Full wwPDB EM Validation Report (i)

Nov 16, 2022 – 04:05 PM JST

PDB ID	:	6M6I
EMDB ID	:	EMD-30125
Title	:	Structure of HSV2 B-capsid portal vertex
Authors	:	Wang, X.X.; Wang, N.
Deposited on	:	2020-03-14
Resolution	:	4.05 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 (i) 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 (i)) were used in the production of this report:

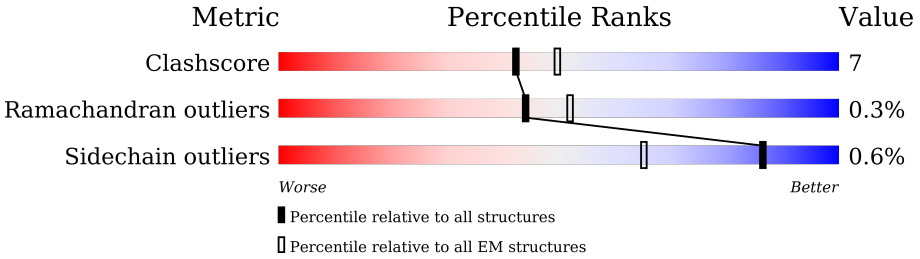
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.05 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	1374	14% 77% 21% • •
1	B	1374	13% 80% 19% •
1	C	1374	25% 82% 17% •
1	D	1374	15% 83% 16% •
1	E	1374	11% 82% 16% •
1	F	1374	15% 80% 18% • •
2	G	81	49% 94% 6%
3	H	83	46% 90% 10%

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Mol	Chain	Length	Quality of chain
4	I	318	27% 76% 18% 6%
4	J	318	29% 83% 14% •
5	K	466	20% 47% 14% 39%
6	L	112	70% 82% 8% 10%
6	M	112	68% 78% 12% 10%
6	N	112	60% 75% 15% 10%
6	O	112	62% 79% 12% 10%
6	P	112	83% 79% 11% 10%
6	Q	112	87% 80% 10% 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 72384 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 Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1350	9971	6319	1810	1789	53	0	0
1	B	1362	10205	6478	1846	1827	54	0	0
1	C	1362	10217	6483	1843	1837	54	0	0
1	D	1360	10197	6472	1845	1826	54	0	0
1	E	1345	10106	6423	1827	1802	54	0	0
1	F	1351	9972	6341	1803	1777	51	0	0

- Molecule 2 is a protein called Coiled coils chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	G	81	405	243	81	81	0	0

- Molecule 3 is a protein called Coiled coils chain 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	H	83	415	249	83	83	0	0

- Molecule 4 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	299	2078	1341	373	357	7	0	0
4	J	307	2175	1405	392	370	8	0	0

- Molecule 5 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	285	2005	1281	360	348	16	0	0

- Molecule 6 is a protein called Small capsomere-interacting protein.

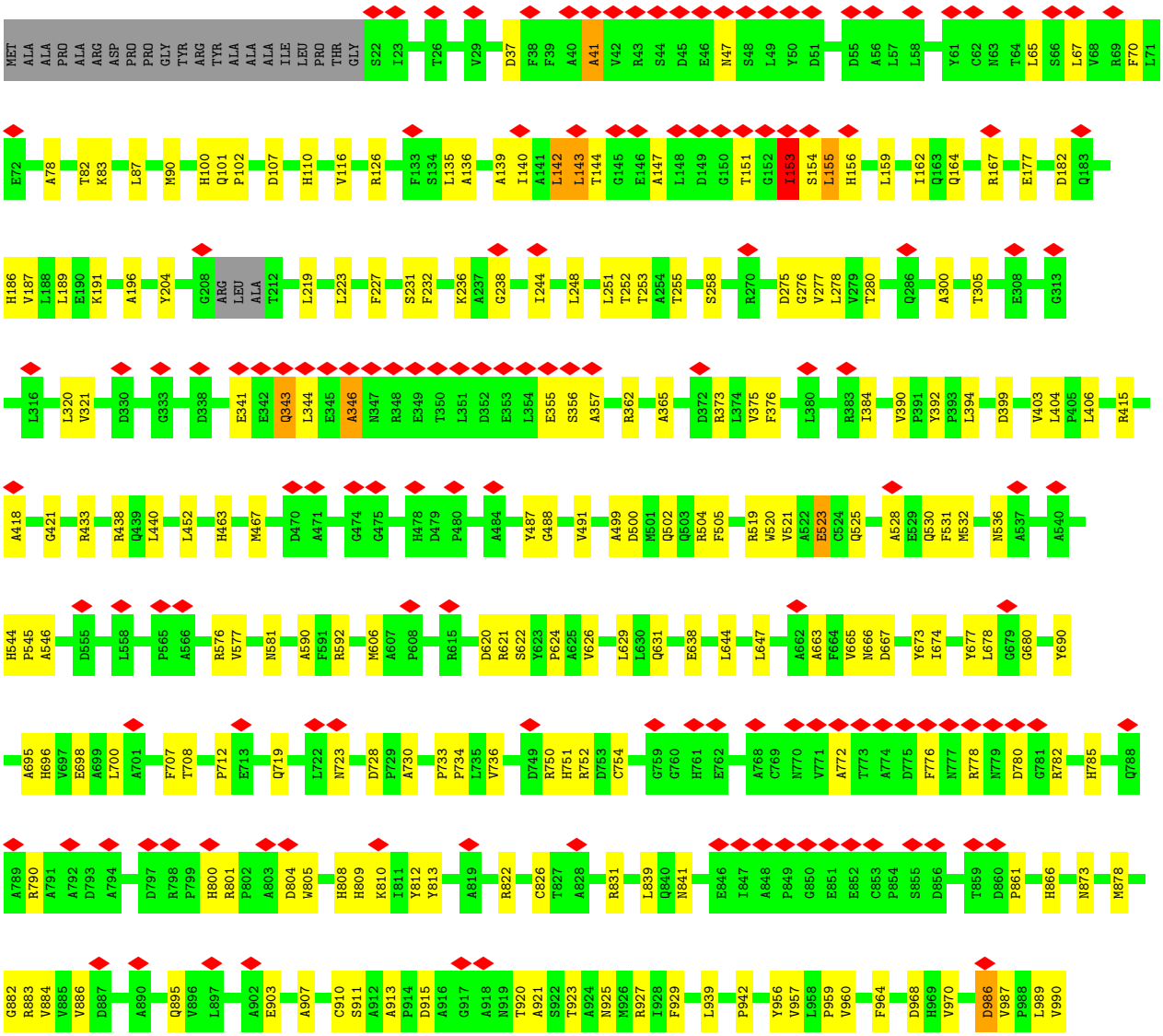
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	L	101	773	489	143	138	3	0	0
6	M	101	773	489	143	138	3	0	0
6	N	101	773	489	143	138	3	0	0
6	O	101	773	489	143	138	3	0	0
6	P	101	773	489	143	138	3	0	0
6	Q	101	773	489	143	138	3	0	0

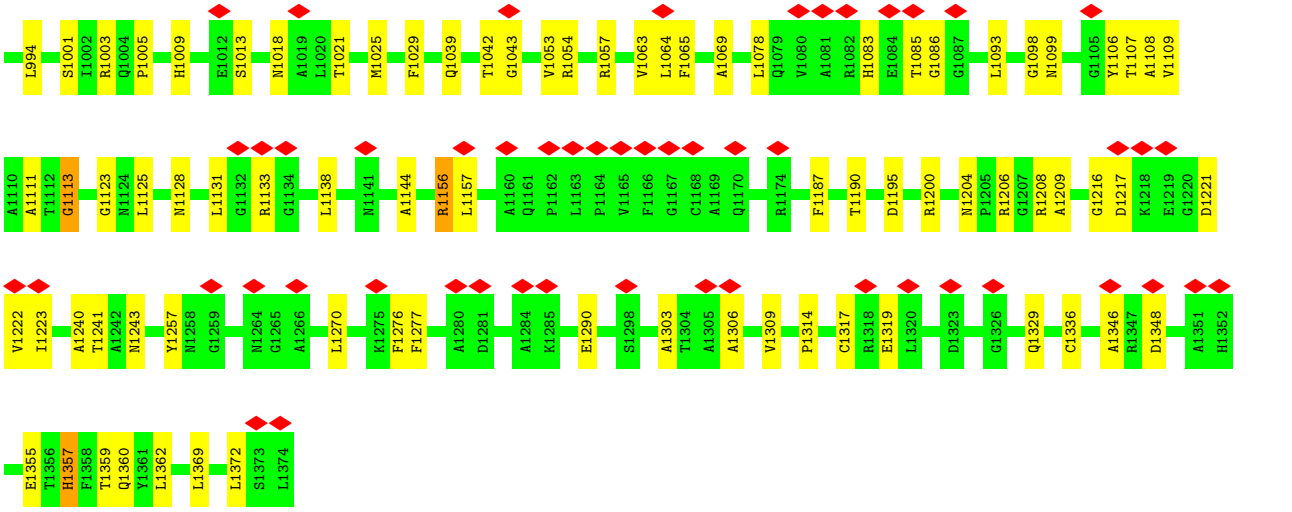
3 Residue-property plots (i)

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: Major capsid protein

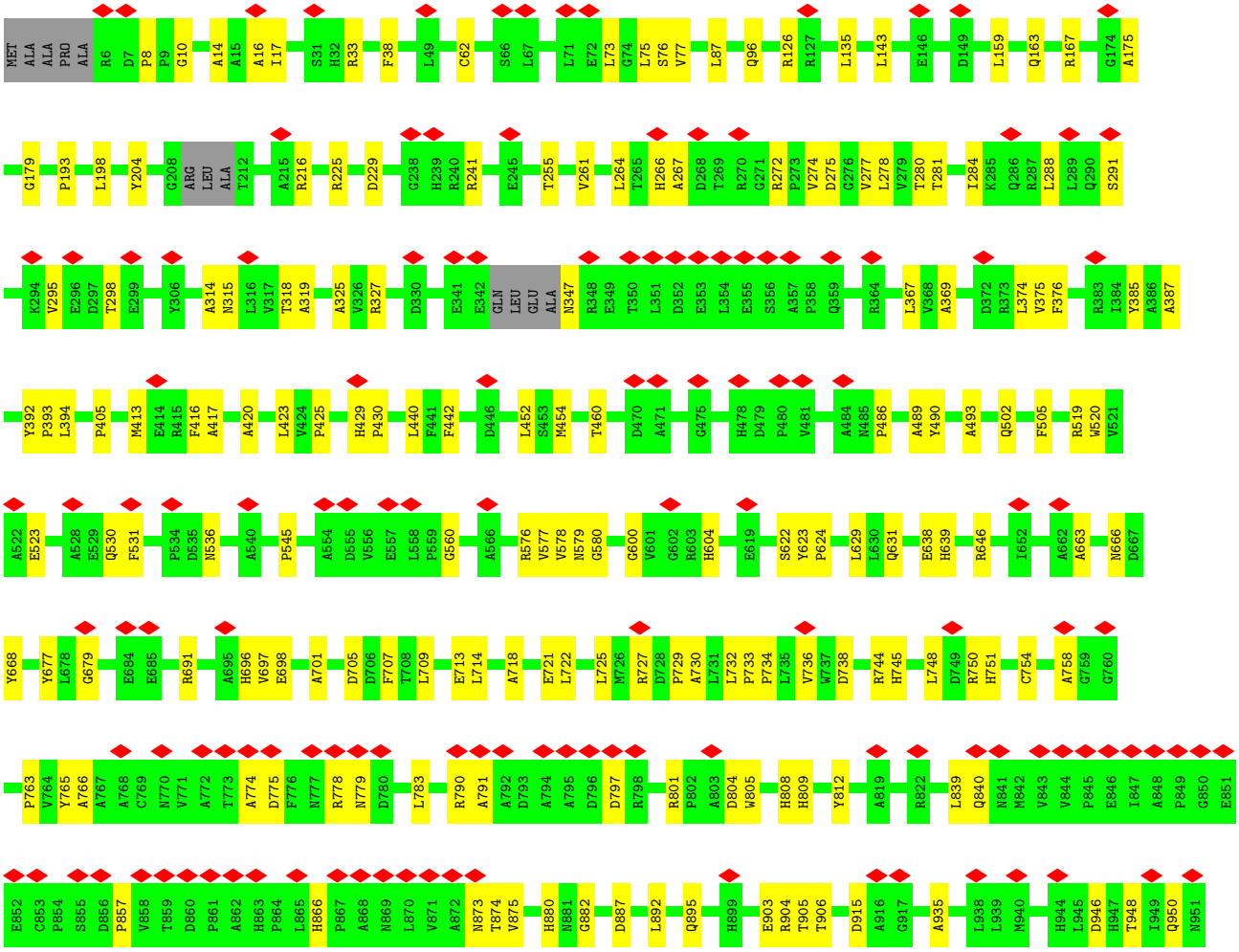
Chain A:

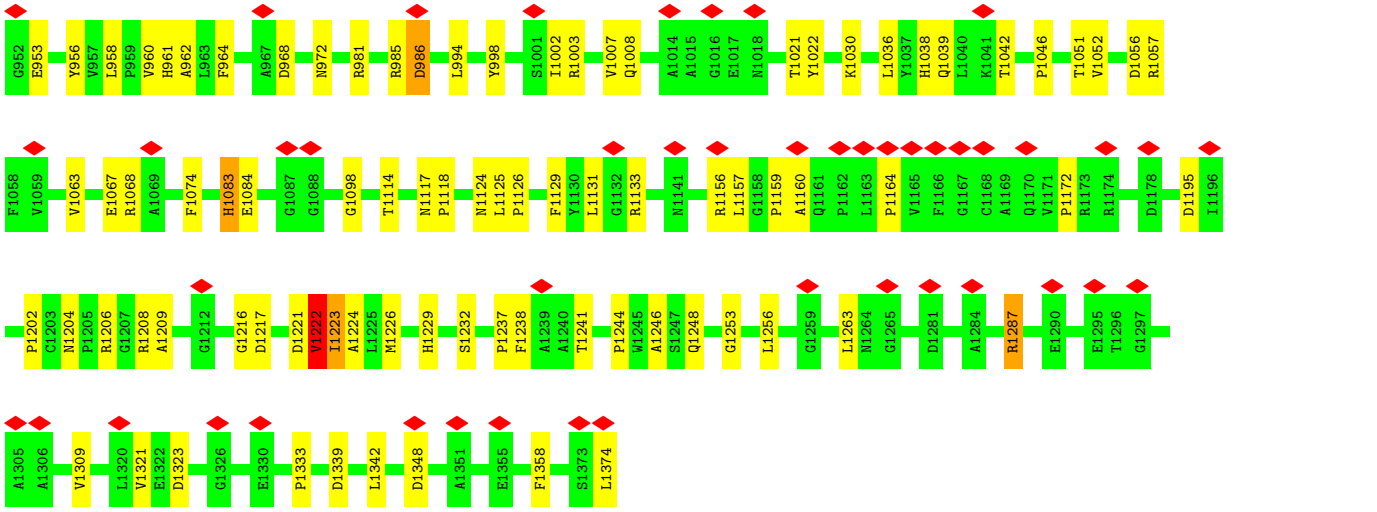




- Molecule 1: Major capsid protein

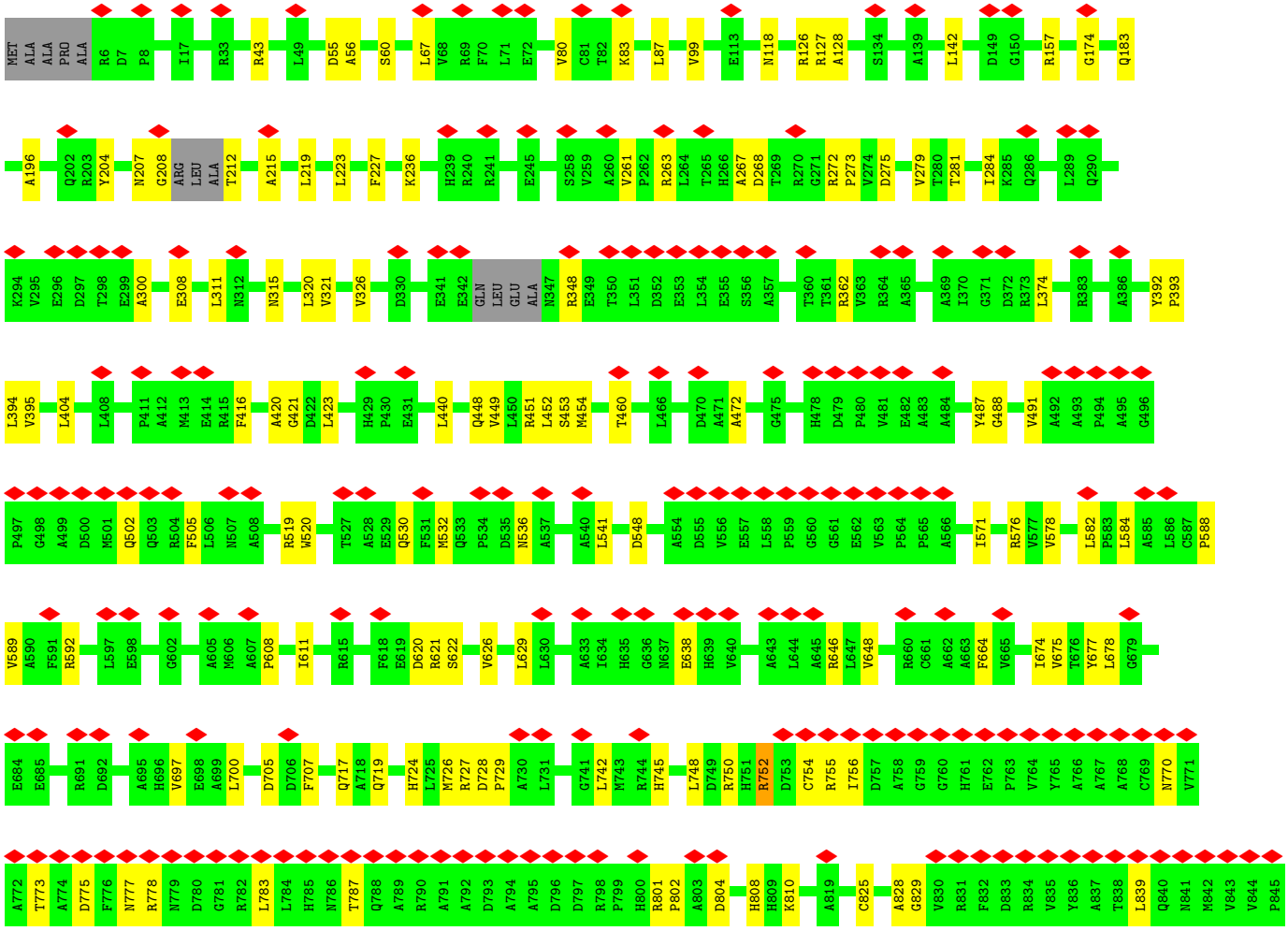
Chain B: 13% 80% 19%

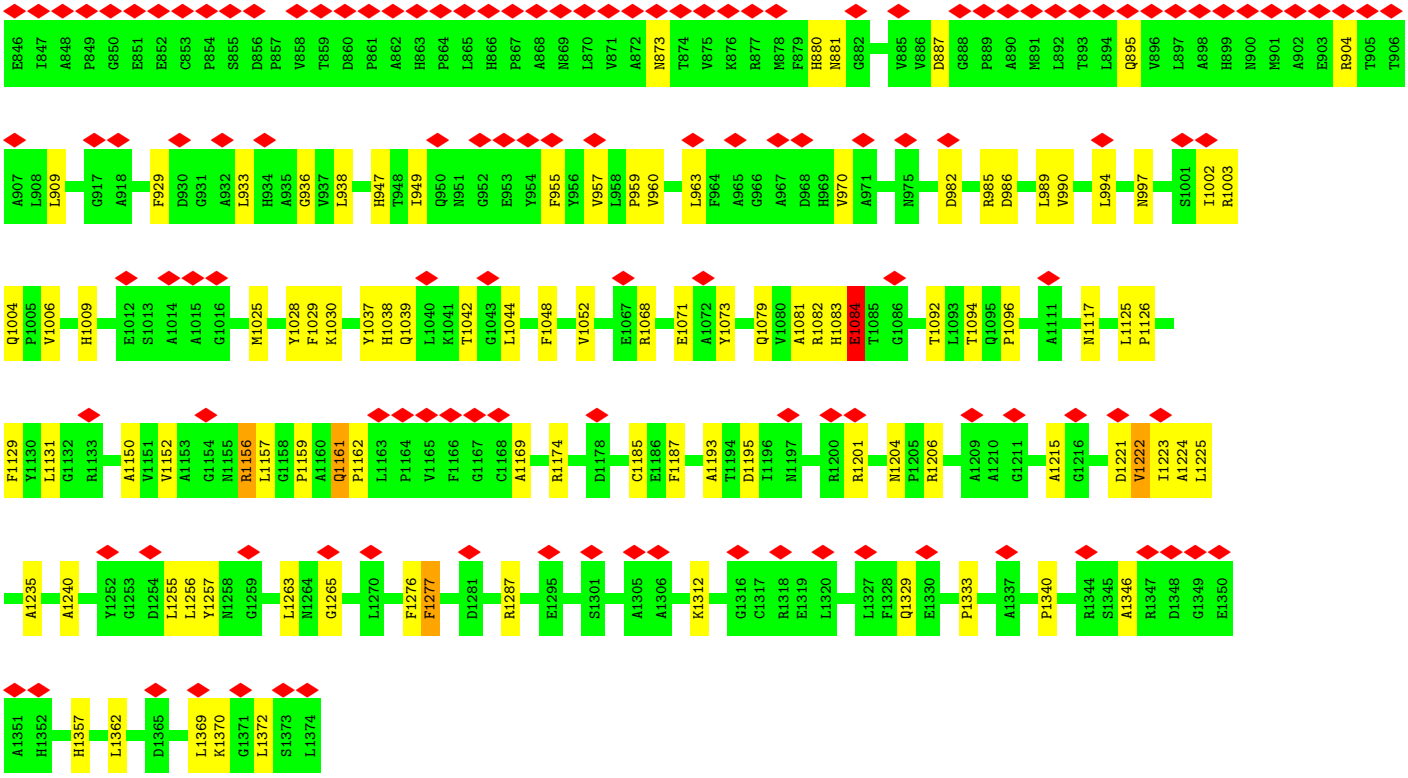




- Molecule 1: Major capsid protein

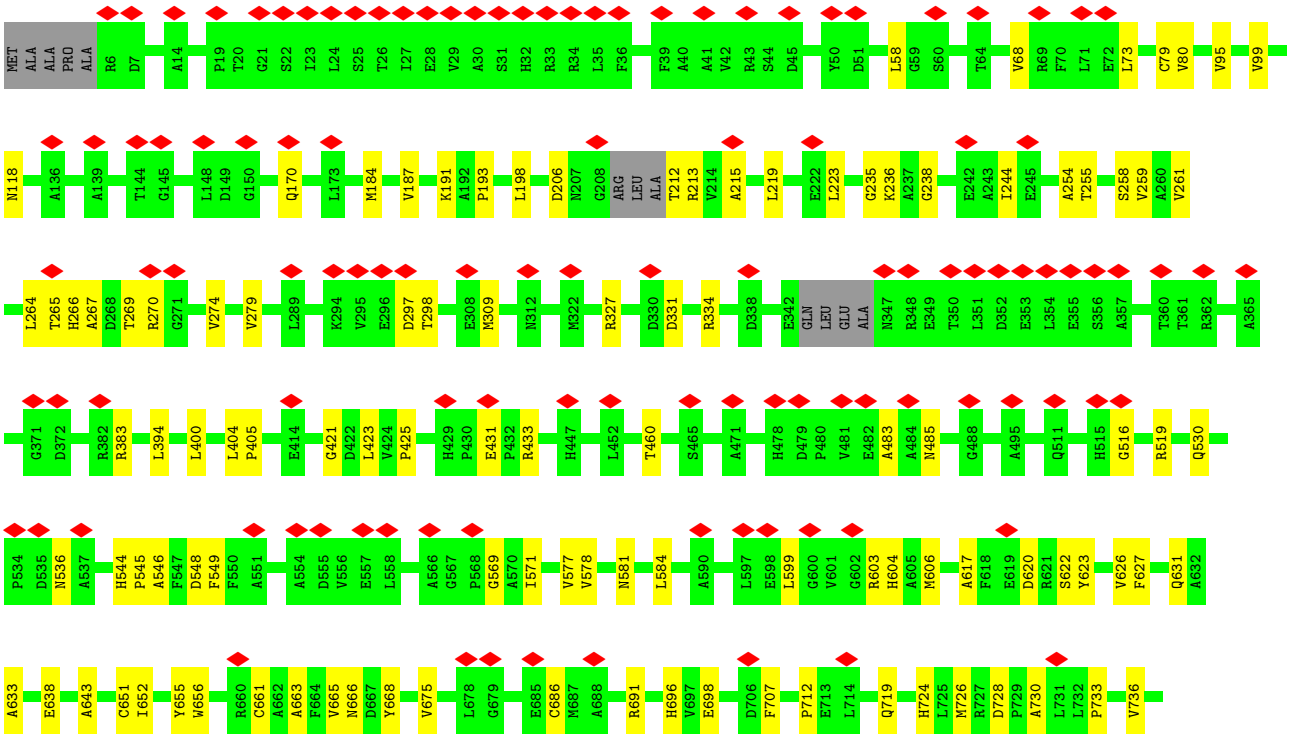
Chain C:

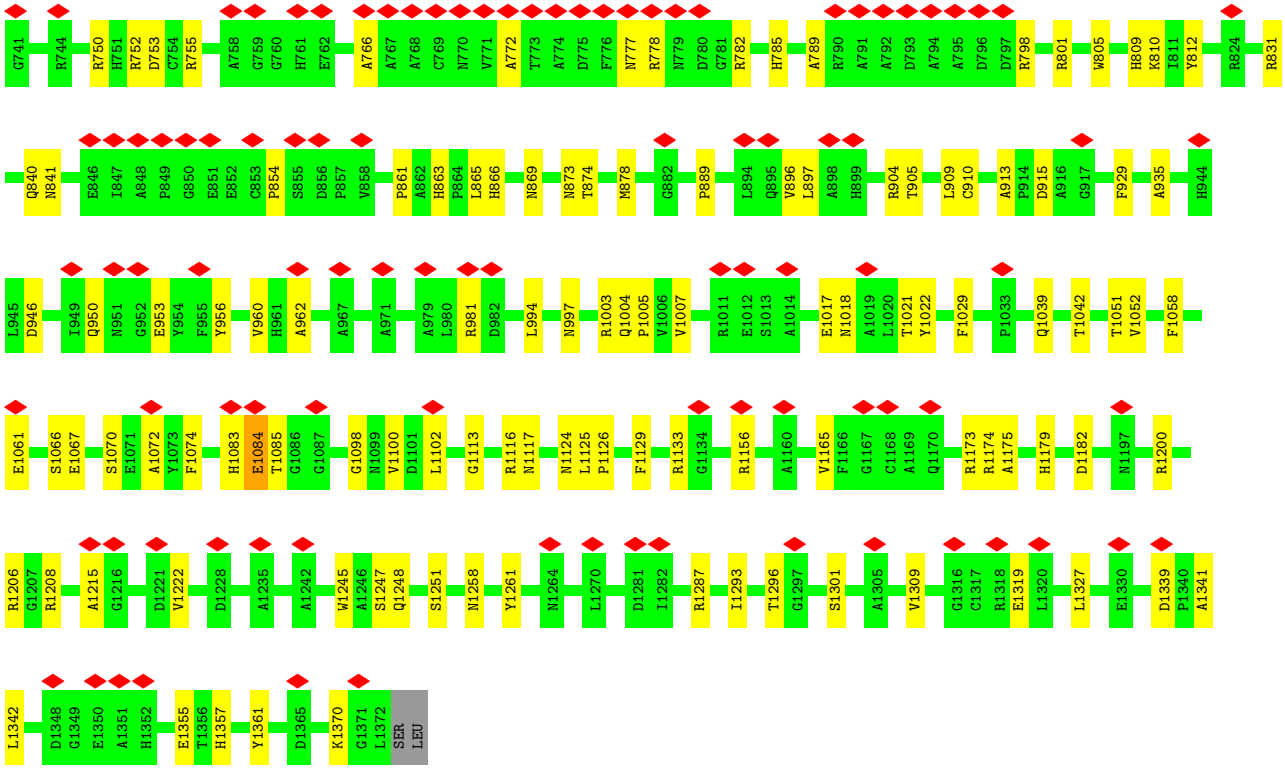




- Molecule 1: Major capsid protein

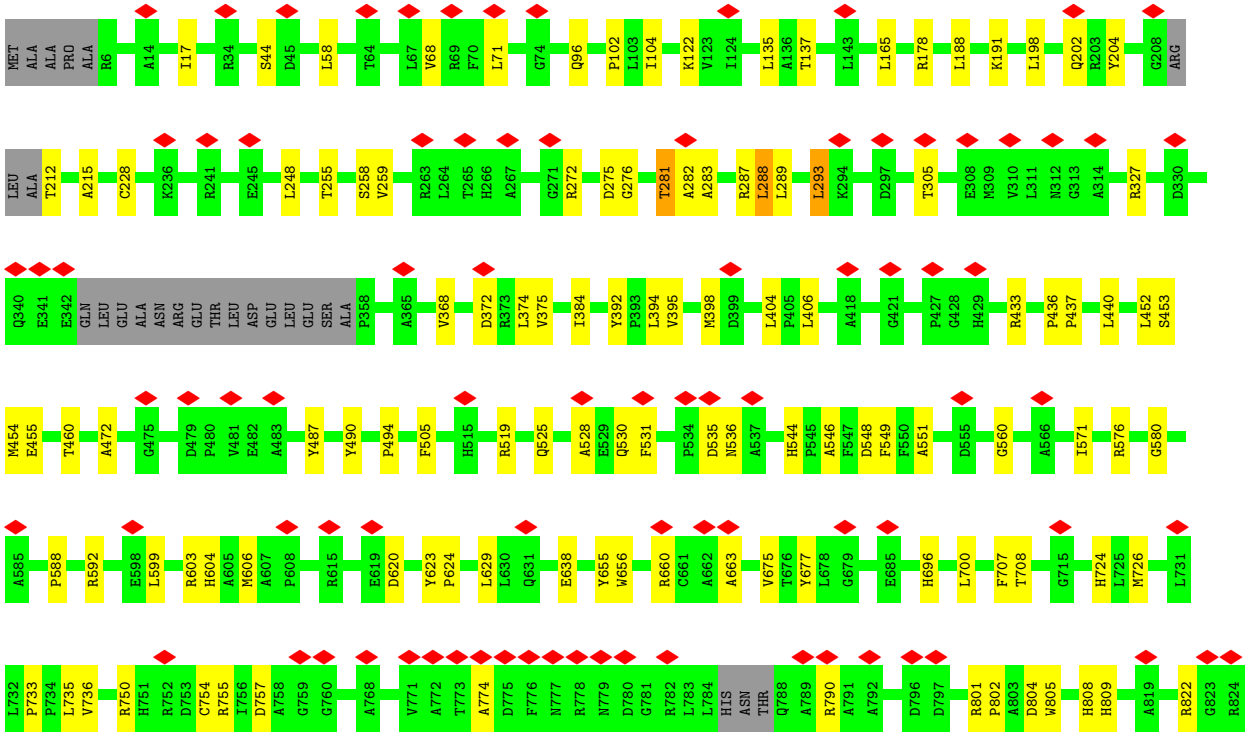
Chain D:

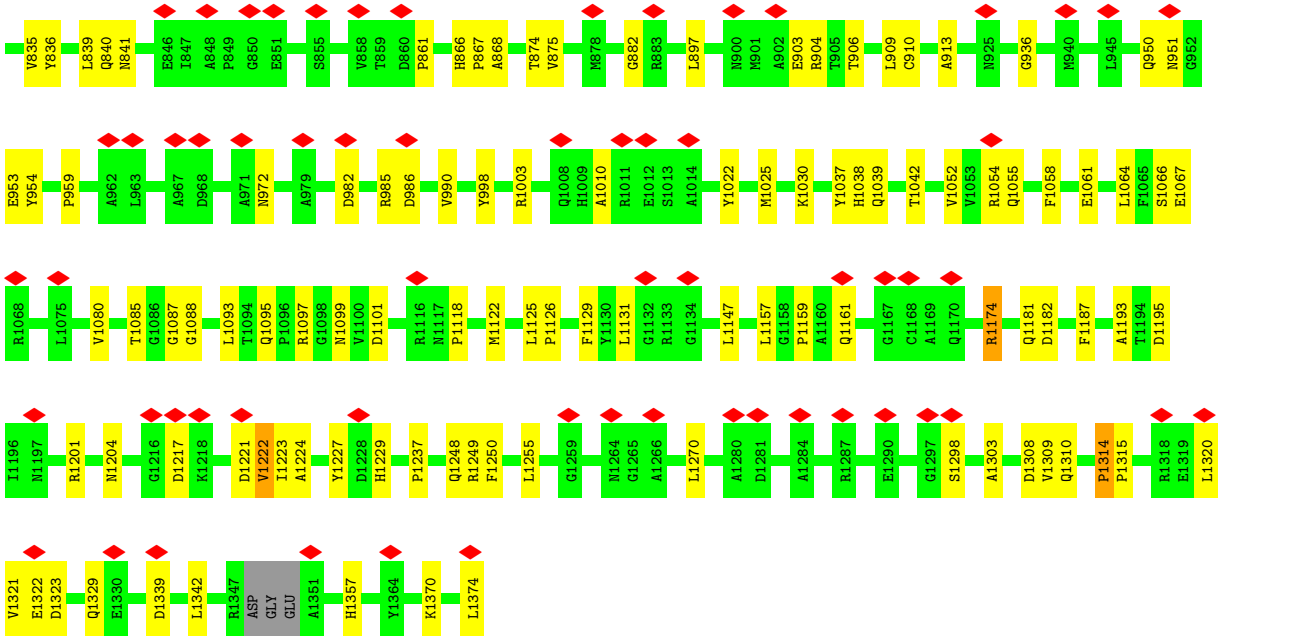




- Molecule 1: Major capsid protein

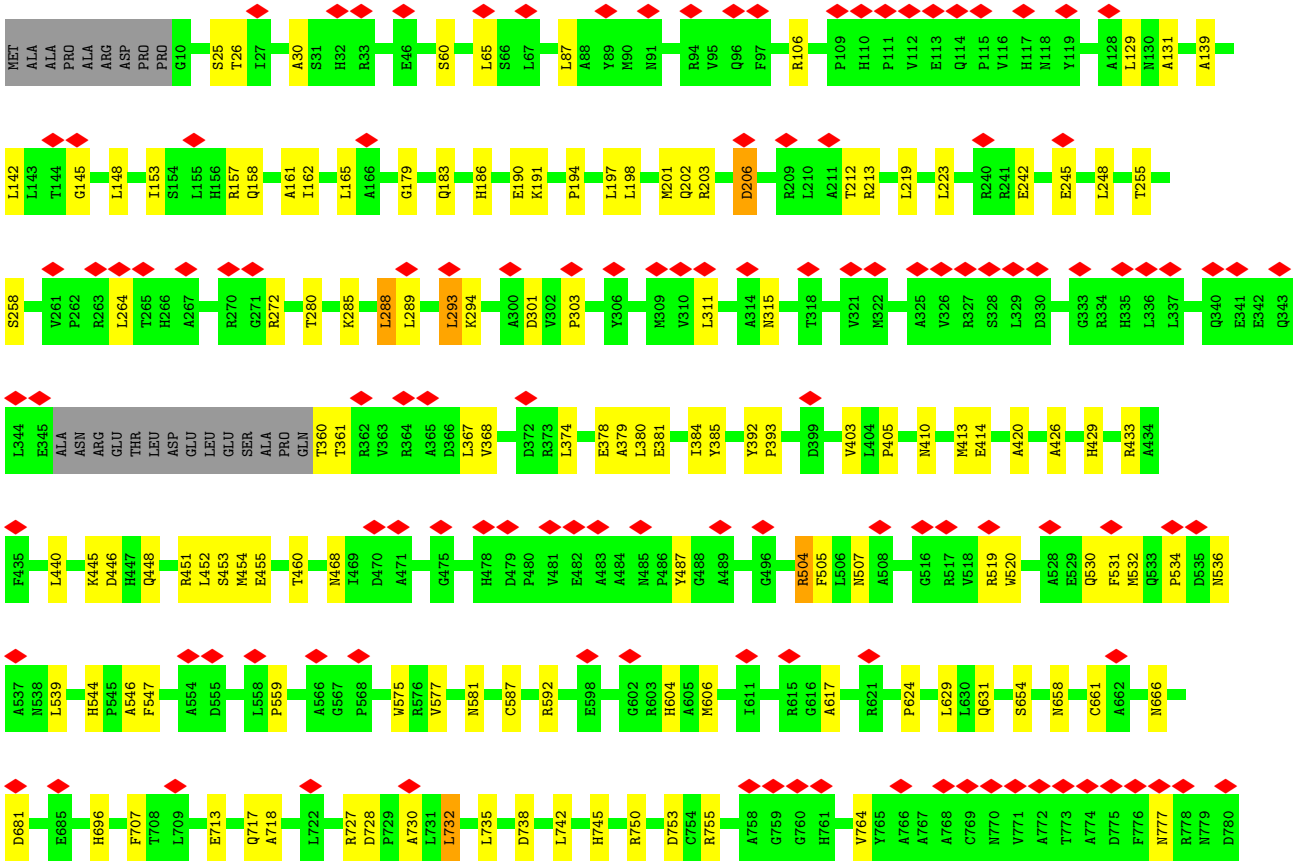
Chain E:

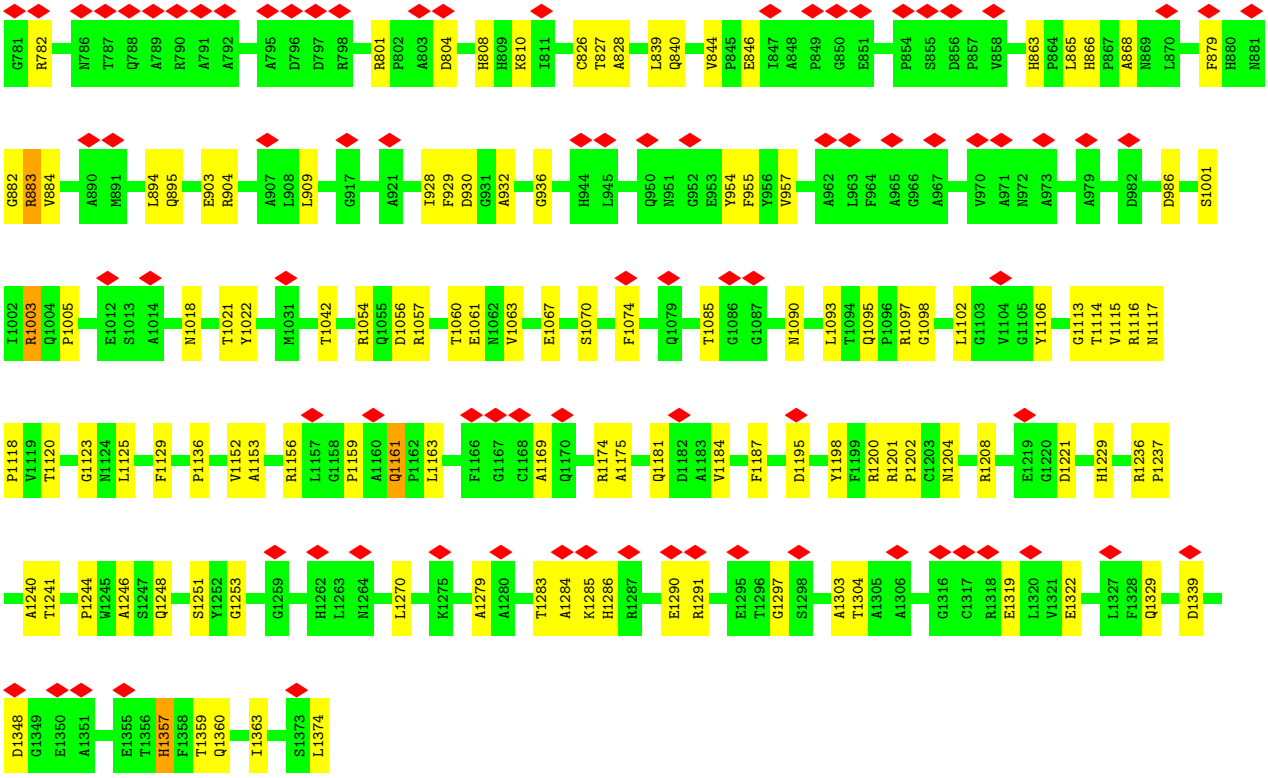




- Molecule 1: Major capsid protein

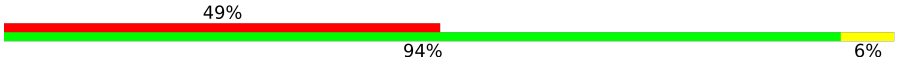
Chain F:

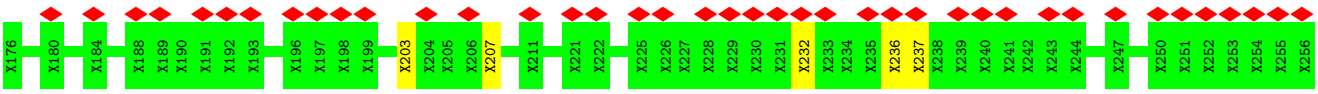




- Molecule 2: Coiled coils chain 1

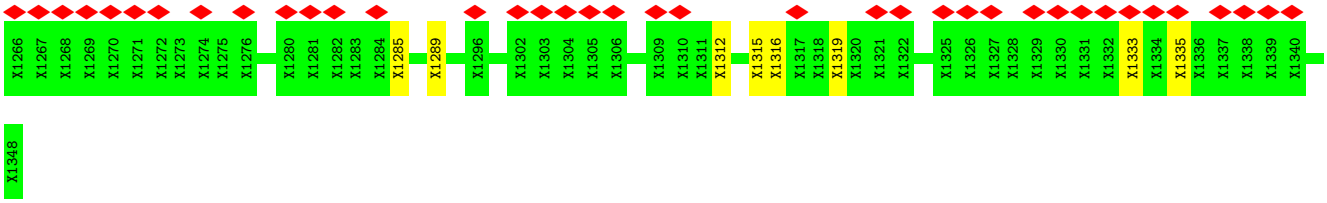
Chain G:





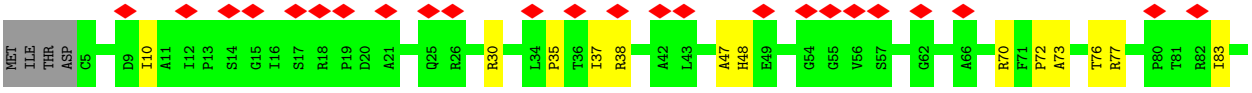
- Molecule 3: Coiled coils chain 2

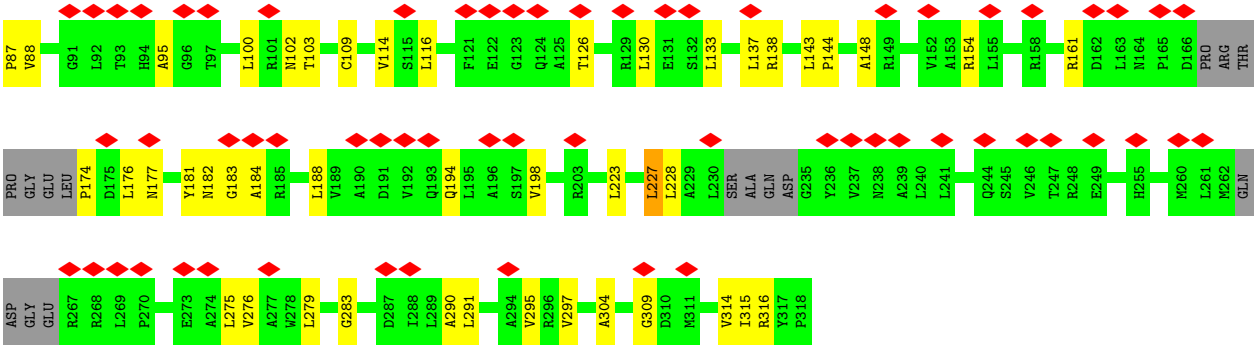
Chain H:



- Molecule 4: Triplex capsid protein 2

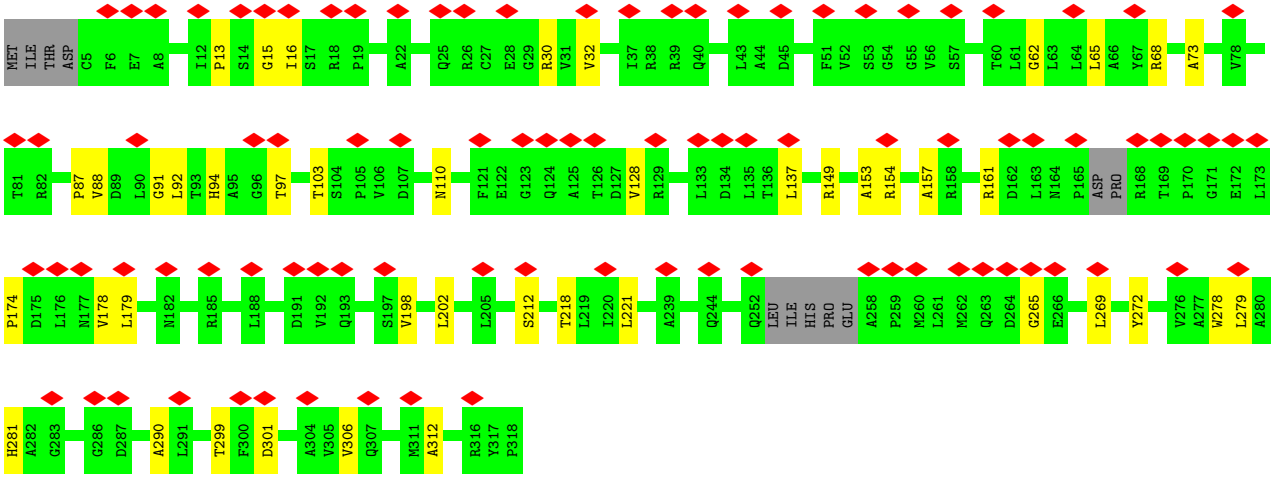
Chain I:





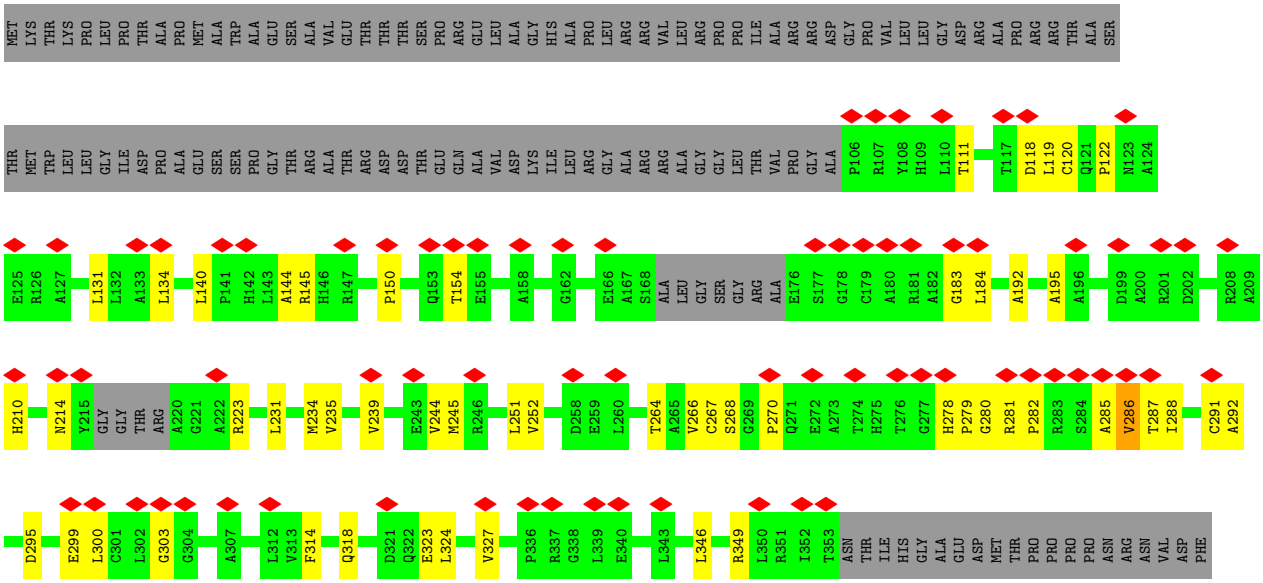
- Molecule 4: Triplex capsid protein 2

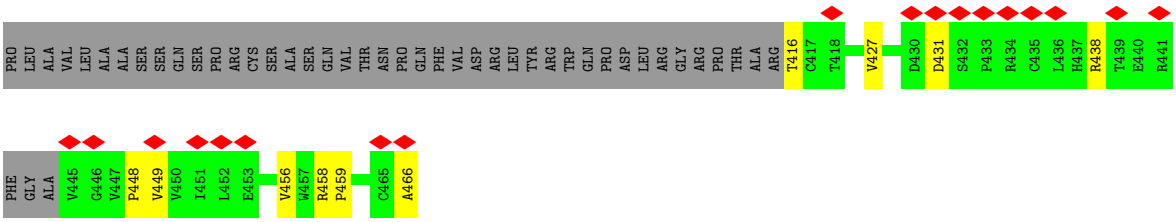
Chain J:



- Molecule 5: Triplex capsid protein 1

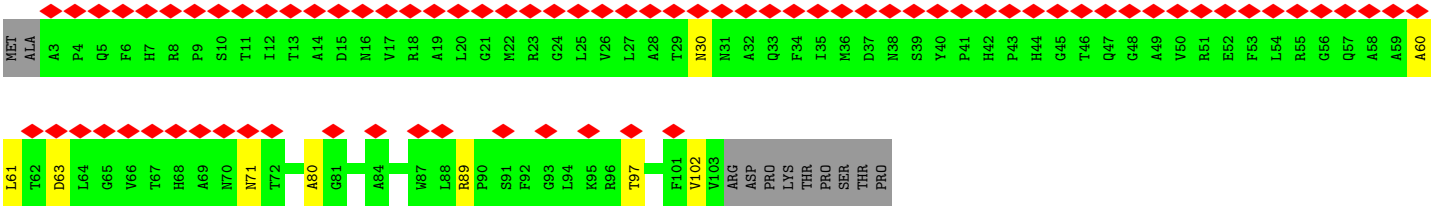
Chain K:





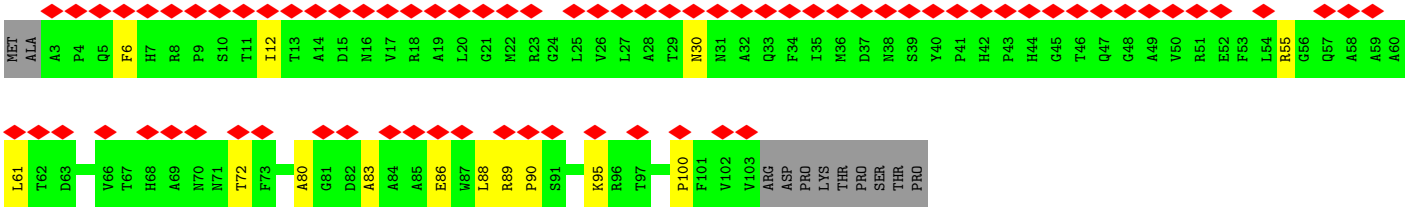
• Molecule 6: Small capsomere-interacting protein

Chain L:



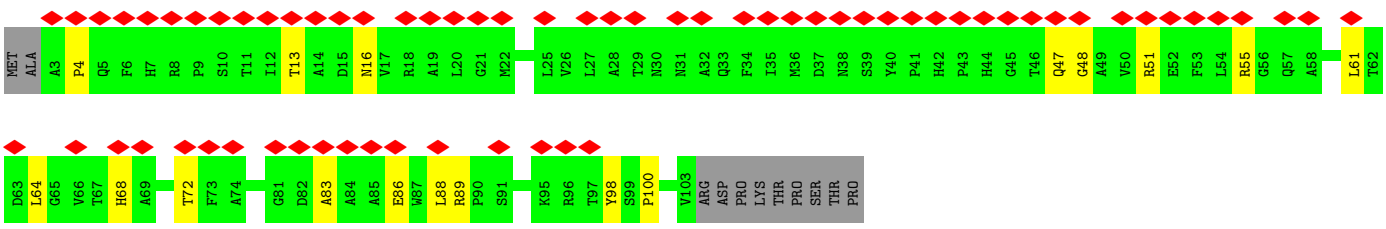
• Molecule 6: Small capsomere-interacting protein

Chain M:



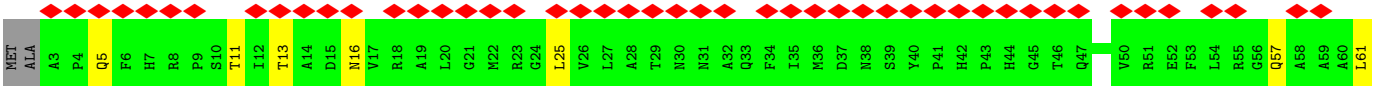
• Molecule 6: Small capsomere-interacting protein

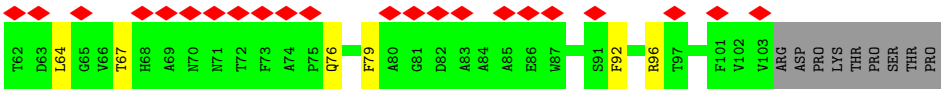
Chain N:



• Molecule 6: Small capsomere-interacting protein

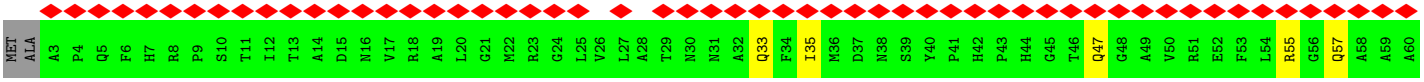
Chain O:

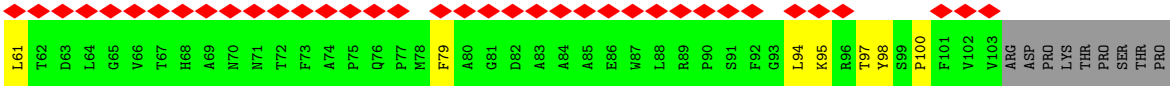




- Molecule 6: Small capsomere-interacting protein

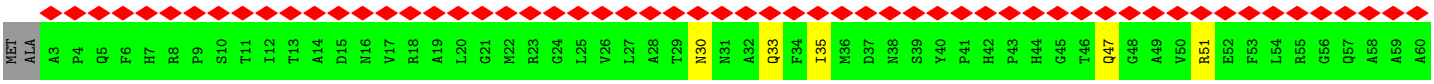
Chain P:

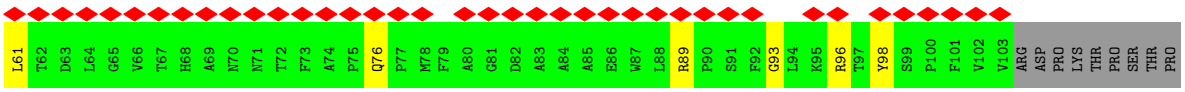




- Molecule 6: Small capsomere-interacting protein

Chain Q:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22158	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 ($e^-/Å^2$)	30.0, 30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k), FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.232	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	414.0, 414.0, 414.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.43	0/10213	0.64	3/13973 (0.0%)
1	B	0.40	0/10460	0.62	4/14301 (0.0%)
1	C	0.39	0/10472	0.61	3/14317 (0.0%)
1	D	0.39	0/10451	0.60	0/14287
1	E	0.42	0/10357	0.62	2/14152 (0.0%)
1	F	0.43	0/10221	0.64	3/13989 (0.0%)
4	I	0.34	0/2114	0.65	0/2909
4	J	0.33	0/2215	0.62	0/3047
5	K	0.34	0/2052	0.66	1/2814 (0.0%)
6	L	0.27	0/795	0.47	0/1084
6	M	0.29	0/795	0.54	0/1084
6	N	0.29	0/795	0.53	0/1084
6	O	0.28	0/795	0.51	0/1084
6	P	0.27	0/795	0.48	0/1084
6	Q	0.27	0/795	0.47	0/1084
All	All	0.40	0/73325	0.62	16/100293 (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	9
1	B	0	4
1	C	0	9
1	D	0	11
1	E	0	6
1	F	0	6
2	G	0	1
4	I	0	2
4	J	0	1
5	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	51

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1348	ASP	CB-CG-OD1	9.75	127.07	118.30
1	A	1348	ASP	CB-CG-OD1	9.08	126.48	118.30
1	F	293	LEU	C-N-CA	7.21	139.74	121.70
1	A	159	LEU	CA-CB-CG	5.52	127.99	115.30
1	F	293	LEU	CA-CB-CG	5.50	127.95	115.30
5	K	346	LEU	CA-CB-CG	5.44	127.82	115.30
1	C	1277	PHE	CB-CG-CD1	5.42	124.59	120.80
1	C	949	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	F	1348	ASP	CB-CG-OD1	5.35	123.11	118.30
1	E	986	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	986	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	986	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	986	ASP	CB-CG-OD2	5.15	122.94	118.30
1	E	259	VAL	CG1-CB-CG2	-5.12	102.72	110.90
1	B	892	LEU	CA-CB-CG	5.11	127.04	115.30
1	B	732	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1113	GLY	Peptide
1	A	1222	VAL	Peptide
1	A	1357	HIS	Peptide
1	A	346	ALA	Peptide
1	A	355	GLU	Peptide
1	A	357	ALA	Peptide
1	A	523	GLU	Peptide
1	A	65	LEU	Peptide
1	A	956	TYR	Peptide
1	B	1083	HIS	Peptide
1	B	1222	VAL	Peptide
1	B	16	ALA	Peptide
1	B	520	TRP	Peptide
1	C	1002	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	C	1083	HIS	Peptide
1	C	1084	GLU	Peptide
1	C	1161	GLN	Peptide
1	C	1169	ALA	Peptide
1	C	1222	VAL	Peptide
1	C	1357	HIS	Peptide
1	C	43	ARG	Peptide
1	C	752	ARG	Peptide
1	D	1083	HIS	Peptide
1	D	1084	GLU	Peptide
1	D	1113	GLY	Peptide
1	D	1222	VAL	Peptide
1	D	1357	HIS	Peptide
1	D	258	SER	Peptide
1	D	265	THR	Peptide
1	D	752	ARG	Peptide
1	D	753	ASP	Peptide
1	D	79	CYS	Peptide
1	D	956	TYR	Peptide
1	E	1161	GLN	Peptide
1	E	1314	PRO	Peptide
1	E	1357	HIS	Peptide
1	E	258	SER	Peptide
1	E	281	THR	Peptide
1	E	44	SER	Peptide
1	F	1113	GLY	Peptide
1	F	1161	GLN	Peptide
1	F	1357	HIS	Peptide
1	F	206	ASP	Peptide
1	F	293	LEU	Peptide
1	F	520	TRP	Peptide
2	G	237	UNK	Peptide
4	I	103	THR	Peptide
4	I	315	ILE	Peptide
4	J	15	GLY	Peptide
5	K	119	LEU	Peptide
5	K	140	LEU	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	9971	0	9605	220	0
1	B	10205	0	9940	162	0
1	C	10217	0	9945	151	0
1	D	10197	0	9934	134	0
1	E	10106	0	9891	137	0
1	F	9972	0	9623	151	0
2	G	405	0	86	2	0
3	H	415	0	89	4	0
4	I	2078	0	2053	32	0
4	J	2175	0	2213	28	0
5	K	2005	0	1876	39	0
6	L	773	0	748	9	0
6	M	773	0	748	10	0
6	N	773	0	748	13	0
6	O	773	0	748	9	0
6	P	773	0	748	11	0
6	Q	773	0	748	9	0
All	All	72384	0	69743	1021	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 7.

All (1021) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LEU:CG	1:A:140:ILE:HG23	1.34	1.58
1:A:135:LEU:CD1	1:A:140:ILE:HG12	1.40	1.50
1:A:135:LEU:HG	1:A:140:ILE:CG2	1.39	1.47
1:A:135:LEU:CG	1:A:140:ILE:CG2	1.91	1.47
1:A:135:LEU:CD1	1:A:140:ILE:CG1	1.95	1.42
1:A:143:LEU:CG	1:A:162:ILE:HG22	1.53	1.36
1:A:135:LEU:HD11	1:A:140:ILE:CG1	1.57	1.31
1:A:135:LEU:CD1	1:A:140:ILE:CG2	2.11	1.29
1:A:135:LEU:HD11	1:A:140:ILE:CB	1.62	1.27
1:A:143:LEU:HG	1:A:162:ILE:CG2	1.65	1.27
1:A:135:LEU:CD2	1:A:140:ILE:HG23	1.64	1.26
5:K:280:GLY:HA2	5:K:285:ALA:CB	1.71	1.21
1:A:135:LEU:CD1	1:A:140:ILE:HG23	1.68	1.17
1:A:143:LEU:HB3	1:A:162:ILE:CG2	1.75	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HB3	1:A:162:ILE:HG21	1.27	1.15
1:A:135:LEU:HD12	1:A:140:ILE:CG1	1.65	1.14
1:A:135:LEU:HD11	1:A:140:ILE:CG2	1.77	1.10
1:A:143:LEU:CG	1:A:162:ILE:CG2	2.26	1.08
1:A:143:LEU:CB	1:A:162:ILE:CG2	2.34	1.06
5:K:280:GLY:HA2	5:K:285:ALA:HB3	1.05	1.04
5:K:280:GLY:CA	5:K:285:ALA:HB3	1.89	1.01
1:A:135:LEU:HG	1:A:140:ILE:HG21	1.01	1.01
1:A:135:LEU:HD21	1:A:140:ILE:HG23	1.42	0.98
1:A:143:LEU:CB	1:A:162:ILE:HB	1.96	0.95
1:A:143:LEU:HB2	1:A:162:ILE:HB	1.52	0.90
1:A:135:LEU:CG	1:A:140:ILE:HG21	1.80	0.89
1:A:135:LEU:CD1	1:A:140:ILE:CB	2.36	0.89
1:A:143:LEU:CB	1:A:162:ILE:CB	2.53	0.85
1:A:135:LEU:CD1	1:A:140:ILE:HG13	2.07	0.85
1:A:143:LEU:HB3	1:A:162:ILE:CB	2.07	0.85
1:A:135:LEU:HD11	1:A:140:ILE:HG13	1.59	0.84
1:A:143:LEU:HD22	1:A:143:LEU:O	1.83	0.77
1:A:153:ILE:HD13	1:A:153:ILE:N	2.00	0.75
1:E:790:ARG:HD3	6:O:79:PHE:HB2	1.69	0.75
1:A:143:LEU:HG	1:A:162:ILE:HG22	0.78	0.75
1:A:135:LEU:HD12	1:A:140:ILE:HG12	0.74	0.74
1:A:232:PHE:HA	1:A:1113:GLY:HA2	1.70	0.73
1:D:997:ASN:HD21	1:D:1004:GLN:HB2	1.54	0.72
6:O:13:THR:H	6:O:16:ASN:HD22	1.37	0.71
1:B:267:ALA:HB1	1:B:274:VAL:HB	1.73	0.70
1:F:532:MET:HA	1:F:1240:ALA:H	1.56	0.70
1:D:99:VAL:HG13	1:D:118:ASN:HD22	1.57	0.69
1:A:143:LEU:CD1	1:A:162:ILE:HG22	2.21	0.69
1:A:135:LEU:HD11	1:A:140:ILE:HG23	1.46	0.69
1:A:1054:ARG:HH22	1:A:1123:GLY:H	1.40	0.69
1:A:730:ALA:HB2	1:A:750:ARG:HH12	1.58	0.68
1:C:519:ARG:HH22	1:C:541:LEU:HB2	1.59	0.68
1:E:576:ARG:HA	1:E:1003:ARG:HH12	1.59	0.67
1:C:707:PHE:HA	1:C:1042:THR:HG21	1.75	0.67
1:B:751:HIS:HE1	1:B:754:CYS:HB2	1.60	0.66
1:D:1124:ASN:O	1:D:1156:ARG:NH2	2.29	0.66
1:C:578:VAL:HG23	1:C:1003:ARG:HH22	1.60	0.66
1:C:957:VAL:HG22	1:C:959:PRO:HD3	1.78	0.66
1:A:78:ALA:HB2	1:A:277:VAL:HG21	1.77	0.66
1:D:981:ARG:HH22	1:E:802:PRO:HB3	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:THR:HG22	1:B:367:LEU:H	1.61	0.66
1:B:986:ASP:OD1	1:C:705:ASP:HB3	1.95	0.66
1:F:530:GLN:O	1:F:536:ASN:ND2	2.29	0.66
1:A:143:LEU:CB	1:A:162:ILE:HG21	2.08	0.66
1:E:460:THR:HG21	1:E:1187:PHE:HB2	1.76	0.66
1:A:343:GLN:HB3	1:B:159:LEU:HD13	1.78	0.65
5:K:244:VAL:HG12	5:K:245:MET:HG3	1.76	0.65
1:B:576:ARG:HA	1:B:1003:ARG:HH12	1.62	0.65
1:C:520:TRP:HB3	1:C:1004:GLN:HG2	1.78	0.64
1:A:37:ASP:HA	1:A:41:ALA:HB3	1.79	0.64
1:E:1217:ASP:N	1:E:1221:ASP:OD2	2.30	0.64
1:A:1346:ALA:HB2	1:A:1362:LEU:HD11	1.79	0.64
1:C:829:GLY:HA2	1:C:936:GLY:HA2	1.80	0.64
1:E:398:MET:HG3	1:E:1322:GLU:HB3	1.79	0.64
1:B:420:ALA:HB2	1:C:421:GLY:HA3	1.79	0.63
1:A:135:LEU:HD11	1:A:140:ILE:CA	2.28	0.63
1:C:261:VAL:HG12	1:C:263:ARG:H	1.64	0.63
1:B:452:LEU:HD13	1:B:1052:VAL:HG21	1.81	0.63
1:E:707:PHE:HA	1:E:1042:THR:HG21	1.80	0.63
1:A:1156:ARG:NH2	1:F:1237:PRO:O	2.32	0.63
1:C:530:GLN:O	1:C:536:ASN:ND2	2.31	0.63
1:C:804:ASP:O	1:C:808:HIS:ND1	2.30	0.62
1:F:544:HIS:HB3	1:F:547:PHE:HB2	1.81	0.62
1:A:957:VAL:HG22	1:A:959:PRO:HD3	1.82	0.62
1:D:191:LYS:NZ	1:D:1070:SER:O	2.32	0.62
1:A:920:THR:OG1	1:A:921:ALA:N	2.32	0.62
1:D:193:PRO:HG2	1:D:198:LEU:HD12	1.82	0.62
1:D:730:ALA:HB2	1:D:750:ARG:HH12	1.65	0.62
1:A:135:LEU:CD2	1:A:140:ILE:CG2	2.52	0.62
1:C:1204:ASN:ND2	1:C:1329:GLN:O	2.29	0.62
1:B:857:PRO:O	1:B:866:HIS:ND1	2.31	0.62
1:C:1215:ALA:O	1:C:1287:ARG:NH1	2.33	0.62
1:C:80:VAL:HG13	1:C:263:ARG:HH21	1.65	0.62
1:E:867:PRO:HG3	6:N:98:TYR:HB2	1.80	0.62
1:A:135:LEU:HD21	1:A:140:ILE:CG2	2.25	0.61
1:A:404:LEU:HB3	1:A:440:LEU:HD21	1.82	0.61
1:B:264:LEU:O	1:B:1068:ARG:NH2	2.34	0.61
1:A:772:ALA:HA	6:M:55:ARG:HE	1.65	0.61
1:A:280:THR:HG22	1:A:1063:VAL:HG13	1.82	0.61
1:C:754:CYS:SG	1:C:755:ARG:N	2.74	0.61
1:D:279:VAL:HG12	1:D:394:LEU:HD11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:530:GLN:O	1:D:536:ASN:ND2	2.32	0.61
1:F:1125:LEU:HD23	1:F:1184:VAL:HG22	1.81	0.61
1:D:485:ASN:ND2	1:D:516:GLY:O	2.34	0.61
1:F:381:GLU:HA	1:F:385:TYR:HB2	1.83	0.60
1:F:903:GLU:HG2	1:F:904:ARG:HG2	1.83	0.60
1:B:96:GLN:HG2	1:C:60:SER:HA	1.82	0.60
1:E:950:GLN:HB3	1:E:953:GLU:HB2	1.82	0.60
1:A:144:THR:O	1:A:144:THR:HG22	2.01	0.60
4:I:10:ILE:HB	4:I:83:ILE:HB	1.83	0.60
4:I:95:ALA:HB3	4:I:316:ARG:HH12	1.67	0.60
1:A:204:TYR:OH	1:B:1117:ASN:ND2	2.34	0.60
1:D:549:PHE:HB3	1:D:571:ILE:HD11	1.83	0.60
1:E:733:PRO:HG2	1:E:736:VAL:HG22	1.84	0.60
5:K:134:LEU:HA	5:K:245:MET:HG2	1.83	0.60
1:E:708:THR:HA	1:E:1038:HIS:HB3	1.83	0.59
1:E:1174:ARG:NH2	1:E:1182:ASP:OD2	2.35	0.59
1:F:1060:THR:HG22	1:F:1115:VAL:HG12	1.84	0.59
1:C:775:ASP:HB3	1:C:778:ARG:HE	1.66	0.59
5:K:210:HIS:HD2	5:K:214:ASN:HD22	1.49	0.59
1:C:472:ALA:HB2	1:C:1255:LEU:HD11	1.85	0.59
1:E:1157:LEU:HD21	1:E:1309:VAL:HG11	1.84	0.59
1:A:776:PHE:HA	1:A:903:GLU:HB2	1.85	0.59
1:B:968:ASP:O	1:B:972:ASN:ND2	2.35	0.59
1:C:55:ASP:OD1	1:C:55:ASP:N	2.35	0.59
1:C:272:ARG:HD3	1:C:374:LEU:HD13	1.85	0.59
1:C:1346:ALA:HB2	1:C:1362:LEU:HD11	1.85	0.59
1:E:525:GLN:NE2	1:E:535:ASP:O	2.36	0.59
1:F:728:ASP:O	1:F:810:LYS:NZ	2.34	0.59
1:C:620:ASP:OD1	1:D:691:ARG:NH1	2.36	0.59
1:F:301:ASP:OD1	1:F:360:THR:N	2.36	0.59
1:A:1187:PHE:O	1:A:1257:TYR:OH	2.19	0.58
1:A:135:LEU:HD11	1:A:140:ILE:H	1.67	0.58
1:E:805:TRP:O	1:E:809:HIS:ND1	2.34	0.58
1:C:204:TYR:OH	1:D:1117:ASN:ND2	2.36	0.58
1:E:1030:LYS:O	1:E:1039:GLN:NE2	2.31	0.58
1:A:778:ARG:NH1	1:A:903:GLU:OE2	2.37	0.58
1:F:735:LEU:HD22	1:F:936:GLY:HA3	1.85	0.58
1:E:624:PRO:HB3	1:E:882:GLY:HA3	1.86	0.58
1:A:143:LEU:HG	1:A:162:ILE:CB	2.33	0.58
1:C:588:PRO:HD3	1:C:1193:ALA:HB2	1.86	0.58
1:F:707:PHE:HA	1:F:1042:THR:HG21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1054:ARG:NH1	1:E:1122:MET:O	2.36	0.58
6:N:13:THR:OG1	6:N:16:ASN:ND2	2.37	0.58
1:E:599:LEU:O	1:E:603:ARG:NH1	2.37	0.58
1:E:293:LEU:HD13	1:E:368:VAL:HG11	1.84	0.57
1:B:413:MET:HG2	1:C:1340:PRO:HD2	1.85	0.57
1:B:775:ASP:HB3	1:B:778:ARG:HD2	1.86	0.57
1:D:548:ASP:OD1	1:D:1003:ARG:NH2	2.37	0.57
1:A:841:ASN:ND2	1:A:873:ASN:O	2.37	0.57
1:B:578:VAL:HA	1:B:1030:LYS:HA	1.85	0.57
1:E:638:GLU:OE1	1:E:801:ARG:NH2	2.36	0.57
1:F:1279:ALA:O	1:F:1283:THR:OG1	2.22	0.57
1:A:135:LEU:HD11	1:A:140:ILE:N	2.18	0.57
1:B:622:SER:OG	1:C:675:VAL:O	2.20	0.57
1:D:831:ARG:NH2	1:D:953:GLU:O	2.36	0.57
1:B:204:TYR:OH	1:C:1117:ASN:ND2	2.37	0.57
1:E:530:GLN:O	1:E:536:ASN:ND2	2.35	0.57
4:I:275:LEU:HD22	4:J:157:ALA:HB2	1.86	0.57
1:B:1204:ASN:HD22	1:B:1209:ALA:HA	1.69	0.57
1:B:1217:ASP:H	1:B:1221:ASP:HB2	1.69	0.57
1:A:780:ASP:OD2	1:A:782:ARG:NH1	2.38	0.57
1:B:961:HIS:HB3	1:B:964:PHE:HD2	1.70	0.57
1:C:142:LEU:HD21	1:C:157:ARG:HB3	1.87	0.57
1:E:440:LEU:HD23	1:E:452:LEU:HD12	1.86	0.57
1:A:1195:ASP:OD1	1:A:1195:ASP:N	2.37	0.57
4:I:154:ARG:NH1	4:I:176:LEU:O	2.38	0.57
1:A:438:ARG:NH2	1:A:1043:GLY:O	2.38	0.57
1:E:1066:SER:OG	1:E:1067:GLU:N	2.37	0.57
1:A:153:ILE:HD13	1:A:153:ILE:H	1.68	0.56
1:C:621:ARG:NH2	1:D:698:GLU:OE2	2.36	0.56
1:F:717:GLN:HE22	1:F:750:ARG:HD3	1.70	0.56
1:A:136:ALA:O	1:A:139:ALA:HB3	2.05	0.56
1:E:1221:ASP:OD1	1:E:1221:ASP:N	2.37	0.56
1:F:194:PRO:HG2	1:F:197:LEU:HD12	1.87	0.56
1:B:905:THR:HA	1:B:935:ALA:HB3	1.88	0.56
1:C:787:THR:O	1:C:801:ARG:NH2	2.38	0.56
1:F:272:ARG:HD2	1:F:374:LEU:HB2	1.88	0.56
1:F:440:LEU:HB3	1:F:452:LEU:HB2	1.86	0.56
4:I:297:VAL:HG22	4:I:314:VAL:HG22	1.87	0.56
6:M:6:PHE:HA	6:M:12:ILE:HD11	1.88	0.56
1:A:1200:ARG:NH2	1:A:1355:GLU:OE2	2.38	0.56
1:B:87:LEU:O	1:B:126:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ASP:OD1	1:D:334:ARG:NH2	2.38	0.56
1:E:656:TRP:O	1:E:660:ARG:NH1	2.39	0.56
1:F:828:ALA:HB1	1:F:955:PHE:HB3	1.86	0.56
1:B:646:ARG:NH2	1:B:887:ASP:OD2	2.38	0.56
1:C:982:ASP:OD1	1:C:985:ARG:NH2	2.39	0.56
1:C:279:VAL:HG12	1:C:394:LEU:HD11	1.88	0.56
5:K:291:CYS:HA	5:K:449:VAL:HG23	1.88	0.56
1:C:460:THR:HG23	1:C:1129:PHE:HE2	1.71	0.56
1:D:696:HIS:HE1	1:D:1021:THR:HG21	1.71	0.56
1:D:766:ALA:HB2	1:D:782:ARG:HH11	1.69	0.56
4:J:218:THR:HA	4:J:221:LEU:HD23	1.88	0.56
5:K:235:VAL:HB	5:K:323:GLU:HB3	1.88	0.56
1:A:673:TYR:OH	1:A:801:ARG:NH2	2.39	0.56
1:A:1078:LEU:HD12	1:A:1093:LEU:HD23	1.88	0.56
1:A:1157:LEU:HD21	1:A:1309:VAL:HG11	1.87	0.56
1:C:646:ARG:NH2	1:C:887:ASP:OD2	2.38	0.56
1:B:175:ALA:O	1:B:179:GLY:N	2.38	0.55
1:B:277:VAL:HG22	1:B:376:PHE:HB2	1.88	0.55
1:D:889:PRO:HB2	6:P:100:PRO:HG2	1.88	0.55
1:E:228:CYS:O	1:E:1370:LYS:NZ	2.39	0.55
1:E:472:ALA:HB2	1:E:1255:LEU:HD11	1.88	0.55
1:F:433:ARG:NH2	1:F:1339:ASP:OD2	2.38	0.55
1:B:1232:SER:OG	1:C:1174:ARG:NH1	2.37	0.55
1:E:68:VAL:HG21	1:E:384:ILE:HG22	1.89	0.55
1:A:499:ALA:HB1	1:A:831:ARG:HH11	1.70	0.55
1:A:700:LEU:HD22	1:A:1025:MET:HG2	1.88	0.55
1:B:840:GLN:HB2	6:L:61:LEU:HD21	1.87	0.55
1:C:1079:GLN:HG3	1:C:1094:THR:HG23	1.86	0.55
1:E:1204:ASN:ND2	1:E:1329:GLN:O	2.35	0.55
1:A:1276:PHE:HA	1:A:1329:GLN:HE22	1.71	0.55
1:D:638:GLU:OE1	1:D:801:ARG:NH2	2.38	0.55
1:F:1152:VAL:HG11	1:F:1159:PRO:HD2	1.87	0.55
1:B:1157:LEU:HD21	1:B:1309:VAL:HG11	1.89	0.55
1:D:707:PHE:HA	1:D:1042:THR:HG21	1.87	0.55
1:B:629:LEU:HB3	1:B:839:LEU:HD21	1.88	0.55
1:B:1124:ASN:O	1:B:1156:ARG:NH2	2.38	0.55
1:B:696:HIS:HE1	1:B:1021:THR:HG21	1.71	0.55
1:C:957:VAL:HG21	1:C:970:VAL:HA	1.88	0.55
1:D:1074:PHE:N	1:D:1098:GLY:O	2.38	0.55
1:A:754:CYS:HA	1:A:910:CYS:HA	1.89	0.55
1:B:1208:ARG:HB2	1:B:1241:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:895:GLN:HA	6:Q:61:LEU:HD13	1.89	0.55
1:E:433:ARG:NH2	1:E:1339:ASP:OD2	2.40	0.55
1:E:1221:ASP:HA	1:F:1175:ALA:HB1	1.87	0.55
1:F:1181:GLN:NE2	1:F:1304:THR:O	2.36	0.55
1:A:530:GLN:O	1:A:536:ASN:ND2	2.32	0.55
1:B:1237:PRO:O	1:C:1156:ARG:NH2	2.39	0.55
1:E:822:ARG:NH1	1:E:1010:ALA:O	2.39	0.55
1:E:1227:TYR:CG	1:E:1249:ARG:HG3	2.42	0.55
1:F:258:SER:OG	1:F:1102:LEU:O	2.25	0.55
1:F:617:ALA:HB2	1:F:661:CYS:HB3	1.89	0.55
1:B:981:ARG:HH22	1:C:802:PRO:HB3	1.72	0.55
1:B:1133:ARG:NH1	1:B:1164:PRO:O	2.34	0.55
1:B:1222:VAL:O	1:B:1224:ALA:N	2.41	0.54
1:C:404:LEU:HB2	1:C:1052:VAL:HB	1.88	0.54
1:D:259:VAL:HG21	1:D:1102:LEU:HD12	1.89	0.54
1:E:1227:TYR:CD1	1:E:1249:ARG:HG3	2.42	0.54
1:D:95:VAL:HG22	1:E:58:LEU:HB2	1.88	0.54
6:P:95:LYS:HB3	6:P:97:THR:HG23	1.90	0.54
1:A:187:VAL:HG11	1:A:1099:ASN:HD21	1.72	0.54
1:C:502:GLN:HA	1:C:505:PHE:HB3	1.89	0.54
1:F:1195:ASP:OD1	1:F:1195:ASP:N	2.39	0.54
1:A:151:THR:HB	1:A:155:LEU:HD22	1.89	0.54
4:I:181:TYR:HB3	4:I:184:ALA:HB3	1.89	0.54
1:B:216:ARG:NH2	1:B:1287:ARG:O	2.41	0.54
1:D:1066:SER:OG	1:D:1067:GLU:N	2.40	0.54
1:F:242:GLU:HA	1:F:245:GLU:HB2	1.89	0.54
1:F:460:THR:HG23	1:F:1129:PHE:HE2	1.73	0.54
1:F:577:VAL:HG21	1:F:1001:SER:HA	1.88	0.54
1:B:531:PHE:HE1	1:B:1244:PRO:HD3	1.72	0.54
1:E:398:MET:N	1:E:1058:PHE:O	2.41	0.54
1:A:1083:HIS:HB3	1:A:1085:THR:HG22	1.89	0.54
1:F:1106:TYR:OH	1:F:1290:GLU:O	2.25	0.54
1:F:1357:HIS:O	1:F:1360:GLN:N	2.41	0.54
6:L:30:ASN:OD1	6:Q:89:ARG:NH2	2.41	0.54
1:B:774:ALA:HB1	1:B:903:GLU:HB3	1.88	0.54
4:J:154:ARG:HG3	4:J:179:LEU:HD11	1.89	0.54
1:A:415:ARG:HH12	1:A:590:ALA:HB1	1.71	0.54
1:A:960:VAL:HG12	1:A:994:LEU:HD13	1.88	0.54
1:B:545:PRO:O	1:B:576:ARG:NH1	2.41	0.54
1:B:873:ASN:ND2	6:L:30:ASN:OD1	2.40	0.54
1:D:778:ARG:HG2	1:D:904:ARG:HE	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:110:ASN:ND2	4:J:299:THR:OG1	2.41	0.54
1:B:77:VAL:HG23	1:B:266:HIS:HB3	1.90	0.54
1:C:275:ASP:HB3	1:C:1068:ARG:HD2	1.90	0.54
4:J:87:PRO:O	4:J:91:GLY:N	2.36	0.54
1:B:707:PHE:HA	1:B:1042:THR:HG21	1.90	0.53
1:B:709:LEU:H	1:B:1038:HIS:HD2	1.56	0.53
1:C:578:VAL:HA	1:C:1030:LYS:HA	1.89	0.53
1:E:96:GLN:NE2	1:F:60:SER:OG	2.42	0.53
4:J:128:VAL:HG12	4:J:137:LEU:HB2	1.89	0.53
1:A:667:ASP:OD1	1:A:813:TYR:OH	2.26	0.53
1:C:448:GLN:NE2	1:C:449:VAL:O	2.40	0.53
1:E:1095:GLN:OE1	1:E:1097:ARG:NH2	2.41	0.53
1:F:587:CYS:SG	1:F:592:ARG:NH2	2.81	0.53
1:A:252:THR:HG23	1:A:373:ARG:HD2	1.89	0.53
1:B:76:SER:OG	1:B:266:HIS:NE2	2.35	0.53
1:C:236:LYS:NZ	1:C:1370:LYS:O	2.39	0.53
1:F:280:THR:HG23	1:F:1063:VAL:HG22	1.90	0.53
1:F:1270:LEU:HD22	1:F:1303:ALA:HB2	1.90	0.53
1:A:100:HIS:NE2	1:B:62:CYS:SG	2.77	0.53
1:B:1256:LEU:HA	1:B:1263:LEU:HD12	1.90	0.53
1:A:1208:ARG:HB2	1:A:1241:THR:HG22	1.91	0.53
1:E:460:THR:HG23	1:E:1129:PHE:HE2	1.73	0.53
4:I:38:ARG:NH2	4:J:301:ASP:O	2.41	0.53
5:K:278:HIS:N	5:K:279:PRO:CD	2.72	0.53
1:A:440:LEU:HB3	1:A:452:LEU:HB2	1.90	0.53
1:D:712:PRO:O	1:D:719:GLN:NE2	2.38	0.53
1:A:707:PHE:HA	1:A:1042:THR:HG21	1.91	0.53
1:B:751:HIS:CE1	1:B:754:CYS:HB2	2.43	0.53
1:E:204:TYR:OH	1:F:1117:ASN:ND2	2.41	0.53
1:F:1057:ARG:HH22	1:F:1319:GLU:HB3	1.74	0.53
3:H:1333:UNK:C	3:H:1335:UNK:N	2.72	0.53
6:L:89:ARG:NH2	6:M:30:ASN:OD1	2.42	0.53
1:D:631:GLN:OE1	1:D:666:ASN:ND2	2.41	0.53
1:E:629:LEU:HB3	1:E:839:LEU:HD21	1.91	0.53
5:K:427:VAL:HB	5:K:456:VAL:HB	1.91	0.53
1:B:960:VAL:HG12	1:B:994:LEU:HD13	1.91	0.53
1:B:1321:VAL:HG13	1:B:1323:ASP:HB2	1.91	0.53
1:C:1265:GLY:O	1:C:1312:LYS:NZ	2.42	0.53
1:F:863:HIS:HB3	1:F:866:HIS:HB2	1.91	0.53
5:K:118:ASP:O	5:K:223:ARG:NH1	2.42	0.53
1:B:961:HIS:HE2	1:B:1002:ILE:HB	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:544:HIS:CD2	1:E:546:ALA:H	2.27	0.52
4:I:102:ASN:HB3	4:I:309:GLY:H	1.73	0.52
1:A:231:SER:O	1:A:236:LYS:NZ	2.30	0.52
1:B:225:ARG:NH1	1:B:229:ASP:OD2	2.38	0.52
1:C:717:GLN:HE21	1:C:748:LEU:HD22	1.74	0.52
1:F:303:PRO:HB3	1:F:360:THR:HG23	1.92	0.52
1:F:559:PRO:HB2	1:F:755:ARG:HH12	1.73	0.52
5:K:134:LEU:HB3	5:K:183:GLY:HA2	1.90	0.52
1:A:734:PRO:HG2	1:A:964:PHE:HE2	1.74	0.52
1:A:1217:ASP:N	1:A:1221:ASP:OD2	2.39	0.52
1:B:604:HIS:O	1:B:1022:TYR:OH	2.26	0.52
1:A:1086:GLY:C	5:K:278:HIS:HE1	2.13	0.52
1:D:236:LYS:NZ	1:D:1370:LYS:O	2.42	0.52
1:E:580:GLY:HA2	1:E:592:ARG:HH12	1.74	0.52
1:F:606:MET:HB2	1:F:1018:ASN:HD21	1.75	0.52
1:F:1246:ALA:HA	1:F:1253:GLY:HA3	1.91	0.52
3:H:1285:UNK:O	3:H:1289:UNK:N	2.42	0.52
1:A:626:VAL:HG12	1:A:878:MET:HG3	1.91	0.52
1:C:947:HIS:HB2	6:P:79:PHE:HD1	1.75	0.52
1:D:544:HIS:HD2	1:D:546:ALA:H	1.58	0.52
1:D:1293:ILE:HG22	1:D:1327:LEU:HD11	1.91	0.52
1:F:696:HIS:HE1	1:F:1021:THR:HG21	1.75	0.52
1:A:621:ARG:NH1	1:B:698:GLU:OE2	2.43	0.52
1:A:826:CYS:O	1:A:939:LEU:N	2.41	0.52
1:B:744:ARG:NH2	1:B:801:ARG:O	2.40	0.52
1:D:622:SER:OG	1:E:675:VAL:O	2.23	0.52
4:I:72:PRO:HG2	4:I:88:VAL:HB	1.92	0.52
1:A:252:THR:HG22	1:A:253:THR:HG23	1.91	0.52
1:B:73:LEU:HD23	1:B:75:LEU:H	1.75	0.52
1:E:1125:LEU:HD12	1:E:1126:PRO:HD2	1.90	0.52
1:F:826:CYS:SG	1:F:827:THR:N	2.83	0.52
4:I:73:ALA:HA	4:I:87:PRO:HA	1.91	0.52
4:I:279:LEU:HD22	4:J:153:ALA:HB2	1.91	0.52
5:K:438:ARG:HA	5:K:448:PRO:HA	1.91	0.52
1:C:638:GLU:OE2	1:C:677:TYR:OH	2.22	0.52
1:D:626:VAL:HG12	1:D:878:MET:HG3	1.92	0.52
1:A:155:LEU:O	1:A:155:LEU:HG	2.07	0.52
1:B:729:PRO:O	1:B:745:HIS:ND1	2.43	0.52
1:D:269:THR:HG21	1:D:298:THR:HB	1.92	0.52
1:A:622:SER:HB2	1:B:679:GLY:HA3	1.92	0.51
1:B:385:TYR:HD2	1:B:392:TYR:HD1	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:GLN:OE1	1:B:666:ASN:ND2	2.43	0.51
1:B:790:ARG:NH1	6:L:80:ALA:O	2.43	0.51
1:B:1118:PRO:HD3	1:B:1374:LEU:HD13	1.92	0.51
1:A:663:ALA:N	1:A:690:TYR:OH	2.43	0.51
1:C:629:LEU:HB3	1:C:839:LEU:HD21	1.93	0.51
1:E:835:VAL:HG22	1:E:954:TYR:HD1	1.75	0.51
1:E:1055:GLN:HB3	1:E:1310:GLN:HE22	1.75	0.51
1:D:1182:ASP:HB2	1:D:1309:VAL:HA	1.91	0.51
1:B:758:ALA:HB1	1:B:779:ASN:HA	1.92	0.51
1:B:778:ARG:HG2	1:B:904:ARG:HE	1.76	0.51
1:C:1052:VAL:HG22	1:C:1187:PHE:HE1	1.75	0.51
1:D:404:LEU:O	1:D:1052:VAL:N	2.40	0.51
1:D:840:GLN:NE2	6:P:57:GLN:OE1	2.43	0.51
1:F:219:LEU:O	1:F:223:LEU:N	2.43	0.51
1:F:713:GLU:HG2	1:F:718:ALA:HA	1.92	0.51
1:A:343:GLN:N	1:A:343:GLN:OE1	2.44	0.51
1:D:604:HIS:O	1:D:1022:TYR:OH	2.26	0.51
1:E:836:TYR:HE1	1:E:897:LEU:HD22	1.74	0.51
4:I:116:LEU:HD21	4:I:143:LEU:HB2	1.93	0.51
1:C:440:LEU:HB3	1:C:452:LEU:HD12	1.92	0.51
1:C:700:LEU:HD22	1:C:1025:MET:HG2	1.93	0.51
1:D:255:THR:OG1	1:D:1067:GLU:OE2	2.23	0.51
1:F:954:TYR:HE1	6:M:90:PRO:HG3	1.76	0.51
1:A:90:MET:O	1:A:126:ARG:NH1	2.43	0.51
1:E:904:ARG:NH1	1:E:906:THR:OG1	2.44	0.51
3:H:1312:UNK:O	3:H:1316:UNK:N	2.44	0.51
1:B:241:ARG:NH1	1:B:291:SER:O	2.44	0.51
1:C:622:SER:OG	1:D:675:VAL:O	2.28	0.51
1:D:198:LEU:HD22	1:D:254:ALA:HB1	1.92	0.51
1:D:405:PRO:HA	1:D:1051:THR:HA	1.93	0.51
1:D:873:ASN:OD1	6:O:92:PHE:N	2.42	0.51
1:E:1201:ARG:HH12	1:F:446:ASP:HB3	1.75	0.51
1:F:1095:GLN:OE1	1:F:1097:ARG:NH2	2.44	0.51
1:A:238:GLY:HA2	1:A:244:ILE:HD11	1.93	0.51
1:C:729:PRO:HG2	1:C:748:LEU:HD11	1.93	0.51
1:D:264:LEU:HD22	1:D:266:HIS:HB2	1.93	0.51
1:D:643:ALA:HB1	1:D:896:VAL:HG21	1.93	0.51
1:F:25:SER:OG	1:F:26:THR:N	2.43	0.51
5:K:131:LEU:HD11	5:K:251:LEU:HD12	1.93	0.51
1:A:463:HIS:HE2	1:A:1133:ARG:HG2	1.76	0.50
1:A:606:MET:HB2	1:A:1018:ASN:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:ILE:O	1:D:656:TRP:N	2.41	0.50
1:E:1080:VAL:HG22	1:E:1093:LEU:HG	1.92	0.50
1:B:272:ARG:HG2	1:B:374:LEU:HD11	1.92	0.50
1:C:728:ASP:O	1:C:810:LYS:NZ	2.44	0.50
1:E:982:ASP:OD1	1:E:985:ARG:NH1	2.45	0.50
1:E:1195:ASP:N	1:E:1195:ASP:OD1	2.45	0.50
1:A:390:VAL:HG22	1:F:106:ARG:HH11	1.76	0.50
1:A:644:LEU:HD23	1:A:647:LEU:HD23	1.92	0.50
1:B:425:PRO:HB2	1:B:429:HIS:HB2	1.93	0.50
1:E:519:ARG:NE	1:E:998:TYR:OH	2.45	0.50
1:F:629:LEU:HB3	1:F:839:LEU:HD21	1.93	0.50
4:J:265:GLY:HA3	5:K:150:PRO:HG2	1.94	0.50
1:A:521:VAL:HG21	1:A:987:VAL:HG22	1.93	0.50
1:E:1339:ASP:HB2	1:E:1342:LEU:HG	1.93	0.50
1:F:380:LEU:HB3	1:F:384:ILE:HD11	1.92	0.50
6:N:4:PRO:HD3	6:N:16:ASN:HB3	1.93	0.50
1:A:399:ASP:OD1	1:A:399:ASP:N	2.43	0.50
1:D:755:ARG:N	1:D:910:CYS:SG	2.84	0.50
1:D:950:GLN:HB3	1:D:953:GLU:HG3	1.94	0.50
1:E:1222:VAL:O	1:E:1224:ALA:N	2.45	0.50
1:A:191:LYS:NZ	1:A:1107:THR:OG1	2.36	0.50
1:B:766:ALA:N	1:B:783:LEU:O	2.44	0.50
1:B:1246:ALA:HA	1:B:1253:GLY:HA3	1.93	0.50
1:F:191:LYS:NZ	1:F:1070:SER:O	2.41	0.50
1:F:727:ARG:NH1	1:F:804:ASP:OD1	2.44	0.50
1:F:742:LEU:HA	1:F:745:HIS:HB3	1.93	0.50
4:J:68:ARG:NH2	4:J:290:ALA:O	2.45	0.50
1:A:544:HIS:HD2	1:A:546:ALA:H	1.60	0.50
1:C:592:ARG:HD2	1:C:1009:HIS:CD2	2.46	0.50
1:C:777:ASN:ND2	6:Q:47:GLN:OE1	2.45	0.50
1:F:264:LEU:HD23	1:F:303:PRO:HB2	1.94	0.50
5:K:192:ALA:HA	5:K:195:ALA:HB2	1.94	0.50
6:Q:76:GLN:O	6:Q:96:ARG:NH2	2.40	0.50
1:A:1369:LEU:HD13	1:A:1372:LEU:HD12	1.94	0.50
1:C:1152:VAL:HG11	1:C:1159:PRO:HD2	1.93	0.50
1:D:404:LEU:HB2	1:D:1052:VAL:HB	1.94	0.50
1:D:1017:GLU:O	1:D:1021:THR:OG1	2.25	0.50
4:I:114:VAL:HG11	4:I:291:LEU:HB3	1.94	0.50
1:A:164:GLN:OE1	1:A:167:ARG:NH2	2.44	0.50
1:B:135:LEU:HD21	1:B:143:LEU:HD21	1.93	0.50
1:E:1037:TYR:OH	1:E:1147:LEU:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:144:PRO:O	4:I:148:ALA:N	2.45	0.50
1:D:863:HIS:O	1:D:869:ASN:ND2	2.45	0.49
1:A:728:ASP:O	1:A:810:LYS:NZ	2.45	0.49
1:B:804:ASP:O	1:B:808:HIS:ND1	2.45	0.49
1:B:874:THR:OG1	1:B:875:VAL:N	2.44	0.49
1:C:420:ALA:HB2	1:D:421:GLY:HA3	1.94	0.49
1:C:959:PRO:HG2	1:C:990:VAL:HA	1.94	0.49
4:I:194:GLN:O	4:I:198:VAL:N	2.41	0.49
4:J:161:ARG:NH1	4:J:174:PRO:O	2.45	0.49
5:K:431:ASP:OD1	5:K:431:ASP:N	2.41	0.49
1:B:1339:ASP:HB2	1:B:1342:LEU:HG	1.94	0.49
1:D:633:ALA:HB1	1:D:897:LEU:HD21	1.92	0.49
4:I:227:LEU:HD13	4:I:228:LEU:H	1.77	0.49
5:K:270:PRO:HA	5:K:456:VAL:HA	1.94	0.49
1:A:907:ALA:HB1	1:A:994:LEU:HD21	1.94	0.49
1:B:738:ASP:N	1:B:738:ASP:OD1	2.44	0.49
1:C:392:TYR:HB3	1:C:395:VAL:HG12	1.92	0.49
1:C:970:VAL:HG11	1:C:989:LEU:HB2	1.95	0.49
1:D:577:VAL:HG12	1:D:578:VAL:HG13	1.93	0.49
1:D:1206:ARG:NH2	1:D:1208:ARG:O	2.44	0.49
1:E:1181:GLN:HE21	1:E:1310:GLN:HA	1.77	0.49
1:F:487:TYR:HE1	1:F:505:PHE:HZ	1.59	0.49
1:F:1118:PRO:HD3	1:F:1374:LEU:HD22	1.93	0.49
5:K:145:ARG:HA	5:K:154:THR:HB	1.94	0.49
1:B:730:ALA:HB2	1:B:750:ARG:HH12	1.78	0.49
1:C:99:VAL:HG13	1:C:118:ASN:HB2	1.94	0.49
1:D:1200:ARG:NH2	1:D:1355:GLU:OE2	2.44	0.49
1:F:460:THR:HG21	1:F:1187:PHE:HB2	1.94	0.49
4:I:109:CYS:HB2	4:I:304:ALA:HB1	1.93	0.49
4:I:177:ASN:HB3	4:I:188:LEU:HB3	1.94	0.49
4:J:281:HIS:HE1	5:K:466:ALA:HB2	1.78	0.49
6:N:83:ALA:N	6:N:86:GLU:OE2	2.44	0.49
1:A:629:LEU:HB3	1:A:839:LEU:HD21	1.94	0.49
1:A:751:HIS:CE1	1:A:754:CYS:HB2	2.48	0.49
1:B:1195:ASP:N	1:B:1195:ASP:OD1	2.45	0.49
1:D:778:ARG:H	1:D:904:ARG:HE	1.60	0.49
5:K:318:GLN:OE1	5:K:416:THR:N	2.45	0.49
1:B:713:GLU:HG2	1:B:718:ALA:HA	1.94	0.49
1:C:756:ILE:HG12	1:C:783:LEU:HD11	1.94	0.49
1:E:840:GLN:HB2	6:O:61:LEU:HD11	1.95	0.49
6:N:88:LEU:HD12	6:N:89:ARG:HG2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:O:76:GLN:O	6:O:96:ARG:NH2	2.35	0.49
1:A:320:LEU:HD12	1:A:321:VAL:HG23	1.94	0.49
1:A:925:ASN:O	1:A:927:ARG:NH1	2.44	0.49
1:C:584:LEU:HD13	1:C:589:VAL:HB	1.94	0.49
1:F:532:MET:HG3	1:F:534:PRO:HD2	1.95	0.49
1:F:624:PRO:HB3	1:F:882:GLY:HA3	1.94	0.49
1:F:1297:GLY:HA2	1:F:1322:GLU:HA	1.94	0.49
1:A:532:MET:HA	1:A:1240:ALA:H	1.77	0.49
1:B:579:ASN:ND2	1:B:1046:PRO:O	2.38	0.49
5:K:122:PRO:HB3	5:K:251:LEU:HD11	1.93	0.49
1:A:487:TYR:OH	1:A:990:VAL:N	2.46	0.49
1:B:315:ASN:O	1:B:319:ALA:N	2.39	0.49
1:D:599:LEU:O	1:D:603:ARG:NH1	2.44	0.49
1:D:909:LEU:HD11	1:D:929:PHE:HB3	1.94	0.49
1:F:539:LEU:O	1:F:1248:GLN:NE2	2.41	0.49
1:A:1001:SER:O	1:A:1003:ARG:NH1	2.46	0.48
1:B:1030:LYS:O	1:B:1039:GLN:NE2	2.41	0.48
1:C:460:THR:HG21	1:C:1187:PHE:HB2	1.95	0.48
1:D:405:PRO:O	1:D:1361:TYR:OH	2.26	0.48
1:E:392:TYR:HD2	1:E:395:VAL:HG12	1.76	0.48
1:F:410:ASN:ND2	1:F:414:GLU:O	2.46	0.48
1:F:433:ARG:O	1:F:1359:THR:OG1	2.29	0.48
4:J:32:VAL:N	4:J:73:ALA:O	2.42	0.48
5:K:278:HIS:N	5:K:279:PRO:HD2	2.28	0.48
1:B:523:GLU:HB3	1:B:1008:GLN:HG2	1.95	0.48
1:B:638:GLU:OE2	1:B:677:TYR:OH	2.23	0.48
1:C:219:LEU:O	1:C:223:LEU:N	2.45	0.48
1:C:770:ASN:H	1:C:773:THR:HB	1.77	0.48
1:D:261:VAL:HG12	1:D:264:LEU:H	1.78	0.48
1:F:604:HIS:O	1:F:1022:TYR:OH	2.26	0.48
1:B:14:ALA:HA	1:B:17:ILE:HD12	1.94	0.48
1:C:1222:VAL:O	1:C:1224:ALA:N	2.46	0.48
5:K:286:VAL:C	5:K:288:ILE:H	2.17	0.48
1:C:1037:TYR:CZ	1:C:1150:ALA:HB1	2.49	0.48
4:J:62:GLY:HA2	4:J:65:LEU:HD12	1.95	0.48
1:D:238:GLY:HA2	1:D:244:ILE:HD11	1.94	0.48
1:D:861:PRO:HA	1:D:866:HIS:CG	2.48	0.48
1:F:285:LYS:HZ1	1:F:378:GLU:HA	1.79	0.48
1:C:582:LEU:HD21	1:C:1048:PHE:HB3	1.96	0.48
1:C:648:VAL:HG13	1:C:664:PHE:HE2	1.78	0.48
1:C:1225:LEU:HD23	1:D:1175:ALA:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:805:TRP:O	1:D:809:HIS:ND1	2.34	0.48
1:E:535:ASP:H	1:F:1153:ALA:HB3	1.79	0.48
1:F:777:ASN:ND2	6:N:47:GLN:OE1	2.46	0.48
1:A:680:GLY:O	1:F:658:ASN:ND2	2.47	0.48
1:B:275:ASP:HA	1:B:1068:ARG:HD2	1.95	0.48
1:B:460:THR:HG23	1:B:1129:PHE:HE2	1.78	0.48
1:C:1221:ASP:OD2	1:D:1173:ARG:NH1	2.40	0.48
1:D:1248:GLN:HB2	1:D:1251:SER:HB3	1.96	0.48
1:E:255:THR:OG1	1:E:1067:GLU:OE2	2.31	0.48
1:F:804:ASP:O	1:F:808:HIS:ND1	2.39	0.48
1:A:696:HIS:HE1	1:A:1021:THR:HG21	1.78	0.48
1:A:942:PRO:HB2	1:A:968:ASP:HB2	1.94	0.48
1:D:80:VAL:HB	1:D:1072:ALA:HA	1.95	0.48
1:E:841:ASN:O	1:E:874:THR:OG1	2.27	0.48
1:F:717:GLN:HE22	1:F:750:ARG:HH11	1.62	0.48
1:A:433:ARG:O	1:A:1359:THR:OG1	2.31	0.48
1:A:778:ARG:NE	1:A:780:ASP:OD1	2.47	0.48
1:C:1129:PHE:HZ	1:C:1257:TYR:HE1	1.62	0.48
1:E:754:CYS:HA	1:E:910:CYS:HA	1.95	0.48
1:A:631:GLN:OE1	1:A:666:ASN:ND2	2.47	0.48
1:E:638:GLU:OE2	1:E:677:TYR:OH	2.32	0.48
1:E:755:ARG:N	1:E:909:LEU:O	2.46	0.48
1:B:763:PRO:HB2	1:B:765:TYR:HE1	1.79	0.47
1:C:674:ILE:HG23	1:C:678:LEU:HD12	1.95	0.47
1:C:909:LEU:HD11	1:C:929:PHE:HB3	1.95	0.47
1:B:733:PRO:HG2	1:B:736:VAL:HG22	1.96	0.47
1:D:433:ARG:HH22	1:D:1341:ALA:HB3	1.79	0.47
1:E:1131:LEU:HD23	1:E:1159:PRO:HG3	1.96	0.47
4:I:30:ARG:NH1	4:I:126:THR:OG1	2.47	0.47
1:A:491:VAL:HG21	1:A:929:PHE:HD2	1.79	0.47
1:A:712:PRO:O	1:A:719:GLN:NE2	2.43	0.47
1:A:592:ARG:HD2	1:A:1009:HIS:CD2	2.49	0.47
1:A:1057:ARG:NH2	1:A:1319:GLU:OE2	2.47	0.47
1:D:724:HIS:CD2	1:D:726:MET:H	2.32	0.47
1:D:1061:GLU:OE2	1:D:1116:ARG:NH1	2.48	0.47
1:F:129:LEU:HD11	1:F:183:GLN:HG3	1.96	0.47
1:F:131:ALA:N	1:F:1093:LEU:O	2.44	0.47
1:F:531:PHE:HE1	1:F:1244:PRO:HD3	1.80	0.47
1:C:697:VAL:HG12	1:C:808:HIS:HD2	1.79	0.47
1:D:1125:LEU:HD12	1:D:1126:PRO:HD2	1.96	0.47
1:F:202:GLN:O	1:F:206:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:ALA:HB1	1:A:376:PHE:HE1	1.79	0.47
1:B:33:ARG:O	1:B:33:ARG:NH2	2.45	0.47
1:D:905:THR:OG1	1:D:935:ALA:O	2.28	0.47
1:E:178:ARG:NH1	1:E:384:ILE:O	2.47	0.47
5:K:292:ALA:HB3	5:K:295:ASP:HB2	1.96	0.47
1:A:70:PHE:N	1:A:177:GLU:OE2	2.41	0.47
1:A:502:GLN:HA	1:A:505:PHE:HB3	1.96	0.47
1:C:1201:ARG:H	1:C:1333:PRO:HG2	1.79	0.47
1:C:1206:ARG:HB3	1:C:1277:PHE:CE1	2.49	0.47
1:D:184:MET:HA	1:D:187:VAL:HG22	1.96	0.47
1:D:460:THR:HG23	1:D:1129:PHE:HE2	1.80	0.47
1:D:724:HIS:HD2	1:D:726:MET:H	1.62	0.47
1:D:946:ASP:HA	1:E:677:TYR:HE1	1.80	0.47
1:E:528:ALA:H	1:E:531:PHE:HD2	1.61	0.47
1:F:840:GLN:HB2	6:N:61:LEU:HD11	1.96	0.47
5:K:267:CYS:SG	5:K:268:SER:OG	2.59	0.47
6:P:33:GLN:HG2	6:P:35:ILE:H	1.80	0.47
1:A:107:ASP:O	1:A:110:HIS:ND1	2.47	0.47
1:C:87:LEU:O	1:C:126:ARG:NH1	2.48	0.47
1:E:700:LEU:HD22	1:E:1025:MET:HG2	1.97	0.47
1:E:135:LEU:HD21	1:E:165:LEU:HD13	1.96	0.47
1:F:440:LEU:HD23	1:F:452:LEU:HD12	1.95	0.47
5:K:111:THR:HG23	5:K:266:VAL:HA	1.96	0.47
1:E:874:THR:OG1	1:E:875:VAL:N	2.48	0.47
1:F:581:ASN:HB3	1:F:1003:ARG:HB2	1.97	0.47
1:A:1270:LEU:HD22	1:A:1303:ALA:HB2	1.97	0.46
1:B:295:VAL:HB	1:B:369:ALA:H	1.80	0.46
1:C:488:GLY:H	1:C:520:TRP:HH2	1.62	0.46
1:E:272:ARG:HH11	1:E:374:LEU:HD12	1.80	0.46
1:E:606:MET:HG3	1:E:696:HIS:CD2	2.50	0.46
5:K:278:HIS:HB3	5:K:279:PRO:HD3	1.97	0.46
1:A:101:GLN:HB2	1:A:116:VAL:HG23	1.96	0.46
1:A:674:ILE:HG23	1:A:678:LEU:HD12	1.97	0.46
1:A:680:GLY:H	1:F:883:ARG:HH21	1.61	0.46
1:A:1306:ALA:HA	1:F:212:THR:HB	1.96	0.46
1:C:719:GLN:OE1	1:C:1038:HIS:NE2	2.42	0.46
1:F:445:LYS:HG3	1:F:1118:PRO:HG2	1.97	0.46
1:B:578:VAL:HG23	1:B:580:GLY:H	1.79	0.46
1:B:948:THR:HA	6:Q:93:GLY:HA3	1.97	0.46
1:C:548:ASP:OD1	1:C:576:ARG:NE	2.44	0.46
1:C:1003:ARG:HD2	1:C:1006:VAL:HG23	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1071:GLU:HG3	1:C:1073:TYR:HB2	1.98	0.46
4:I:161:ARG:NH1	4:I:174:PRO:O	2.33	0.46
1:B:295:VAL:HG21	1:B:369:ALA:HB3	1.96	0.46
1:D:750:ARG:HE	1:D:915:ASP:HA	1.81	0.46
1:E:1085:THR:OG1	1:E:1088:GLY:O	2.31	0.46
1:F:1061:GLU:OE2	1:F:1116:ARG:NE	2.44	0.46
1:A:102:PRO:HD2	1:B:387:ALA:HB3	1.97	0.46
1:A:278:LEU:HG	1:A:1065:PHE:HD1	1.79	0.46
5:K:314:PHE:HE1	5:K:327:VAL:HG13	1.81	0.46
1:A:1131:LEU:HD11	1:A:1157:LEU:HB3	1.96	0.46
1:B:278:LEU:HD13	1:B:375:VAL:HG11	1.96	0.46
1:C:1369:LEU:HD13	1:C:1372:LEU:HD12	1.97	0.46
1:D:1258:ASN:HB3	1:D:1261:TYR:HD2	1.80	0.46
1:E:212:THR:HB	1:E:215:ALA:HB3	1.96	0.46
1:E:281:THR:O	1:E:283:ALA:N	2.48	0.46
1:E:1270:LEU:HD22	1:E:1303:ALA:HB2	1.98	0.46
1:F:451:ARG:NH2	1:F:453:SER:OG	2.48	0.46
4:I:130:LEU:HD12	4:I:133:LEU:HD11	1.97	0.46
1:A:500:ASP:O	1:A:504:ARG:N	2.43	0.46
1:B:1238:PHE:HA	1:C:1156:ARG:HH22	1.81	0.46
1:C:825:CYS:HB2	1:C:938:LEU:HD11	1.96	0.46
1:F:581:ASN:HD22	1:F:1005:PRO:HD2	1.81	0.46
6:O:5:GLN:H	6:O:11:THR:HG21	1.80	0.46
1:A:403:VAL:HG22	1:A:1053:VAL:HG22	1.98	0.46
1:B:797:ASP:OD1	1:B:797:ASP:N	2.49	0.46
1:B:998:TYR:HA	1:B:1003:ARG:HE	1.80	0.46
1:C:997:ASN:HD21	1:C:1004:GLN:HB2	1.80	0.46
1:E:102:PRO:HB3	1:F:65:LEU:HD11	1.96	0.46
1:E:122:LYS:NZ	1:E:1101:ASP:O	2.43	0.46
1:E:1227:TYR:CE2	1:E:1249:ARG:HG2	2.51	0.46
1:F:403:VAL:HG12	1:F:405:PRO:HD3	1.97	0.46
1:F:738:ASP:OD2	1:F:801:ARG:NH2	2.49	0.46
4:J:306:VAL:HG11	4:J:312:ALA:HB2	1.97	0.46
1:A:528:ALA:H	1:A:531:PHE:HD2	1.63	0.46
1:A:581:ASN:HD22	1:A:1005:PRO:HD2	1.81	0.46
1:A:620:ASP:OD1	1:B:691:ARG:NH1	2.40	0.46
1:C:880:HIS:NE2	6:P:98:TYR:HB3	2.31	0.46
1:C:128:ALA:HA	1:C:1096:PRO:HA	1.97	0.46
1:E:724:HIS:CD2	1:E:726:MET:H	2.33	0.46
1:A:1357:HIS:O	1:A:1360:GLN:N	2.48	0.45
1:B:714:LEU:HB2	1:B:722:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1296:THR:HG21	1:D:1327:LEU:HD12	1.98	0.45
1:E:998:TYR:HA	1:E:1003:ARG:HE	1.81	0.45
1:F:453:SER:O	1:F:455:GLU:N	2.49	0.45
4:I:290:ALA:HB2	4:J:279:LEU:HD21	1.98	0.45
1:A:1125:LEU:HD11	1:A:1157:LEU:HG	1.97	0.45
1:B:915:ASP:OD1	1:B:915:ASP:N	2.50	0.45
1:C:750:ARG:O	1:C:752:ARG:NH2	2.49	0.45
1:C:933:LEU:HG	1:C:960:VAL:HG11	1.98	0.45
1:D:212:THR:HB	1:D:215:ALA:HB3	1.97	0.45
1:F:139:ALA:HB2	1:F:161:ALA:HB1	1.97	0.45
5:K:252:VAL:N	5:K:264:THR:O	2.45	0.45
1:A:251:LEU:HD21	1:A:1111:ALA:HB2	1.99	0.45
1:C:1195:ASP:OD1	1:C:1195:ASP:N	2.48	0.45
1:D:544:HIS:CD2	1:D:546:ALA:H	2.33	0.45
1:D:606:MET:HB2	1:D:1018:ASN:HD21	1.80	0.45
1:F:255:THR:OG1	1:F:1067:GLU:OE2	2.30	0.45
1:B:624:PRO:HB3	1:B:882:GLY:HA3	1.98	0.45
1:E:494:PRO:HB2	1:E:757:ASP:HA	1.98	0.45
1:E:604:HIS:O	1:E:1022:TYR:OH	2.25	0.45
1:B:600:GLY:HA2	1:B:1022:TYR:HD2	1.81	0.45
1:C:1131:LEU:HA	1:C:1159:PRO:HG3	1.98	0.45
1:D:617:ALA:HB2	1:D:661:CYS:HB3	1.98	0.45
1:F:865:LEU:HD21	1:F:879:PHE:HB3	1.97	0.45
1:F:1251:SER:O	1:F:1251:SER:OG	2.29	0.45
1:A:219:LEU:O	1:A:223:LEU:N	2.48	0.45
1:A:502:GLN:HE22	1:A:970:VAL:HG13	1.82	0.45
1:A:1128:ASN:ND2	1:A:1157:LEU:O	2.46	0.45
1:D:620:ASP:OD2	1:D:655:TYR:OH	2.29	0.45
1:E:198:LEU:O	1:E:202:GLN:N	2.36	0.45
1:F:285:LYS:HZ2	1:F:379:ALA:H	1.64	0.45
1:F:839:LEU:HB3	1:F:894:LEU:HD21	1.98	0.45
1:A:418:ALA:HA	1:B:423:LEU:HD23	1.99	0.45
1:A:433:ARG:NH1	1:F:413:MET:O	2.46	0.45
1:B:1216:GLY:O	1:B:1287:ARG:NH2	2.45	0.45
1:F:1204:ASN:ND2	1:F:1329:GLN:O	2.49	0.45
1:A:920:THR:HG22	1:A:1138:LEU:HD23	1.98	0.45
1:C:541:LEU:HD22	1:C:571:ILE:HD12	1.99	0.45
1:E:1321:VAL:HG13	1:E:1323:ASP:HB2	1.98	0.45
1:A:1257:TYR:HB2	1:A:1277:PHE:HD2	1.82	0.45
1:B:440:LEU:HD23	1:B:452:LEU:HD12	1.99	0.45
1:C:728:ASP:OD2	1:C:1030:LYS:NZ	2.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:ALA:HB3	1:D:274:VAL:HB	1.98	0.45
1:D:841:ASN:O	1:D:874:THR:OG1	2.27	0.45
1:E:588:PRO:HD3	1:E:1193:ALA:HB2	1.99	0.45
1:E:951:ASN:ND2	1:E:972:ASN:O	2.43	0.45
1:F:1061:GLU:HG3	1:F:1114:THR:HB	1.98	0.45
1:F:1085:THR:OG1	1:F:1090:ASN:ND2	2.50	0.45
3:H:1315:UNK:O	3:H:1319:UNK:N	2.50	0.45
1:A:196:ALA:HB1	1:A:227:PHE:HA	1.99	0.45
1:A:606:MET:HG3	1:A:696:HIS:CD2	2.52	0.45
1:D:68:VAL:HG12	1:D:383:ARG:HH21	1.82	0.45
1:A:258:SER:HB3	1:A:1069:ALA:HB3	1.98	0.44
1:A:404:LEU:HD12	1:A:1336:CYS:HB3	1.98	0.44
1:B:284:ILE:O	1:B:288:LEU:N	2.43	0.44
1:B:1160:ALA:HB2	1:B:1172:PRO:HG3	1.98	0.44
1:D:777:ASN:ND2	6:P:47:GLN:OE1	2.42	0.44
1:F:446:ASP:HB2	1:F:448:GLN:HB2	1.98	0.44
5:K:458:ARG:HA	5:K:459:PRO:HD3	1.85	0.44
1:A:577:VAL:H	1:A:1003:ARG:HH12	1.64	0.44
1:C:532:MET:HA	1:C:1240:ALA:H	1.81	0.44
2:G:232:UNK:O	2:G:236:UNK:N	2.50	0.44
1:A:392:TYR:CE2	1:A:394:LEU:HB2	2.52	0.44
1:A:752:ARG:O	1:A:911:SER:OG	2.28	0.44
1:C:578:VAL:HG21	1:C:1028:TYR:HD1	1.82	0.44
1:D:623:TYR:OH	1:D:663:ALA:O	2.31	0.44
1:E:137:THR:OG1	1:E:1087:GLY:O	2.33	0.44
1:F:360:THR:OG1	1:F:361:THR:N	2.51	0.44
4:I:100:LEU:HD12	4:I:314:VAL:HG21	1.99	0.44
1:A:276:GLY:HA3	1:A:375:VAL:HG13	2.00	0.44
1:B:718:ALA:HB3	1:B:721:GLU:HG3	2.00	0.44
1:E:104:ILE:HG23	1:F:179:GLY:HA2	2.00	0.44
1:A:986:ASP:OD2	1:B:705:ASP:HB3	2.17	0.44
1:B:486:PRO:HB2	1:B:489:ALA:HB3	2.00	0.44
1:E:750:ARG:NH2	1:E:913:ALA:O	2.50	0.44
1:F:654:SER:HB3	1:F:884:VAL:HG13	2.00	0.44
6:M:72:THR:HB	6:M:100:PRO:HB2	2.00	0.44
1:A:87:LEU:HD21	1:A:1098:GLY:H	1.81	0.44
1:D:777:ASN:HA	1:D:904:ARG:HD3	1.99	0.44
1:A:251:LEU:HD23	1:A:251:LEU:HA	1.83	0.44
1:B:1056:ASP:OD1	1:B:1057:ARG:N	2.47	0.44
1:C:275:ASP:OD1	1:C:275:ASP:N	2.49	0.44
1:C:1003:ARG:HG3	1:C:1006:VAL:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:GLY:H	1:D:238:GLY:HA3	1.83	0.44
1:F:504:ARG:HA	1:F:507:ASN:HB2	1.99	0.44
1:F:846:GLU:HA	6:N:68:HIS:CE1	2.53	0.44
1:F:1283:THR:O	1:F:1285:LYS:N	2.49	0.44
6:L:71:ASN:O	6:L:102:VAL:N	2.44	0.44
1:D:656:TRP:CD2	1:D:686:CYS:HB3	2.53	0.44
1:A:970:VAL:HG11	1:A:989:LEU:HB2	1.98	0.44
1:C:315:ASN:ND2	1:C:326:VAL:O	2.43	0.44
1:C:348:ARG:HE	1:D:170:GLN:HE22	1.65	0.44
1:C:1029:PHE:HE2	1:C:1044:LEU:HD13	1.83	0.44
1:D:750:ARG:NH2	1:D:913:ALA:O	2.51	0.44
1:A:467:MET:HG3	1:A:923:THR:HG21	1.99	0.43
1:B:730:ALA:HB2	1:B:750:ARG:HH22	1.82	0.43
1:B:1131:LEU:HD23	1:B:1159:PRO:HG3	1.99	0.43
1:E:490:TYR:OH	1:E:560:GLY:O	2.28	0.43
1:E:548:ASP:OD1	1:E:576:ARG:NE	2.51	0.43
1:A:182:ASP:O	1:A:186:HIS:ND1	2.41	0.43
1:A:895:GLN:HA	6:M:61:LEU:HD13	2.00	0.43
1:B:697:VAL:HG12	1:B:808:HIS:HD2	1.83	0.43
1:C:1125:LEU:HD12	1:C:1126:PRO:HD2	2.00	0.43
1:E:1314:PRO:HA	1:E:1315:PRO:HD3	1.85	0.43
1:F:866:HIS:CD2	1:F:868:ALA:H	2.37	0.43
1:A:83:LYS:HG3	1:A:305:THR:HG21	2.00	0.43
1:D:728:ASP:O	1:D:810:LYS:NZ	2.51	0.43
1:E:1118:PRO:HD3	1:E:1374:LEU:HD13	1.99	0.43
1:F:186:HIS:O	1:F:190:GLU:N	2.49	0.43
1:F:1163:LEU:HD23	1:F:1169:ALA:HB2	2.00	0.43
5:K:131:LEU:HB3	5:K:184:LEU:HD22	2.00	0.43
6:O:25:LEU:HD21	6:O:57:GLN:HG2	2.00	0.43
1:A:189:LEU:HD12	1:A:1064:LEU:HD13	2.01	0.43
1:A:785:HIS:HE2	1:A:800:HIS:HD2	1.66	0.43
1:B:193:PRO:HG2	1:B:198:LEU:HD12	2.00	0.43
1:B:904:ARG:NH1	1:B:906:THR:OG1	2.51	0.43
1:B:1125:LEU:HD12	1:B:1126:PRO:HD2	2.00	0.43
1:C:828:ALA:HB1	1:C:955:PHE:HB3	1.99	0.43
1:D:960:VAL:HA	1:D:994:LEU:HD13	2.00	0.43
5:K:281:ARG:N	5:K:282:PRO:CD	2.81	0.43
1:B:950:GLN:HB3	1:B:953:GLU:HB3	2.01	0.43
1:C:268:ASP:N	1:C:272:ARG:O	2.47	0.43
1:D:1133:ARG:NH1	1:D:1165:VAL:O	2.51	0.43
1:D:1339:ASP:HB2	1:D:1342:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1161:GLN:H	1:F:1161:GLN:HG2	1.57	0.43
1:B:429:HIS:HA	1:B:430:PRO:HD3	1.86	0.43
1:E:472:ALA:HA	1:E:1250:PHE:HB3	1.99	0.43
1:F:198:LEU:HA	1:F:201:MET:HB3	2.01	0.43
1:F:1221:ASP:OD1	1:F:1221:ASP:N	2.44	0.43
1:A:154:SER:C	1:A:156:HIS:H	2.22	0.43
1:A:421:GLY:HA3	1:F:420:ALA:HB2	1.99	0.43
1:B:493:ALA:HB2	1:B:560:GLY:HA2	2.01	0.43
1:B:805:TRP:CE2	1:B:809:HIS:HE1	2.37	0.43
1:C:1082:ARG:NH2	1:C:1084:GLU:OE2	2.52	0.43
1:F:681:ASP:OD1	1:F:681:ASP:N	2.45	0.43
6:L:60:ALA:HA	6:L:63:ASP:HB2	1.99	0.43
1:A:790:ARG:NH1	6:M:80:ALA:O	2.52	0.43
1:A:1106:TYR:OH	1:A:1290:GLU:OE1	2.33	0.43
1:C:724:HIS:HD1	1:C:1029:PHE:HD1	1.66	0.43
1:D:665:VAL:O	1:D:812:TYR:OH	2.29	0.43
1:D:789:ALA:HB1	6:P:79:PHE:CG	2.53	0.43
1:D:854:PRO:HB2	1:D:863:HIS:HD2	1.84	0.43
1:F:285:LYS:HG3	1:F:289:LEU:HD23	2.00	0.43
6:O:64:LEU:O	6:O:67:THR:OG1	2.30	0.43
1:A:915:ASP:N	1:A:915:ASP:OD1	2.50	0.43
1:A:1029:PHE:HB3	1:A:1039:GLN:NE2	2.34	0.43
1:A:1054:ARG:NH1	1:A:1123:GLY:O	2.51	0.43
1:B:416:PHE:HB2	1:C:423:LEU:HA	2.01	0.43
1:C:1052:VAL:HG13	1:C:1185:CYS:HB3	2.00	0.43
1:D:785:HIS:NE2	1:D:798:ARG:O	2.52	0.43
1:D:904:ARG:NH1	1:D:905:THR:O	2.51	0.43
6:Q:33:GLN:HG2	6:Q:35:ILE:H	1.82	0.43
1:B:490:TYR:OH	1:B:560:GLY:O	2.37	0.43
1:E:276:GLY:HA3	1:E:375:VAL:HG13	2.00	0.43
1:E:620:ASP:OD2	1:E:655:TYR:OH	2.31	0.43
1:E:1227:TYR:CG	1:E:1249:ARG:CG	3.02	0.43
1:F:248:LEU:HD21	1:F:288:LEU:HD11	2.00	0.43
1:C:127:ARG:HD2	1:C:183:GLN:HE21	1.84	0.42
1:C:196:ALA:HB1	1:C:227:PHE:HA	1.99	0.42
1:C:960:VAL:HG12	1:C:994:LEU:HD13	2.01	0.42
1:D:483:ALA:HB2	1:D:569:GLY:HA3	2.01	0.42
1:E:790:ARG:HH11	6:O:79:PHE:HD2	1.67	0.42
1:F:367:LEU:HD12	1:F:374:LEU:HG	2.01	0.42
1:F:1056:ASP:HA	1:F:1120:THR:HG21	2.01	0.42
4:I:276:VAL:HG11	4:J:154:ARG:HE	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:269:LEU:HB3	4:J:272:TYR:HB3	2.01	0.42
1:B:76:SER:HG	1:B:266:HIS:CD2	2.35	0.42
1:B:405:PRO:HA	1:B:1051:THR:HA	2.02	0.42
1:B:530:GLN:HG3	1:B:536:ASN:ND2	2.33	0.42
1:B:734:PRO:HB3	1:B:960:VAL:HG21	2.01	0.42
1:C:452:LEU:HD13	1:C:1052:VAL:HG21	2.01	0.42
1:E:453:SER:O	1:E:455:GLU:N	2.52	0.42
1:F:575:TRP:HE3	1:F:928:ILE:HD11	1.83	0.42
1:F:1198:TYR:CD1	1:F:1236:ARG:HD2	2.54	0.42
1:A:677:TYR:HD1	6:M:95:LYS:HE2	1.85	0.42
1:A:695:ALA:HA	1:A:698:GLU:HB2	2.02	0.42
1:B:701:ALA:O	1:B:727:ARG:NH2	2.45	0.42
1:B:1229:HIS:CE1	1:B:1248:GLN:HG2	2.53	0.42
1:C:608:PRO:HA	1:C:611:ILE:HD12	2.00	0.42
1:C:742:LEU:HA	1:C:745:HIS:HB3	2.01	0.42
1:C:963:LEU:HD21	1:C:1006:VAL:HG12	2.01	0.42
1:D:627:PHE:CE1	1:D:651:CYS:HB3	2.54	0.42
1:D:772:ALA:HA	6:P:55:ARG:HE	1.84	0.42
1:E:735:LEU:HD22	1:E:936:GLY:HA3	2.01	0.42
1:F:1200:ARG:HG2	1:F:1363:ILE:HG23	2.01	0.42
4:J:154:ARG:NH1	4:J:178:VAL:O	2.43	0.42
1:A:300:ALA:HA	1:A:362:ARG:HA	2.00	0.42
1:A:1204:ASN:HD22	1:A:1209:ALA:HA	1.84	0.42
1:B:8:PRO:O	1:B:10:GLY:N	2.46	0.42
1:B:281:THR:HG22	1:B:392:TYR:HE2	1.85	0.42
1:C:451:ARG:HG2	1:C:453:SER:HB3	2.00	0.42
1:D:309:MET:SD	1:D:327:ARG:NH1	2.92	0.42
1:D:584:LEU:HG	1:D:1005:PRO:HB3	2.00	0.42
1:E:436:PRO:HA	1:E:437:PRO:HD3	1.89	0.42
1:E:1229:HIS:CE1	1:E:1248:GLN:HG2	2.53	0.42
1:F:294:LYS:H	1:F:368:VAL:HG12	1.84	0.42
1:A:545:PRO:O	1:A:576:ARG:NH1	2.40	0.42
1:A:1054:ARG:NH2	1:A:1123:GLY:H	2.14	0.42
1:B:880:HIS:CE1	6:Q:98:TYR:HB3	2.54	0.42
1:C:626:VAL:HA	1:C:629:LEU:HD12	2.02	0.42
1:D:606:MET:HG3	1:D:696:HIS:CD2	2.53	0.42
1:E:452:LEU:HA	1:E:452:LEU:HD23	1.81	0.42
1:E:544:HIS:HD2	1:E:546:ALA:H	1.66	0.42
1:E:551:ALA:HA	1:E:571:ILE:HA	2.02	0.42
1:E:1099:ASN:N	1:E:1099:ASN:OD1	2.52	0.42
1:F:142:LEU:HD23	1:F:158:GLN:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:LEU:HB2	1:F:392:TYR:HE1	1.83	0.42
1:F:1054:ARG:HD2	1:F:1123:GLY:HA2	2.01	0.42
4:J:30:ARG:HH12	4:J:103:THR:HG21	1.85	0.42
1:A:204:TYR:HD2	1:A:219:LEU:HD13	1.84	0.42
1:A:255:THR:HG21	1:A:1109:VAL:H	1.85	0.42
1:A:581:ASN:HB2	1:A:1003:ARG:NH2	2.34	0.42
1:A:621:ARG:NH2	1:B:698:GLU:OE1	2.52	0.42
1:A:822:ARG:NH2	1:A:1013:SER:O	2.52	0.42
1:B:639:HIS:CE1	1:B:791:ALA:HB2	2.55	0.42
4:I:283:GLY:O	4:J:149:ARG:NH1	2.52	0.42
1:C:207:ASN:OD1	1:C:208:GLY:N	2.53	0.42
1:C:300:ALA:HB1	1:C:362:ARG:HD2	2.00	0.42
1:F:1074:PHE:N	1:F:1098:GLY:O	2.48	0.42
5:K:144:ALA:HA	5:K:239:VAL:HG21	2.02	0.42
1:A:1216:GLY:N	1:A:1221:ASP:OD2	2.53	0.42
1:B:729:PRO:HB2	1:B:748:LEU:HD11	2.02	0.42
1:C:487:TYR:OH	1:C:990:VAL:N	2.53	0.42
1:C:959:PRO:HB2	1:C:990:VAL:HG22	2.01	0.42
1:D:840:GLN:HB2	6:P:61:LEU:HD21	2.01	0.42
1:D:1206:ARG:NH1	1:D:1247:SER:O	2.53	0.42
4:J:212:SER:HB2	4:J:278:TRP:CD1	2.55	0.42
1:B:895:GLN:HA	6:L:61:LEU:HD13	2.02	0.42
1:C:416:PHE:HB2	1:D:423:LEU:HA	2.02	0.42
1:C:1081:ALA:HB3	1:C:1092:THR:HG22	2.02	0.42
1:E:188:LEU:HD23	1:E:191:LYS:HD3	2.02	0.42
1:F:87:LEU:HD22	1:F:1074:PHE:HB3	2.01	0.42
5:K:300:LEU:HB3	5:K:303:GLY:HA3	2.01	0.42
6:N:48:GLY:HA2	6:N:51:ARG:HD2	2.01	0.42
1:A:861:PRO:HA	1:A:866:HIS:CG	2.55	0.42
1:A:1138:LEU:HD12	1:A:1144:ALA:HA	2.02	0.42
1:B:261:VAL:HG12	1:B:264:LEU:H	1.83	0.42
1:B:1206:ARG:NH2	1:B:1208:ARG:O	2.50	0.42
1:C:83:LYS:HB2	1:C:308:GLU:HG2	2.02	0.42
1:C:212:THR:HB	1:C:215:ALA:HB3	2.01	0.42
1:C:320:LEU:HD12	1:C:321:VAL:HG23	2.01	0.42
1:D:219:LEU:O	1:D:223:LEU:N	2.53	0.42
1:E:406:LEU:HD23	1:E:406:LEU:HA	1.90	0.42
1:F:539:LEU:HD23	1:F:1229:HIS:HB3	2.00	0.42
6:M:83:ALA:HB3	6:M:86:GLU:HG2	2.01	0.42
6:N:72:THR:HG22	6:N:100:PRO:HB2	2.02	0.42
1:A:665:VAL:O	1:A:812:TYR:OH	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:TYR:OH	1:B:663:ALA:O	2.30	0.41
1:B:668:TYR:HB2	1:B:812:TYR:CD2	2.55	0.41
1:B:946:ASP:OD1	1:B:946:ASP:N	2.53	0.41
1:D:962:ALA:HB3	1:D:1007:VAL:HG21	2.02	0.41
1:E:623:TYR:OH	1:E:663:ALA:O	2.24	0.41
1:E:1298:SER:HB2	1:E:1320:LEU:HD22	2.02	0.41
1:F:544:HIS:HD2	1:F:546:ALA:H	1.68	0.41
1:F:753:ASP:N	1:F:753:ASP:OD1	2.52	0.41
1:F:909:LEU:HD11	1:F:929:PHE:HB3	2.01	0.41
6:M:88:LEU:HD12	6:M:89:ARG:HG2	2.02	0.41
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.85	0.41
1:B:502:GLN:HA	1:B:505:PHE:HB3	2.02	0.41
1:B:956:TYR:HE2	1:B:958:LEU:HD22	1.85	0.41
1:B:985:ARG:HH12	1:C:727:ARG:HD2	1.86	0.41
1:C:311:LEU:HD22	1:C:315:ASN:HB3	2.01	0.41
1:D:1029:PHE:HB3	1:D:1039:GLN:NE2	2.35	0.41
1:E:372:ASP:OD1	1:E:372:ASP:N	2.52	0.41
1:E:394:LEU:HD21	1:E:1064:LEU:HD13	2.01	0.41
1:F:440:LEU:HD12	1:F:440:LEU:HA	1.89	0.41
1:F:730:ALA:HA	1:F:745:HIS:HD1	1.84	0.41
4:I:48:HIS:CD2	4:I:138:ARG:HD3	2.55	0.41
1:A:142:LEU:O	1:A:142:LEU:HD22	2.20	0.41
1:A:488:GLY:H	1:A:520:TRP:HH2	1.67	0.41
1:A:638:GLU:HB2	1:A:801:ARG:HH22	1.85	0.41
1:A:884:VAL:HG12	1:A:886:VAL:HG23	2.02	0.41
1:B:1074:PHE:N	1:B:1098:GLY:O	2.48	0.41
1:C:1256:LEU:HA	1:C:1263:LEU:HD12	2.03	0.41
1:D:73:LEU:HD12	1:D:73:LEU:HA	1.92	0.41
1:D:485:ASN:OD1	1:D:485:ASN:N	2.53	0.41
1:E:17:ILE:HG22	1:E:17:ILE:O	2.19	0.41
1:E:289:LEU:HA	1:E:293:LEU:HD12	2.01	0.41
1:F:1286:HIS:HE1	1:F:1291:ARG:HB3	1.84	0.41
5:K:299:GLU:HG2	5:K:300:LEU:H	1.85	0.41
1:A:384:ILE:H	1:A:384:ILE:HG13	1.80	0.41
1:C:1161:GLN:HG3	1:C:1162:PRO:HD2	2.02	0.41
1:D:270:ARG:NH1	1:D:297:ASP:OD1	2.54	0.41
1:D:545:PRO:HG3	1:D:1245:TRP:CD2	2.55	0.41
1:D:1301:SER:OG	1:D:1319:GLU:OE1	2.39	0.41
1:E:1237:PRO:HB2	1:F:1156:ARG:NH1	2.35	0.41
1:F:165:LEU:HD23	1:F:165:LEU:HA	1.89	0.41
4:I:35:PRO:HA	4:I:70:ARG:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:276:VAL:HG21	4:J:154:ARG:HD3	2.02	0.41
1:A:752:ARG:HH22	1:A:913:ALA:HB2	1.84	0.41
1:A:778:ARG:NH1	1:A:782:ARG:O	2.53	0.41
1:B:255:THR:OG1	1:B:1067:GLU:OE2	2.27	0.41
1:B:417:ALA:HB2	1:B:1358:PHE:CE1	2.56	0.41
1:B:1223:ILE:O	1:B:1226:MET:N	2.51	0.41
1:C:1029:PHE:HB3	1:C:1039:GLN:NE2	2.35	0.41
1:E:487:TYR:HE1	1:E:505:PHE:HZ	1.68	0.41
1:E:530:GLN:HG3	1:E:536:ASN:ND2	2.34	0.41
1:F:153:ILE:O	1:F:157:ARG:N	2.46	0.41
1:F:158:GLN:O	1:F:162:ILE:N	2.50	0.41
4:I:182:ASN:OD1	4:I:183:GLY:N	2.52	0.41
1:A:708:THR:OG1	1:A:723:ASN:ND2	2.42	0.41
1:A:804:ASP:O	1:A:808:HIS:ND1	2.36	0.41
1:B:392:TYR:CE2	1:B:394:LEU:HB2	2.55	0.41
1:B:452:LEU:HA	1:B:452:LEU:HD23	1.86	0.41
1:B:962:ALA:HB3	1:B:1007:VAL:HG21	2.01	0.41
1:B:1202:PRO:HA	1:B:1333:PRO:HD3	2.02	0.41
1:C:1235:ALA:O	1:D:1179:HIS:NE2	2.37	0.41
1:D:668:TYR:HB2	1:D:812:TYR:CD2	2.55	0.41
1:E:248:LEU:HD21	1:E:288:LEU:HD11	2.03	0.41
1:E:275:ASP:N	1:E:275:ASP:OD1	2.53	0.41
1:E:1066:SER:HG	1:E:1067:GLU:N	2.19	0.41
4:J:212:SER:HB2	4:J:278:TRP:HD1	1.85	0.41
1:A:154:SER:C	1:A:156:HIS:N	2.73	0.41
1:B:1083:HIS:CD2	1:B:1084:GLU:H	2.39	0.41
1:D:581:ASN:HB3	1:D:1003:ARG:HE	1.86	0.41
1:E:804:ASP:O	1:E:808:HIS:ND1	2.43	0.41
1:A:1125:LEU:HD21	1:A:1309:VAL:HG13	2.02	0.41
1:B:8:PRO:HG2	1:B:38:PHE:HB2	2.03	0.41
1:B:163:GLN:HB3	1:B:167:ARG:HH21	1.85	0.41
1:B:325:ALA:HB3	1:C:56:ALA:HB2	2.03	0.41
1:D:425:PRO:HD3	1:D:431:GLU:OE1	2.21	0.41
1:F:145:GLY:HA2	1:F:148:LEU:HD13	2.03	0.41
1:F:385:TYR:CE2	1:F:393:PRO:HD3	2.56	0.41
1:F:452:LEU:HD23	1:F:452:LEU:HA	1.80	0.41
1:F:631:GLN:OE1	1:F:666:ASN:ND2	2.54	0.41
1:F:930:ASP:OD1	1:F:1001:SER:OG	2.35	0.41
2:G:203:UNK:O	2:G:207:UNK:N	2.54	0.41
4:I:47:ALA:HA	4:I:137:LEU:HD23	2.02	0.41
4:I:76:THR:OG1	4:I:77:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:231:LEU:HA	5:K:234:MET:HE3	2.03	0.41
1:A:143:LEU:HD13	1:A:143:LEU:C	2.41	0.41
1:A:244:ILE:HG23	1:A:248:LEU:HD13	2.03	0.41
1:A:523:GLU:O	1:A:525:GLN:N	2.54	0.41
1:A:624:PRO:HB3	1:A:882:GLY:HA3	2.03	0.41
1:A:733:PRO:HG2	1:A:736:VAL:HG22	2.02	0.41
1:A:1190:THR:HG22	1:A:1243:ASN:ND2	2.36	0.41
1:A:1206:ARG:HB3	1:A:1277:PHE:CE1	2.56	0.41
1:C:281:THR:HG22	1:C:284:ILE:HD12	2.02	0.41
1:C:778:ARG:HB3	1:C:904:ARG:HE	1.85	0.41
1:D:863:HIS:CE1	1:D:865:LEU:HB2	2.56	0.41
1:D:1215:ALA:HB3	1:D:1287:ARG:HE	1.86	0.41
1:E:281:THR:HG21	1:E:1061:GLU:HB3	2.03	0.41
1:E:861:PRO:HA	1:E:866:HIS:CD2	2.56	0.41
1:F:895:GLN:HA	6:N:61:LEU:HD13	2.02	0.41
4:I:223:LEU:O	4:I:227:LEU:N	2.54	0.41
4:J:88:VAL:HG13	4:J:92:LEU:HD22	2.03	0.41
1:A:1314:PRO:HG2	1:A:1317:CYS:HB3	2.02	0.41
1:B:280:THR:HG22	1:B:1063:VAL:HG12	2.03	0.41
1:C:1157:LEU:HD23	1:C:1157:LEU:HA	1.85	0.41
1:C:1276:PHE:HA	1:C:1329:GLN:HE22	1.86	0.41
1:D:58:LEU:HD23	1:D:58:LEU:HA	1.88	0.41
1:D:213:ARG:NH2	1:E:1308:ASP:OD2	2.54	0.41
1:E:71:LEU:HD13	1:E:305:THR:HA	2.02	0.41
4:J:16:ILE:HD13	4:J:16:ILE:HA	1.88	0.41
1:A:406:LEU:HD21	1:A:452:LEU:HB3	2.02	0.40
1:B:314:ALA:O	1:B:318:THR:OG1	2.28	0.40
1:C:392:TYR:HA	1:C:393:PRO:HD3	1.97	0.40
1:D:400:LEU:HD12	1:D:1058:PHE:HE2	1.86	0.40
1:D:606:MET:H	1:D:1018:ASN:ND2	2.19	0.40
1:E:549:PHE:HB3	1:E:571:ILE:HD11	2.03	0.40
1:E:774:ALA:HB1	1:E:903:GLU:HB3	2.03	0.40
1:E:1227:TYR:CD2	1:E:1249:ARG:HG2	2.56	0.40
1:F:311:LEU:O	1:F:315:ASN:N	2.49	0.40
1:F:764:VAL:HG13	1:F:782:ARG:HE	1.85	0.40
1:A:275:ASP:N	1:A:275:ASP:OD1	2.53	0.40
1:A:883:ARG:NH2	6:L:97:THR:OG1	2.52	0.40
1:C:491:VAL:HG21	1:C:929:PHE:HD2	1.86	0.40
1:C:724:HIS:CD2	1:C:726:MET:H	2.38	0.40
1:C:881:ASN:HD21	6:P:94:LEU:HD23	1.86	0.40
1:D:206:ASP:OD1	1:D:206:ASP:N	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:LEU:O	1:E:1052:VAL:N	2.49	0.40
1:F:468:ASN:HD21	1:F:1136:PRO:HB2	1.85	0.40
1:F:732:LEU:HD13	1:F:932:ALA:HB2	2.03	0.40
1:B:577:VAL:HG11	1:B:725:LEU:HD13	2.03	0.40
1:C:67:LEU:HD22	1:C:174:GLY:HA3	2.03	0.40
1:C:267:ALA:HA	1:C:273:PRO:HA	2.02	0.40
1:C:873:ASN:ND2	6:Q:30:ASN:OD1	2.44	0.40
1:D:733:PRO:HG2	1:D:736:VAL:HG22	2.03	0.40
1:E:959:PRO:HB2	1:E:990:VAL:HG22	2.03	0.40
1:F:844:VAL:HB	6:N:64:LEU:HD21	2.03	0.40
1:F:1208:ARG:HB2	1:F:1241:THR:HG22	2.03	0.40
4:J:198:VAL:O	4:J:202:LEU:N	2.46	0.40
1:A:805:TRP:O	1:A:809:HIS:ND1	2.41	0.40
1:B:392:TYR:HA	1:B:393:PRO:HD3	1.84	0.40
1:B:442:PHE:HE1	1:B:452:LEU:HG	1.85	0.40
1:E:836:TYR:O	1:E:840:GLN:HG2	2.21	0.40
1:F:426:ALA:HB3	1:F:429:HIS:ND1	2.36	0.40
4:J:94:HIS:HB3	4:J:97:THR:H	1.85	0.40
1:A:440:LEU:O	1:A:452:LEU:N	2.46	0.40
1:C:777:ASN:O	6:Q:51:ARG:NH2	2.50	0.40
1:E:866:HIS:CD2	1:E:868:ALA:H	2.40	0.40
5:K:324:LEU:HD23	5:K:349:ARG:HE	1.87	0.40
6:N:51:ARG:HB3	6:N:55:ARG:HH12	1.87	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	1346/1374 (98%)	1192 (89%)	146 (11%)	8 (1%)	25 63
1	B	1356/1374 (99%)	1236 (91%)	117 (9%)	3 (0%)	47 80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1356/1374 (99%)	1227 (90%)	126 (9%)	3 (0%)	47	80
1	D	1354/1374 (98%)	1241 (92%)	111 (8%)	2 (0%)	51	84
1	E	1335/1374 (97%)	1206 (90%)	125 (9%)	4 (0%)	41	75
1	F	1347/1374 (98%)	1198 (89%)	145 (11%)	4 (0%)	41	75
4	I	291/318 (92%)	250 (86%)	41 (14%)	0	100	100
4	J	301/318 (95%)	265 (88%)	35 (12%)	1 (0%)	41	75
5	K	275/466 (59%)	231 (84%)	41 (15%)	3 (1%)	14	51
6	L	99/112 (88%)	93 (94%)	6 (6%)	0	100	100
6	M	99/112 (88%)	93 (94%)	6 (6%)	0	100	100
6	N	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
6	O	99/112 (88%)	93 (94%)	6 (6%)	0	100	100
6	P	99/112 (88%)	96 (97%)	3 (3%)	0	100	100
6	Q	99/112 (88%)	94 (95%)	5 (5%)	0	100	100
All	All	9555/10018 (95%)	8609 (90%)	918 (10%)	28 (0%)	44	75

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1223	ILE
1	B	1223	ILE
1	C	1223	ILE
1	D	1084	GLU
1	E	454	MET
1	E	1223	ILE
5	K	286	VAL
1	A	147	ALA
1	B	454	MET
1	C	1084	GLU
1	F	454	MET
1	F	1284	ALA
5	K	120	CYS
1	A	47	ASN
1	C	454	MET
1	D	1085	THR
1	E	282	ALA
1	F	30	ALA
1	A	153	ILE

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Mol	Chain	Res	Type
5	K	287	THR
1	A	41	ALA
1	A	346	ALA
1	A	356	SER
1	E	1222	VAL
1	F	1202	PRO
1	A	1108	ALA
1	B	1222	VAL
4	J	13	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	A	968/1080 (90%)	958 (99%)	10 (1%)	76	86
1	B	1016/1080 (94%)	1010 (99%)	6 (1%)	86	92
1	C	1020/1080 (94%)	1019 (100%)	1 (0%)	93	97
1	D	1015/1080 (94%)	1012 (100%)	3 (0%)	92	95
1	E	1010/1080 (94%)	1005 (100%)	5 (0%)	88	93
1	F	966/1080 (89%)	954 (99%)	12 (1%)	71	83
4	I	195/264 (74%)	192 (98%)	3 (2%)	65	80
4	J	214/264 (81%)	214 (100%)	0	100	100
5	K	182/365 (50%)	182 (100%)	0	100	100
6	L	78/88 (89%)	78 (100%)	0	100	100
6	M	78/88 (89%)	78 (100%)	0	100	100
6	N	78/88 (89%)	78 (100%)	0	100	100
6	O	78/88 (89%)	78 (100%)	0	100	100
6	P	78/88 (89%)	78 (100%)	0	100	100
6	Q	78/88 (89%)	78 (100%)	0	100	100
All	All	7054/7901 (89%)	7014 (99%)	40 (1%)	86	92

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

Mol	Chain	Res	Type
1	A	67	LEU
1	A	82	THR
1	A	142	LEU
1	A	143	LEU
1	A	153	ILE
1	A	155	LEU
1	A	341	GLU
1	A	343	GLN
1	A	519	ARG
1	A	1156	ARG
1	B	327	ARG
1	B	347	ASN
1	B	519	ARG
1	B	1036	LEU
1	B	1114	THR
1	B	1287	ARG
1	C	1156	ARG
1	D	519	ARG
1	D	1100	VAL
1	D	1174	ARG
1	E	287	ARG
1	E	288	LEU
1	E	293	LEU
1	E	327	ARG
1	E	1174	ARG
1	F	203	ARG
1	F	213	ARG
1	F	288	LEU
1	F	504	ARG
1	F	519	ARG
1	F	732	LEU
1	F	883	ARG
1	F	957	VAL
1	F	986	ASP
1	F	1003	ARG
1	F	1174	ARG
1	F	1201	ARG
4	I	37	ILE
4	I	227	LEU
4	I	295	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	ASN
1	A	581	ASN
1	A	657	ASN
1	A	696	HIS
1	A	777	ASN
1	A	800	HIS
1	A	1018	ASN
1	A	1045	HIS
1	A	1179	HIS
1	A	1204	ASN
1	A	1264	ASN
1	A	1329	GLN
1	B	168	ASN
1	B	183	GLN
1	B	347	ASN
1	B	581	ASN
1	B	696	HIS
1	B	751	HIS
1	B	770	ASN
1	B	800	HIS
1	B	947	HIS
1	B	1008	GLN
1	B	1018	ASN
1	B	1117	ASN
1	B	1286	HIS
1	B	1310	GLN
1	C	168	ASN
1	C	429	HIS
1	C	604	HIS
1	C	696	HIS
1	C	717	GLN
1	C	777	ASN
1	C	972	ASN
1	C	1018	ASN
1	C	1117	ASN
1	C	1310	GLN
1	C	1329	GLN
1	D	118	ASN
1	D	168	ASN
1	D	170	GLN
1	D	544	HIS
1	D	581	ASN

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Mol	Chain	Res	Type
1	D	604	HIS
1	D	696	HIS
1	D	997	ASN
1	D	1018	ASN
1	D	1117	ASN
1	D	1124	ASN
1	D	1197	ASN
1	D	1357	HIS
1	E	96	GLN
1	E	286	GLN
1	E	315	ASN
1	E	544	HIS
1	E	658	ASN
1	E	696	HIS
1	E	717	GLN
1	E	880	HIS
1	E	934	HIS
1	E	1018	ASN
1	E	1045	HIS
1	E	1310	GLN
1	F	478	HIS
1	F	581	ASN
1	F	658	ASN
1	F	696	HIS
1	F	717	GLN
1	F	724	HIS
1	F	1008	GLN
1	F	1009	HIS
1	F	1018	ASN
1	F	1062	ASN
1	F	1090	ASN
1	F	1117	ASN
1	F	1197	ASN
1	F	1264	ASN
1	F	1286	HIS
4	I	48	HIS
4	J	110	ASN
4	J	281	HIS
5	K	142	HIS
5	K	210	HIS
5	K	278	HIS
6	L	16	ASN

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Mol	Chain	Res	Type
6	L	44	HIS
6	M	16	ASN
6	M	44	HIS
6	N	16	ASN
6	N	68	HIS
6	O	16	ASN
6	O	44	HIS
6	P	16	ASN
6	Q	16	ASN
6	Q	47	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

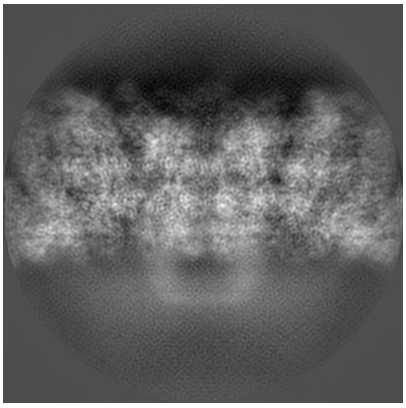
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30125. These allow visual inspection of the internal detail of the map and identification of artifacts.

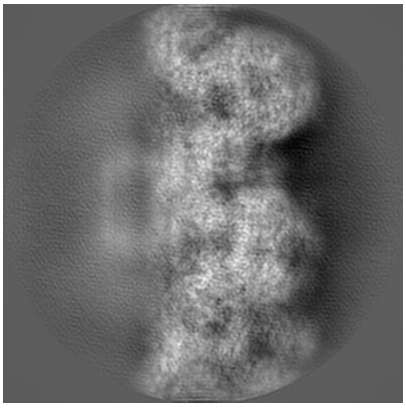
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

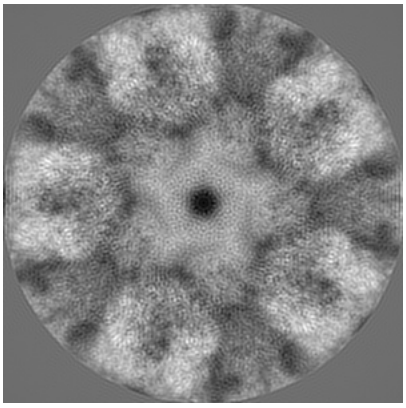
6.1.1 Primary map



X



Y

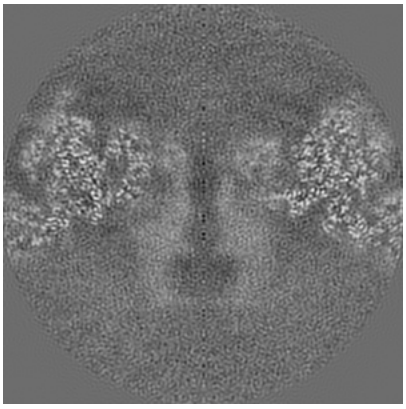


Z

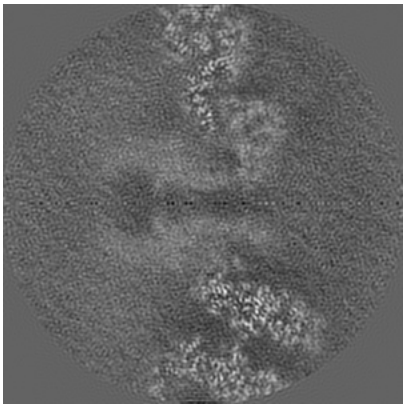
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

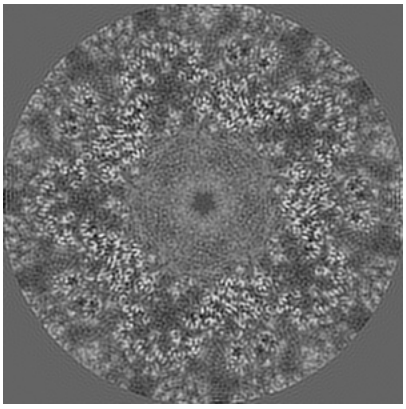
6.2.1 Primary map



X Index: 150



Y Index: 150

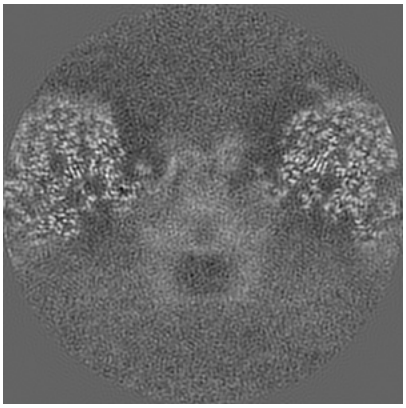


Z Index: 150

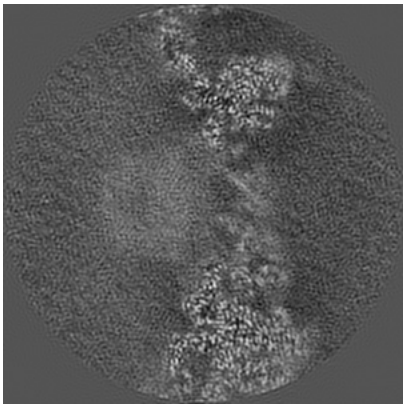
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

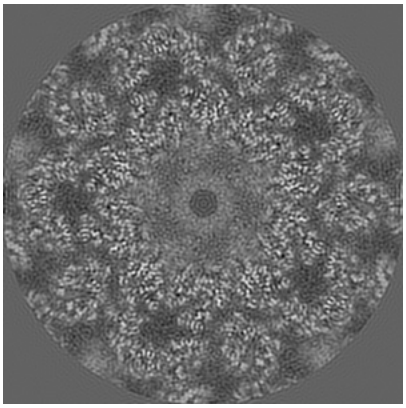
6.3.1 Primary map



X Index: 136



Y Index: 123

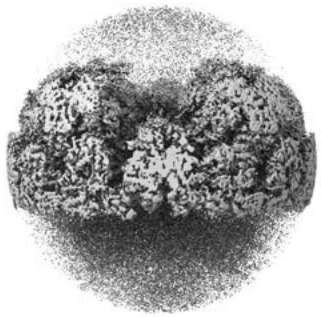


Z Index: 156

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

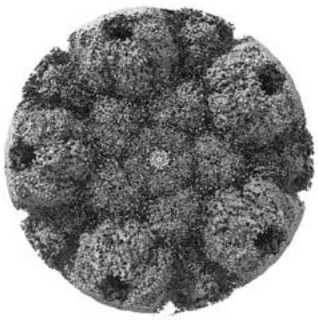
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

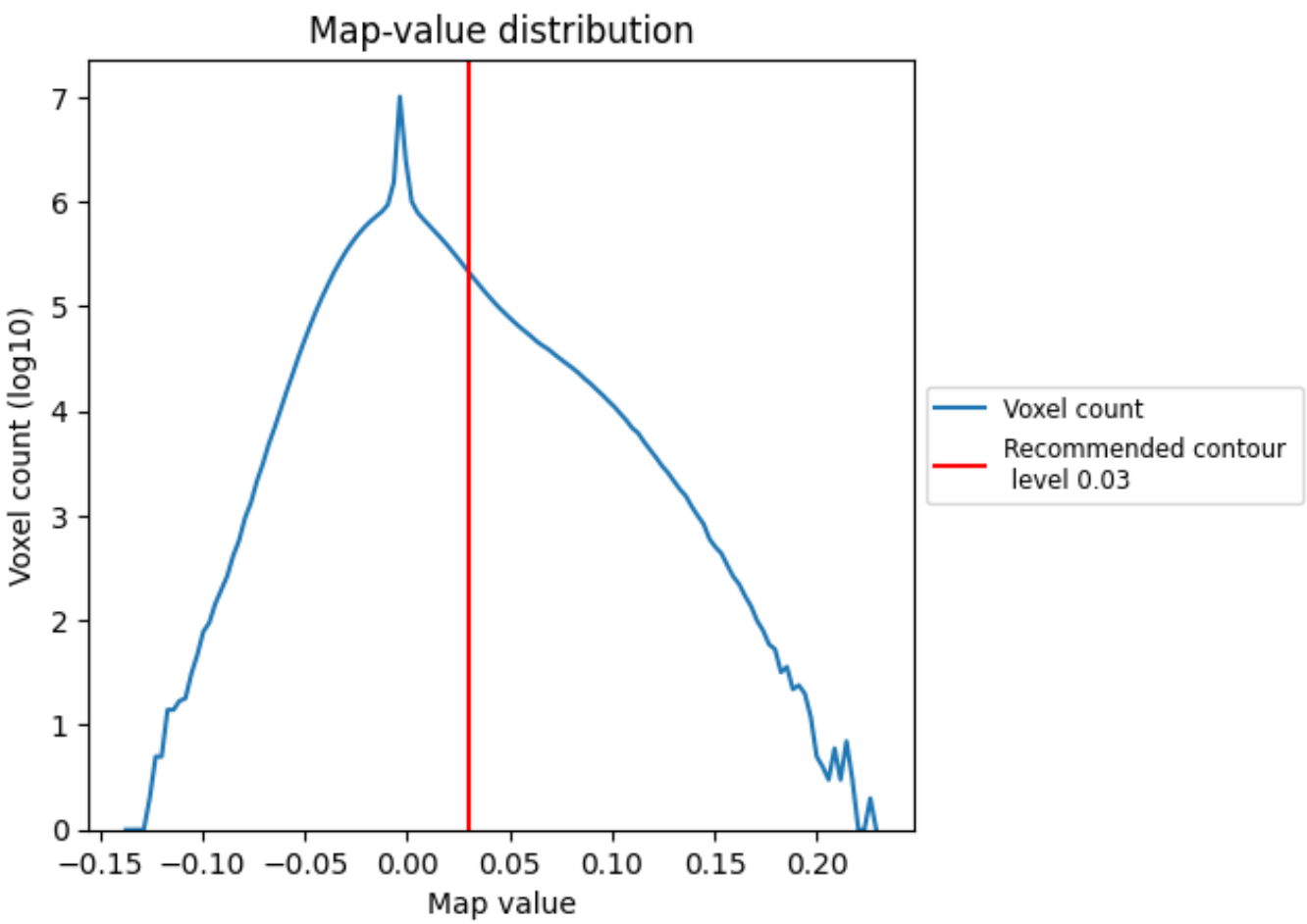
6.5 Mask visualisation (i)

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

7 Map analysis (i)

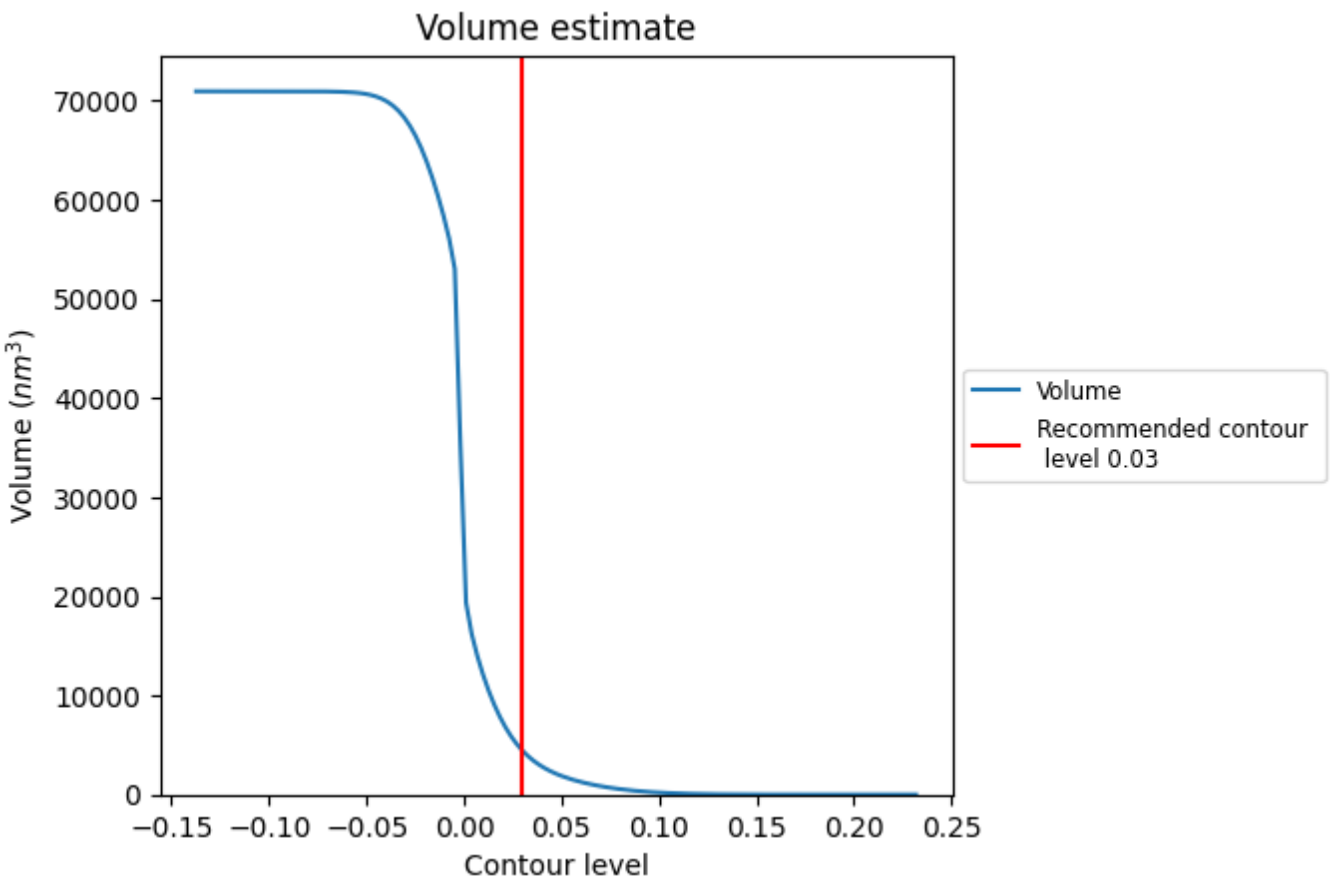
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

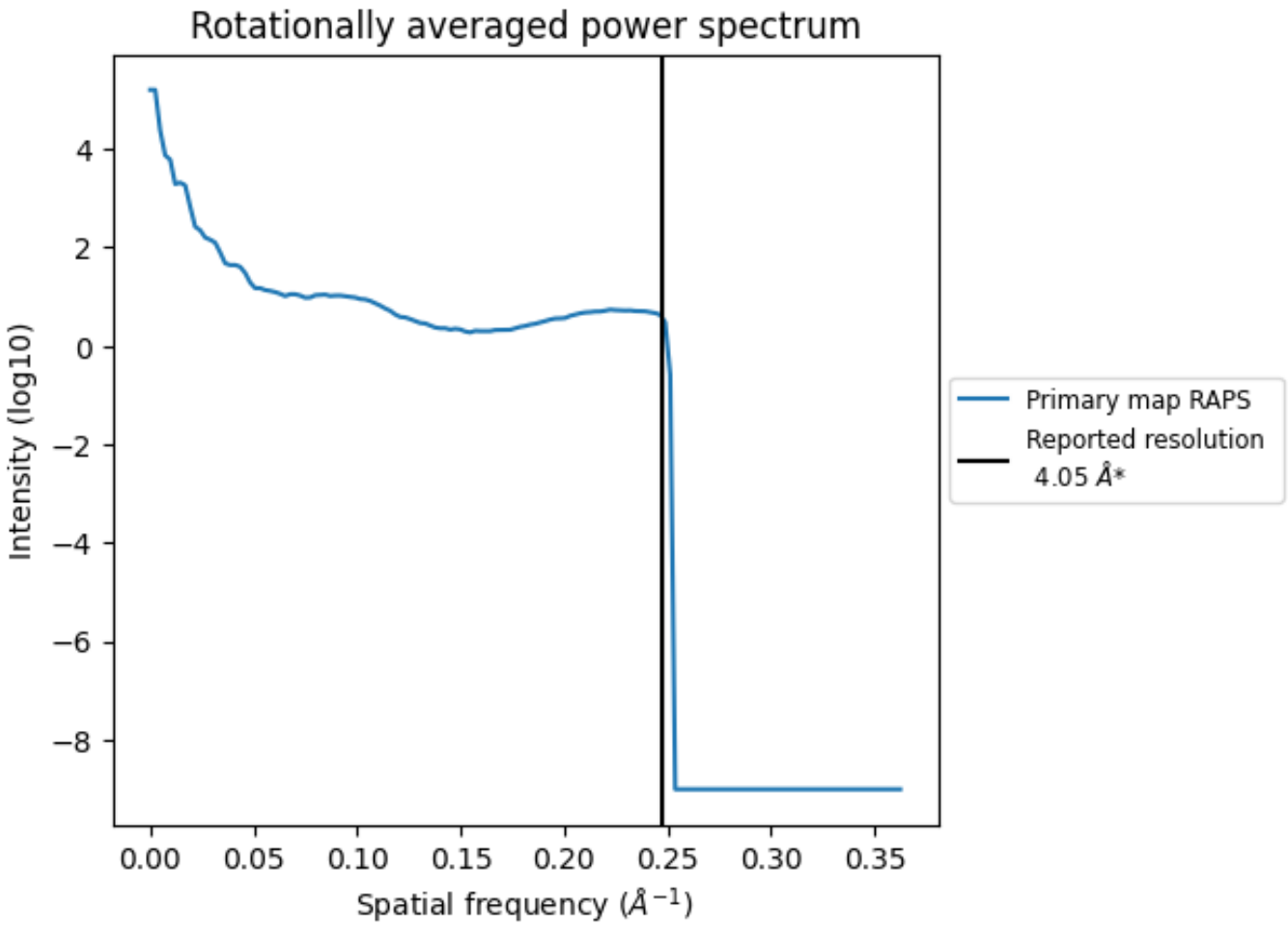
7.2 Volume estimate (i)



The volume at the recommended contour level is 4430 nm^3; this corresponds to an approximate mass of 4002 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 0.247 Å^{-1}

8 Fourier-Shell correlation (i)

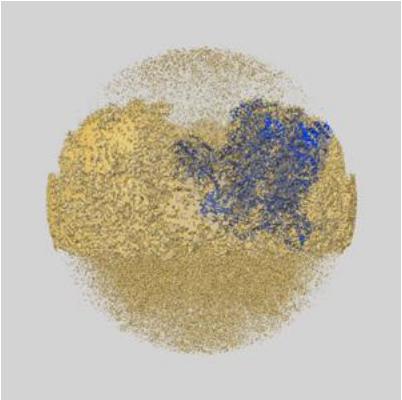
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit (i)

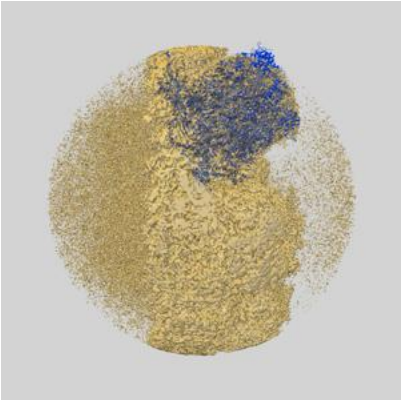
This section contains information regarding the fit between EMDB map EMD-30125 and PDB model 6M6I. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

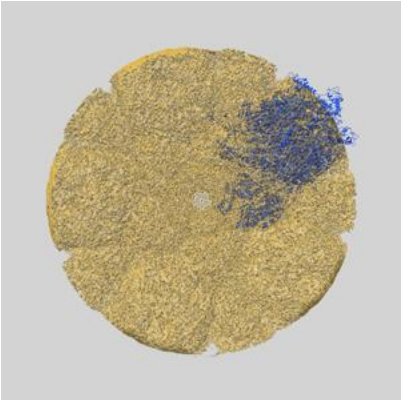
9.1.1 Map-model overlay (i)



X

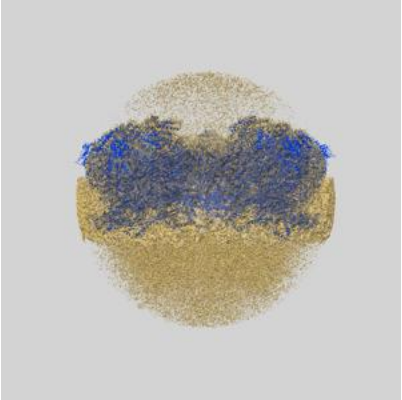


Y

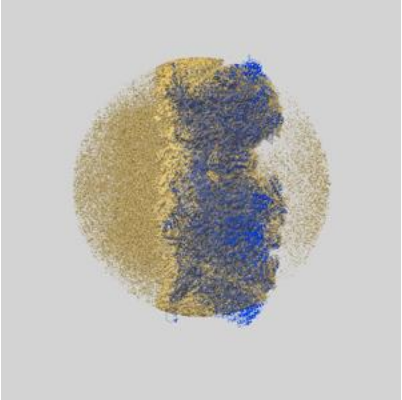


Z

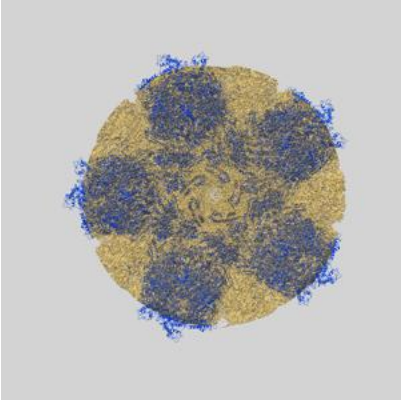
9.1.2 Map-model assembly overlay (i)



X



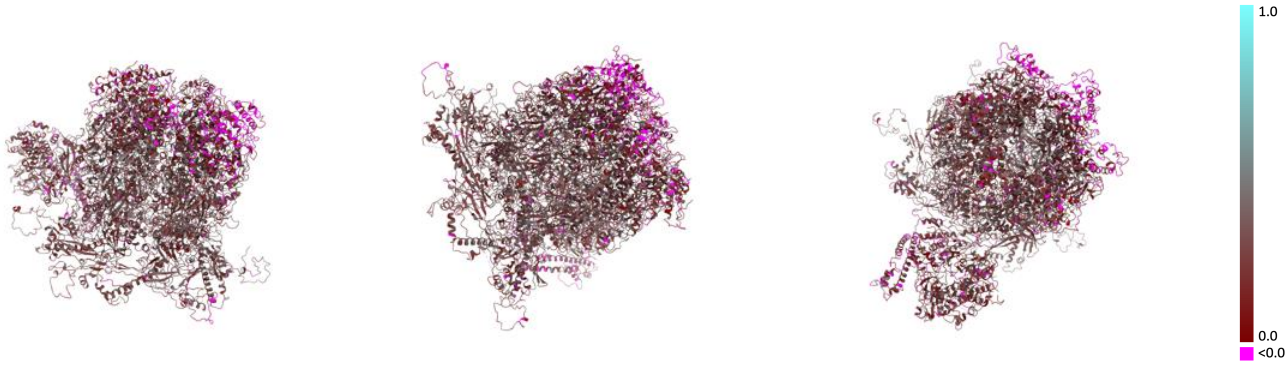
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

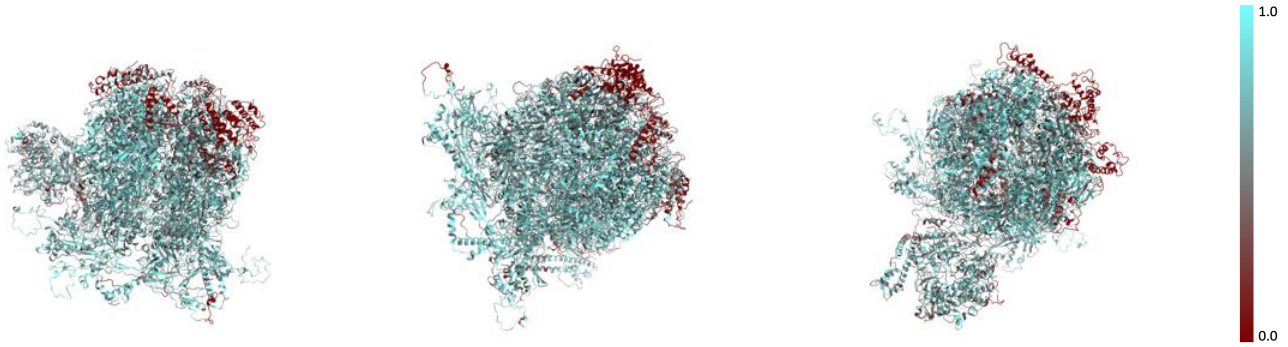
9.2 Q-score mapped to coordinate model (i)



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.

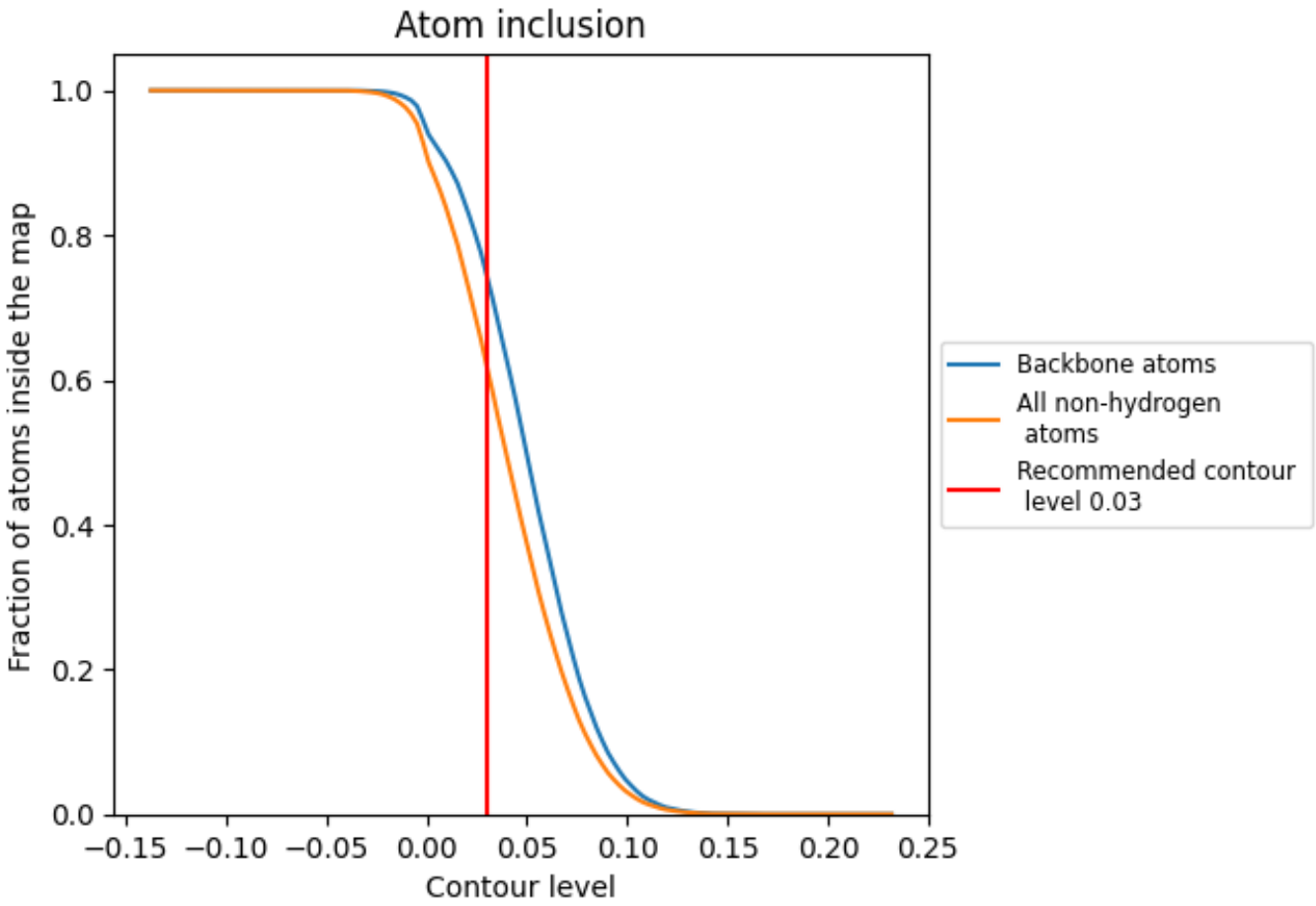
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6191	0.2570
A	0.6724	0.2780
B	0.6762	0.2730
C	0.5798	0.2450
D	0.6680	0.2690
E	0.6923	0.2940
F	0.6649	0.2900
G	0.4914	0.1460
H	0.5036	0.1160
I	0.5759	0.2340
J	0.5544	0.2340
K	0.5620	0.1760
L	0.1825	0.0630
M	0.2460	0.1540
N	0.3056	0.1820
O	0.3280	0.1590
P	0.0728	0.0270
Q	0.0489	-0.0000