Full wwPDB EM Validation Report ⓘ

Sep 3, 2024 – 04:33 PM JST

PDB ID	:	8XKV
EMDB ID	:	EMD-38428
Title	:	Cryo-EM structure of the Ycf2-FtsHi motor complex from Arabidopsis in Apo state
Authors	:	Liang, K.; Zhan, X.; Xu, Q.; Wu, J.; Yan, Z.
Deposited on	:	2023-12-25
Resolution	:	3.30 Å(reported)

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

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

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

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

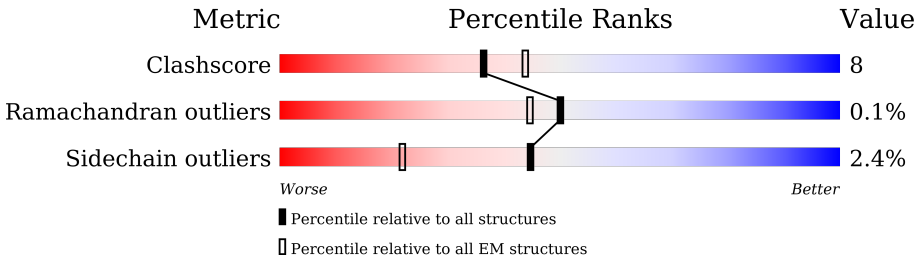
EMDB validation analysis	:	0.0.1.dev112
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.38.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	855	7% 66% 18% · 15%
2	B	1008	14% 66% 17% · 17%
3	C	1320	42% 57% 13% 30%
4	D	2294	· 28% 7% 65%
5	E	946	20% 42% 11% 47%
6	F	876	5% 41% 13% 45%
7	G	396	· 53% 19% · 28%
8	H	348	14% · 84%

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Mol	Chain	Length	Quality of chain
9	I	403	62% 16% 21%
9	J	403	63% 15% 21%
10	K	80	75% 66% 18% 16%
11	L	18	94% 83% 17%
12	M	11	64% 64% 36%
13	N	37	84% 81% 19%
14	O	17	53% 82% 18%
15	P	19	100% 100%
16	R	328	38% 64% 17% 19%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 45453 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 Probable inactive ATP-dependent zinc metalloprotease FTSHI 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	730	5841	3718	1000	1103	20	0	0

- Molecule 2 is a protein called ATP-dependent zinc metalloprotease FTSH 12, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	841	6849	4388	1191	1241	29	0	0

- Molecule 3 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	921	7494	4775	1299	1386	34	0	0

- Molecule 4 is a protein called Protein Ycf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	805	6659	4314	1145	1173	27	0	0

- Molecule 5 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	498	3884	2454	690	729	11	0	0

- Molecule 6 is a protein called Probable inactive ATP-dependent zinc metalloprotease FTSHI 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	478	Total	C	N	O	S	0	0
			3744	2356	667	701	20		

- Molecule 7 is a protein called AtTam46.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	285	Total	C	N	O	S	0	0
			2375	1615	370	379	11		

- Molecule 8 is a protein called At4g28210.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	54	Total	C	N	O	S	0	0
			459	310	76	72	1		

- Molecule 9 is a protein called Malate dehydrogenase, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	317	Total	C	N	O	S	0	0
			2363	1503	396	457	7		
9	J	317	Total	C	N	O	S	0	0
			2363	1503	396	457	7		

- Molecule 10 is a protein called Aspartyl/glutamyl-tRNA (Asn/Gln) amidotransferase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	67	Total	C	N	O	S	0	0
			555	359	98	97	1		

- Molecule 11 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	18	Total	C	N	O	S	0	0
			131	89	21	20	1		

- Molecule 12 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	11	Total	C	N	O	0	0
			84	59	13	12		

- Molecule 13 is a protein called UNK.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	37	Total	C	N	O	S	0	0
			246	159	45	41	1		

- Molecule 14 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	17	Total	C	N	O	0	0
			132	89	25	18		

- Molecule 15 is a protein called UNK.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	19	Total	C	N	O	0	0
			95	57	19	19		

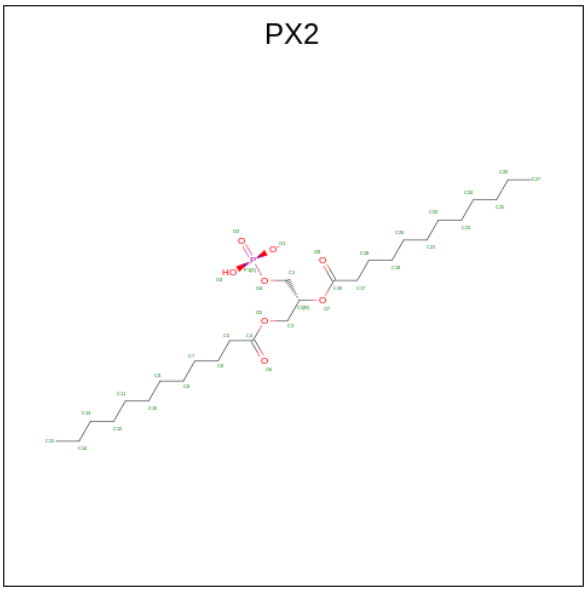
- Molecule 16 is a protein called Embryo defective 2737.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	267	Total	C	N	O	S	0	0
			2151	1371	367	397	16		

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
17	B	1	Total	Zn	0
			1	1	
17	R	2	Total	Zn	0
			2	2	

- Molecule 18 is 1,2-DILAUROYL-SN-GLYCERO-3-PHOSPHATE (three-letter code: PX2) (formula: $C_{27}H_{52}O_8P$).



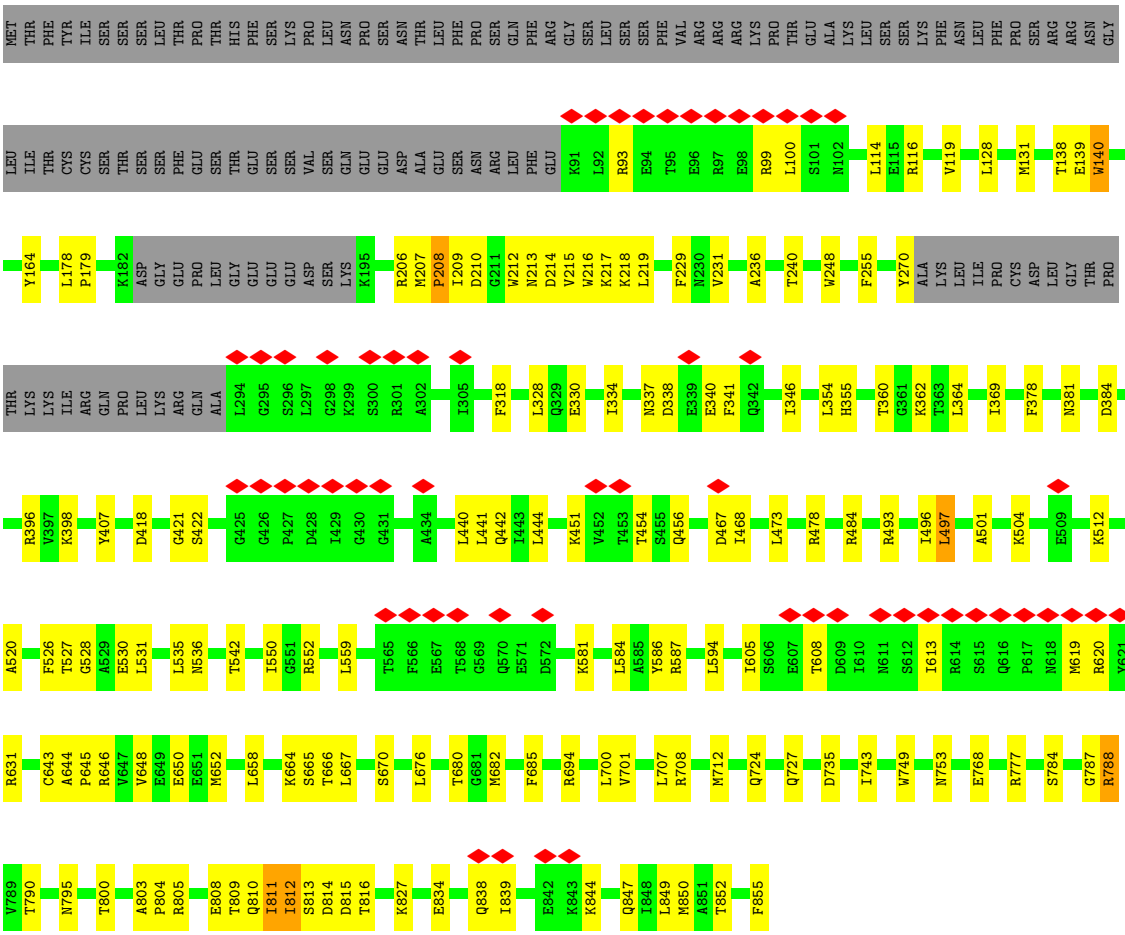
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
18	G	1	25	16	8	1	0

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.

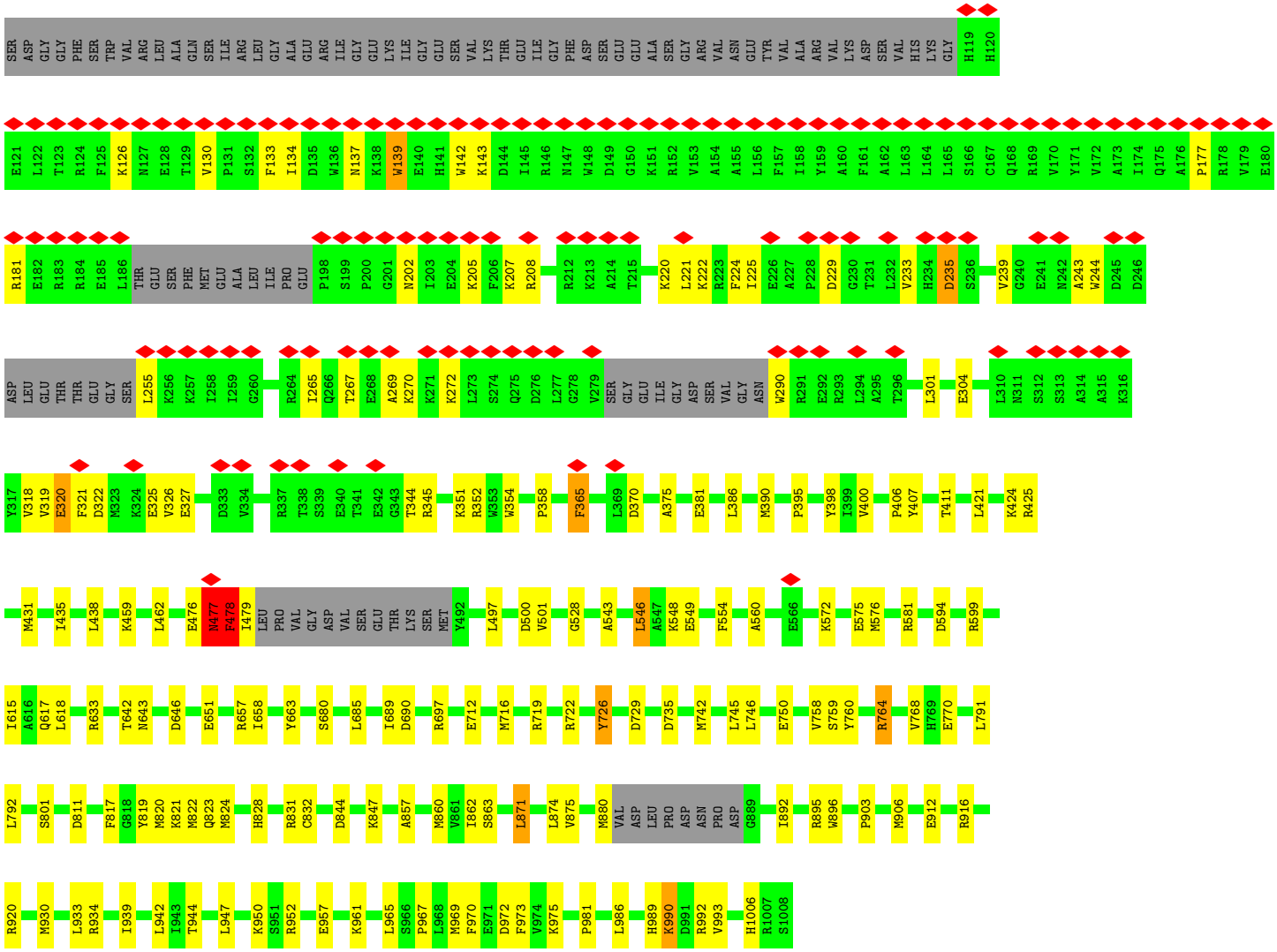
• Molecule 1: Probable inactive ATP-dependent zinc metalloprotease FTSHI 4, chloroplastic

Chain A:



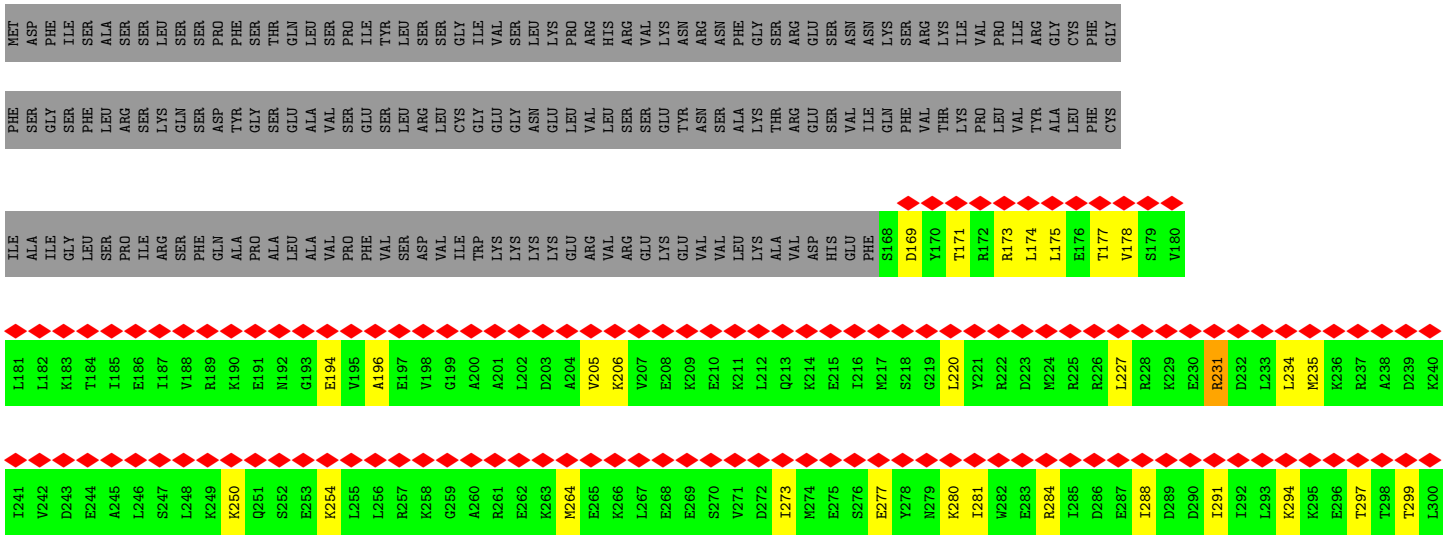
• Molecule 2: ATP-dependent zinc metalloprotease FTSH 12, chloroplastic

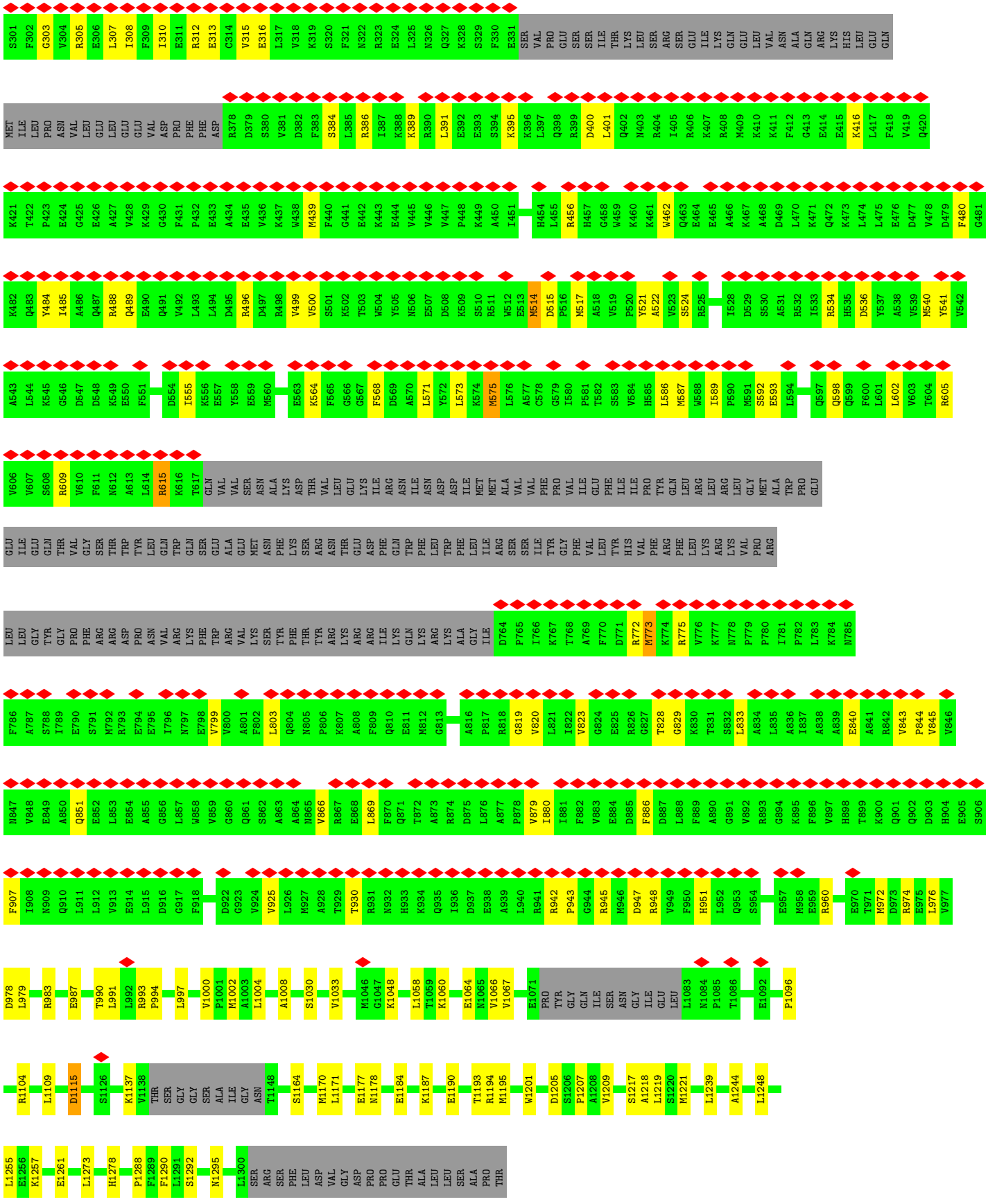
Chain B:



• Molecule 3: Probable inactive ATP-dependent zinc metalloprotease FTSHI 5, chloroplastic

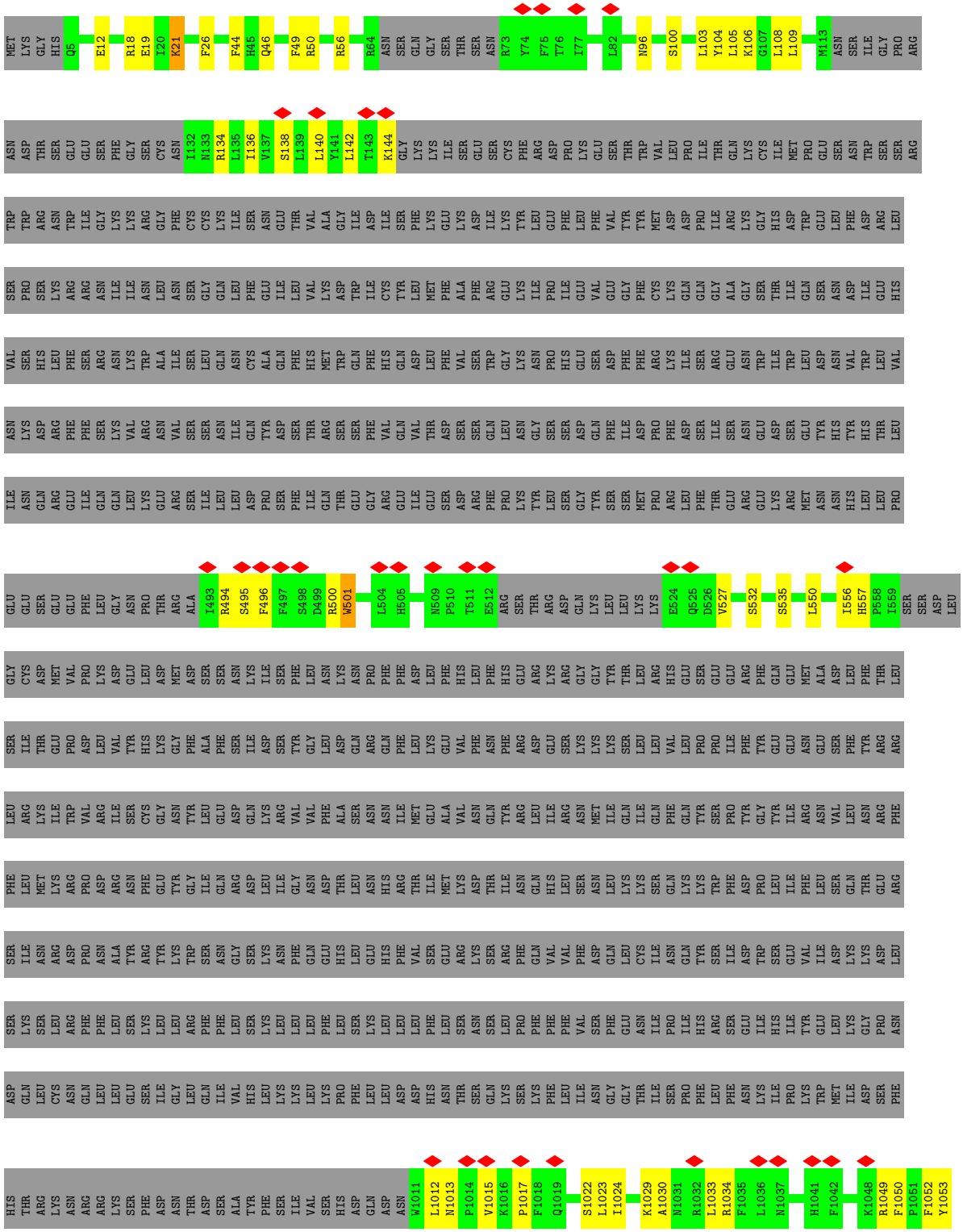
Chain C:

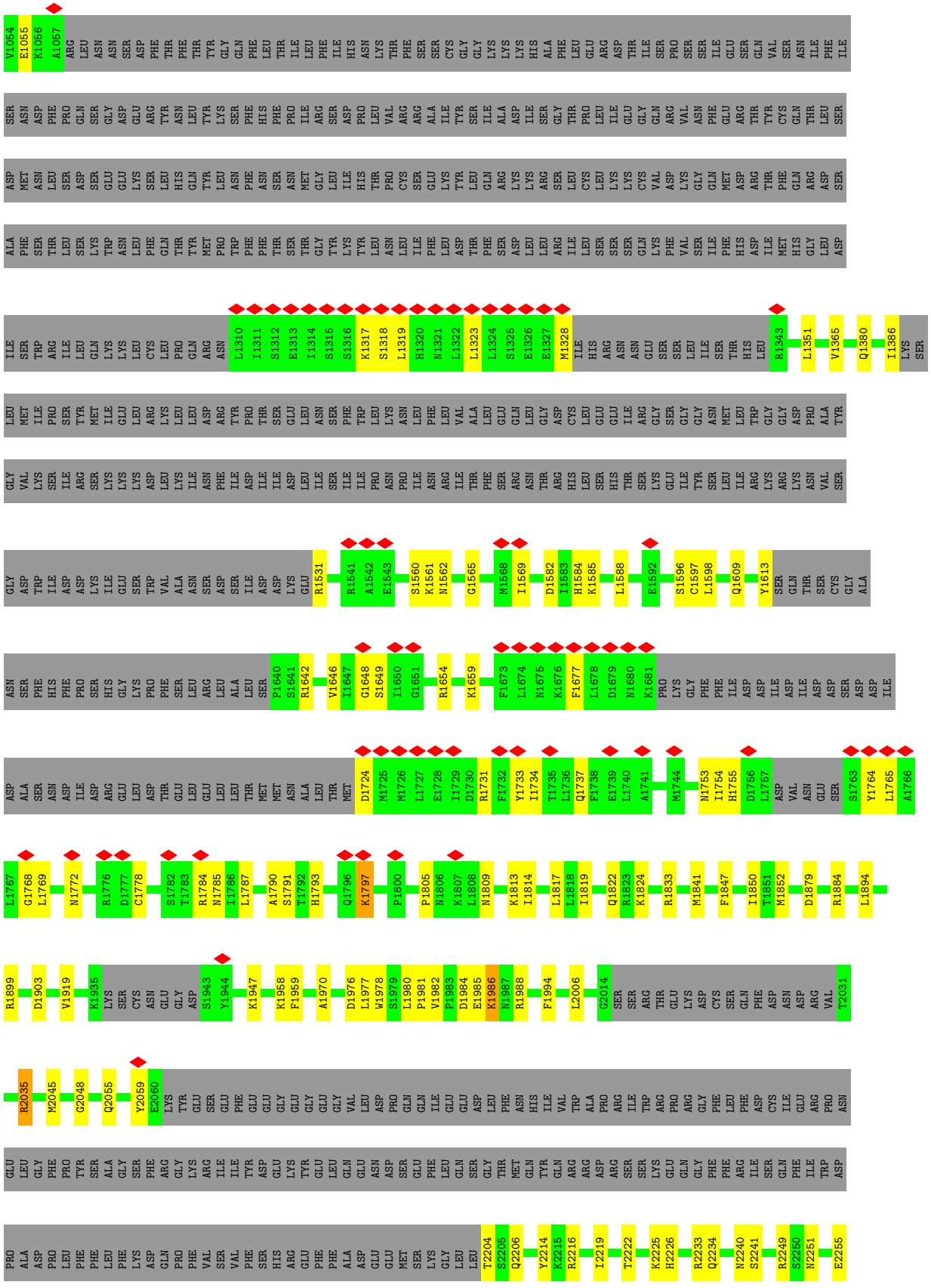


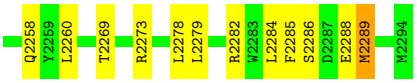

S301 F302 G303 V304 R305 E306 L307 I308 F309 I310 E311 R312 E313 C314 V315 E316 L317 V318 K319 S320 F321 N322 R323 E324 L325 N326 Q327 K328 S329 F330 E331 SER VAL PRO GLU SER SER ILE THR LYS LEU SER ARG SER GLU ILE LYS GLN GLU LEU VAL ASN ALA GLN ARG LYS HIS LEU GLU GLN
MET ILE LEU PRO ASN VAL LEU GLU GLU LEU GLU VAL ASP PRO PHE PHE ASP R378 D379 S380 V381 D382 F383 S384 L385 R386 I387 K388 K389 R390 L391 E392 E393 S394 K395 K396 L397 Q398 R399 D400 L401 Q402 N403 R404 I405 R406 K407 R408 M409 K410 K411 F412 G413 E414 E415 K416 L417 F418 V419 Q420
K421 T422 P423 E424 G425 E426 A427 V428 K429 G430 F431 P432 E433 A434 E435 V436 K437 W438 M439 F440 G441 E442 K443 E444 V445 V446 V447 P448 K449 A450 I451 H454 L455 R456 H457 G458 W459 K460 K461 W462 Q463 E464 E465 A466 K467 A468 D469 L470 K471 Q472 K473 L474 L475 E476 D477 V478 D479 F480 G481
K482 Q483 Y484 I485 A486 Q487 R488 Q489 E490 Q491 V492 L493 L494 D495 R496 D497 R498 V499 V500 S501 K502 T503 W504 Y505 N506 E507 D508 K509 S510 R511 W512 E513 M514 D515 P516 M517 A518 V519 P520 Y521 A522 V523 S524 R525 I528 D529 S530 A531 R532 I533 R534 H535 D536 Y537 A538 V539 M540 Y541 V542
A543 L544 K545 G546 D547 D548 K549 E550 F551 D554 I555 K556 E557 Y558 E559 M560 E563 K564 F565 G566 G567 F568 D569 A570 L571 Y572 L573 K574 M575 L576 A577 C578 G579 I580 P581 T582 S583 V584 H585 L586 M587 W588 I589 P590 M591 S592 E593 L594 Q597 Q598 Q599 F600 L601 L602 V603 T604 R605
V606 V607 S608 R609 V610 F611 N612 A613 L614 R615 K616 T617 GLN VAL VAL SER ASN ALA LYS ASP THR VAL LEU GLU LYS ILE ARG ASN ILE ASN ASP ASP ILE MET MET ALA VAL VAL PHE PRO VAL ILE GLU PHE ILE ILE PRO TYR GLN LEU ARG LEU ARG LEU GLY MET ALA TRP PRO GLU
GLU ILE GLU GLN THR VAL GLY SER THR TRP TYR LEU GLN TRP GLN SER GLU ALA GLU MET ASN PHE LYS SER ARG ASN THR GLU ASP PHE GLN TRP PHE LEU TRP PHE LEU ILE ARG SER SER ILE TYR GLY PHE VAL LEU TYR HIS VAL PHE ARG PHE LEU LYS ARG LYS VAL PRO ARG
LEU LEU GLY TYR GLY PRO PHE ARG ARG ASP PRO ASN VAL ARG LYS PHE TRP ARG VAL LYS SER TYR PHE THR TYR ARG LYS ARG ARG ILE LYS GLN LYS ARG LYS ALA GLY ILE D764 P765 I766 K767 T768 A769 F770 D771 R772 M773 K774 R775 V776 K777 N778 P779 P780 I781 P782 L783 K784 N785
F786 A787 S788 I789 E790 S791 M792 R793 E794 E795 I796 N797 E798 V799 V800 A801 F802 L803 Q804 N805 P806 K807 A808 F809 Q810 E811 M812 G813 A816 P817 R818 G819 V820 L821 I822 V823 G824 E825 R826 G827 T828 G829 K830 T831 S832 L833 A834 L835 A836 I837 A838 A839 E840 A841 R842 V843 P844 V845 V846
N847 V848 E849 A850 Q851 E852 L853 E854 A855 G856 L857 W858 V859 G860 Q861 S862 A863 A864 N865 V866 R867 E868 L869 F870 Q871 T872 A873 R874 D875 L876 A877 P878 V879 I880 I881 F882 V883 E884 D885 F886 D887 L888 F889 A890 G891 V892 R893 G894 K895 F896 V897 H898 T899 K900 Q901 Q902 D903 H904 E905 S906
F907 I908 N909 Q910 L911 L912 V913 E914 L915 D916 G917 F918 D922 G923 V924 V925 L926 M927 A928 T929 T930 R931 N932 H933 K934 Q935 I936 D937 E938 A939 L940 R941 R942 P943 G944 R945 M946 D947 R948 V949 F950 H951 L952 Q953 S954 E957 M958 E959 R960 E970 T971 M972 D973 R974 E975 L976 V977
D978 L979 R983 E987 T990 L991 L992 R993 P994 L997 V1000 P1001 M1002 A1003 L1004 A1008 S1030 V1033 M1046 G1047 K1048 L1058 T1059 K1060 E1064 N1065 V1066 V1067 E1071 PRO TYR GLY GLN ILE SER ASN GLY ILE GLU LEU L1083 N1084 P1085 T1086 E1092 P1096
R1104 L1109 D1115 S1126 K1137 V1138 THR SER GLY GLY SER ALA ILE GLY ASN T1148 S1164 M1170 L1171 E1177 N1178 E1184 K1187 E1190 T1193 R1194 M1195 W1201 D1205 S1206 P1207 A1208 V1209 S1217 A1218 L1219 S1220 M1221 L1239 A1244 L1248
L1255 E1256 K1257 E1261 L1273 H1278 P1288 F1289 F1290 L1291 S1292 N1295 L1300 SER ARG SER PHE LEU ASP VAL GLY ASP PRO PRO GLU THR ALA LEU LEU SER ALA PRO THR

• Molecule 4: Protein Ycf2

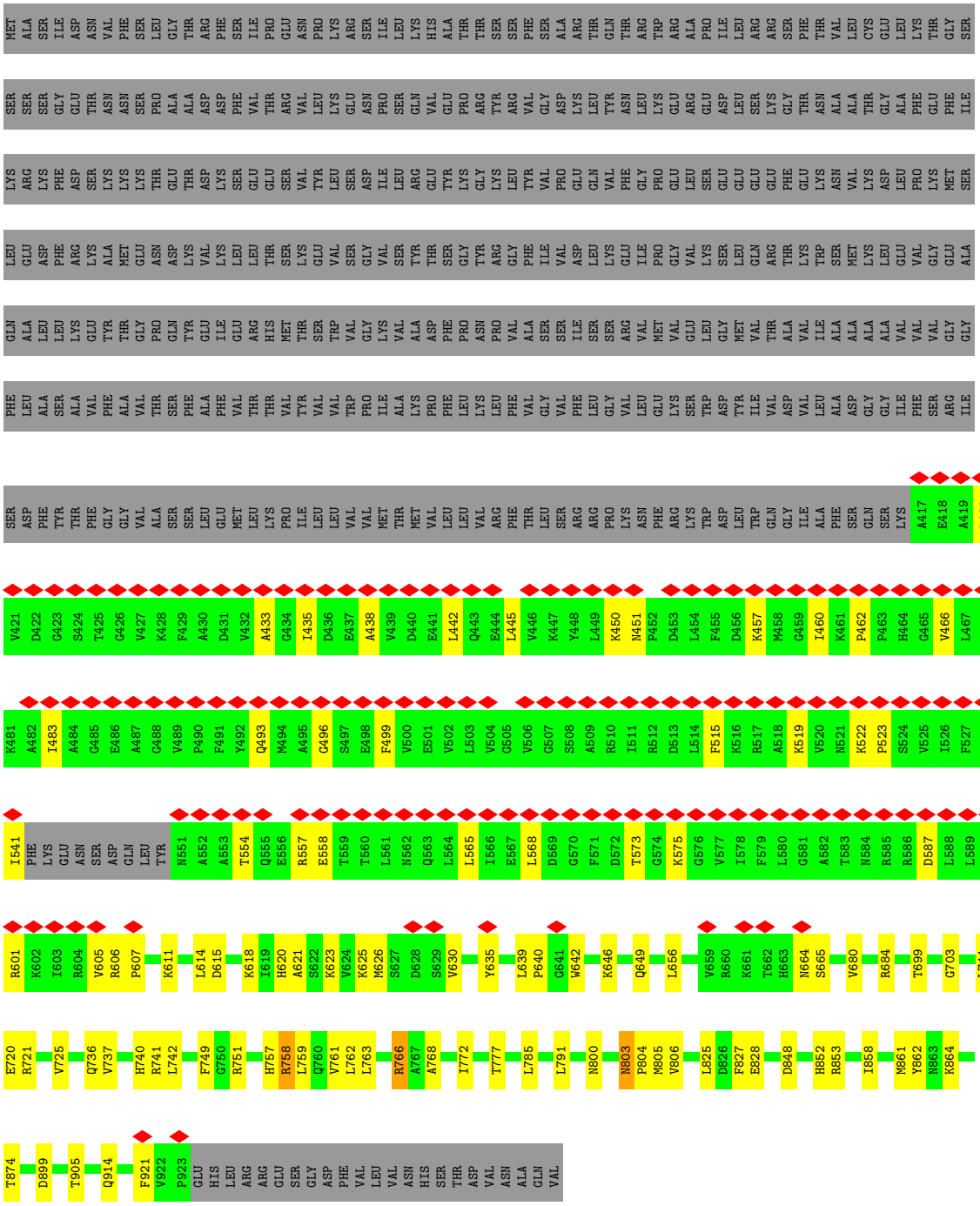
Chain D:



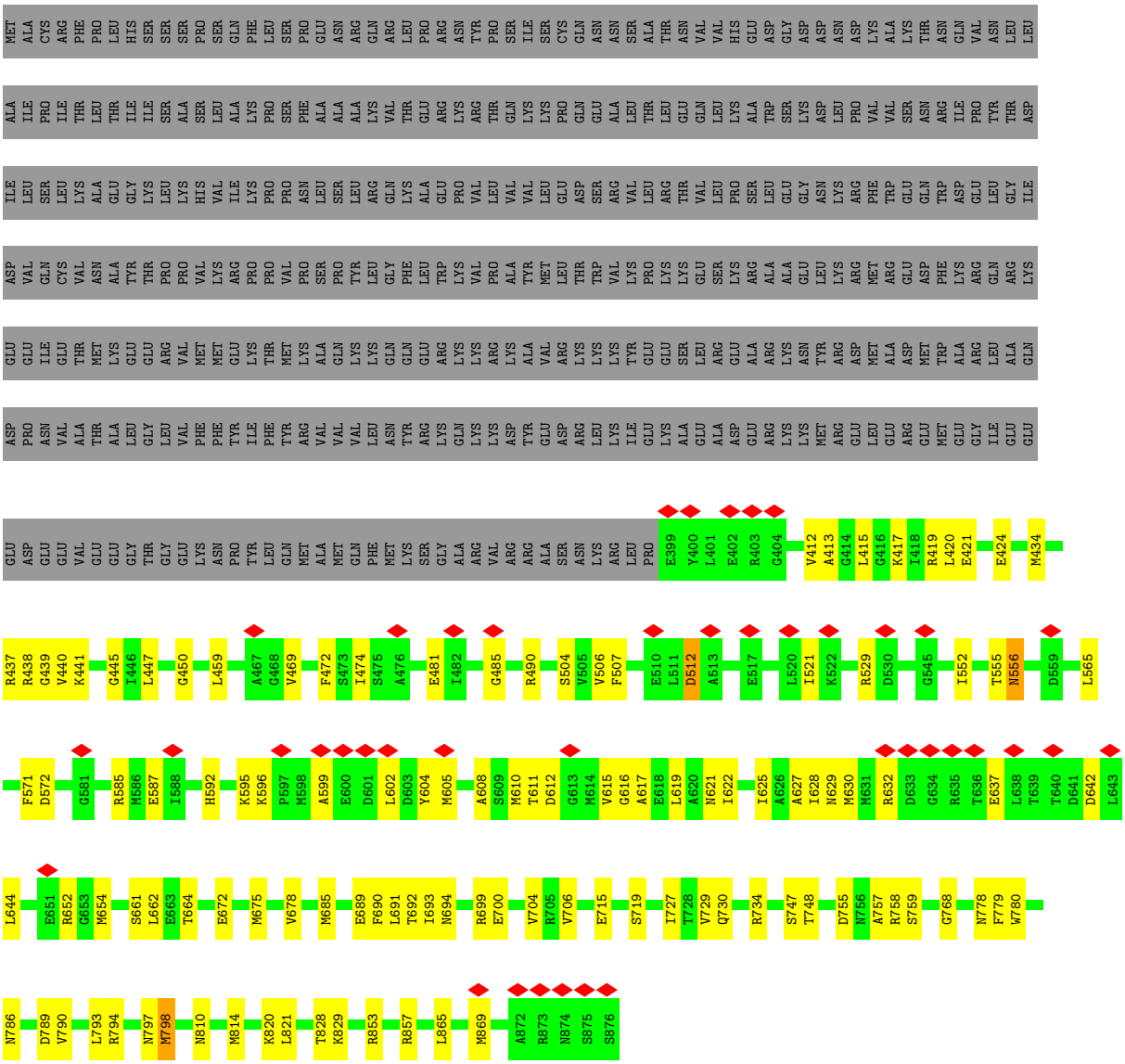




• Molecule 5: Probable inactive ATP-dependent zinc metalloprotease FTSHI 1, chloroplastic

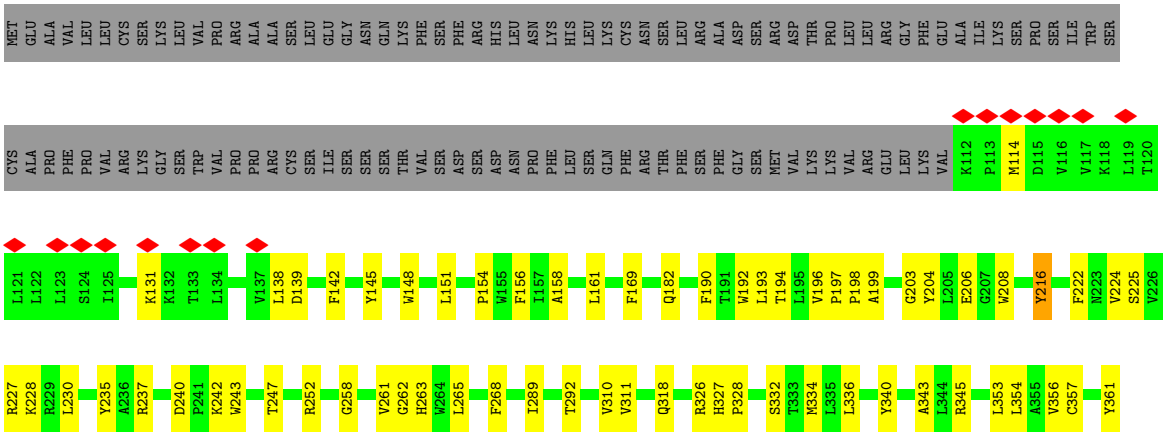


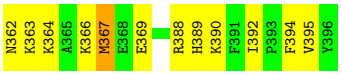
• Molecule 6: Probable inactive ATP-dependent zinc metalloprotease FTSHI 2, chloroplastic



• Molecule 7: AtTam46

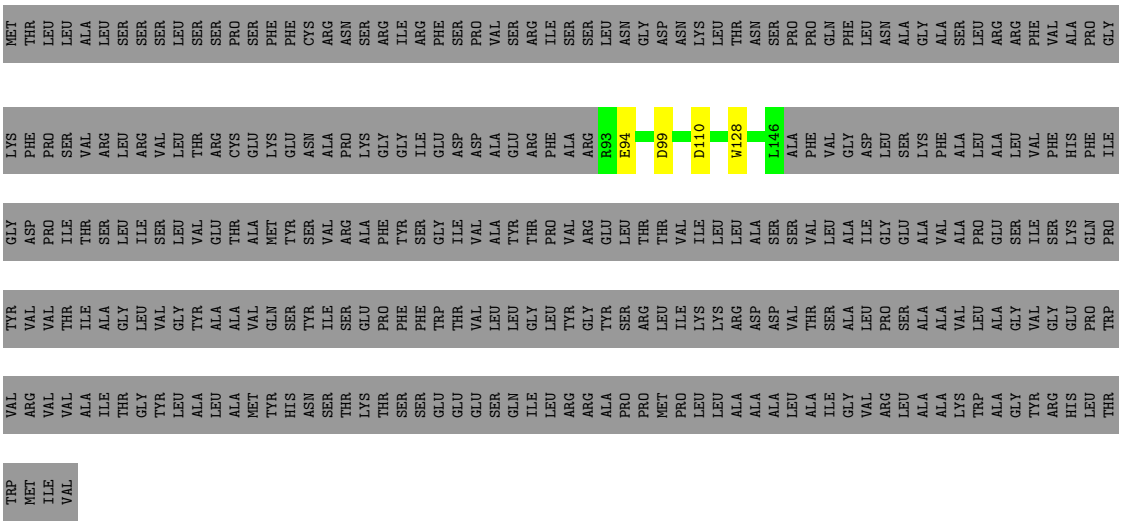
Chain G:





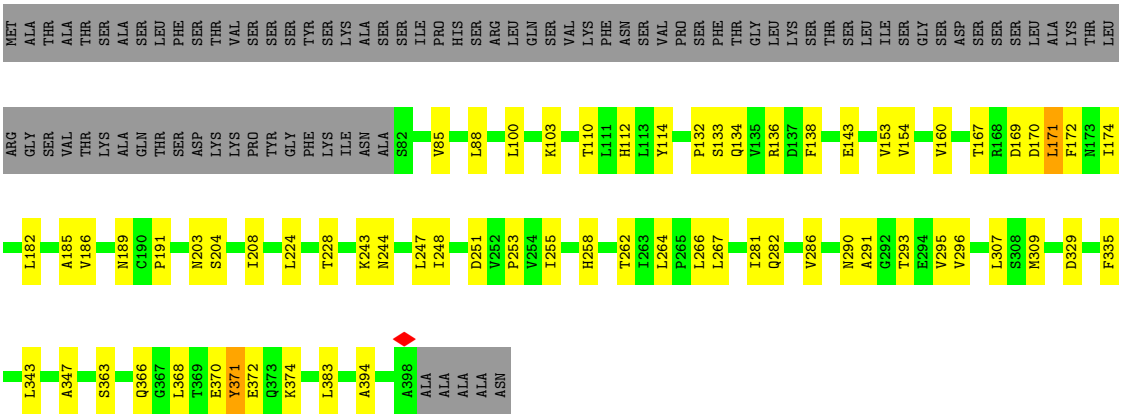
• Molecule 8: At4g28210

Chain H:



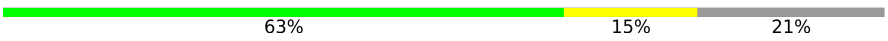
• Molecule 9: Malate dehydrogenase, chloroplastic

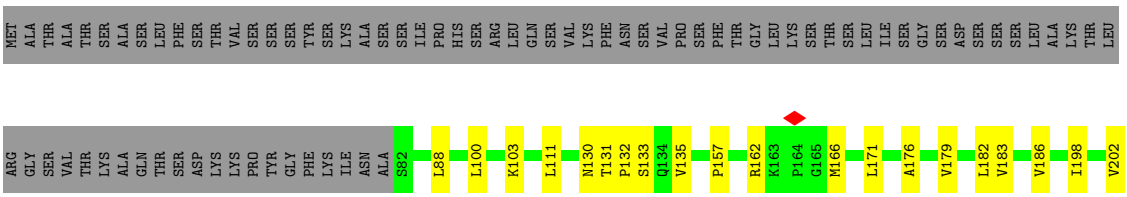
Chain I:



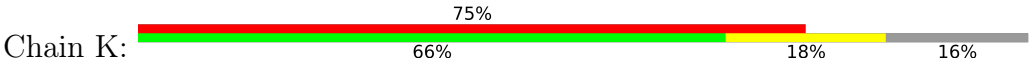
• Molecule 9: Malate dehydrogenase, chloroplastic

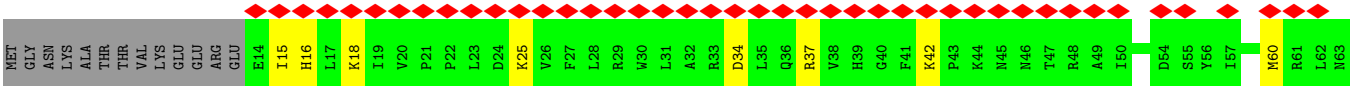
Chain J:



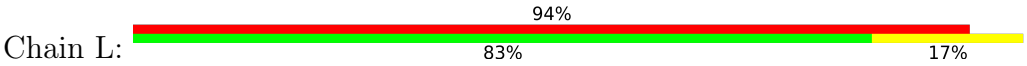


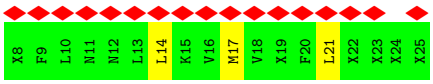
• Molecule 10: Aspartyl/glutamyl-tRNA (Asn/Gln) amidotransferase subunit B



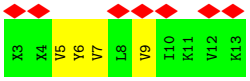


• Molecule 11: UNK

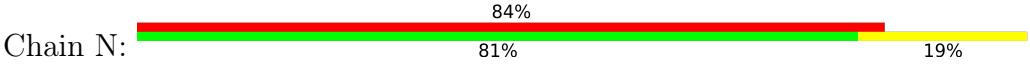


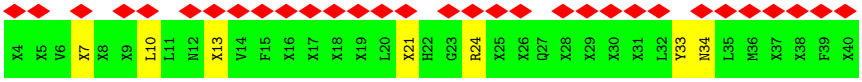


• Molecule 12: UNK

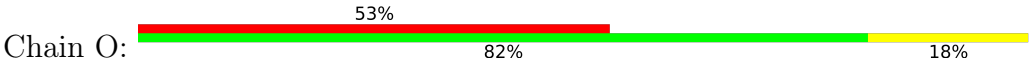


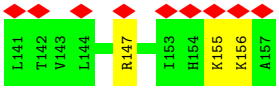
• Molecule 13: UNK



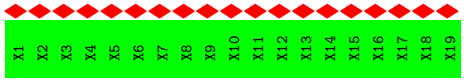


• Molecule 14: UNK

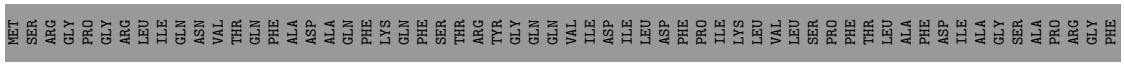


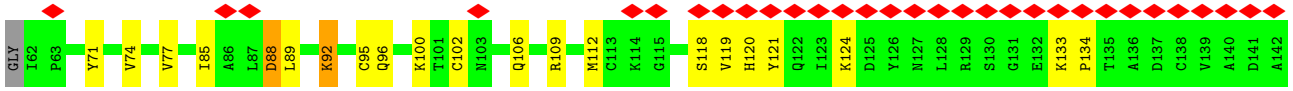


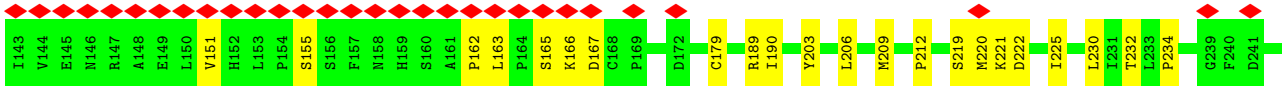
• Molecule 15: UNK

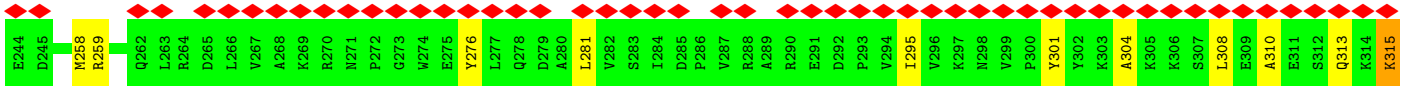


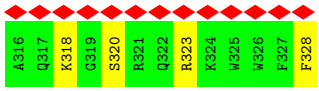
• Molecule 16: Embryo defective 2737











4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	340640	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.960	Depositor
Minimum map value	-2.634	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.086	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	391.32, 391.32, 391.32	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PX2, ZN

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	A	0.26	0/5952	0.53	1/8038 (0.0%)
2	B	0.26	0/6992	0.60	6/9419 (0.1%)
3	C	0.26	0/7627	0.55	2/10262 (0.0%)
4	D	0.26	0/6804	0.55	1/9177 (0.0%)
5	E	0.35	2/3956 (0.1%)	0.59	3/5361 (0.1%)
6	F	0.25	0/3798	0.56	1/5115 (0.0%)
7	G	0.40	2/2470 (0.1%)	0.66	5/3375 (0.1%)
8	H	0.28	0/477	0.52	0/651
9	I	0.30	1/2399 (0.0%)	0.58	3/3261 (0.1%)
9	J	0.25	0/2399	0.48	0/3261
10	K	0.25	0/570	0.59	1/772 (0.1%)
11	L	0.26	0/101	0.49	0/133
12	M	0.24	0/74	0.51	0/99
13	N	0.25	0/142	0.54	0/179
14	O	0.24	0/132	0.79	0/175
16	R	0.27	0/2206	0.56	2/2986 (0.1%)
All	All	0.28	5/46099 (0.0%)	0.57	25/62264 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	4
4	D	0	2
5	E	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	523	PRO	CG-CD	-12.69	1.08	1.50
7	G	198	PRO	CG-CD	-11.80	1.11	1.50
5	E	523	PRO	N-CD	7.17	1.57	1.47
7	G	198	PRO	N-CD	5.96	1.56	1.47
9	I	191	PRO	CG-CD	-5.35	1.33	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	523	PRO	N-CD-CG	-13.51	82.93	103.20
9	I	191	PRO	CA-N-CD	-12.29	94.29	111.50
7	G	198	PRO	CA-N-CD	-12.26	94.34	111.50
7	G	198	PRO	N-CD-CG	-12.11	85.03	103.20
5	E	523	PRO	CA-N-CD	-12.02	94.67	111.50
9	I	191	PRO	N-CD-CG	-8.17	90.94	103.20
7	G	197	PRO	C-N-CD	8.07	145.34	128.40
7	G	198	PRO	CA-CB-CG	-7.00	90.70	104.00
2	B	822	MET	CA-CB-CG	6.72	124.72	113.30
7	G	193	LEU	CA-CB-CG	6.66	130.62	115.30
5	E	523	PRO	CA-CB-CG	-6.55	91.55	104.00
16	R	220	MET	CA-CB-CG	6.53	124.40	113.30
3	C	575	MET	CG-SD-CE	6.48	110.57	100.20
2	B	824	MET	CA-CB-CG	6.35	124.10	113.30
2	B	546	LEU	CA-CB-CG	5.89	128.84	115.30
16	R	206	LEU	CA-CB-CG	5.78	128.59	115.30
4	D	2289	MET	CA-CB-CG	5.71	123.00	113.30
2	B	871	LEU	CA-CB-CG	5.68	128.36	115.30
9	I	171	LEU	CA-CB-CG	5.38	127.67	115.30
10	K	69	ASP	CB-CG-OD1	5.34	123.11	118.30
6	F	798	MET	CA-CB-CG	5.27	122.26	113.30
2	B	745	LEU	CA-CB-CG	5.24	127.36	115.30
2	B	764	ARG	CA-CB-CG	5.20	124.85	113.40
1	A	497	LEU	CA-CB-CG	5.14	127.13	115.30
3	C	517	MET	CA-CB-CG	5.02	121.84	113.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	811	ILE	Peptide
2	B	476	GLU	Peptide
2	B	477	ASN	Peptide

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Mol	Chain	Res	Type	Group
2	B	478	PHE	Peptide
2	B	990	LYS	Peptide
4	D	1982	VAL	Peptide
4	D	495	SER	Peptide
5	E	803	ASN	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	A	5841	0	5859	116	0
2	B	6849	0	6890	116	0
3	C	7494	0	7625	102	0
4	D	6659	0	6763	115	0
5	E	3884	0	3935	66	0
6	F	3744	0	3823	83	0
7	G	2375	0	2353	55	0
8	H	459	0	455	3	0
9	I	2363	0	2437	37	0
9	J	2363	0	2437	41	0
10	K	555	0	561	9	0
11	L	131	0	122	4	0
12	M	84	0	98	3	0
13	N	246	0	174	4	0
14	O	132	0	161	2	0
15	P	95	0	21	0	0
16	R	2151	0	2123	44	0
17	B	1	0	0	0	0
17	R	2	0	0	0	0
18	G	25	0	23	10	0
All	All	45453	0	45860	688	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 (688) 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)
7:G:199:ALA:CB	18:G:401:PX2:H7	2.06	0.85
2:B:764:ARG:HH21	2:B:768:VAL:HB	1.48	0.78
7:G:199:ALA:HB1	18:G:401:PX2:C4	2.15	0.77
7:G:199:ALA:O	18:G:401:PX2:H4	1.86	0.75
1:A:838:GLN:HG2	1:A:839:ILE:HG12	1.69	0.73
16:R:120:HIS:HB3	16:R:163:LEU:HB2	1.72	0.72
7:G:199:ALA:HB1	18:G:401:PX2:C5	2.18	0.72
3:C:489:GLN:NE2	11:L:17:MET:SD	2.63	0.71
5:E:759:LEU:HD13	5:E:791:LEU:HD23	1.73	0.71
1:A:784:SER:HB3	9:J:251:ASP:HB3	1.73	0.70
1:A:381:ASN:HB3	1:A:384:ASP:HB2	1.74	0.70
2:B:406:PRO:HG3	16:R:209:MET:HB3	1.73	0.70
1:A:811:ILE:HD12	4:D:2255:GLU:HG3	1.73	0.69
2:B:370:ASP:OD1	2:B:411:THR:OG1	2.11	0.69
4:D:1034:ARG:HH12	16:R:219:SER:HB2	1.57	0.68
1:A:214:ASP:O	1:A:217:LYS:HB3	1.92	0.68
5:E:800:ASN:ND2	5:E:805:MET:SD	2.67	0.68
3:C:1096:PRO:HB3	3:C:1178:ASN:HD21	1.60	0.67
4:D:557:HIS:O	4:D:1052:PHE:HA	1.94	0.67
1:A:207:MET:SD	1:A:207:MET:N	2.66	0.67
3:C:972:MET:O	3:C:974:ARG:NH1	2.28	0.67
4:D:2006:LEU:HD13	4:D:2249:ARG:HB3	1.77	0.66
16:R:222:ASP:HB3	16:R:225:ILE:HB	1.77	0.66
6:F:595:LYS:HG3	6:F:596:LYS:HE3	1.78	0.66
3:C:194:GLU:HG3	3:C:196:ALA:H	1.61	0.66
2:B:972:ASP:HB3	2:B:975:LYS:HD3	1.78	0.65
3:C:499:VAL:HG21	3:C:522:ALA:HB2	1.76	0.65
1:A:418:ASP:HB2	1:A:468:ILE:HD11	1.77	0.65
1:A:504:LYS:HE3	1:A:535:LEU:HB3	1.77	0.65
4:D:1819:ILE:HD11	4:D:1852:MET:HE1	1.78	0.65
7:G:158:ALA:O	7:G:192:TRP:NE1	2.31	0.64
3:C:851:GLN:NE2	4:D:1764:TYR:O	2.30	0.64
4:D:2006:LEU:HB3	4:D:2249:ARG:HD2	1.78	0.64
16:R:96:GLN:O	16:R:189:ARG:NH1	2.31	0.64
2:B:139:TRP:HE1	16:R:304:ALA:HB3	1.63	0.63
2:B:222:LYS:HG2	2:B:318:VAL:HB	1.79	0.63
7:G:199:ALA:CB	18:G:401:PX2:C5	2.74	0.63
7:G:247:THR:HB	7:G:252:ARG:HD3	1.79	0.63
1:A:255:PHE:HB3	16:R:74:VAL:HG12	1.81	0.63
2:B:581:ARG:NH2	2:B:617:GLN:OE1	2.32	0.63
16:R:102:CYS:SG	16:R:179:CYS:CB	2.87	0.63
1:A:694:ARG:NH2	2:B:896:TRP:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:844:PRO:HG2	3:C:879:VAL:HG12	1.81	0.62
1:A:138:THR:HG23	1:A:140:TRP:H	1.64	0.62
9:I:85:VAL:HG22	9:I:153:VAL:HB	1.82	0.62
2:B:177:PRO:HB2	2:B:181:ARG:HH21	1.65	0.61
7:G:362:ASN:OD1	7:G:390:LYS:NZ	2.34	0.61
1:A:504:LYS:HD3	6:F:438:ARG:HH22	1.65	0.61
4:D:1755:HIS:HB2	4:D:1797:LYS:HD3	1.82	0.61
5:E:435:ILE:HG22	5:E:438:ALA:HB3	1.82	0.61
5:E:445:LEU:HD21	5:E:466:VAL:HG21	1.82	0.61
2:B:395:PRO:HB3	7:G:151:LEU:HD21	1.81	0.61
4:D:1013:ASN:ND2	4:D:1015:VAL:O	2.33	0.60
6:F:630:MET:SD	6:F:630:MET:N	2.73	0.60
2:B:344:THR:HG22	4:D:527:VAL:HB	1.83	0.60
4:D:1841:MET:SD	4:D:1841:MET:N	2.74	0.60
7:G:388:ARG:O	7:G:388:ARG:NH1	2.34	0.60
9:I:343:LEU:HD13	9:I:383:LEU:HD23	1.84	0.60
4:D:1597:CYS:SG	4:D:1598:LEU:N	2.73	0.60
2:B:375:ALA:H	2:B:390:MET:HA	1.67	0.60
9:I:282:GLN:OE1	9:I:371:TYR:OH	2.20	0.60
1:A:724:GLN:HA	1:A:727:GLN:HG2	1.84	0.60
3:C:976:LEU:HD12	3:C:979:LEU:HD13	1.84	0.60
2:B:354:TRP:CZ2	18:G:401:PX2:C16	2.84	0.60
3:C:1209:VAL:HG21	5:E:785:LEU:HB3	1.82	0.60
3:C:1244:ALA:O	3:C:1248:LEU:HB2	2.02	0.60
7:G:199:ALA:HB1	18:G:401:PX2:O5	2.02	0.60
16:R:102:CYS:SG	16:R:179:CYS:HB2	2.42	0.60
5:E:720:GLU:OE2	5:E:758:ARG:NH1	2.35	0.59
2:B:791:LEU:HD11	2:B:947:LEU:HB3	1.84	0.59
9:I:132:PRO:O	9:I:134:GLN:NE2	2.35	0.59
2:B:770:GLU:OE1	2:B:801:SER:OG	2.19	0.59
5:E:720:GLU:HA	5:E:742:LEU:HD21	1.84	0.59
9:J:343:LEU:HD22	9:J:387:ILE:HD12	1.83	0.59
1:A:787:GLY:HA2	1:A:800:THR:O	2.01	0.59
3:C:174:LEU:HD21	3:C:310:ILE:HG21	1.83	0.59
4:D:18:ARG:HA	4:D:21:LYS:HE3	1.84	0.59
4:D:1642:ARG:NH1	4:D:1778:CYS:O	2.36	0.59
16:R:112:MET:SD	16:R:112:MET:N	2.75	0.59
1:A:808:GLU:OE1	4:D:2035:ARG:NH2	2.37	0.58
7:G:392:ILE:HB	7:G:395:VAL:HB	1.85	0.58
6:F:629:ASN:ND2	6:F:642:ASP:OD1	2.32	0.58
1:A:341:PHE:HB3	1:A:346:ILE:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ASN:ND2	6:F:441:LYS:O	2.36	0.58
2:B:322:ASP:O	2:B:325:GLU:N	2.36	0.58
5:E:499:PHE:O	5:E:557:ARG:NH2	2.37	0.58
1:A:542:THR:HG21	1:A:550:ILE:HA	1.86	0.58
2:B:875:VAL:HG12	2:B:903:PRO:HA	1.86	0.58
2:B:351:LYS:NZ	7:G:206:GLU:OE1	2.32	0.57
6:F:793:LEU:HD23	6:F:794:ARG:HH12	1.68	0.57
9:J:282:GLN:OE1	9:J:371:TYR:OH	2.22	0.57
6:F:652:ARG:HH22	6:F:699:ARG:HH11	1.50	0.57
1:A:749:TRP:O	1:A:753:ASN:ND2	2.37	0.57
1:A:114:LEU:HD13	4:D:550:LEU:HD11	1.86	0.57
1:A:213:ASN:ND2	16:R:209:MET:O	2.38	0.57
2:B:208:ARG:HG2	2:B:243:ALA:HA	1.85	0.57
4:D:138:SER:HA	4:D:142:LEU:HD13	1.86	0.57
5:E:476:LYS:HG2	5:E:605:VAL:HG21	1.86	0.57
1:A:338:ASP:OD1	1:A:338:ASP:N	2.36	0.57
6:F:592:HIS:O	6:F:595:LYS:NZ	2.38	0.57
7:G:326:ARG:NH1	7:G:369:GLU:OE1	2.35	0.57
2:B:528:GLY:HA3	2:B:658:ILE:HD13	1.87	0.57
4:D:2278:LEU:HD13	4:D:2284:LEU:HD22	1.85	0.57
7:G:258:GLY:HA3	7:G:356:VAL:HG21	1.87	0.57
4:D:1380:GLN:O	16:R:71:TYR:OH	2.22	0.57
6:F:415:LEU:HB3	6:F:419:ARG:HB2	1.87	0.57
6:F:616:GLY:HA2	6:F:619:LEU:HD12	1.86	0.57
2:B:615:ILE:HD11	2:B:657:ARG:HD3	1.87	0.57
2:B:863:SER:HA	2:B:895:ARG:HH22	1.70	0.57
2:B:722:ARG:HD3	2:B:726:TYR:CE1	2.41	0.56
5:E:763:LEU:HD13	5:E:862:TYR:HD1	1.71	0.56
9:J:246:LYS:HZ2	9:J:248:ILE:HB	1.70	0.56
2:B:497:LEU:HD22	2:B:501:VAL:HG11	1.86	0.56
1:A:100:LEU:HD13	2:B:265:ILE:HD13	1.88	0.56
3:C:1008:ALA:HA	3:C:1066:VAL:HG21	1.87	0.56
4:D:1584:HIS:NE2	4:D:1785:ASN:O	2.39	0.56
6:F:793:LEU:O	6:F:797:ASN:ND2	2.39	0.56
9:J:262:THR:HA	9:J:379:LEU:HB2	1.88	0.56
9:I:100:LEU:HD13	9:J:307:LEU:HB3	1.86	0.56
16:R:221:LYS:HA	16:R:258:MET:HE3	1.87	0.56
4:D:1805:PRO:O	4:D:1809:ASN:ND2	2.39	0.56
4:D:2234:GLN:NE2	6:F:786:ASN:OD1	2.32	0.56
16:R:118:SER:O	16:R:155:SER:OG	2.24	0.56
3:C:227:LEU:HD12	3:C:288:ILE:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:514:MET:SD	3:C:515:ASP:N	2.79	0.55
4:D:1654:ARG:NH2	4:D:1753:ASN:OD1	2.38	0.55
4:D:1734:ILE:HB	4:D:1769:LEU:HD22	1.88	0.55
6:F:747:SER:OG	6:F:748:THR:N	2.38	0.55
2:B:134:ILE:HG12	16:R:162:PRO:HD2	1.87	0.55
3:C:1217:SER:OG	3:C:1218:ALA:N	2.38	0.55
4:D:2216:ARG:NH2	6:F:759:SER:OG	2.39	0.55
2:B:989:HIS:HD2	4:D:1977:LEU:HB3	1.72	0.55
1:A:708:ARG:O	1:A:712:MET:HG2	2.06	0.55
2:B:735:ASP:OD2	2:B:952:ARG:NH2	2.27	0.55
3:C:828:THR:HG22	3:C:993:ARG:HG2	1.89	0.55
1:A:652:MET:SD	1:A:652:MET:N	2.80	0.55
2:B:479:ILE:HB	2:B:554:PHE:HB3	1.89	0.55
7:G:262:GLY:HA3	7:G:353:LEU:HD13	1.88	0.55
3:C:521:TYR:O	3:C:524:SER:OG	2.22	0.55
7:G:310:VAL:HG12	7:G:311:VAL:HG23	1.89	0.55
9:J:293:THR:HA	9:J:296:VAL:HG22	1.89	0.55
1:A:519:VAL:HG23	1:A:559:LEU:HD11	1.88	0.54
1:A:813:SER:HB2	1:A:815:ASP:H	1.72	0.54
4:D:1754:ILE:HD12	4:D:1754:ILE:H	1.72	0.54
6:F:692:THR:OG1	6:F:694:ASN:ND2	2.40	0.54
7:G:203:GLY:O	18:G:401:PX2:O8	2.26	0.54
9:J:103:LYS:HZ1	9:J:131:THR:HB	1.70	0.54
4:D:1754:ILE:HD11	4:D:1790:ALA:HB1	1.90	0.54
9:J:203:ASN:HD21	9:J:262:THR:HG21	1.71	0.54
1:A:501:ALA:O	1:A:512:LYS:NZ	2.41	0.54
9:J:183:VAL:HA	9:J:186:VAL:HG22	1.89	0.54
1:A:664:LYS:HG3	1:A:667:LEU:HD22	1.90	0.54
10:K:60:MET:SD	10:K:65:SER:OG	2.65	0.54
1:A:682:MET:SD	1:A:682:MET:N	2.78	0.54
9:I:329:ASP:OD1	9:I:329:ASP:N	2.41	0.54
1:A:178:LEU:HD12	1:A:179:PRO:HD2	1.88	0.53
4:D:2233:ARG:NH1	6:F:779:PHE:O	2.36	0.53
3:C:234:LEU:HD22	3:C:281:ILE:HG23	1.91	0.53
4:D:2285:PHE:N	4:D:2288:GLU:OE1	2.40	0.53
5:E:568:LEU:HB3	5:E:598:ARG:HG2	1.90	0.53
9:I:247:LEU:HD13	9:J:132:PRO:HB3	1.91	0.53
3:C:384:SER:HB2	16:R:276:TYR:HD2	1.73	0.53
6:F:438:ARG:HG3	6:F:440:VAL:HG23	1.89	0.53
1:A:608:THR:HB	1:A:743:ILE:HG13	1.91	0.53
4:D:1648:GLY:HA3	4:D:1814:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:220:LEU:HD21	3:C:299:THR:HG21	1.91	0.53
6:F:654:MET:SD	6:F:654:MET:N	2.76	0.53
6:F:755:ASP:HA	6:F:758:ARG:HG2	1.90	0.53
1:A:527:THR:HG22	1:A:530:GLU:HG2	1.90	0.53
2:B:134:ILE:HD12	2:B:137:ASN:HB3	1.91	0.53
4:D:1596:SER:OG	4:D:1597:CYS:N	2.41	0.53
7:G:139:ASP:HB3	7:G:142:PHE:HB3	1.91	0.53
2:B:354:TRP:HE1	7:G:154:PRO:HG3	1.74	0.53
3:C:484:TYR:OH	3:C:488:ARG:NH1	2.41	0.53
3:C:820:VAL:HG12	3:C:948:ARG:HB2	1.90	0.53
2:B:651:GLU:O	2:B:657:ARG:NH1	2.40	0.52
5:E:460:ILE:HD11	6:F:628:ILE:HG22	1.91	0.52
5:E:711:LEU:HD13	5:E:757:HIS:HB3	1.90	0.52
6:F:828:THR:OG1	6:F:829:LYS:N	2.43	0.52
9:I:167:THR:HG23	9:I:169:ASP:H	1.73	0.52
1:A:387:GLU:HA	6:F:485:GLY:HA3	1.90	0.52
2:B:916:ARG:NH2	9:J:327:ASP:OD2	2.42	0.52
1:A:248:TRP:HZ3	16:R:77:VAL:HG13	1.75	0.52
1:A:735:ASP:OD1	6:F:853:ARG:NH2	2.42	0.52
3:C:866:VAL:HG11	3:C:907:PHE:HE1	1.75	0.52
5:E:848:ASP:O	5:E:852:HIS:ND1	2.42	0.52
2:B:758:VAL:HG21	2:B:792:LEU:HD22	1.90	0.52
2:B:823:GLN:HG3	2:B:892:ILE:HD11	1.91	0.52
4:D:136:ILE:HD11	16:R:234:PRO:HG2	1.91	0.52
2:B:697:ARG:NH1	2:B:735:ASP:OD1	2.43	0.52
2:B:992:ARG:NH1	4:D:2258:GLN:OE1	2.42	0.52
3:C:1201:TRP:NE1	5:E:777:THR:OG1	2.43	0.52
1:A:384:ASP:O	1:A:396:ARG:NH1	2.42	0.52
9:I:88:LEU:HD13	9:I:182:LEU:HD22	1.91	0.52
3:C:829:GLY:O	3:C:833:LEU:N	2.40	0.52
9:I:112:HIS:HA	9:I:136:ARG:O	2.10	0.52
2:B:990:LYS:NZ	4:D:1976:ASP:O	2.43	0.51
9:I:208:ILE:HG12	9:I:394:ALA:HB2	1.92	0.51
1:A:850:MET:SD	1:A:852:THR:OG1	2.61	0.51
4:D:1561:LYS:HB2	7:G:230:LEU:HG	1.92	0.51
1:A:501:ALA:HA	1:A:504:LYS:HG3	1.93	0.51
2:B:126:LYS:HE3	16:R:165:SER:H	1.76	0.51
3:C:1190:GLU:OE2	3:C:1194:ARG:NH1	2.44	0.51
4:D:1850:ILE:HG21	4:D:1884:ARG:HH21	1.75	0.51
6:F:585:ARG:NH2	6:F:612:ASP:OD1	2.44	0.51
1:A:800:THR:HG21	1:A:805:ARG:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:46:GLN:NE2	7:G:225:SER:OG	2.44	0.51
4:D:1328:MET:HB2	16:R:100:LYS:HD3	1.93	0.51
4:D:1584:HIS:HD2	4:D:1787:LEU:HD23	1.74	0.51
5:E:565:LEU:HB2	5:E:598:ARG:HH11	1.74	0.51
1:A:330:GLU:HG3	2:B:719:ARG:HH11	1.75	0.51
2:B:950:LYS:NZ	2:B:957:GLU:OE1	2.33	0.51
5:E:640:PRO:HG3	5:E:741:ARG:HD3	1.91	0.51
3:C:1288:PRO:HG2	3:C:1290:PHE:HE2	1.75	0.51
1:A:550:ILE:HD11	6:F:438:ARG:HE	1.74	0.51
2:B:221:LEU:HD13	2:B:319:VAL:HG12	1.92	0.51
16:R:95:CYS:SG	16:R:96:GLN:N	2.83	0.51
16:R:133:LYS:HG2	16:R:134:PRO:HD2	1.91	0.51
16:R:315:LYS:HA	16:R:318:LYS:HD2	1.93	0.51
1:A:338:ASP:OD2	1:A:456:GLN:NE2	2.37	0.51
2:B:989:HIS:CD2	4:D:1977:LEU:HB3	2.45	0.51
3:C:845:VAL:HG12	3:C:880:ILE:HB	1.92	0.51
6:F:689:GLU:HA	6:F:829:LYS:HB2	1.92	0.51
1:A:795:ASN:O	9:J:130:ASN:ND2	2.44	0.50
3:C:1171:LEU:HD11	3:C:1255:LEU:HG	1.93	0.50
4:D:2219:ILE:HB	4:D:2222:THR:HG23	1.92	0.50
16:R:89:LEU:HA	16:R:92:LYS:NZ	2.26	0.50
4:D:1017:PRO:HG2	4:D:1033:LEU:HD21	1.94	0.50
7:G:247:THR:O	7:G:252:ARG:NH1	2.44	0.50
1:A:212:TRP:HA	1:A:215:VAL:HB	1.93	0.50
2:B:939:ILE:HG12	2:B:965:LEU:HD13	1.91	0.50
3:C:803:LEU:HD22	3:C:843:VAL:HG21	1.92	0.50
1:A:608:THR:OG1	1:A:619:MET:SD	2.62	0.50
13:N:7:UNK:HA	13:N:10:LEU:HB3	1.93	0.50
3:C:1115:ASP:HB3	3:C:1137:LYS:HA	1.94	0.50
7:G:357:CYS:O	7:G:361:TYR:HB2	2.12	0.50
9:J:295:VAL:HG11	9:J:305:ALA:HB2	1.93	0.50
4:D:496:PHE:HE2	13:N:24:ARG:HD3	1.76	0.50
10:K:74:ASP:OD1	10:K:74:ASP:N	2.44	0.50
1:A:206:ARG:NH2	16:R:106:GLN:O	2.42	0.50
4:D:532:SER:O	4:D:535:SER:OG	2.28	0.50
2:B:857:ALA:O	2:B:860:MET:HB3	2.11	0.50
16:R:119:VAL:O	16:R:165:SER:HA	2.12	0.50
1:A:328:LEU:HD13	1:A:369:ILE:HD11	1.94	0.50
5:E:442:LEU:HD13	5:E:483:ILE:HD11	1.94	0.50
5:E:800:ASN:HD21	5:E:806:VAL:H	1.60	0.50
3:C:960:ARG:NH2	3:C:990:THR:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:88:LEU:HD13	9:J:182:LEU:HD22	1.94	0.49
16:R:121:TYR:OH	16:R:167:ASP:O	2.30	0.49
6:F:447:LEU:HD11	6:F:555:THR:HG23	1.94	0.49
1:A:587:ARG:HD3	1:A:645:PRO:HB3	1.94	0.49
2:B:930:MET:O	2:B:934:ARG:HG2	2.12	0.49
5:E:462:PRO:HD2	5:E:573:THR:HB	1.94	0.49
6:F:413:ALA:HB1	6:F:587:GLU:HG3	1.95	0.49
6:F:693:ILE:HG23	6:F:821:LEU:HD22	1.93	0.49
1:A:444:LEU:HD22	1:A:478:ARG:HD3	1.95	0.49
1:A:777:ARG:HD3	2:B:912:GLU:HG3	1.93	0.49
2:B:633:ARG:NH2	4:D:12:GLU:OE2	2.45	0.49
9:J:335:PHE:HA	9:J:347:ALA:HA	1.95	0.49
3:C:386:ARG:HA	3:C:389:LYS:HD3	1.94	0.49
6:F:678:VAL:HG13	6:F:729:VAL:HG22	1.93	0.49
7:G:334:MET:HE2	7:G:361:TYR:HD2	1.77	0.49
9:J:351:LYS:NZ	9:J:358:GLU:OE2	2.35	0.49
2:B:973:PHE:HA	4:D:1986:LYS:HD3	1.95	0.49
5:E:861:MET:HA	5:E:864:LYS:HD3	1.93	0.49
1:A:236:ALA:O	1:A:240:THR:HG23	2.11	0.49
2:B:425:ARG:NH1	4:D:96:ASN:OD1	2.45	0.49
4:D:2282:ARG:NH2	8:H:99:ASP:OD1	2.38	0.49
5:E:725:VAL:HG22	5:E:737:VAL:HG23	1.93	0.49
2:B:972:ASP:O	2:B:975:LYS:NZ	2.39	0.49
4:D:557:HIS:NE2	4:D:1055:GLU:OE1	2.43	0.49
4:D:1029:LYS:O	4:D:1029:LYS:NZ	2.37	0.49
2:B:920:ARG:HE	9:J:354:LYS:HZ1	1.60	0.49
9:I:203:ASN:HD21	9:I:262:THR:HG21	1.78	0.49
1:A:334:ILE:HG12	1:A:341:PHE:HD2	1.77	0.49
1:A:643:CYS:HB2	1:A:666:THR:HG22	1.94	0.49
1:A:650:GLU:HG3	1:A:658:LEU:HD21	1.95	0.49
5:E:699:THR:HG23	5:E:772:ILE:HD12	1.95	0.49
1:A:497:LEU:HD21	1:A:520:ALA:HB2	1.95	0.48
6:F:585:ARG:NH2	6:F:608:ALA:O	2.40	0.48
1:A:318:PHE:HB2	1:A:364:LEU:HG	1.95	0.48
1:A:809:THR:HG22	1:A:810:GLN:H	1.78	0.48
4:D:1768:GLY:O	4:D:1772:ASN:ND2	2.46	0.48
5:E:515:PHE:O	5:E:519:LYS:HG2	2.13	0.48
1:A:581:LYS:HE3	1:A:581:LYS:HA	1.95	0.48
1:A:790:THR:OG1	1:A:805:ARG:NH1	2.46	0.48
3:C:1195:MET:HB3	3:C:1201:TRP:HB2	1.96	0.48
9:J:111:LEU:HD23	9:J:135:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2226:HIS:HE1	6:F:778:ASN:HB3	1.78	0.48
5:E:874:THR:HG21	5:E:905:THR:HG23	1.95	0.48
6:F:421:GLU:O	6:F:424:GLU:HB2	2.13	0.48
1:A:216:TRP:HA	1:A:219:LEU:HB2	1.95	0.48
1:A:788:ARG:HB3	2:B:1006:HIS:CE1	2.48	0.48
2:B:759:SER:OG	2:B:760:TYR:N	2.46	0.48
9:J:323:ALA:HB2	9:J:330:VAL:HG11	1.96	0.48
3:C:773:MET:SD	3:C:775:ARG:NH1	2.87	0.48
2:B:811:ASP:HB3	4:D:1899:ARG:HD3	1.96	0.48
4:D:1734:ILE:HD12	4:D:1769:LEU:HB2	1.96	0.48
6:F:585:ARG:HD2	6:F:619:LEU:HD21	1.95	0.48
9:J:351:LYS:HB3	9:J:359:ALA:HB3	1.95	0.48
1:A:337:ASN:ND2	1:A:340:GLU:OE1	2.47	0.48
3:C:1193:THR:HG21	4:D:2048:GLY:HA3	1.96	0.48
1:A:451:LYS:HB2	1:A:454:THR:HG22	1.96	0.47
3:C:983:ARG:O	3:C:987:GLU:HG2	2.14	0.47
4:D:2269:THR:O	4:D:2273:ARG:HG2	2.13	0.47
5:E:466:VAL:HG13	5:E:601:ARG:HB3	1.96	0.47
5:E:713:ARG:NH2	5:E:899:ASP:OD1	2.47	0.47
6:F:450:GLY:O	6:F:556:ASN:ND2	2.46	0.47
1:A:847:GLN:O	7:G:227:ARG:NH2	2.42	0.47
6:F:730:GLN:HB2	6:F:757:ALA:HB2	1.95	0.47
13:N:21:UNK:O	13:N:24:ARG:NH2	2.46	0.47
2:B:685:LEU:HB3	2:B:689:ILE:HG21	1.95	0.47
6:F:727:ILE:HG23	6:F:757:ALA:HB1	1.95	0.47
9:J:343:LEU:HD21	9:J:384:LYS:HA	1.97	0.47
1:A:496:ILE:HD12	1:A:528:GLY:HA2	1.96	0.47
2:B:381:GLU:OE2	2:B:424:LYS:N	2.46	0.47
4:D:1985:GLU:HB3	4:D:1988:ARG:HD2	1.95	0.47
6:F:621:ASN:O	6:F:625:ILE:HG12	2.14	0.47
7:G:261:VAL:O	7:G:265:LEU:HB2	2.15	0.47
2:B:993:VAL:HG12	4:D:1976:ASP:HB3	1.96	0.47
3:C:416:LYS:HB3	3:C:439:MET:HB2	1.95	0.47
3:C:534:ARG:HD3	3:C:541:TYR:HE1	1.80	0.47
4:D:2286:SER:O	4:D:2289:MET:HB2	2.15	0.47
9:I:172:PHE:HE2	9:I:204:SER:HB2	1.79	0.47
2:B:319:VAL:HG22	12:M:7:VAL:HG22	1.96	0.47
2:B:345:ARG:HH22	2:B:375:ALA:HB1	1.80	0.47
2:B:462:LEU:HD21	4:D:1386:ILE:HD13	1.96	0.47
2:B:942:LEU:HD21	2:B:961:LYS:HE3	1.96	0.47
3:C:231:ARG:O	3:C:235:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:312:ARG:HA	3:C:315:VAL:HG22	1.97	0.47
3:C:799:VAL:HG21	3:C:820:VAL:HG11	1.96	0.47
3:C:886:PHE:HB3	3:C:930:THR:HG22	1.96	0.47
4:D:1646:VAL:HG13	4:D:1791:SER:HB2	1.97	0.47
7:G:192:TRP:HA	7:G:196:VAL:HB	1.97	0.47
1:A:116:ARG:HA	1:A:119:VAL:HG22	1.96	0.47
1:A:209:ILE:HG22	1:A:210:ASP:HB3	1.95	0.47
1:A:360:THR:HG22	1:A:362:LYS:HE2	1.97	0.47
1:A:670:SER:HA	1:A:712:MET:HE1	1.96	0.47
3:C:308:ILE:O	3:C:312:ARG:HG2	2.15	0.47
5:E:680:VAL:HG11	5:E:736:GLN:HE22	1.80	0.47
5:E:703:GLY:HA3	5:E:768:ALA:HB2	1.97	0.47
1:A:613:ILE:HG21	6:F:715:GLU:HB3	1.97	0.47
2:B:202:ASN:HA	2:B:205:LYS:HE2	1.96	0.47
2:B:500:ASP:HB3	4:D:1894:LEU:HD12	1.97	0.47
5:E:620:HIS:HA	5:E:623:LYS:HZ3	1.79	0.47
6:F:790:VAL:O	6:F:794:ARG:HG2	2.14	0.47
1:A:138:THR:OG1	1:A:139:GLU:OE1	2.30	0.47
3:C:291:ILE:HA	3:C:294:LYS:HG2	1.97	0.47
3:C:294:LYS:HA	3:C:297:THR:HG22	1.96	0.47
1:A:816:THR:HB	4:D:1959:PHE:HE2	1.80	0.46
2:B:594:ASP:OD1	2:B:594:ASP:N	2.48	0.46
2:B:599:ARG:NH2	2:B:646:ASP:O	2.47	0.46
2:B:847:LYS:HE2	2:B:847:LYS:HB3	1.75	0.46
3:C:500:VAL:HG23	11:L:21:LEU:HD12	1.97	0.46
3:C:602:LEU:O	3:C:605:ARG:HG3	2.15	0.46
7:G:208:TRP:CD2	7:G:343:ALA:HB1	2.51	0.46
7:G:343:ALA:O	7:G:345:ARG:NH1	2.47	0.46
2:B:642:THR:OG1	2:B:643:ASN:N	2.47	0.46
2:B:819:TYR:O	2:B:823:GLN:HG2	2.14	0.46
4:D:2214:TYR:OH	6:F:672:GLU:OE2	2.30	0.46
7:G:328:PRO:O	7:G:332:SER:OG	2.23	0.46
9:J:393:PHE:HA	9:J:396:LYS:HE3	1.96	0.46
1:A:441:LEU:HD22	2:B:560:ALA:HB1	1.98	0.46
3:C:819:GLY:O	3:C:947:ASP:N	2.48	0.46
5:E:442:LEU:HD23	5:E:445:LEU:HD13	1.97	0.46
5:E:827:PHE:HD2	5:E:828:GLU:HG2	1.80	0.46
2:B:207:LYS:HB3	2:B:239:VAL:HG21	1.97	0.46
3:C:1219:LEU:O	3:C:1221:MET:HG2	2.16	0.46
6:F:611:THR:HG21	6:F:622:ILE:HD11	1.97	0.46
9:I:170:ASP:O	9:I:174:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:536:ASP:H	4:D:1323:LEU:HD23	1.81	0.46
3:C:1207:PRO:HG2	5:E:858:ILE:HG22	1.98	0.46
4:D:1649:SER:HB3	4:D:1793:HIS:HB3	1.96	0.46
14:O:155:LYS:HG3	14:O:156:LYS:H	1.81	0.46
1:A:231:VAL:HG21	14:O:155:LYS:HA	1.98	0.46
1:A:467:ASP:N	1:A:467:ASP:OD1	2.49	0.46
2:B:267:THR:HA	2:B:270:LYS:HB2	1.97	0.46
2:B:548:LYS:HD3	2:B:549:GLU:HG3	1.97	0.46
3:C:1109:LEU:HD11	3:C:1273:LEU:HB3	1.97	0.46
4:D:1879:ASP:OD1	4:D:1879:ASP:N	2.39	0.46
6:F:521:ILE:HG22	6:F:529:ARG:HH22	1.81	0.46
6:F:691:LEU:HD13	6:F:704:VAL:HG12	1.96	0.46
9:I:267:LEU:HD12	9:I:281:ILE:HG23	1.97	0.46
1:A:504:LYS:NZ	6:F:439:GLY:O	2.48	0.46
3:C:171:THR:O	3:C:175:LEU:HB2	2.15	0.46
3:C:206:LYS:HD2	3:C:206:LYS:HA	1.71	0.46
3:C:1177:GLU:HB2	4:D:1958:LYS:HB2	1.97	0.46
4:D:56:ARG:HH21	4:D:1588:LEU:HD23	1.81	0.46
1:A:645:PRO:HA	1:A:648:VAL:HG12	1.98	0.46
4:D:1049:ARG:HD2	4:D:1050:PHE:HB2	1.98	0.46
4:D:2226:HIS:CE1	6:F:778:ASN:HB3	2.50	0.46
5:E:538:ARG:NE	5:E:558:GLU:OE1	2.46	0.46
6:F:585:ARG:HG2	6:F:619:LEU:HD11	1.98	0.46
9:I:293:THR:HA	9:I:296:VAL:HG22	1.98	0.46
1:A:515:LEU:HD21	1:A:552:ARG:HG2	1.98	0.46
2:B:981:PRO:HA	4:D:2279:LEU:HD13	1.97	0.46
3:C:978:ASP:OD2	3:C:978:ASP:N	2.41	0.46
4:D:556:ILE:HG22	4:D:1052:PHE:HD2	1.81	0.46
1:A:676:LEU:O	1:A:680:THR:OG1	2.28	0.45
2:B:365:PHE:HB2	2:B:400:VAL:HG21	1.98	0.45
4:D:1365:VAL:HG21	16:R:89:LEU:HD13	1.97	0.45
4:D:1984:ASP:OD1	4:D:1984:ASP:N	2.47	0.45
5:E:625:LYS:HG3	5:E:665:SER:HA	1.97	0.45
1:A:157:LEU:HD11	1:A:219:LEU:HD12	1.97	0.45
3:C:1000:VAL:HG13	3:C:1004:LEU:HD23	1.97	0.45
3:C:1104:ARG:HG3	3:C:1164:SER:HB3	1.98	0.45
16:R:310:ALA:O	16:R:313:GLN:HG3	2.16	0.45
1:A:418:ASP:O	1:A:422:SER:OG	2.32	0.45
1:A:849:LEU:HG	7:G:182:GLN:HB3	1.97	0.45
6:F:507:PHE:HD1	6:F:552:ILE:HG23	1.81	0.45
1:A:827:LYS:HG2	4:D:1919:VAL:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:VAL:HA	2:B:133:PHE:HB3	1.98	0.45
3:C:942:ARG:HE	3:C:945:ARG:HD3	1.81	0.45
9:I:138:PHE:HB3	9:I:143:GLU:HB2	1.97	0.45
16:R:124:LYS:HD3	16:R:151:VAL:HG21	1.97	0.45
4:D:100:SER:HB2	4:D:103:LEU:HB3	1.98	0.45
1:A:128:LEU:HD11	7:G:138:LEU:HA	1.97	0.45
4:D:2279:LEU:HD23	4:D:2279:LEU:HA	1.82	0.45
9:I:291:ALA:O	9:I:295:VAL:HG23	2.17	0.45
9:I:363:SER:HA	9:I:366:GLN:HE22	1.81	0.45
1:A:213:ASN:HD21	16:R:212:PRO:HD3	1.81	0.45
2:B:321:PHE:HB3	2:B:326:VAL:HG21	1.97	0.45
3:C:496:ARG:NH1	11:L:14:LEU:HD22	2.32	0.45
4:D:1365:VAL:HG11	16:R:89:LEU:HD11	1.99	0.45
9:J:305:ALA:HB3	9:J:309:MET:HG3	1.98	0.45
2:B:220:LYS:HG2	2:B:244:TRP:CD1	2.51	0.45
6:F:469:VAL:HB	6:F:504:SER:HA	1.98	0.45
9:I:255:ILE:HD11	9:I:264:LEU:HD23	1.99	0.45
9:J:329:ASP:N	9:J:329:ASP:OD1	2.50	0.45
3:C:571:LEU:O	3:C:575:MET:HE3	2.16	0.45
5:E:606:ARG:HG2	5:E:607:PRO:HD2	1.98	0.45
6:F:661:SER:OG	6:F:662:LEU:N	2.49	0.45
1:A:157:LEU:HD23	1:A:218:LYS:HD2	1.98	0.45
3:C:177:THR:HG22	3:C:205:VAL:HG22	1.99	0.45
7:G:263:HIS:CE1	7:G:353:LEU:HD21	2.52	0.45
9:J:162:ARG:NE	9:J:304:SER:OG	2.47	0.45
4:D:1677:PHE:HE1	4:D:1737:GLN:HE22	1.65	0.44
5:E:611:LYS:HA	5:E:611:LYS:HD2	1.87	0.44
7:G:192:TRP:CE3	7:G:196:VAL:HG11	2.52	0.44
9:J:176:ALA:HA	9:J:179:VAL:HG12	1.99	0.44
1:A:646:ARG:NH1	6:F:768:GLY:O	2.50	0.44
2:B:817:PHE:HA	2:B:820:MET:HG3	1.99	0.44
3:C:308:ILE:HD13	4:D:1319:LEU:HA	1.99	0.44
5:E:420:ARG:NH1	5:E:493:GLN:OE1	2.50	0.44
9:J:166:MET:HE3	9:J:171:LEU:HD13	1.98	0.44
16:R:281:LEU:HD12	16:R:295:ILE:HD11	1.99	0.44
1:A:444:LEU:HD21	1:A:473:LEU:HG	1.99	0.44
2:B:690:ASP:OD1	2:B:690:ASP:N	2.50	0.44
3:C:1205:ASP:OD2	3:C:1295:ASN:ND2	2.49	0.44
6:F:445:GLY:HA3	6:F:571:PHE:HA	2.00	0.44
10:K:25:LYS:HA	10:K:25:LYS:HD2	1.84	0.44
1:A:421:GLY:HA2	1:A:440:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:TRP:HA	2:B:142:TRP:HB2	1.99	0.44
2:B:615:ILE:HD12	2:B:618:LEU:HD12	1.99	0.44
5:E:587:ASP:N	5:E:587:ASP:OD1	2.48	0.44
6:F:417:LYS:O	6:F:420:LEU:HB2	2.17	0.44
6:F:685:MET:HG2	6:F:706:VAL:HG11	2.00	0.44
3:C:280:LYS:HE2	3:C:284:ARG:HG3	2.00	0.44
2:B:680:SER:O	2:B:680:SER:OG	2.31	0.44
3:C:534:ARG:HH12	3:C:589:ILE:HB	1.83	0.44
6:F:481:GLU:OE2	6:F:490:ARG:NH1	2.50	0.44
9:I:307:LEU:HD22	9:J:100:LEU:HD22	1.99	0.44
9:J:103:LYS:NZ	9:J:133:SER:OG	2.50	0.44
10:K:42:LYS:H	10:K:42:LYS:HG2	1.55	0.44
5:E:766:ARG:HA	5:E:766:ARG:HD3	1.79	0.44
6:F:628:ILE:O	6:F:632:ARG:NH1	2.51	0.44
9:I:251:ASP:OD1	9:I:251:ASP:N	2.49	0.44
10:K:18:LYS:HA	10:K:18:LYS:HD2	1.66	0.44
16:R:118:SER:HB3	16:R:165:SER:HB3	1.98	0.44
1:A:814:ASP:OD1	1:A:814:ASP:N	2.42	0.44
3:C:1064:GLU:HA	3:C:1067:VAL:HG22	1.99	0.44
6:F:865:LEU:O	6:F:869:MET:HG3	2.18	0.44
9:J:157:PRO:HA	9:J:198:ILE:HB	1.99	0.44
9:J:343:LEU:HD23	9:J:344:PRO:HD2	1.99	0.44
7:G:161:LEU:HD11	7:G:192:TRP:CD1	2.53	0.44
9:J:253:PRO:HB2	9:J:266:LEU:HB2	2.00	0.44
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.83	0.43
1:A:398:LYS:HB3	1:A:442:GLN:HE21	1.82	0.43
1:A:844:LYS:HB3	7:G:235:TYR:CZ	2.53	0.43
3:C:391:LEU:O	3:C:395:LYS:HG3	2.18	0.43
4:D:1817:LEU:HD23	4:D:1822:GLN:HG2	2.00	0.43
7:G:240:ASP:HB3	7:G:243:TRP:HD1	1.82	0.43
9:I:368:LEU:HB3	9:I:372:GLU:HB2	2.00	0.43
12:M:9:VAL:HG11	16:R:222:ASP:HB2	2.00	0.43
1:A:594:LEU:HD12	1:A:644:ALA:HB2	2.01	0.43
3:C:823:VAL:HG23	3:C:951:HIS:HA	1.99	0.43
4:D:1022:SER:OG	4:D:1023:LEU:N	2.51	0.43
6:F:438:ARG:HD2	6:F:438:ARG:O	2.17	0.43
9:I:253:PRO:HB2	9:I:266:LEU:HB2	1.98	0.43
10:K:15:ILE:O	10:K:16:HIS:ND1	2.51	0.43
1:A:708:ARG:HH22	6:F:779:PHE:HA	1.83	0.43
2:B:225:ILE:HB	2:B:233:VAL:HG13	1.99	0.43
2:B:225:ILE:HD11	2:B:235:ASP:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:906:MET:N	4:D:2240:ASN:OD1	2.39	0.43
2:B:920:ARG:HH21	9:J:354:LYS:HZ3	1.65	0.43
3:C:994:PRO:HA	3:C:997:LEU:HB2	1.99	0.43
9:I:185:ALA:O	9:I:189:ASN:ND2	2.31	0.43
9:I:335:PHE:HA	9:I:347:ALA:HA	2.00	0.43
1:A:550:ILE:HD11	6:F:438:ARG:NE	2.34	0.43
6:F:810:ASN:O	6:F:814:MET:HB2	2.18	0.43
2:B:572:LYS:O	2:B:576:MET:HB2	2.18	0.43
3:C:313:GLU:O	3:C:316:GLU:HG2	2.19	0.43
3:C:573:LEU:HD23	3:C:573:LEU:HA	1.88	0.43
4:D:1980:LEU:HA	4:D:1981:PRO:HD2	1.88	0.43
5:E:914:GLN:H	5:E:914:GLN:HG3	1.67	0.43
6:F:472:PHE:HB3	6:F:474:ILE:HD11	2.00	0.43
6:F:599:ALA:HB2	6:F:637:GLU:HG3	2.01	0.43
16:R:190:ILE:HD12	16:R:190:ILE:HA	1.88	0.43
2:B:764:ARG:HH22	2:B:944:THR:HG21	1.82	0.43
3:C:564:LYS:HE3	3:C:564:LYS:HB2	1.83	0.43
16:R:320:SER:HA	16:R:323:ARG:HG2	2.00	0.43
3:C:943:PRO:HG2	5:E:656:LEU:HD13	2.00	0.43
5:E:646:LYS:O	5:E:649:GLN:HG2	2.18	0.43
2:B:381:GLU:HA	2:B:421:LEU:HD11	2.00	0.43
3:C:485:ILE:HG13	10:K:70:LEU:HD21	2.01	0.43
4:D:1565:GLY:HA2	4:D:1824:LYS:HG2	2.01	0.43
5:E:759:LEU:HG	5:E:861:MET:CE	2.49	0.43
9:J:208:ILE:HA	9:J:394:ALA:HB2	2.01	0.43
1:A:497:LEU:HB3	1:A:531:LEU:HD23	2.00	0.43
3:C:273:ILE:O	3:C:277:GLU:HG2	2.18	0.43
9:I:228:THR:HG22	9:I:258:HIS:HB2	2.01	0.43
10:K:34:ASP:OD1	10:K:37:ARG:NH1	2.52	0.43
1:A:493:ARG:O	1:A:497:LEU:HG	2.19	0.43
2:B:220:LYS:HG2	2:B:244:TRP:HD1	1.84	0.43
4:D:1841:MET:HB3	4:D:1847:PHE:HB3	2.00	0.43
4:D:2204:THR:O	4:D:2204:THR:OG1	2.32	0.43
5:E:496:GLY:HA2	5:E:499:PHE:HD2	1.84	0.43
5:E:522:LYS:HE2	5:E:575:LYS:HD3	2.01	0.43
5:E:539:GLN:HG3	5:E:541:ILE:H	1.83	0.43
2:B:862:ILE:HA	2:B:874:LEU:HD13	2.01	0.42
5:E:630:VAL:HG13	5:E:635:TYR:HE2	1.84	0.42
2:B:746:LEU:HG	2:B:750:GLU:HG3	2.02	0.42
3:C:1239:LEU:HD21	3:C:1292:SER:HB3	2.01	0.42
4:D:134:ARG:HG3	4:D:501:TRP:HZ2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:721:ARG:O	5:E:740:HIS:ND1	2.52	0.42
5:E:762:LEU:HD11	5:E:825:LEU:HD21	2.01	0.42
5:E:804:PRO:HG2	5:E:853:ARG:NH1	2.34	0.42
6:F:691:LEU:HG	6:F:821:LEU:HD21	2.00	0.42
6:F:748:THR:O	6:F:748:THR:OG1	2.34	0.42
9:I:286:VAL:O	9:I:290:ASN:ND2	2.39	0.42
9:J:267:LEU:HD12	9:J:281:ILE:HG23	2.01	0.42
11:L:21:LEU:HD23	11:L:21:LEU:HA	1.86	0.42
2:B:222:LYS:NZ	2:B:320:GLU:HG2	2.34	0.42
2:B:438:LEU:HD12	2:B:438:LEU:HA	1.88	0.42
2:B:933:LEU:HD23	2:B:933:LEU:HA	1.90	0.42
3:C:250:LYS:O	3:C:254:LYS:HG2	2.19	0.42
3:C:979:LEU:HD23	3:C:1060:LYS:HB2	2.01	0.42
3:C:1058:LEU:HD12	3:C:1058:LEU:HA	1.83	0.42
3:C:1190:GLU:OE1	4:D:2055:GLN:NE2	2.53	0.42
4:D:500:ARG:HA	4:D:500:ARG:HD3	1.73	0.42
4:D:1582:ASP:HA	4:D:1585:LYS:HE2	2.02	0.42
6:F:434:MET:HB2	6:F:437:ARG:HH21	1.83	0.42
6:F:572:ASP:OD1	6:F:572:ASP:N	2.44	0.42
6:F:678:VAL:HG11	6:F:729:VAL:HA	2.01	0.42
10:K:66:LEU:HD23	10:K:66:LEU:H	1.84	0.42
1:A:208:PRO:HG2	16:R:109:ARG:HG3	2.02	0.42
1:A:584:LEU:HD11	1:A:613:ILE:HD13	2.01	0.42
2:B:821:LYS:NZ	4:D:1984:ASP:O	2.52	0.42
5:E:614:LEU:O	5:E:618:LYS:HG2	2.19	0.42
5:E:803:ASN:OD1	6:F:734:ARG:NH2	2.36	0.42
6:F:615:VAL:HG13	6:F:617:ALA:H	1.85	0.42
7:G:224:VAL:O	7:G:228:LYS:HG2	2.20	0.42
1:A:93:ARG:NE	2:B:255:LEU:O	2.52	0.42
1:A:834:GLU:O	1:A:838:GLN:HB3	2.20	0.42
2:B:459:LYS:HE2	2:B:459:LYS:HB2	1.86	0.42
5:E:450:LYS:HG3	5:E:451:ASN:OD1	2.19	0.42
5:E:664:ASN:OD1	5:E:664:ASN:N	2.53	0.42
7:G:192:TRP:CE2	7:G:196:VAL:HG21	2.55	0.42
7:G:327:HIS:HD2	7:G:390:LYS:HG2	1.83	0.42
9:I:335:PHE:HD1	9:I:347:ALA:HB2	1.84	0.42
3:C:169:ASP:O	3:C:173:ARG:HG3	2.19	0.42
6:F:412:VAL:HG11	6:F:459:LEU:HD23	2.01	0.42
7:G:366:LYS:HD3	7:G:366:LYS:HA	1.93	0.42
9:J:202:VAL:HG22	9:J:206:VAL:HG23	2.01	0.42
2:B:352:ARG:HA	2:B:354:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:234:LEU:HA	3:C:234:LEU:HD23	1.80	0.42
3:C:303:GLY:O	3:C:307:LEU:HG	2.19	0.42
3:C:305:ARG:HG3	3:C:586:LEU:HD11	2.01	0.42
4:D:105:LEU:HD23	4:D:108:LEU:HD12	2.00	0.42
9:I:248:ILE:HD12	9:I:248:ILE:H	1.85	0.42
16:R:308:LEU:HD23	16:R:308:LEU:HA	1.91	0.42
1:A:735:ASP:OD2	6:F:857:ARG:NH1	2.52	0.42
2:B:572:LYS:HA	2:B:575:GLU:HG2	2.02	0.42
3:C:401:LEU:HD12	3:C:401:LEU:HA	1.81	0.42
3:C:586:LEU:HD13	4:D:1318:SER:HA	2.01	0.42
7:G:199:ALA:CB	18:G:401:PX2:C4	2.90	0.42
7:G:216:TYR:HE1	7:G:336:LEU:HD22	1.84	0.42
2:B:407:TYR:O	2:B:411:THR:HG22	2.20	0.42
3:C:175:LEU:HA	3:C:178:VAL:HG22	2.02	0.42
3:C:1195:MET:HG3	3:C:1201:TRP:HE3	1.85	0.42
5:E:433:ALA:HB1	5:E:615:ASP:HB3	2.01	0.42
7:G:190:PHE:O	7:G:194:THR:OG1	2.33	0.42
7:G:216:TYR:CE1	7:G:336:LEU:HD22	2.54	0.42
9:J:283:GLU:HA	9:J:286:VAL:HG12	2.01	0.42
1:A:355:HIS:CE1	1:A:484:ARG:HB3	2.55	0.42
6:F:512:ASP:N	6:F:512:ASP:OD1	2.52	0.42
16:R:85:ILE:HA	16:R:88:ASP:HB3	2.02	0.42
1:A:701:VAL:HG13	6:F:780:TRP:HB3	2.01	0.41
2:B:269:ALA:HA	2:B:272:LYS:HD2	2.01	0.41
2:B:716:MET:N	2:B:716:MET:SD	2.93	0.41
2:B:967:PRO:HG2	2:B:969:MET:SD	2.59	0.41
3:C:540:MET:HG2	3:C:555:ILE:HD11	2.01	0.41
3:C:1030:SER:HA	3:C:1033:VAL:HG22	2.02	0.41
5:E:725:VAL:HG13	5:E:737:VAL:HB	2.01	0.41
4:D:1569:ILE:HD12	4:D:1569:ILE:HA	1.91	0.41
4:D:1609:GLN:HE21	4:D:1613:TYR:HD2	1.67	0.41
1:A:153:PHE:HZ	1:A:219:LEU:HD11	1.83	0.41
1:A:378:PHE:HZ	1:A:407:TYR:HD1	1.67	0.41
3:C:288:ILE:HD13	3:C:288:ILE:HA	1.90	0.41
4:D:1030:ALA:HB1	12:M:5:VAL:HG11	2.02	0.41
4:D:1562:ASN:OD1	7:G:237:ARG:NH2	2.53	0.41
5:E:460:ILE:HA	6:F:627:ALA:HB1	2.01	0.41
5:E:554:THR:O	5:E:558:GLU:HG2	2.21	0.41
7:G:389:HIS:CD2	7:G:394:PHE:HA	2.56	0.41
9:I:103:LYS:NZ	9:I:133:SER:O	2.52	0.41
4:D:109:LEU:HD23	4:D:109:LEU:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:131:LYS:HE3	7:G:131:LYS:HB2	1.77	0.41
2:B:431:MET:O	2:B:435:ILE:HG12	2.20	0.41
3:C:880:ILE:HA	3:C:925:VAL:O	2.21	0.41
3:C:1184:GLU:O	3:C:1187:LYS:HB2	2.19	0.41
5:E:749:PHE:HE1	6:F:664:THR:HG23	1.84	0.41
6:F:700:GLU:H	6:F:700:GLU:HG2	1.63	0.41
8:H:110:ASP:OD1	8:H:110:ASP:N	2.47	0.41
2:B:358:PRO:HG2	2:B:398:TYR:CD2	2.56	0.41
2:B:828:HIS:HB3	2:B:832:CYS:SG	2.61	0.41
4:D:1024:ILE:HD12	4:D:1024:ILE:HA	1.85	0.41
6:F:602:LEU:HD21	6:F:604:TYR:CZ	2.56	0.41
8:H:94:GLU:H	8:H:94:GLU:HG2	1.67	0.41
9:I:243:LYS:HD3	9:I:243:LYS:HA	1.84	0.41
5:E:639:LEU:HD12	5:E:642:TRP:CE2	2.55	0.41
7:G:145:TYR:HA	7:G:148:TRP:HB2	2.03	0.41
9:I:110:THR:HG23	9:I:134:GLN:HB2	2.03	0.41
9:I:154:VAL:HG11	9:I:186:VAL:HG21	2.03	0.41
9:J:239:VAL:HG21	9:J:252:VAL:HG21	2.02	0.41
13:N:13:UNK:O	16:R:259:ARG:NH1	2.53	0.41
1:A:605:ILE:H	1:A:605:ILE:HG12	1.73	0.41
1:A:803:ALA:HA	1:A:804:PRO:HD3	1.92	0.41
1:A:855:PHE:OXT	7:G:364:LYS:NZ	2.54	0.41
2:B:543:ALA:O	2:B:546:LEU:HB3	2.21	0.41
2:B:712:GLU:O	2:B:716:MET:HG2	2.21	0.41
4:D:1731:ARG:HB2	4:D:1765:LEU:HD21	2.02	0.41
5:E:711:LEU:HD12	5:E:761:VAL:HG23	2.02	0.41
7:G:388:ARG:HH12	7:G:390:LYS:HB2	1.85	0.41
2:B:301:LEU:HA	2:B:304:GLU:HG3	2.03	0.41
2:B:354:TRP:HZ2	18:G:401:PX2:C16	2.34	0.41
3:C:598:GLN:O	3:C:602:LEU:HG	2.20	0.41
4:D:140:LEU:HD21	16:R:230:LEU:HD21	2.03	0.41
4:D:1023:LEU:HD12	4:D:1023:LEU:H	1.85	0.41
4:D:1970:ALA:HA	4:D:2260:LEU:HD13	2.03	0.41
5:E:749:PHE:CE1	6:F:664:THR:HG23	2.55	0.41
6:F:565:LEU:HD23	6:F:565:LEU:HA	1.89	0.41
7:G:354:LEU:HD23	7:G:354:LEU:HA	1.92	0.41
9:I:170:ASP:OD2	9:I:171:LEU:N	2.53	0.41
9:J:203:ASN:ND2	9:J:262:THR:HG21	2.36	0.41
4:D:2055:GLN:O	4:D:2059:TYR:HB2	2.21	0.41
4:D:2206:GLN:NE2	4:D:2216:ARG:O	2.54	0.41
5:E:759:LEU:HG	5:E:861:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:820:LYS:HA	6:F:820:LYS:HD2	1.89	0.41
9:J:206:VAL:HG13	9:J:224:LEU:HD21	2.03	0.41
4:D:105:LEU:HD23	4:D:105:LEU:HA	1.93	0.40
4:D:106:LYS:HD2	4:D:106:LYS:HA	1.88	0.40
5:E:621:ALA:HB1	5:E:626:MET:HG3	2.03	0.40
1:A:707:LEU:HD21	1:A:768:GLU:HB3	2.02	0.40
2:B:477:ASN:O	2:B:478:PHE:HB2	2.21	0.40
3:C:592:SER:OG	3:C:593:GLU:OE2	2.32	0.40
7:G:289:ILE:HA	7:G:292:THR:HG22	2.03	0.40
1:A:812:ILE:H	1:A:812:ILE:HG13	1.61	0.40
2:B:844:ASP:HB2	2:B:847:LYS:HG3	2.03	0.40
4:D:19:GLU:HG2	4:D:26:PHE:HE2	1.86	0.40
4:D:1351:LEU:HD12	4:D:1351:LEU:HA	1.94	0.40
6:F:472:PHE:HB2	6:F:506:VAL:HG12	2.03	0.40
6:F:610:MET:HG2	6:F:644:LEU:HD13	2.03	0.40
1:A:685:PHE:CZ	1:A:700:LEU:HB3	2.57	0.40
2:B:986:LEU:HD22	4:D:2273:ARG:NH2	2.36	0.40
3:C:615:ARG:HD2	3:C:615:ARG:HA	1.78	0.40
3:C:866:VAL:HA	3:C:869:LEU:HB2	2.02	0.40
4:D:103:LEU:HD23	4:D:104:TYR:HD2	1.86	0.40
5:E:721:ARG:HB3	5:E:740:HIS:HD1	1.87	0.40
9:I:160:VAL:HG11	9:I:174:ILE:HD13	2.03	0.40
1:A:440:LEU:O	1:A:444:LEU:HG	2.21	0.40
1:A:811:ILE:HD11	4:D:2251:ASN:HB3	2.03	0.40
2:B:327:GLU:HG3	16:R:232:THR:HG21	2.03	0.40
3:C:568:PHE:HD1	3:C:571:LEU:HD23	1.87	0.40
3:C:605:ARG:HH11	3:C:609:ARG:HD2	1.86	0.40
3:C:1257:LYS:O	3:C:1261:GLU:HG2	2.20	0.40
7:G:363:LYS:O	7:G:367:MET:HE3	2.21	0.40
9:I:371:TYR:HA	9:I:374:LYS:NZ	2.37	0.40
16:R:121:TYR:CE2	16:R:166:LYS:HB2	2.57	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	A	724/855 (85%)	693 (96%)	29 (4%)	2 (0%)	37 66
2	B	829/1008 (82%)	789 (95%)	38 (5%)	2 (0%)	44 71
3	C	911/1320 (69%)	888 (98%)	23 (2%)	0	100 100
4	D	775/2294 (34%)	712 (92%)	63 (8%)	0	100 100
5	E	494/946 (52%)	473 (96%)	21 (4%)	0	100 100
6	F	476/876 (54%)	462 (97%)	14 (3%)	0	100 100
7	G	283/396 (72%)	275 (97%)	8 (3%)	0	100 100
8	H	52/348 (15%)	48 (92%)	4 (8%)	0	100 100
9	I	315/403 (78%)	312 (99%)	3 (1%)	0	100 100
9	J	315/403 (78%)	312 (99%)	3 (1%)	0	100 100
10	K	65/80 (81%)	60 (92%)	5 (8%)	0	100 100
11	L	12/18 (67%)	11 (92%)	1 (8%)	0	100 100
12	M	8/11 (73%)	6 (75%)	2 (25%)	0	100 100
13	N	17/37 (46%)	15 (88%)	2 (12%)	0	100 100
14	O	15/17 (88%)	10 (67%)	5 (33%)	0	100 100
16	R	265/328 (81%)	255 (96%)	10 (4%)	0	100 100
All	All	5556/9340 (60%)	5321 (96%)	231 (4%)	4 (0%)	50 76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	PRO
2	B	477	ASN
2	B	478	PHE
1	A	812	ILE

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	A	628/744 (84%)	615 (98%)	13 (2%)	48 70
2	B	730/872 (84%)	713 (98%)	17 (2%)	45 68
3	C	817/1177 (69%)	799 (98%)	18 (2%)	47 69
4	D	753/2151 (35%)	725 (96%)	28 (4%)	29 56
5	E	423/817 (52%)	417 (99%)	6 (1%)	62 78
6	F	399/757 (53%)	391 (98%)	8 (2%)	50 71
7	G	246/347 (71%)	235 (96%)	11 (4%)	23 52
8	H	46/287 (16%)	45 (98%)	1 (2%)	47 69
9	I	261/332 (79%)	255 (98%)	6 (2%)	45 68
9	J	261/332 (79%)	260 (100%)	1 (0%)	89 93
10	K	62/73 (85%)	61 (98%)	1 (2%)	58 76
11	L	12/12 (100%)	12 (100%)	0	100 100
12	M	9/9 (100%)	8 (89%)	1 (11%)	5 19
13	N	16/16 (100%)	14 (88%)	2 (12%)	3 16
14	O	14/15 (93%)	13 (93%)	1 (7%)	12 37
16	R	236/286 (82%)	230 (98%)	6 (2%)	42 67
All	All	4913/8227 (60%)	4793 (98%)	120 (2%)	45 68

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	ARG
1	A	131	MET
1	A	140	TRP
1	A	164	TYR
1	A	229	PHE
1	A	270	TYR
1	A	354	LEU
1	A	526	PHE
1	A	586	TYR
1	A	620	ARG
1	A	631	ARG
1	A	665	SER
1	A	788	ARG
2	B	139	TRP
2	B	143	LYS
2	B	224	PHE

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Mol	Chain	Res	Type
2	B	229	ASP
2	B	235	ASP
2	B	290	TRP
2	B	320	GLU
2	B	365	PHE
2	B	386	LEU
2	B	663	TYR
2	B	726	TYR
2	B	729	ASP
2	B	742	MET
2	B	831	ARG
2	B	871	LEU
2	B	880	MET
2	B	970	PHE
3	C	231	ARG
3	C	264	MET
3	C	400	ASP
3	C	456	ARG
3	C	462	TRP
3	C	480	PHE
3	C	514	MET
3	C	587	MET
3	C	615	ARG
3	C	772	ARG
3	C	773	MET
3	C	840	GLU
3	C	991	LEU
3	C	1002	MET
3	C	1048	LYS
3	C	1115	ASP
3	C	1170	MET
3	C	1278	HIS
4	D	21	LYS
4	D	44	PHE
4	D	49	PHE
4	D	50	ARG
4	D	144	LYS
4	D	494	ARG
4	D	501	TRP
4	D	1012	LEU
4	D	1053	TYR
4	D	1317	LYS

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Mol	Chain	Res	Type
4	D	1531	ARG
4	D	1560	SER
4	D	1659	LYS
4	D	1724	ASP
4	D	1733	TYR
4	D	1784	ARG
4	D	1797	LYS
4	D	1813	LYS
4	D	1833	ARG
4	D	1903	ASP
4	D	1947	LYS
4	D	1978	TRP
4	D	1986	LYS
4	D	1994	PHE
4	D	2035	ARG
4	D	2045	MET
4	D	2225	LYS
4	D	2241	SER
5	E	457	LYS
5	E	684	ARG
5	E	751	ARG
5	E	758	ARG
5	E	766	ARG
5	E	921	PHE
6	F	512	ASP
6	F	556	ASN
6	F	605	MET
6	F	675	MET
6	F	690	PHE
6	F	719	SER
6	F	789	ASP
6	F	798	MET
7	G	114	MET
7	G	156	PHE
7	G	169	PHE
7	G	204	TYR
7	G	216	TYR
7	G	222	PHE
7	G	242	LYS
7	G	268	PHE
7	G	318	GLN
7	G	340	TYR

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Mol	Chain	Res	Type
7	G	367	MET
8	H	128	TRP
9	I	114	TYR
9	I	224	LEU
9	I	244	ASN
9	I	309	MET
9	I	370	GLU
9	I	371	TYR
9	J	371	TYR
10	K	77	HIS
12	M	6	TYR
13	N	33	TYR
13	N	34	ASN
14	O	147	ARG
16	R	88	ASP
16	R	92	LYS
16	R	203	TYR
16	R	301	TYR
16	R	315	LYS
16	R	328	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN
3	C	1178	ASN
3	C	1225	HIS
4	D	133	ASN
4	D	1609	GLN
5	E	800	ASN
9	I	134	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
18	PX2	G	401	-	24,24,35	1.97	7 (29%)	28,29,40	2.65	14 (50%)

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
18	PX2	G	401	-	-	9/26/26/37	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	G	401	PX2	O5-C4	4.56	1.46	1.33
18	G	401	PX2	O7-C2	-4.23	1.36	1.46
18	G	401	PX2	O8-C16	-4.10	1.10	1.22
18	G	401	PX2	P1-O3	-3.07	1.43	1.54
18	G	401	PX2	O6-C4	-2.74	1.14	1.22
18	G	401	PX2	C17-C16	-2.26	1.44	1.50
18	G	401	PX2	P1-O1	-2.22	1.46	1.54

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	401	PX2	O7-C16-C17	4.70	121.64	111.50
18	G	401	PX2	C19-C18-C17	-4.59	96.67	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	G	401	PX2	O5-C4-C5	4.57	126.25	111.91
18	G	401	PX2	C3-O5-C4	4.02	132.02	117.12
18	G	401	PX2	O1-P1-O4	-3.73	96.82	106.73
18	G	401	PX2	O7-C16-O8	-3.67	114.84	123.70
18	G	401	PX2	O5-C4-O6	-3.64	114.41	123.59
18	G	401	PX2	O7-C2-C3	-3.60	95.35	108.40
18	G	401	PX2	O4-P1-O2	3.38	115.94	106.47
18	G	401	PX2	C8-C7-C6	-2.88	99.80	114.42
18	G	401	PX2	C7-C6-C5	-2.67	103.58	113.19
18	G	401	PX2	C2-O7-C16	2.65	124.31	117.79
18	G	401	PX2	P1-O4-C1	2.48	125.12	118.30
18	G	401	PX2	O1-P1-O2	2.37	119.97	110.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	G	401	PX2	C1-O4-P1-O1
18	G	401	PX2	C1-O4-P1-O2
18	G	401	PX2	C1-O4-P1-O3
18	G	401	PX2	C4-C5-C6-C7
18	G	401	PX2	O8-C16-O7-C2
18	G	401	PX2	C17-C16-O7-C2
18	G	401	PX2	C7-C8-C9-C10
18	G	401	PX2	O6-C4-O5-C3
18	G	401	PX2	C5-C4-O5-C3

There are no ring outliers.

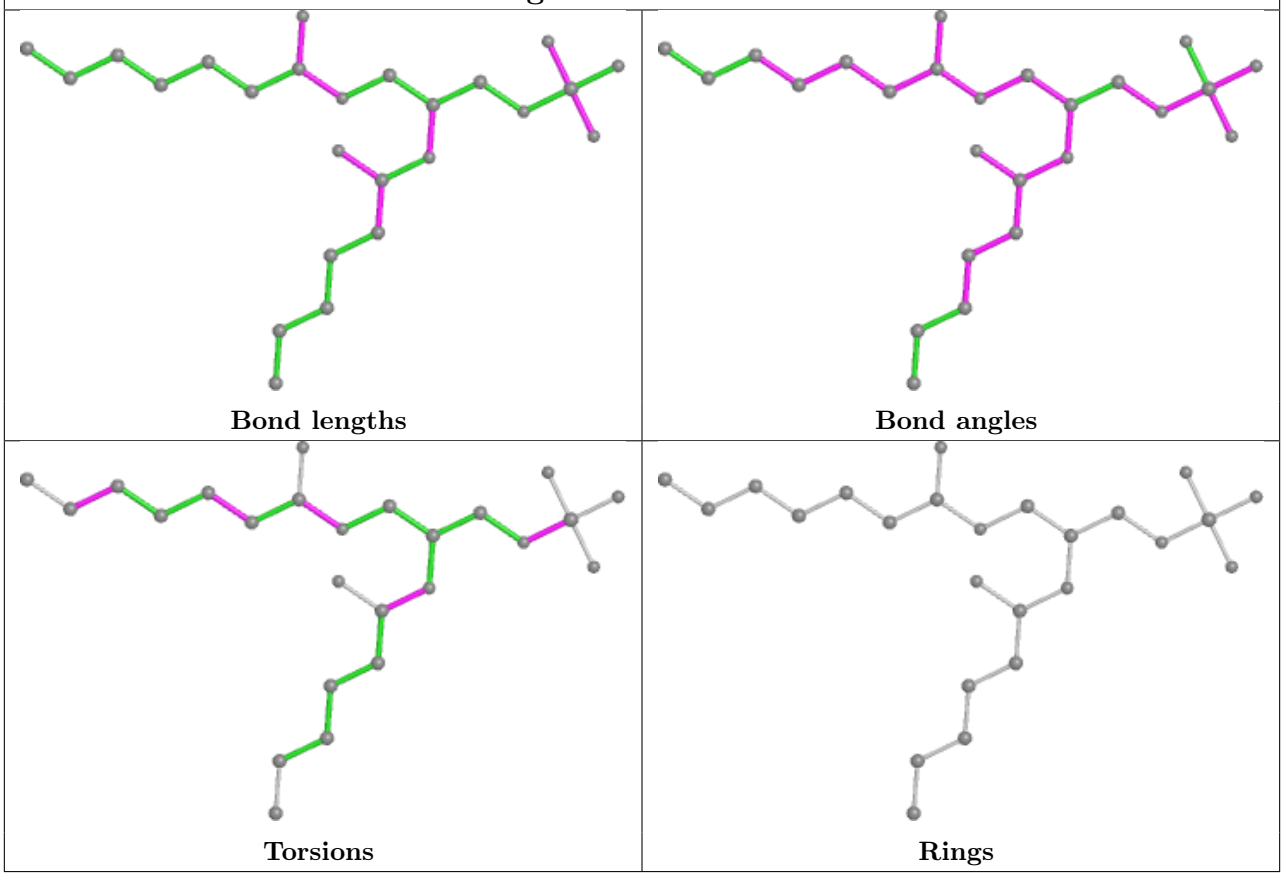
1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	G	401	PX2	10	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 PX2 G 401



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

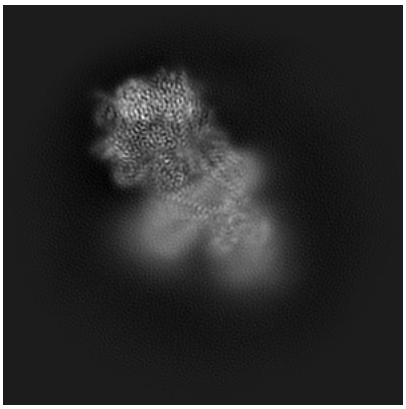
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38428. These allow visual inspection of the internal detail of the map and identification of artifacts.

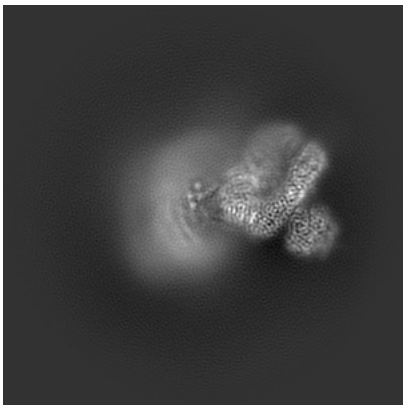
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

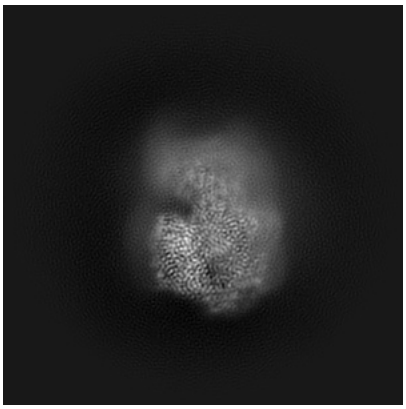
6.1.1 Primary map



X

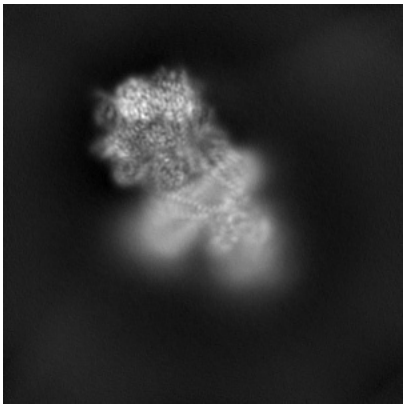


Y

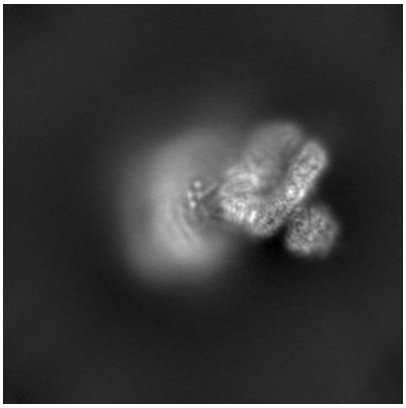


Z

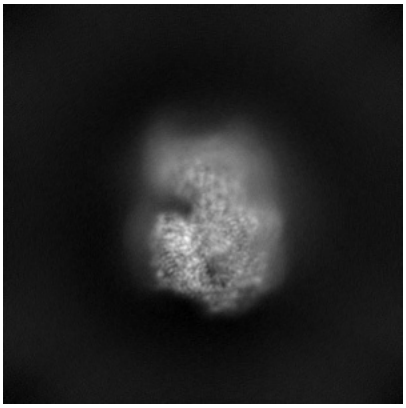
6.1.2 Raw map



X



Y

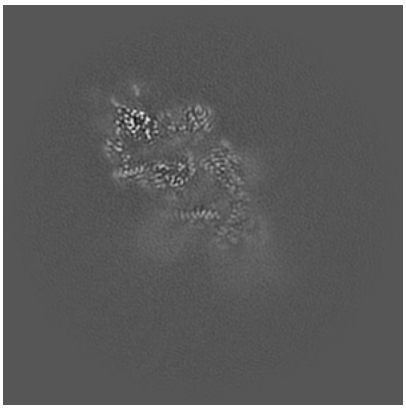


Z

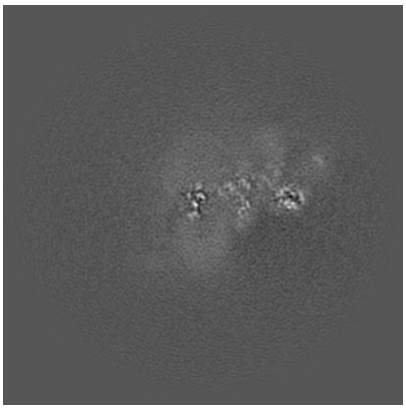
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

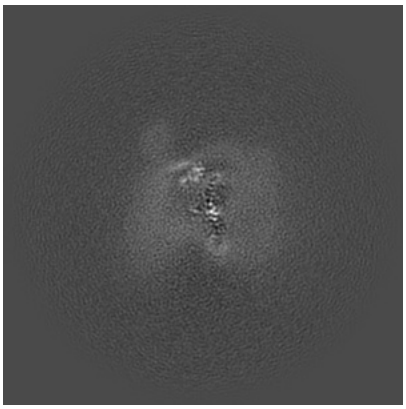
6.2.1 Primary map



X Index: 180

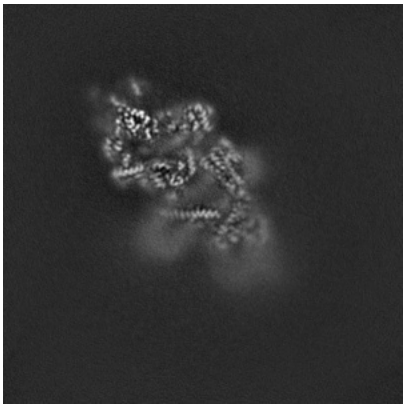


Y Index: 180

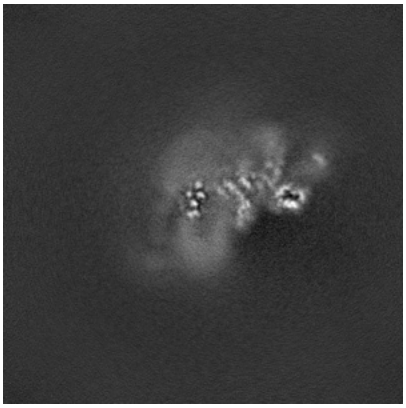


Z Index: 180

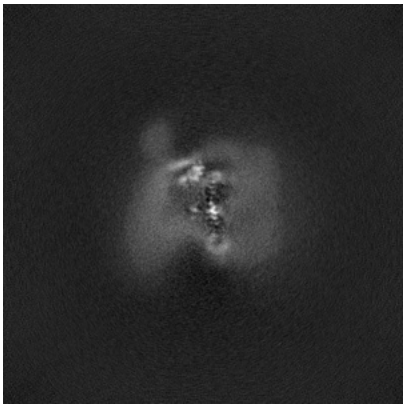
6.2.2 Raw map



X Index: 180



Y Index: 180

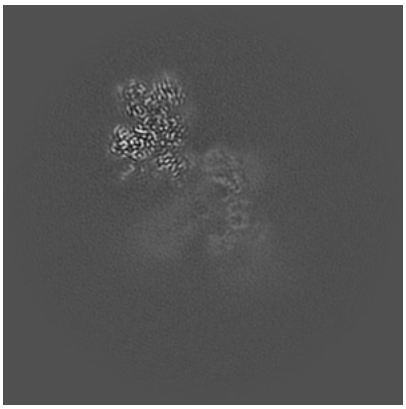


Z Index: 180

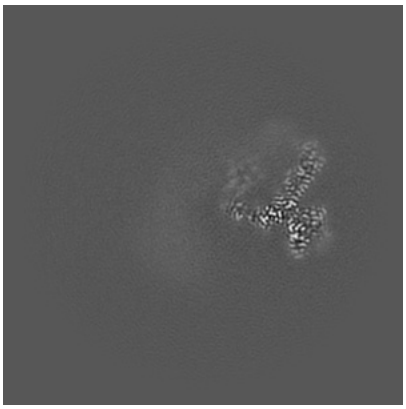
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

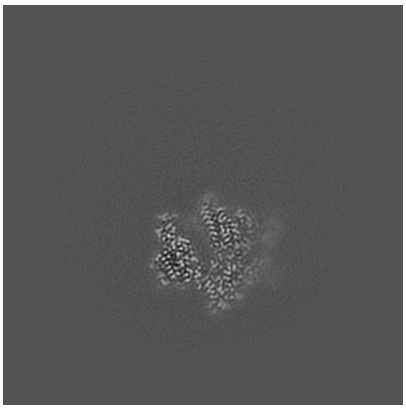
6.3.1 Primary map



X Index: 167

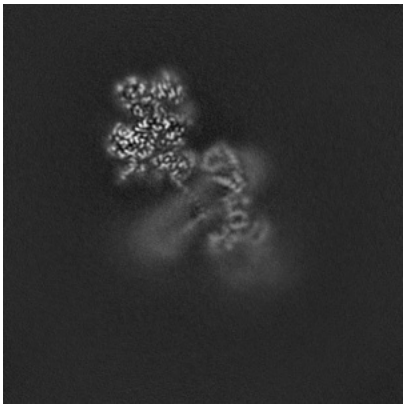


Y Index: 125

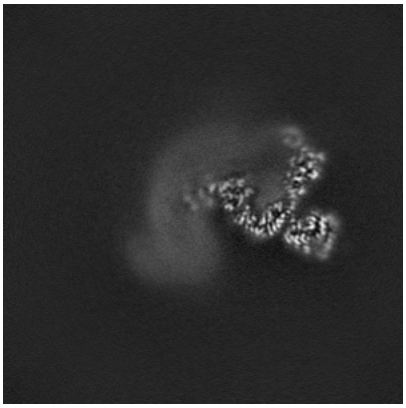


Z Index: 266

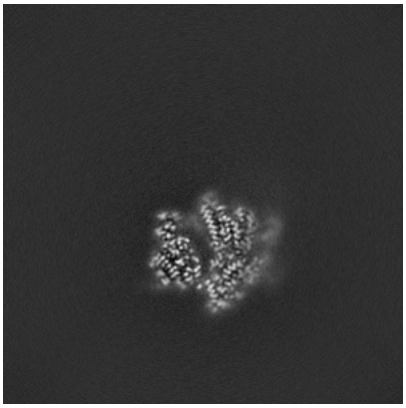
6.3.2 Raw map



X Index: 168



Y Index: 149

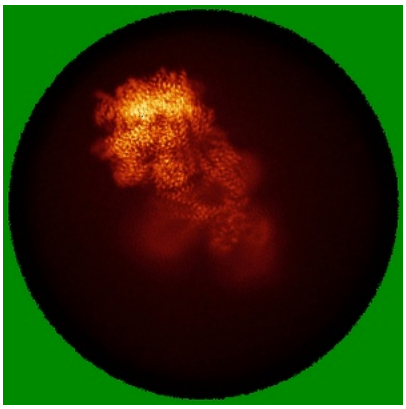


Z Index: 267

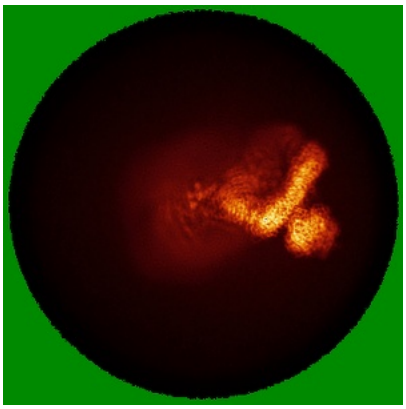
The images above show the largest variance slices of the map in three orthogonal directions.

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

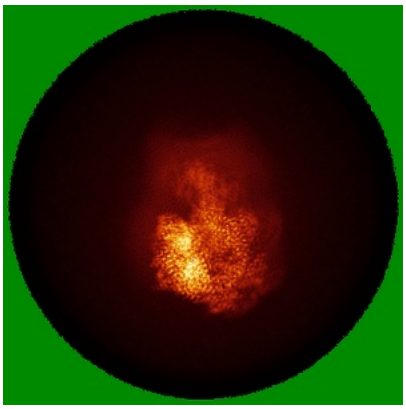
6.4.1 Primary map



X

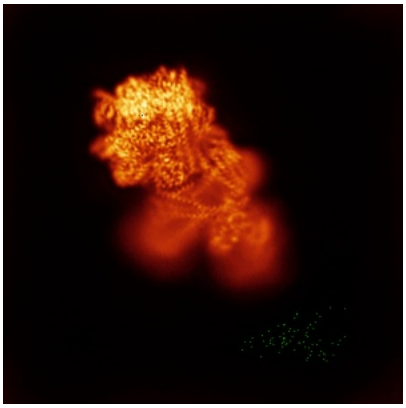


Y

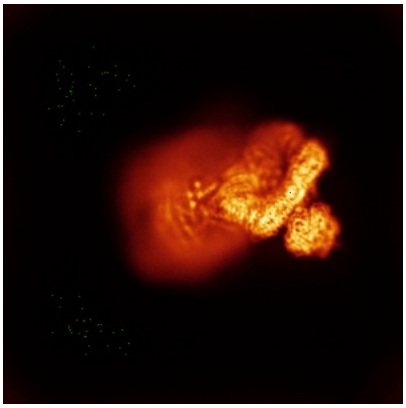


Z

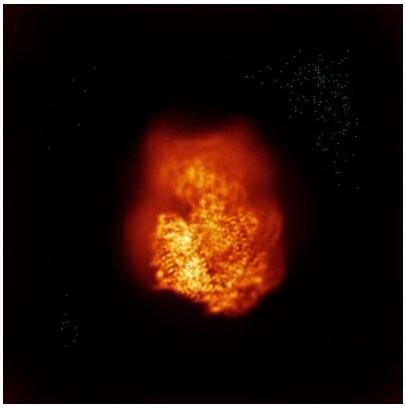
6.4.2 Raw map



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

6.5.2 Raw map

X Y Z

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

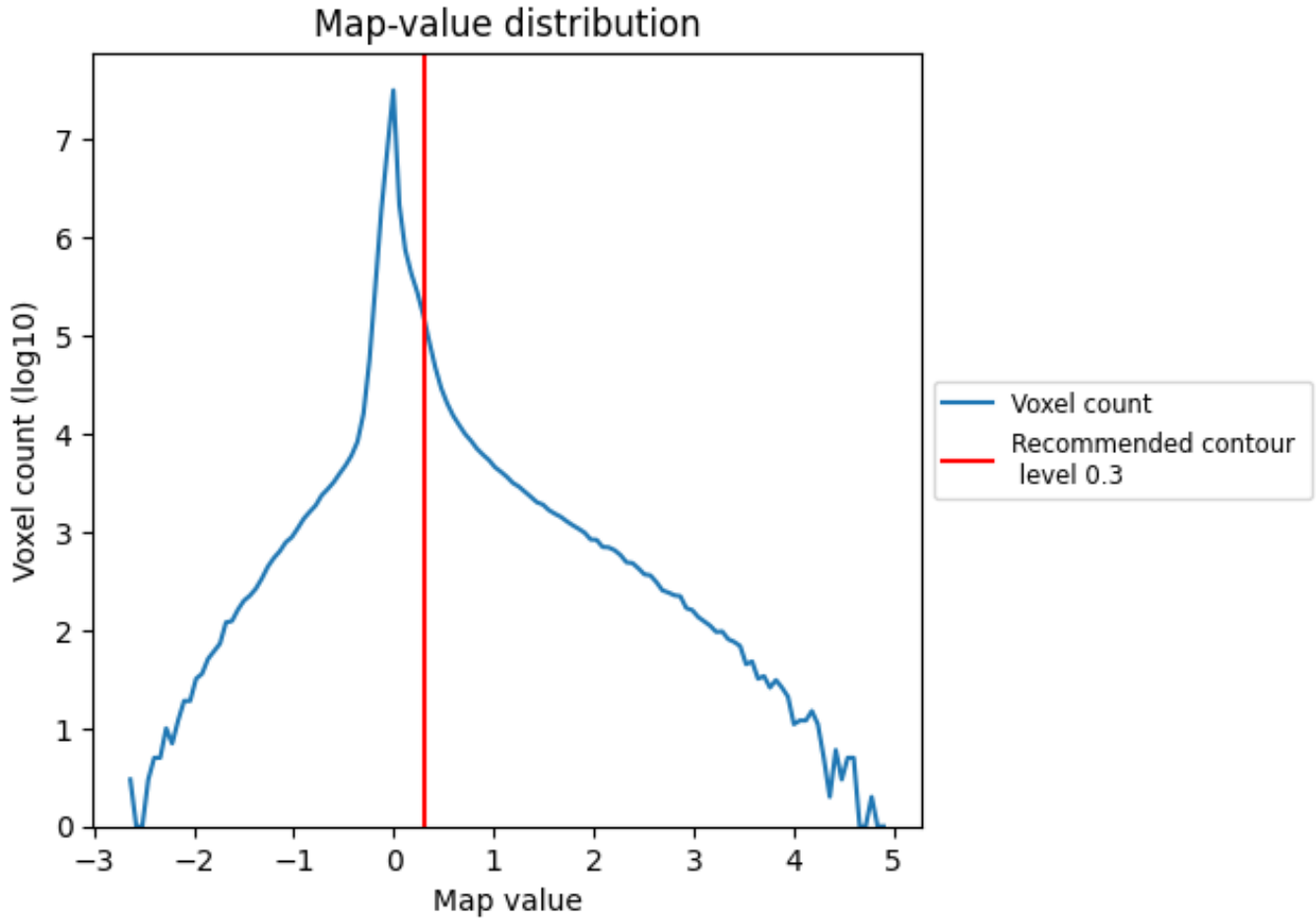
6.6 Mask visualisation (i)

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

7 Map analysis

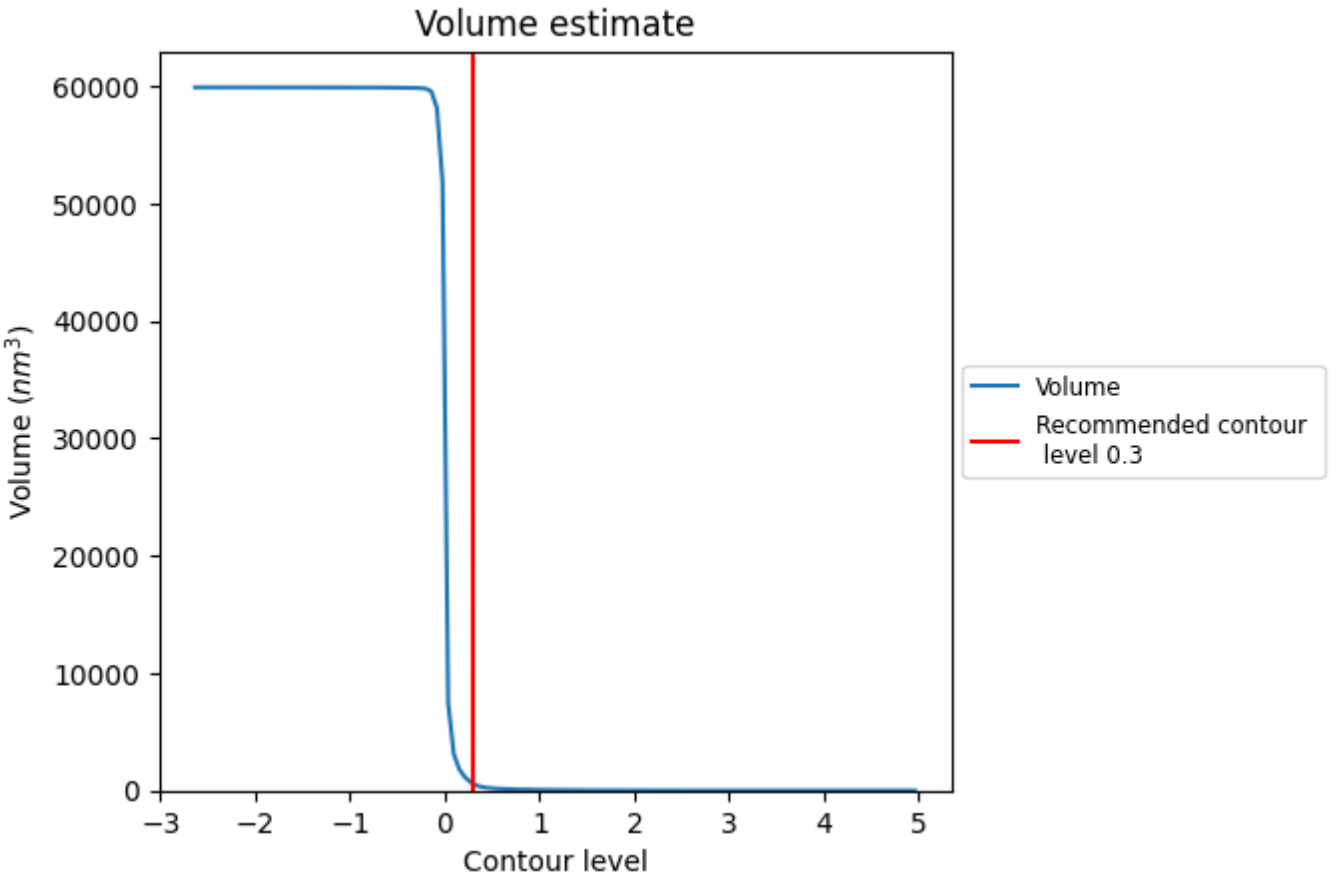
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

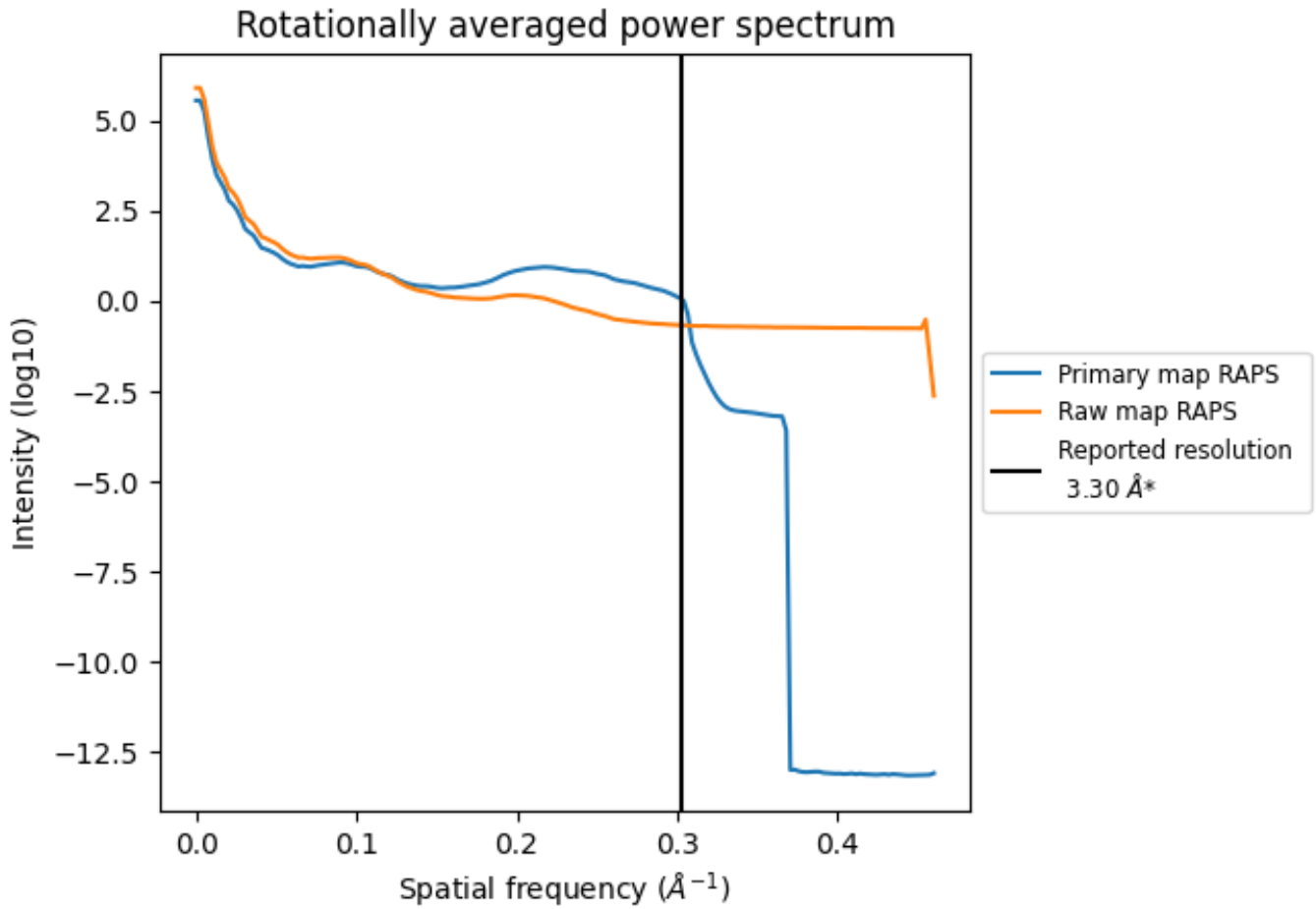
7.2 Volume estimate



The volume at the recommended contour level is 591 nm^3; this corresponds to an approximate mass of 534 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)

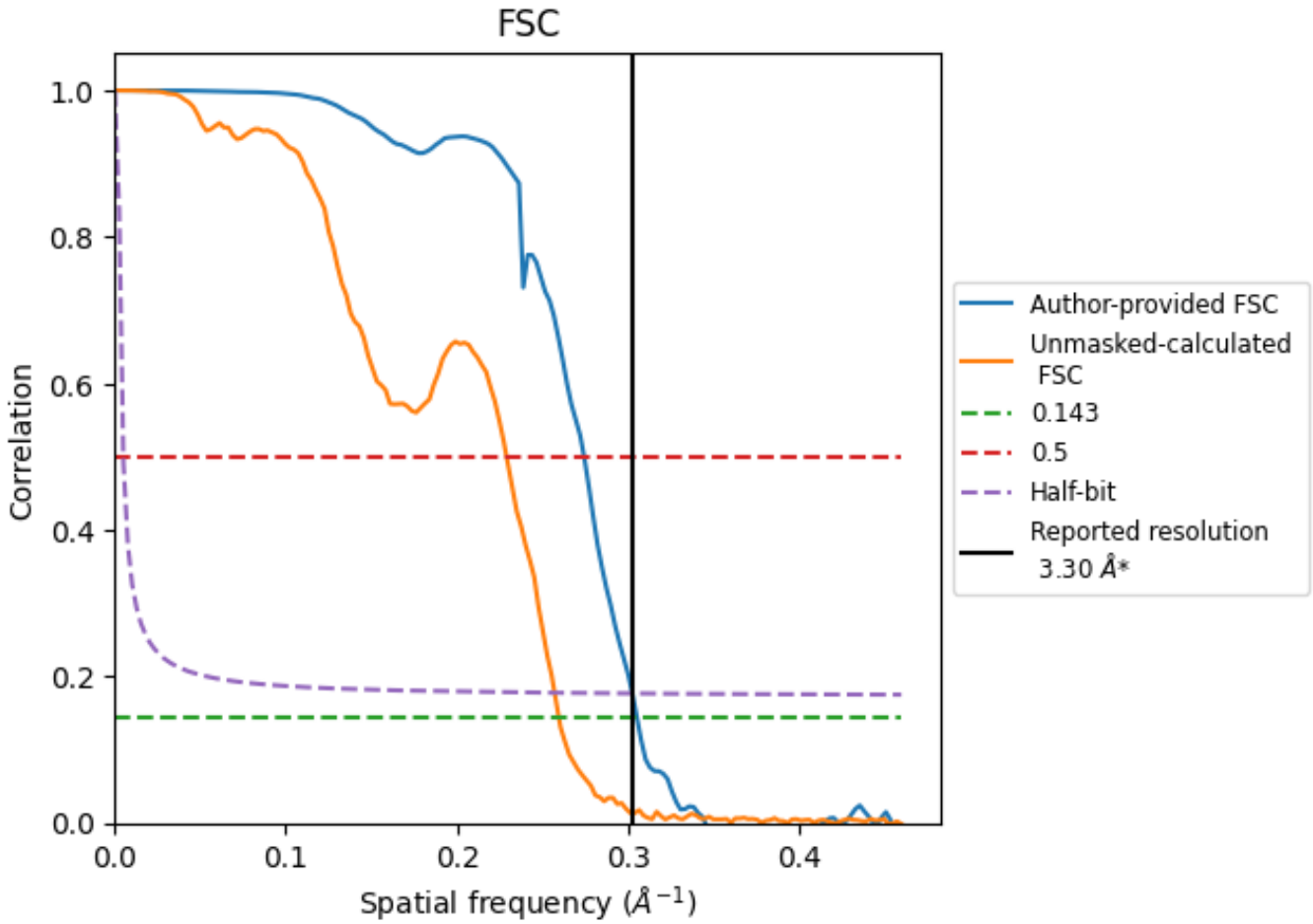


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

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 0.303 Å^{-1}

8.2 Resolution estimates (i)

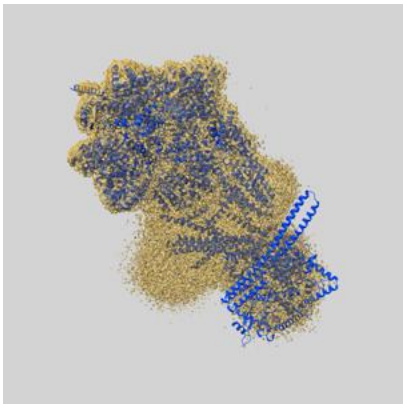
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.64	3.30
Unmasked-calculated*	3.85	4.36	3.89

*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 3.85 differs from the reported value 3.3 by more than 10 %

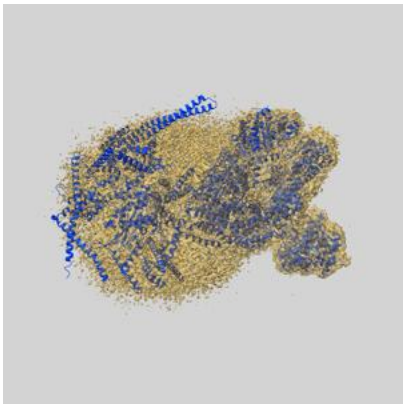
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38428 and PDB model 8XKV. Per-residue inclusion information can be found in section 3 on page 8.

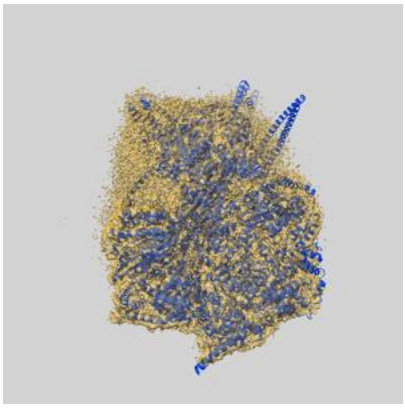
9.1 Map-model overlay



X



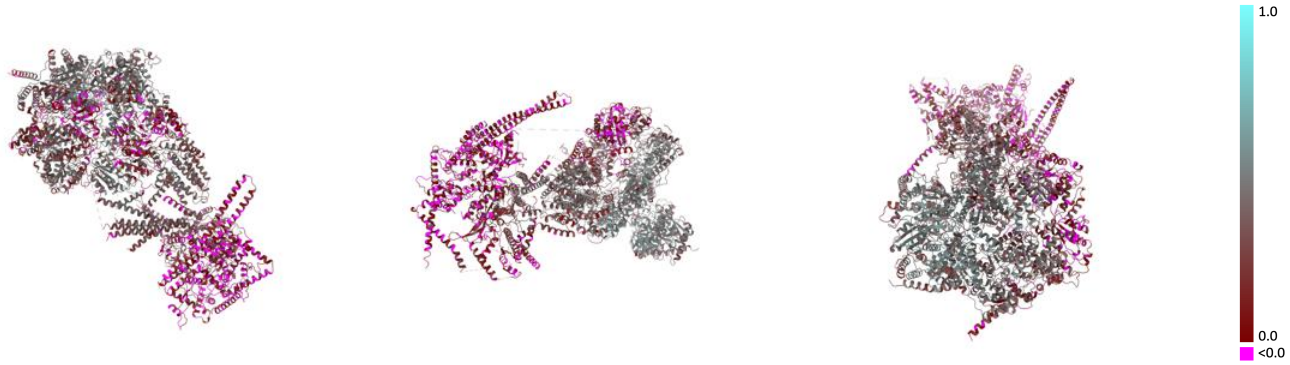
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

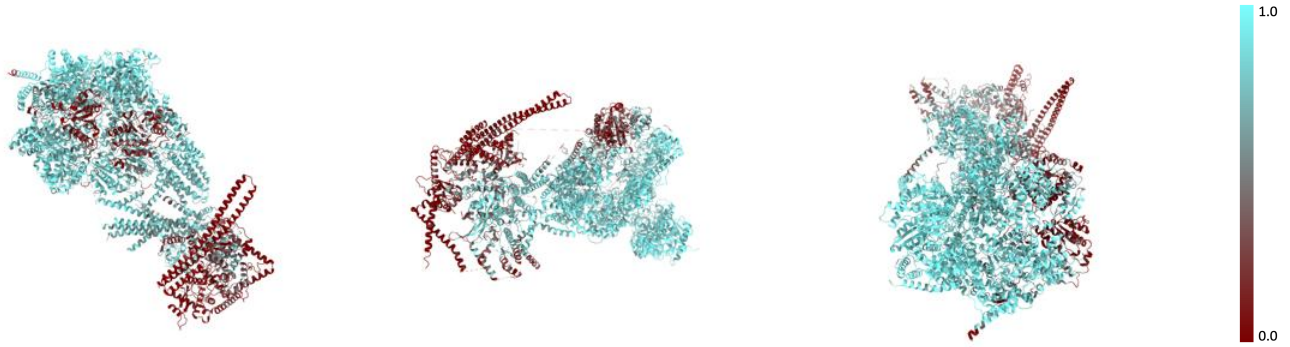
9.2 Q-score mapped to coordinate model (i)



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.

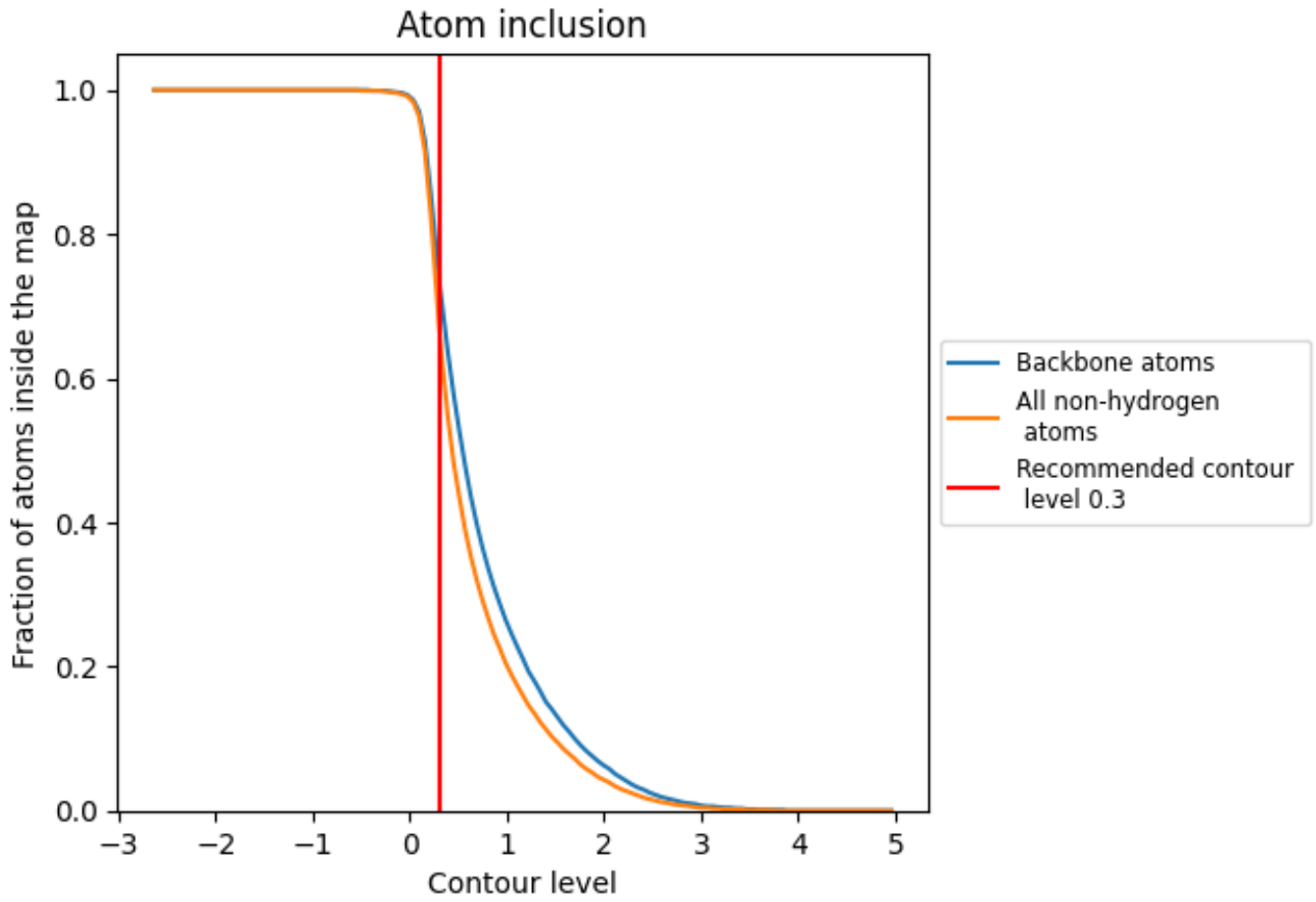
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 67% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6720	0.2920
A	0.7950	0.3270
B	0.7310	0.3420
C	0.3880	0.1760
D	0.7380	0.3150
E	0.5840	0.2760
F	0.7820	0.3230
G	0.8130	0.3060
H	0.8190	0.3520
I	0.9110	0.4420
J	0.9300	0.4600
K	0.1660	0.0530
L	0.0530	-0.0090
M	0.3610	0.0180
N	0.2510	0.0370
O	0.4230	0.1250
P	0.0530	0.0960
R	0.4310	0.1050