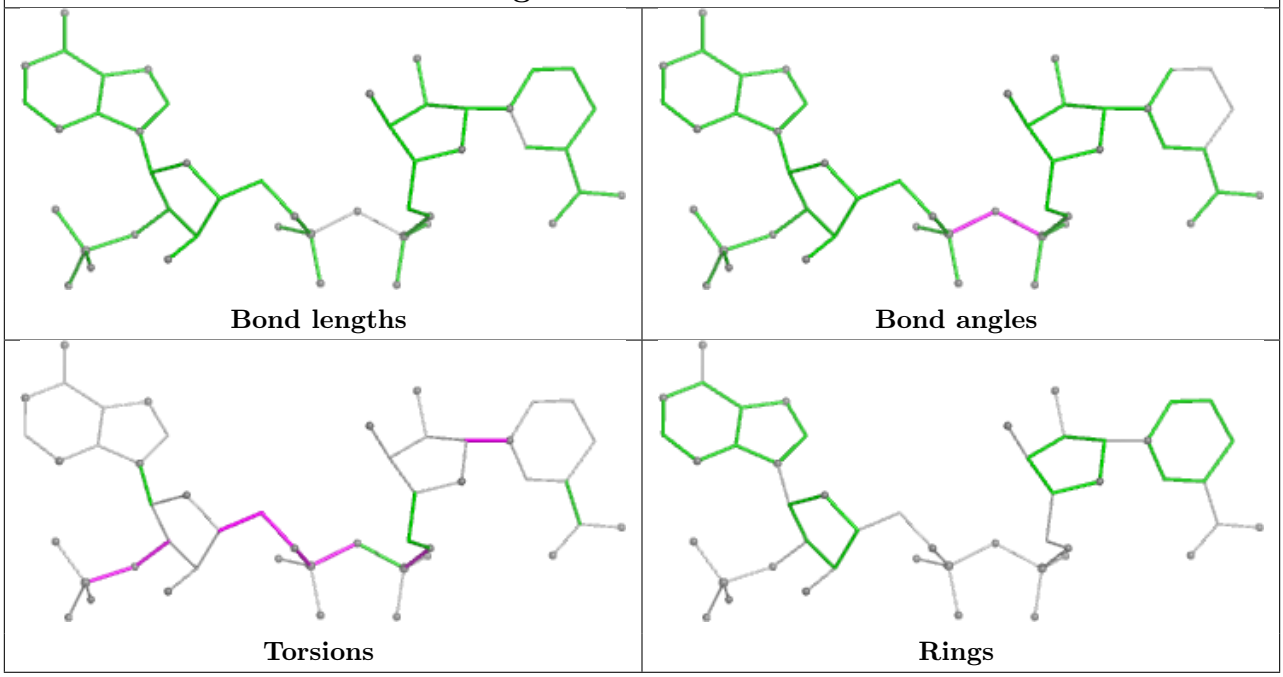
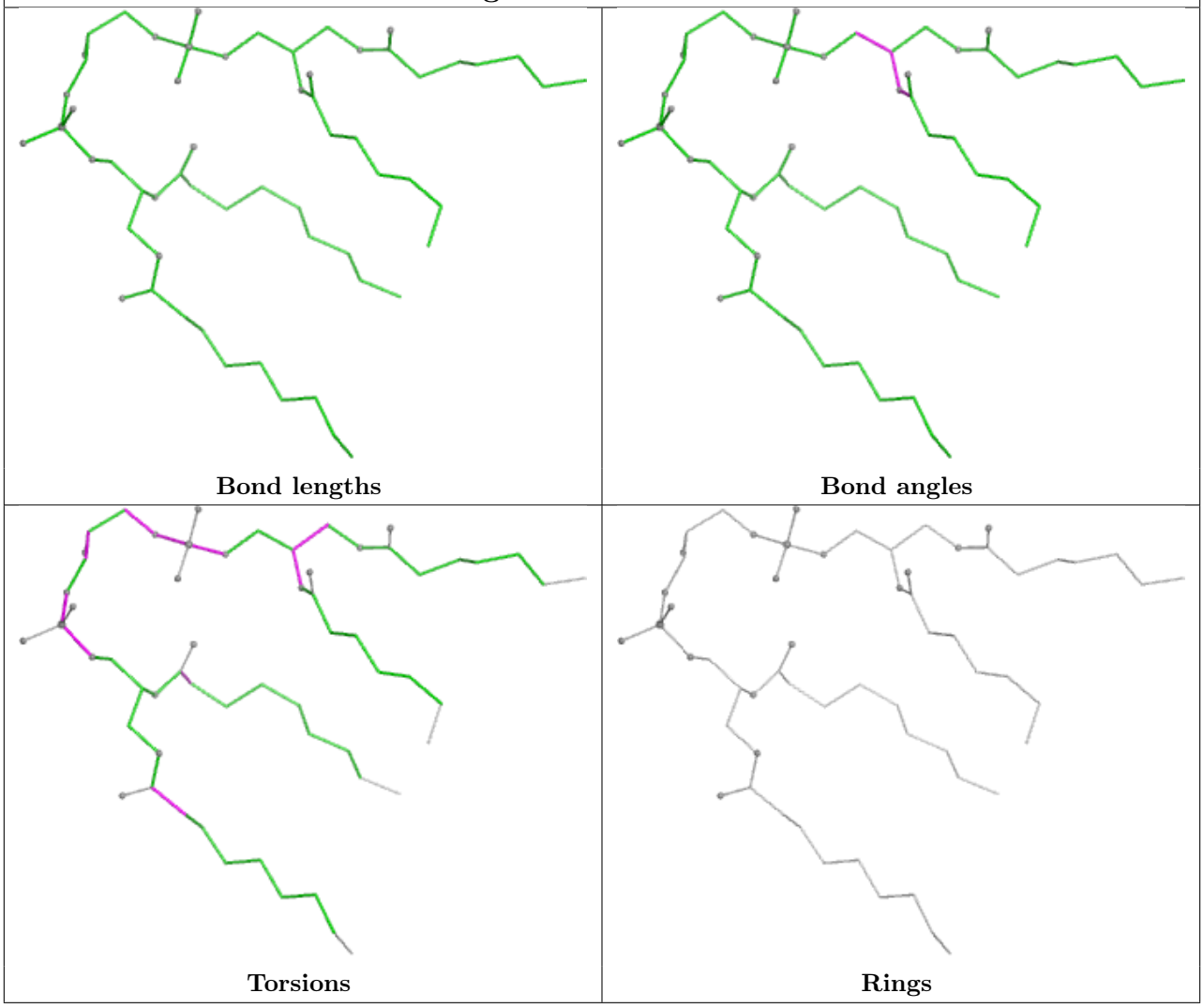
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	S7	300	SF4	1	0
50	AA	101	ZMP	1	0

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

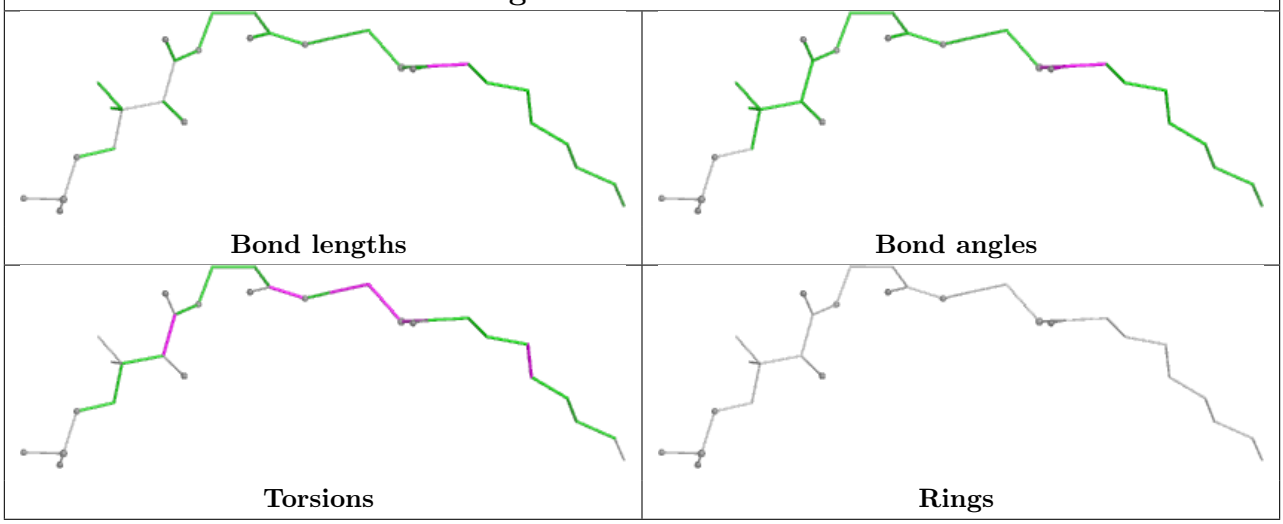
Ligand NDP A9 401



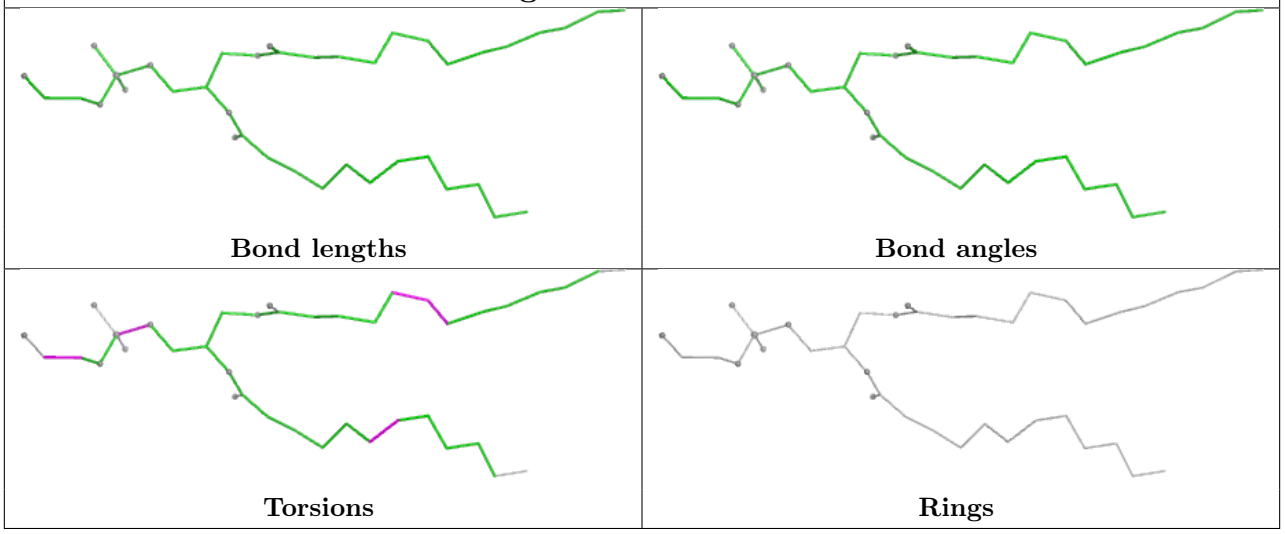
Ligand CDL D5 901



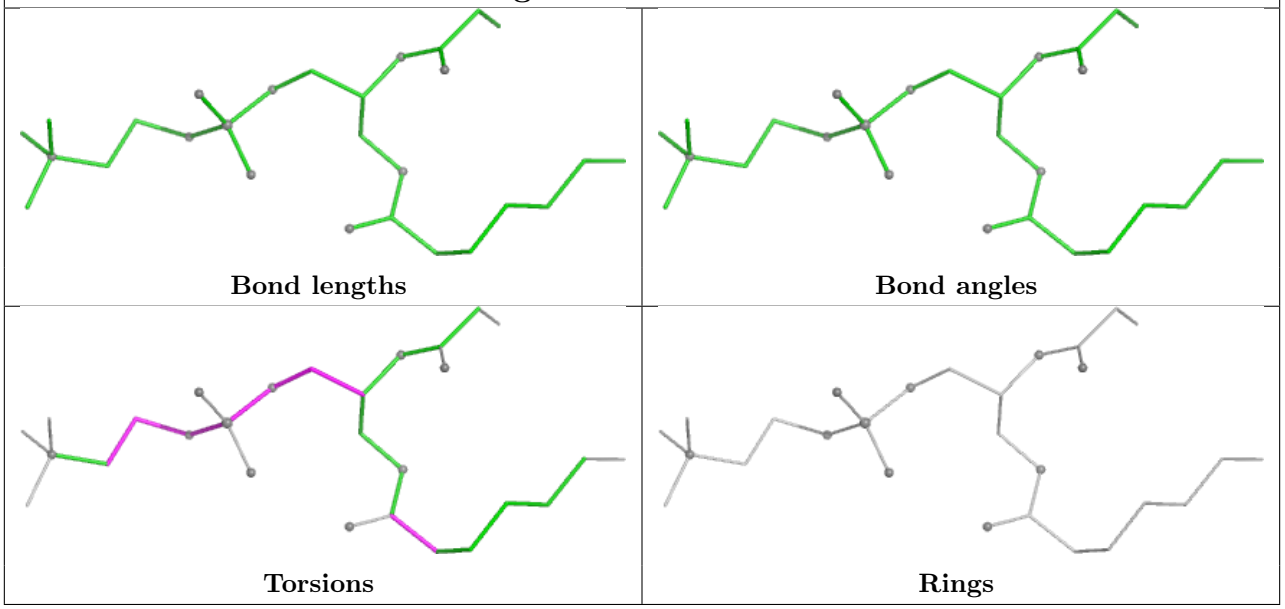
Ligand ZMP AB 101



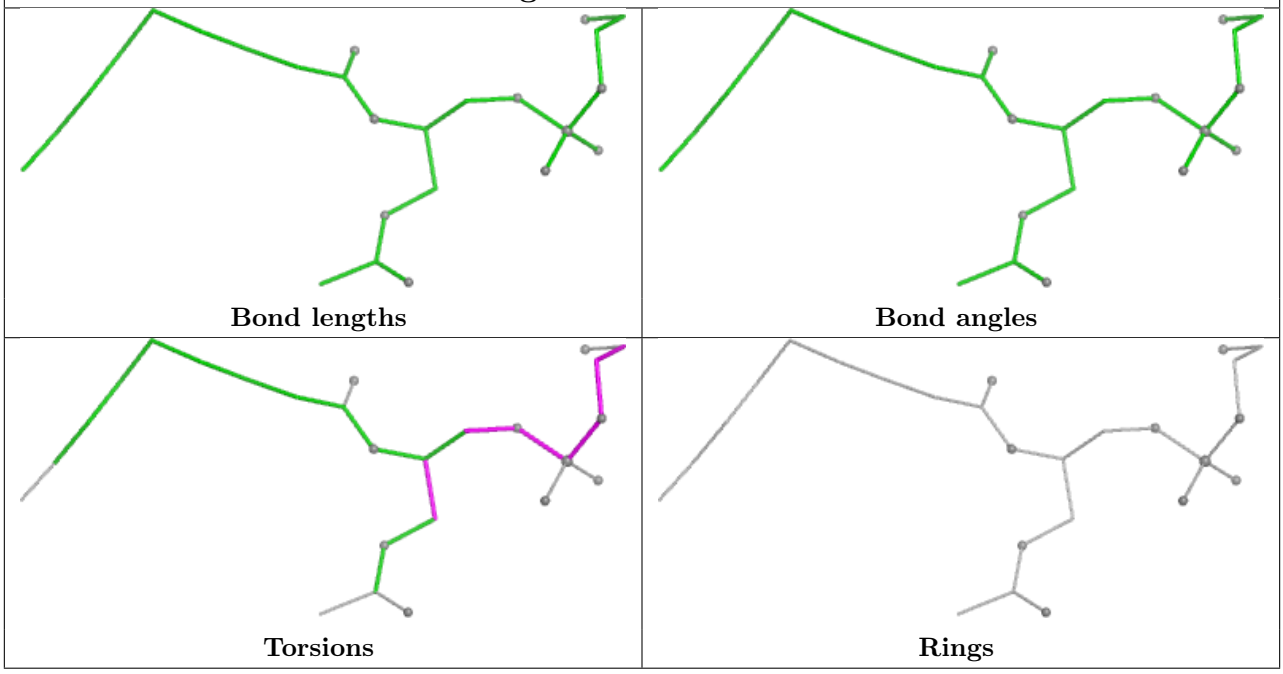
Ligand 3PE D4 501



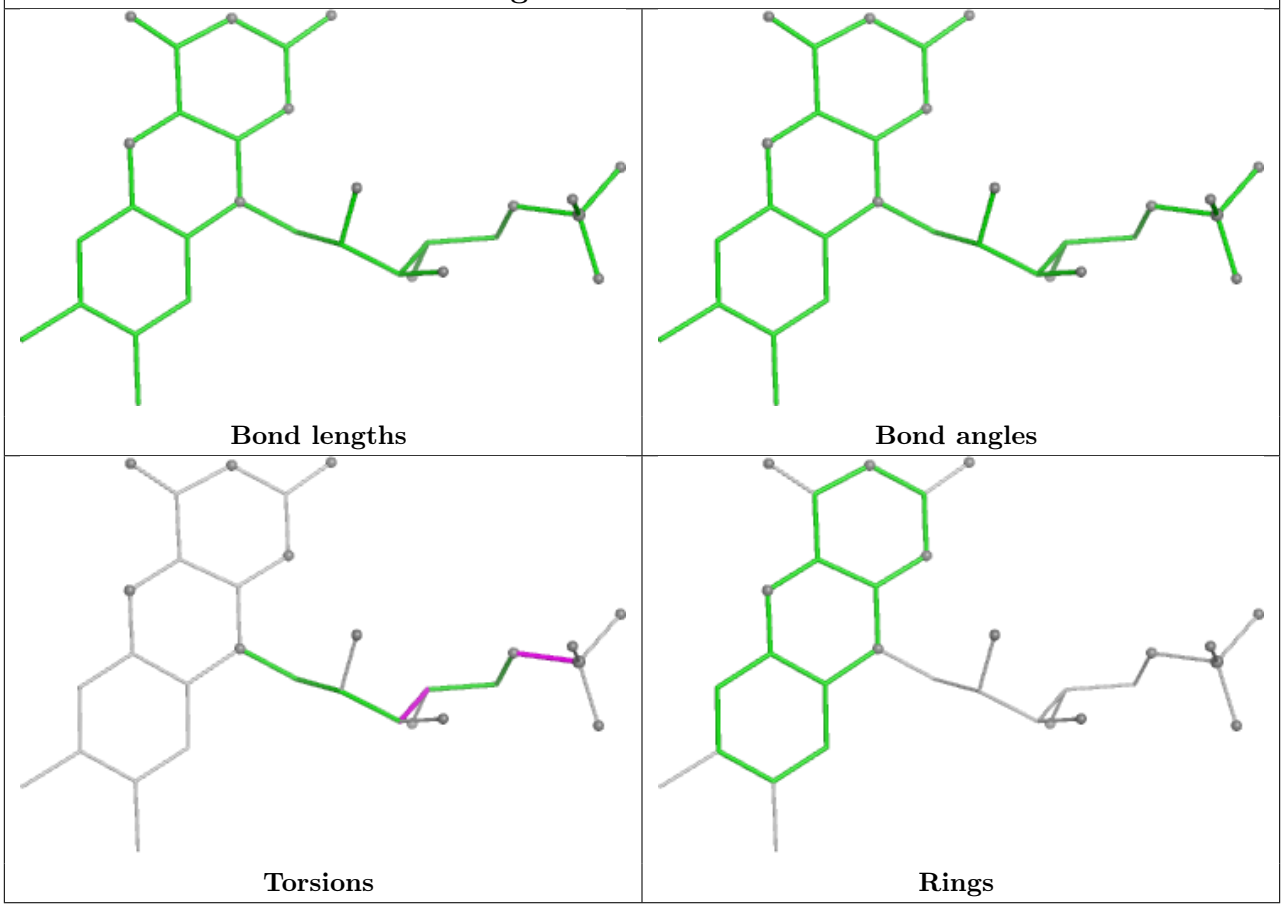
Ligand PC1 AK 201

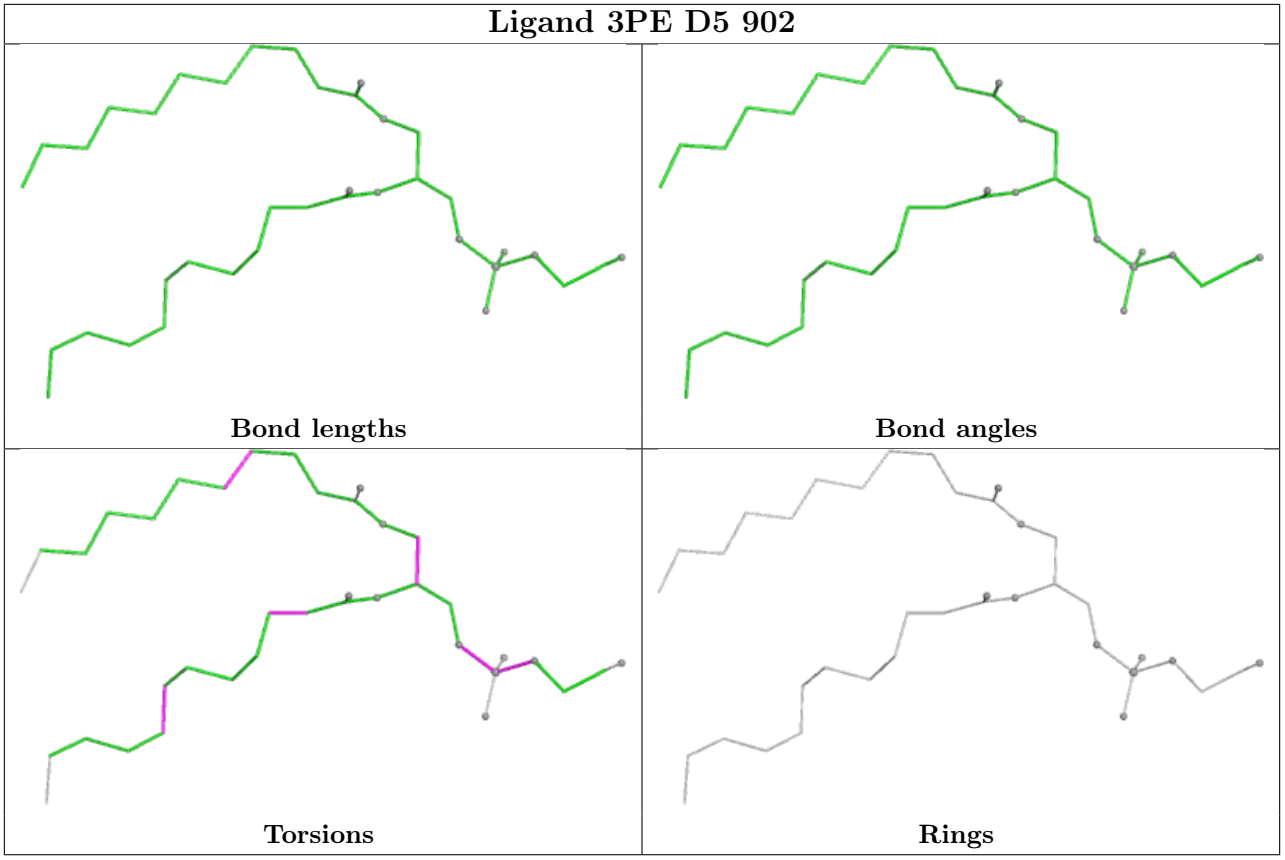


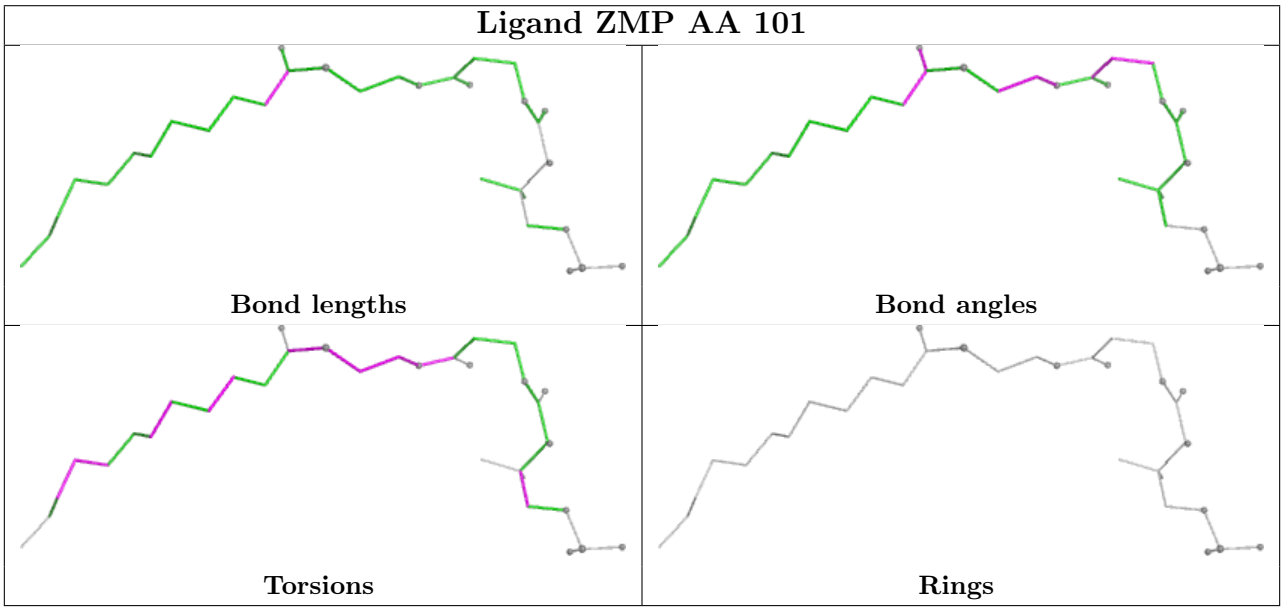
Ligand 3PE D1 501



Ligand FMN V1 501







5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

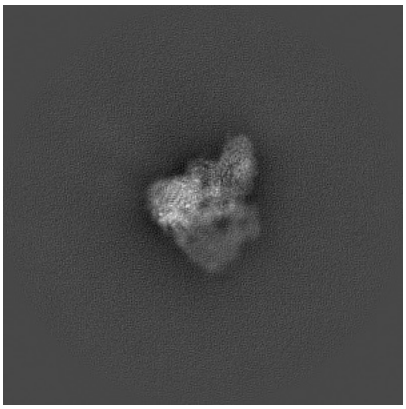
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4500. These allow visual inspection of the internal detail of the map and identification of artifacts.

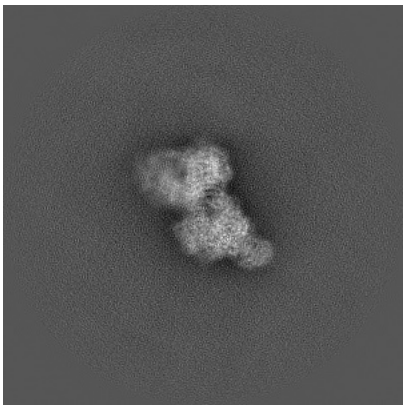
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

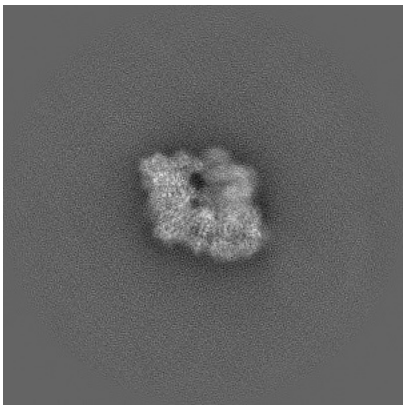
6.1.1 Primary map



X

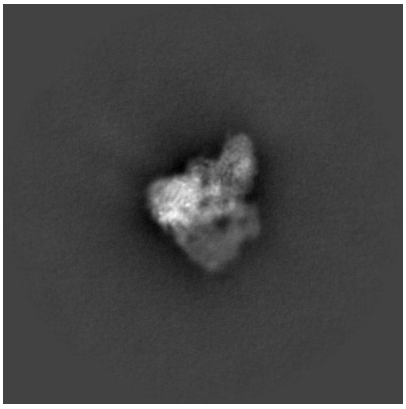


Y

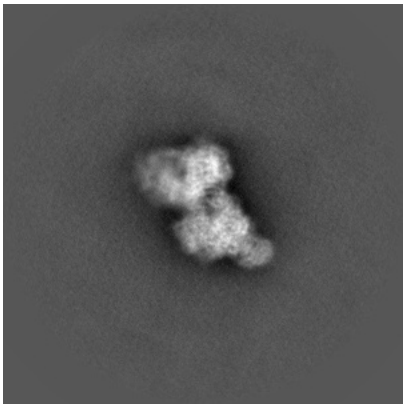


Z

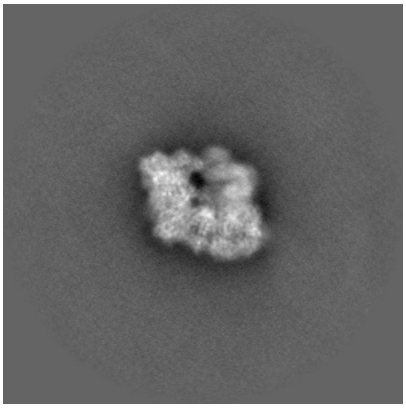
6.1.2 Raw map



X



Y

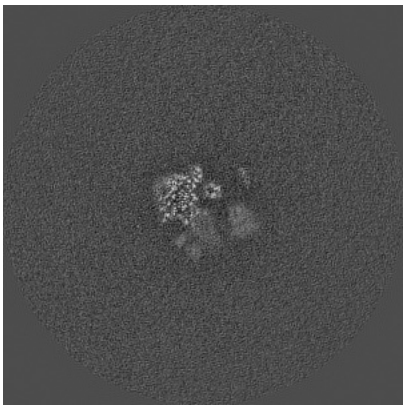


Z

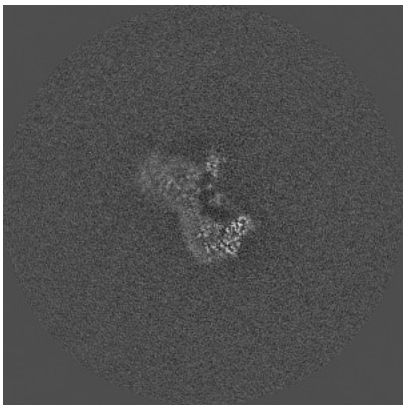
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

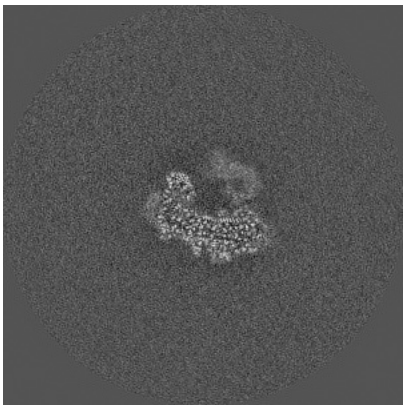
6.2.1 Primary map



X Index: 256

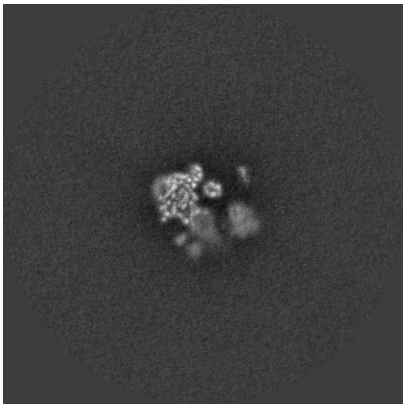


Y Index: 256

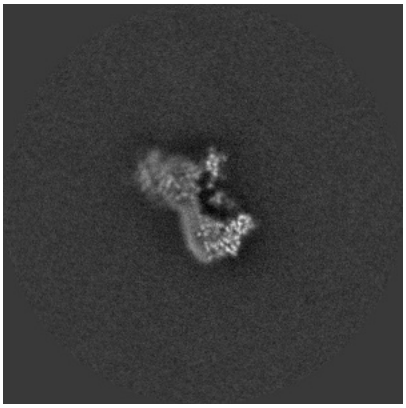


Z Index: 256

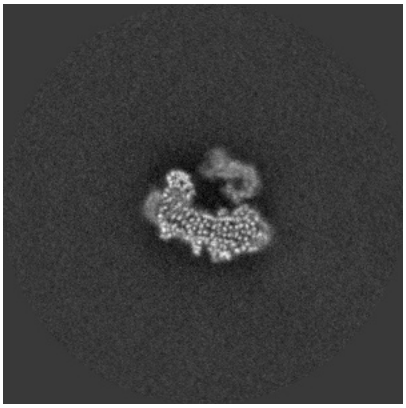
6.2.2 Raw map



X Index: 256



Y Index: 256

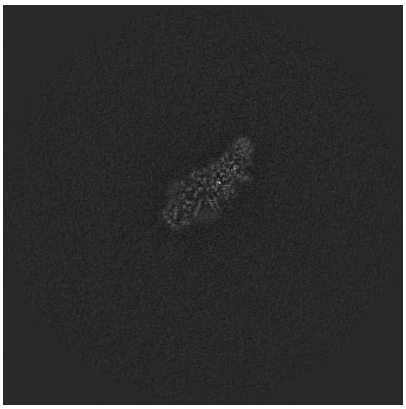


Z Index: 256

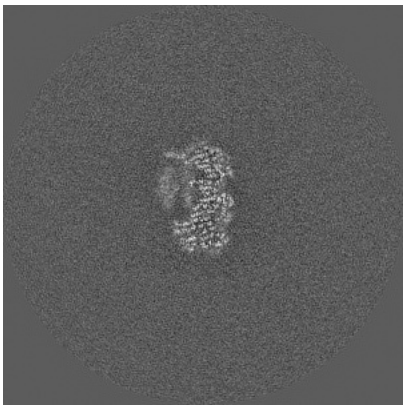
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

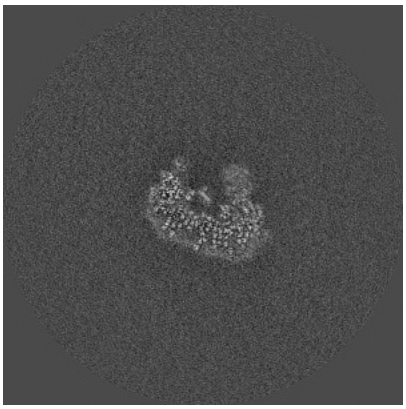
6.3.1 Primary map



X Index: 208

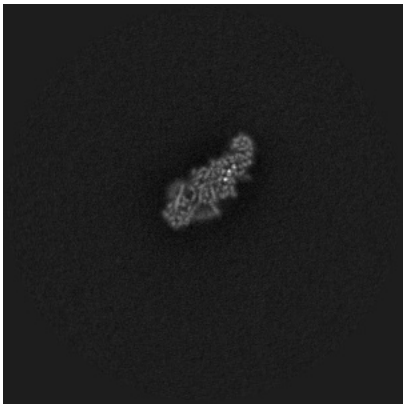


Y Index: 229

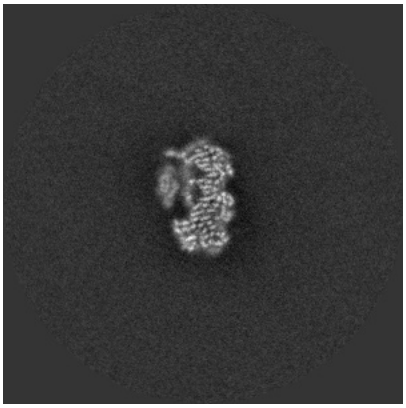


Z Index: 268

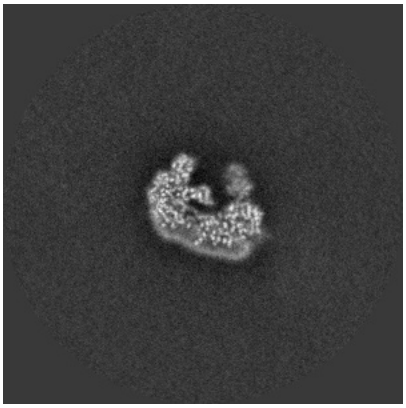
6.3.2 Raw map



X Index: 205



Y Index: 229

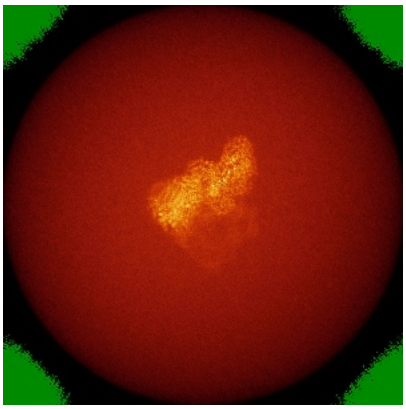


Z Index: 274

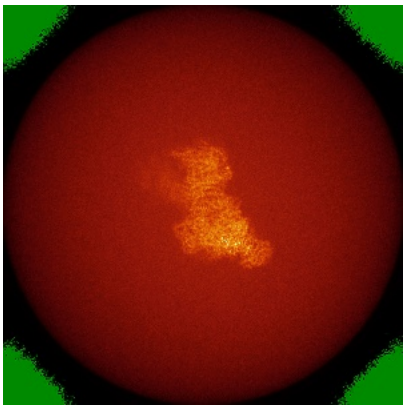
The images above show the largest variance slices of the map in three orthogonal directions.

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

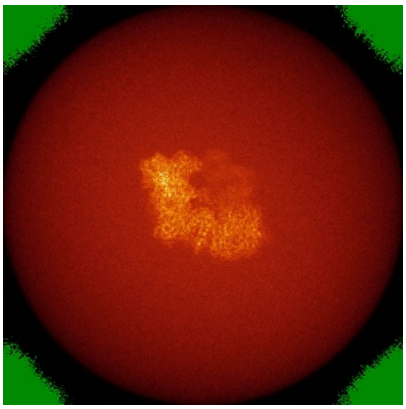
6.4.1 Primary map



X

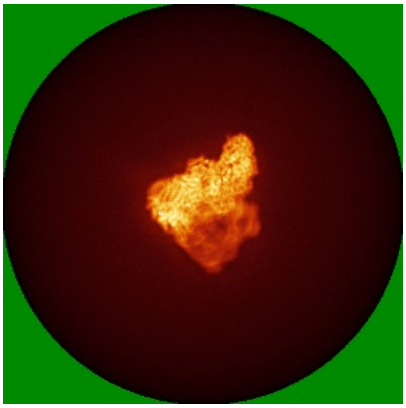


Y

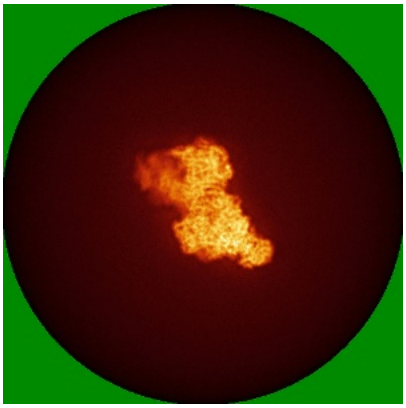


Z

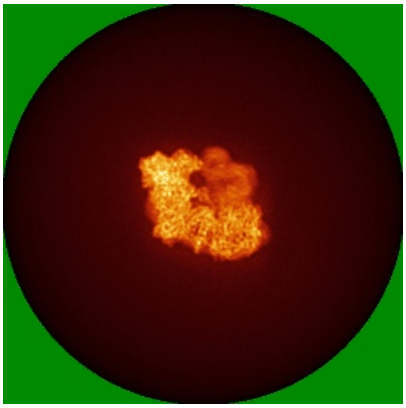
6.4.2 Raw map



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.

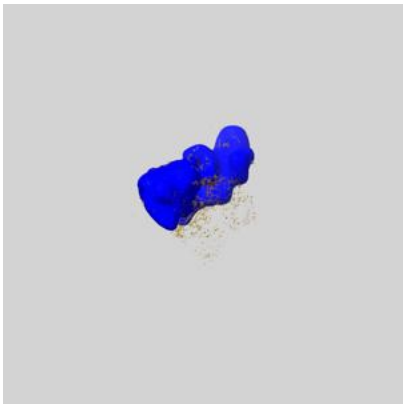
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

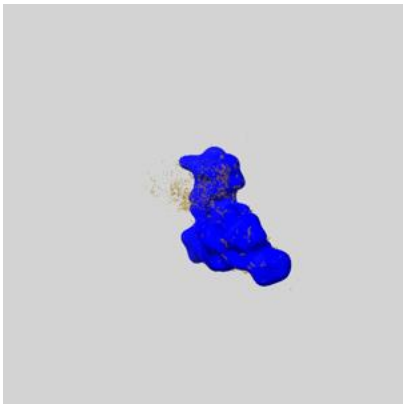
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

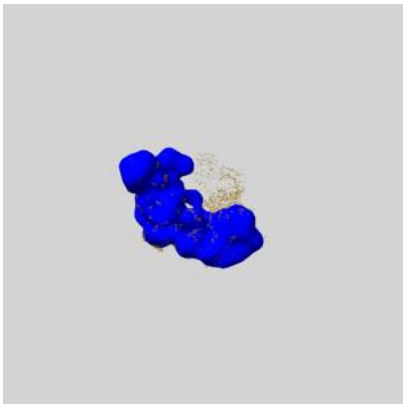
6.6.1 emd_4500_msk_1.map (i)



X



Y

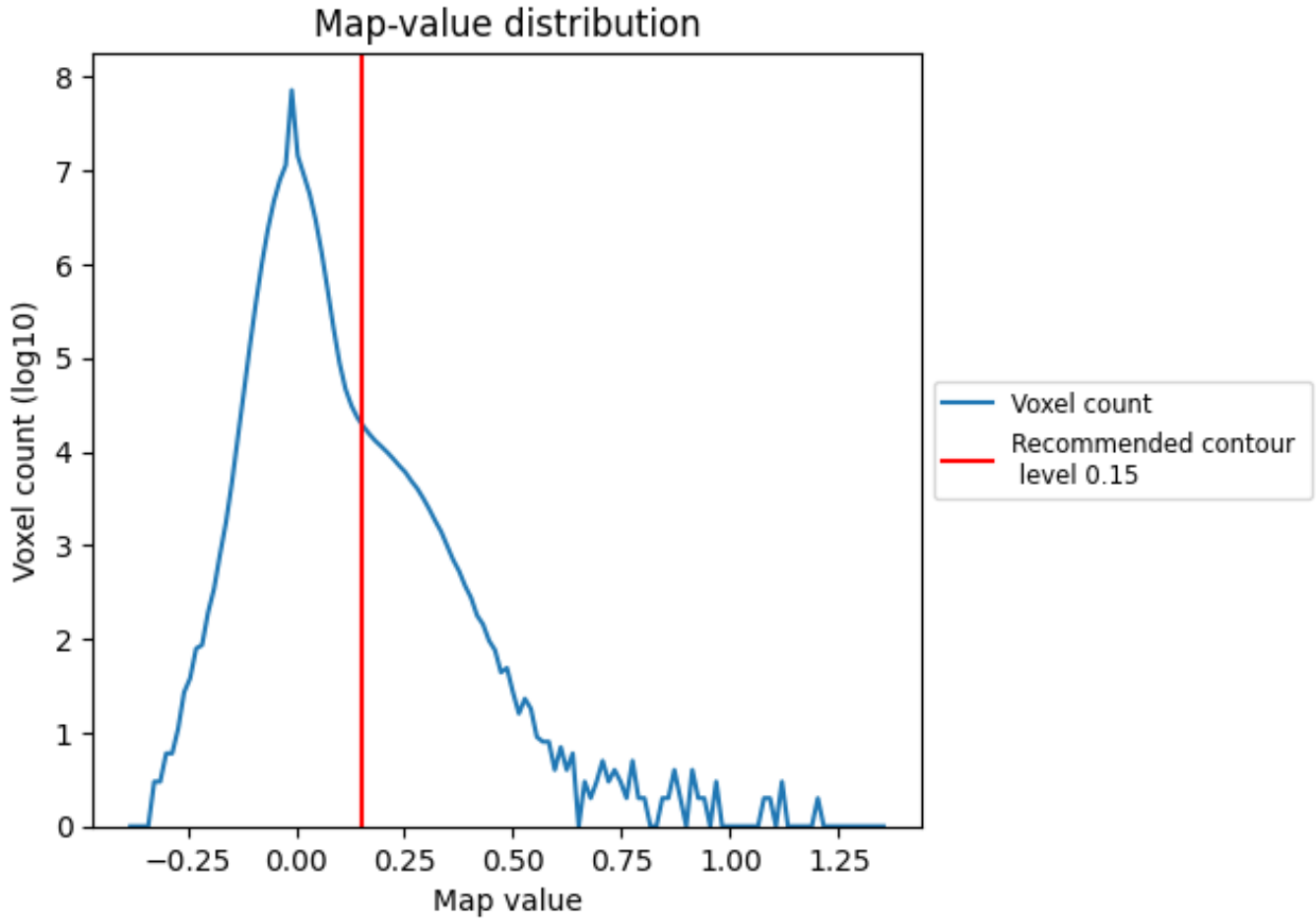


Z

7 Map analysis

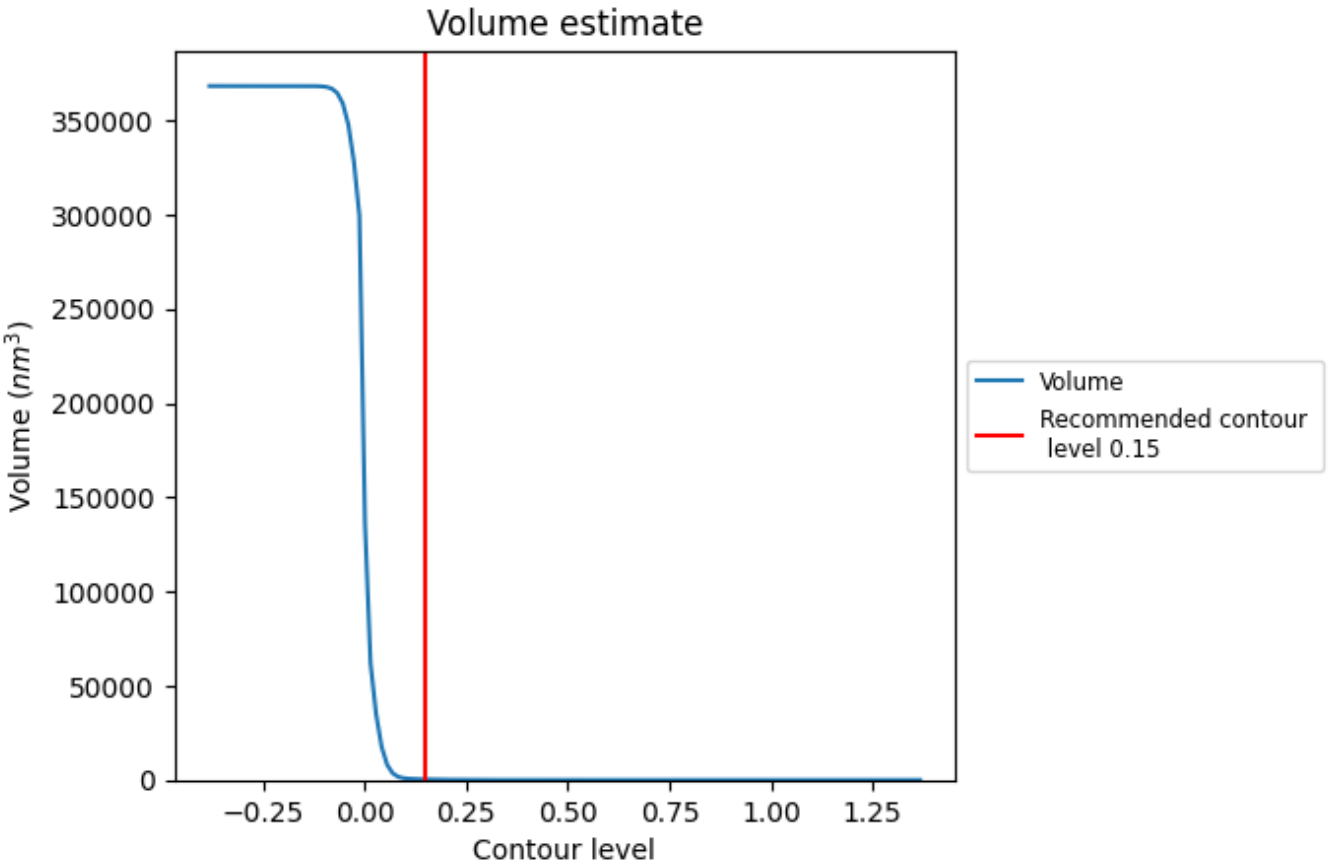
This section contains the results of statistical analysis of the map.

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.

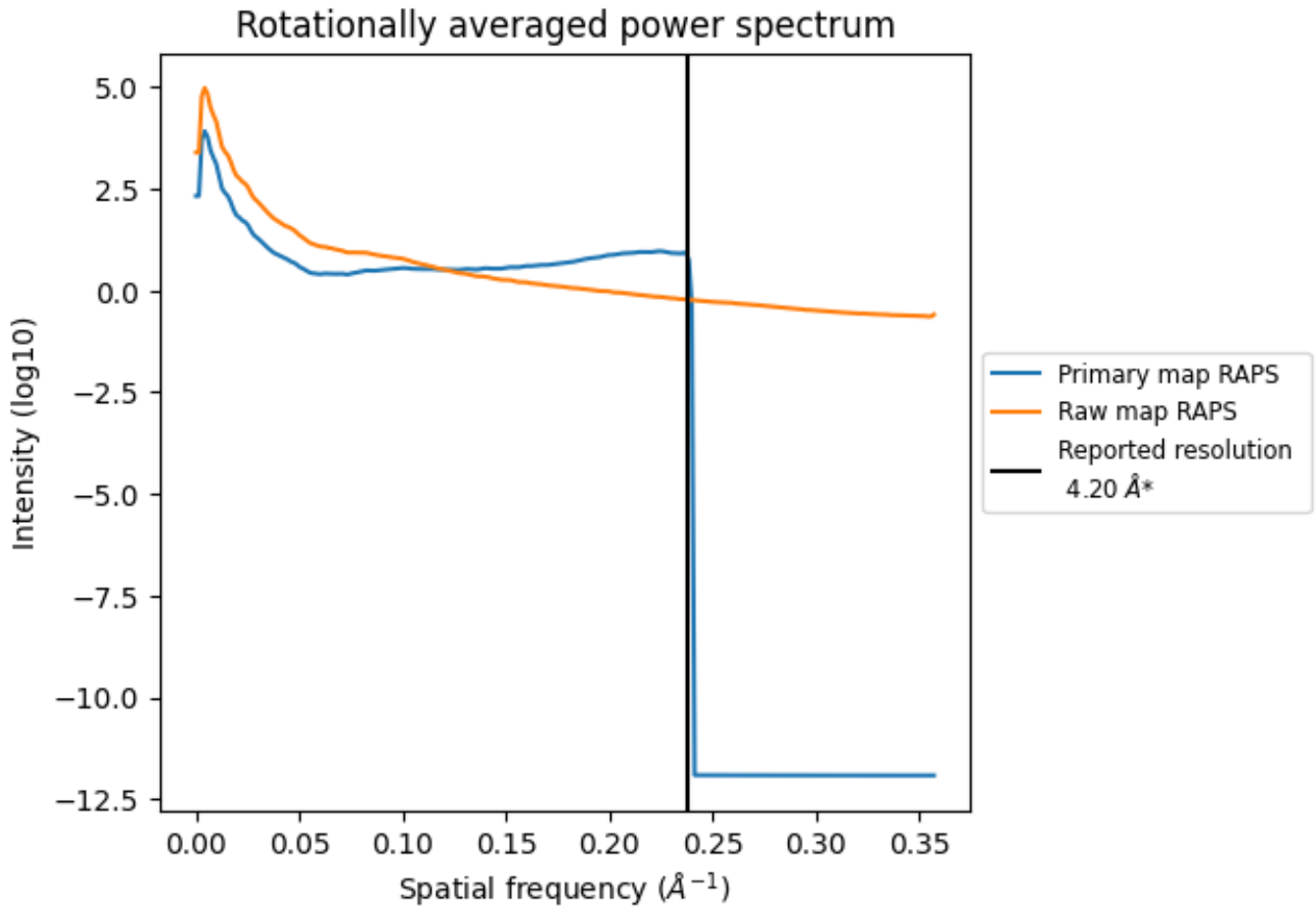
7.2 Volume estimate



The volume at the recommended contour level is 328 nm^3; this corresponds to an approximate mass of 296 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)

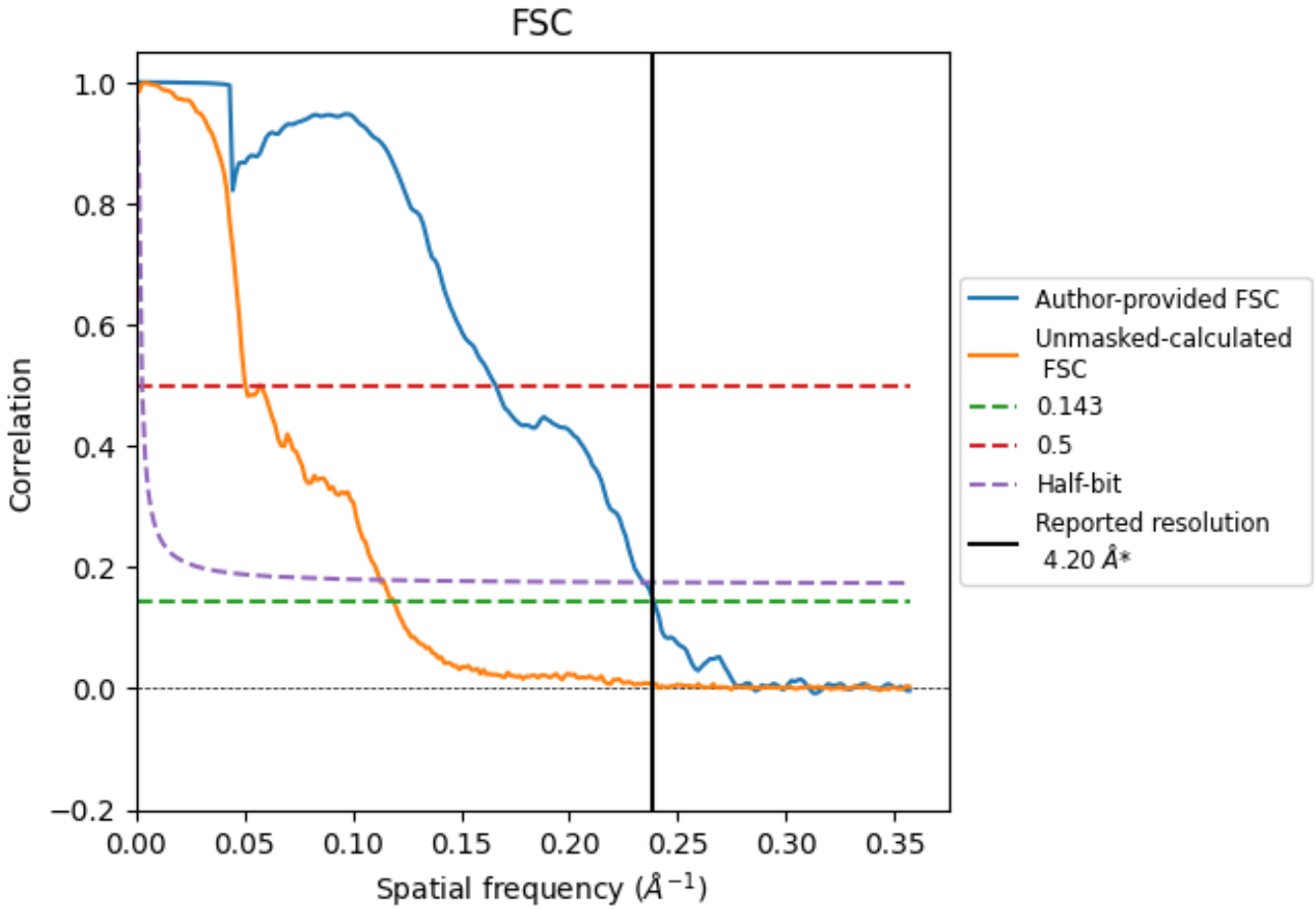


*Reported resolution corresponds to spatial frequency of 0.238 $Å^{-1}$

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 0.238 Å^{-1}

8.2 Resolution estimates (i)

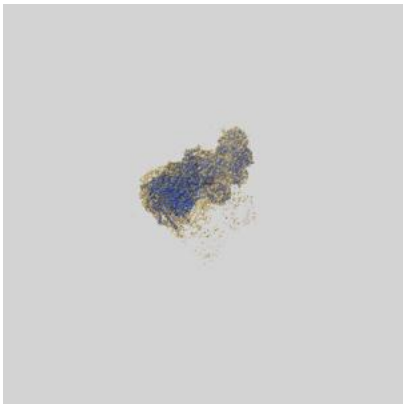
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.18	6.02	4.27
Unmasked-calculated*	8.40	19.80	8.88

*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 8.40 differs from the reported value 4.2 by more than 10 %

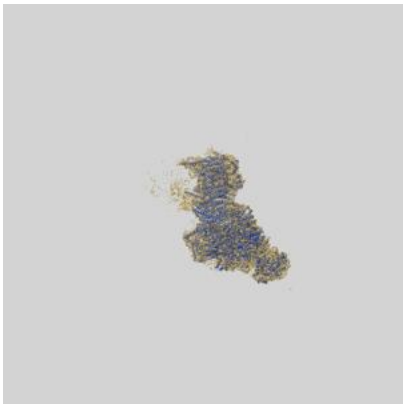
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4500 and PDB model 6QC8. Per-residue inclusion information can be found in section 3 on page 17.

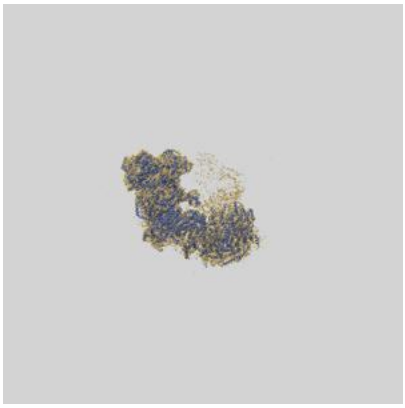
9.1 Map-model overlay



X



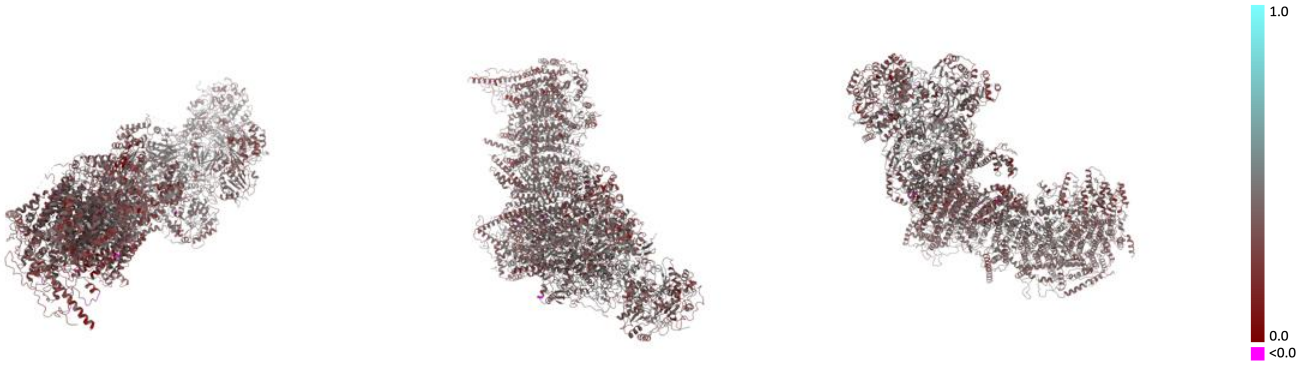
Y



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.

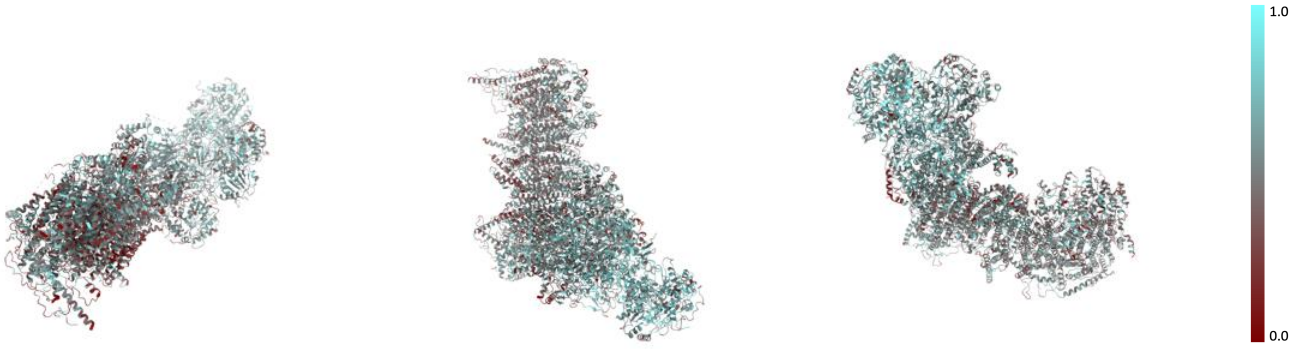
9.2 Q-score mapped to coordinate model (i)



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.

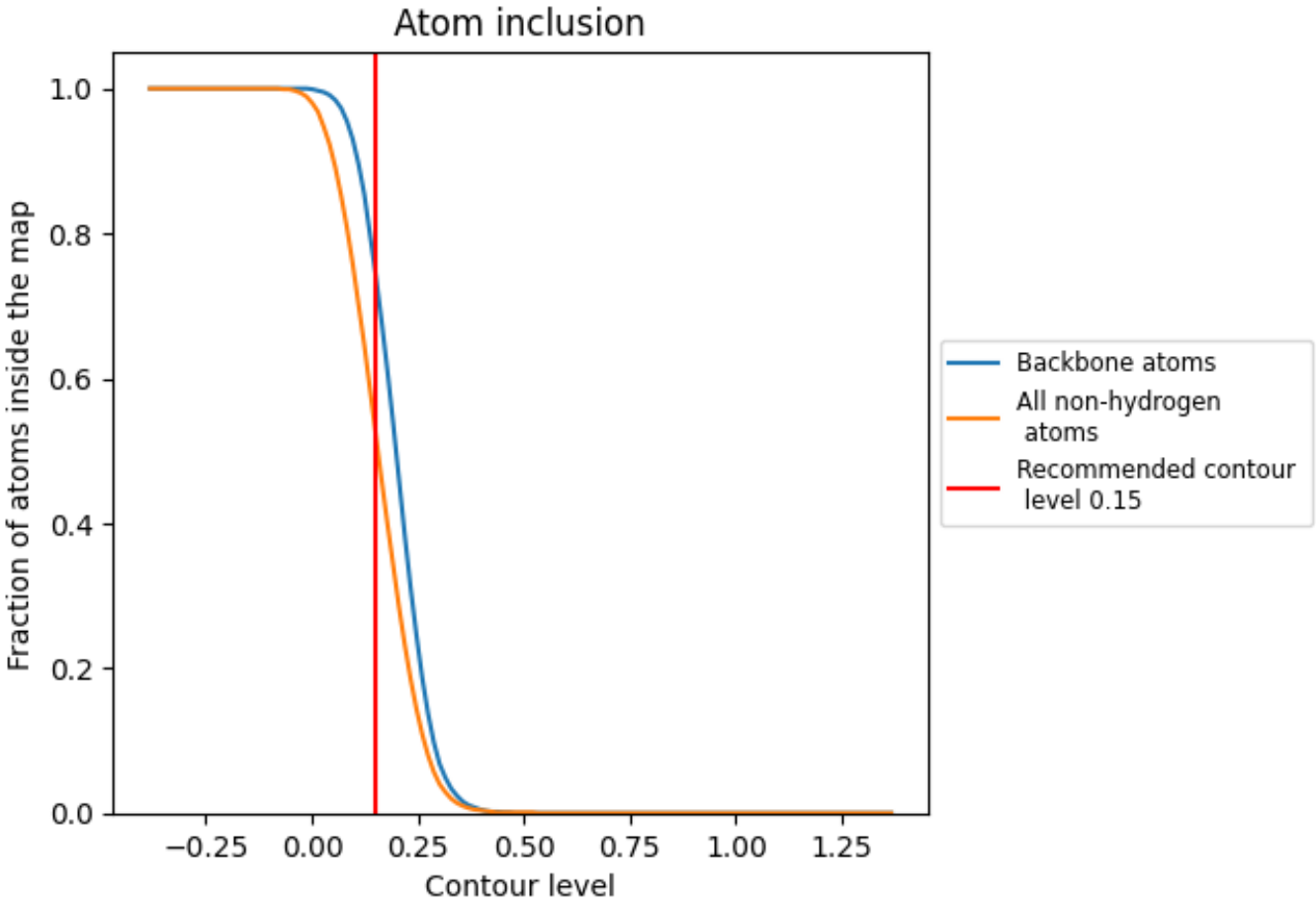
9.3 Atom inclusion mapped to coordinate model (i)



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, 75% of all backbone atoms, 53% 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	0.5270	0.3660
4L	0.4380	0.3710
A1	0.5610	0.3710
A2	0.5840	0.3360
A3	0.5330	0.3650
A5	0.5660	0.3570
A6	0.5380	0.3820
A7	0.4620	0.3790
A8	0.5290	0.3540
A9	0.5410	0.3710
AA	0.4660	0.3170
AB	0.4690	0.3300
AJ	0.5010	0.3510
AK	0.3700	0.3230
AL	0.4570	0.3780
AM	0.5230	0.3490
B1	0.4010	0.3520
B2	0.4560	0.3120
B3	0.4330	0.3230
B4	0.4800	0.3470
B5	0.5330	0.3730
B6	0.4710	0.3370
B7	0.4630	0.2820
B8	0.4770	0.3460
B9	0.5400	0.3490
BJ	0.5300	0.3450
BK	0.4650	0.3640
C1	0.4870	0.3290
C2	0.5130	0.3720
D1	0.4980	0.3700
D2	0.5130	0.3830
D3	0.4250	0.3530
D4	0.4970	0.3860
D5	0.4540	0.3490
D6	0.3950	0.3430

Continued on next page...

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Chain	Atom inclusion	Q-score
S1	0.6050	0.3940
S2	0.5680	0.3870
S3	0.6270	0.4090
S4	0.5850	0.4010
S5	0.5250	0.3370
S6	0.5840	0.4050
S7	0.6200	0.4000
S8	0.6480	0.4010
V1	0.6300	0.3680
V2	0.6110	0.3640
V3	0.6070	0.3810