Full wwPDB EM Validation Report ⓘ

Mar 20, 2024 – 06:29 AM JST

PDB ID	:	6M6A
EMDB ID	:	EMD-30117
Title	:	Cryo-EM structure of Thermus thermophilus Mfd in complex with RNA polymerase
Authors	:	Shi, J.; Wen, A.; Feng, Y.
Deposited on	:	2020-03-14
Resolution	:	5.00 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:

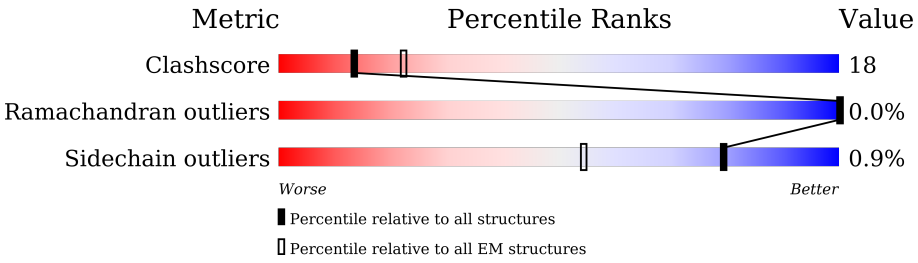
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 5.00 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	315	41% 30% • 28%
1	B	315	42% 28% • 30%
2	C	1119	• 64% 35% •
3	D	1524	53% 32% • 14%
4	E	99	67% 27% • 5%
5	M	978	27% 20% 53%
6	T	63	24% 21% 56%
7	N	63	21% 24% 56%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 28142 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1782	1138	310	332	2		
1	B	222	Total	C	N	O	S	0	0
			1750	1118	304	326	2		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8770	5548	1564	1634	24		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1304	Total	C	N	O	S	0	0
			10293	6515	1825	1921	32		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	94	Total	C	N	O	S	0	0
			761	486	132	139	4		

- Molecule 5 is a protein called Transcription-repair-coupling factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	459	Total	C	N	O	S	0	0
			3635	2327	645	659	4		

- Molecule 6 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	28	Total 574	C 272	N 106	O 168	P 28	0	0

- Molecule 7 is a DNA chain called nontemplate strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	N	28	Total 574	C 272	N 106	O 168	P 28	0	0

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
8	D	2	Total 2	Zn 2	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

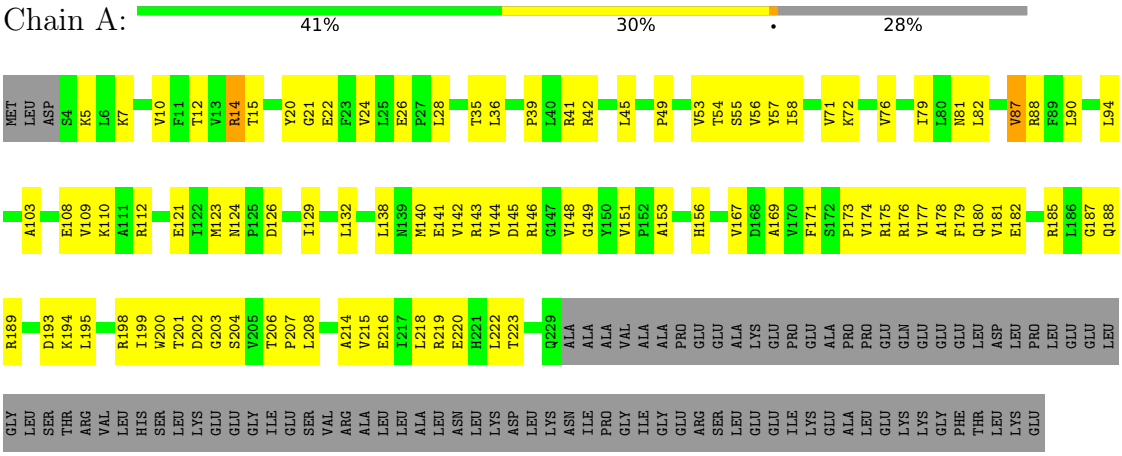
Mol	Chain	Residues	Atoms		AltConf
9	D	1	Total 1	Mg 1	0

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.

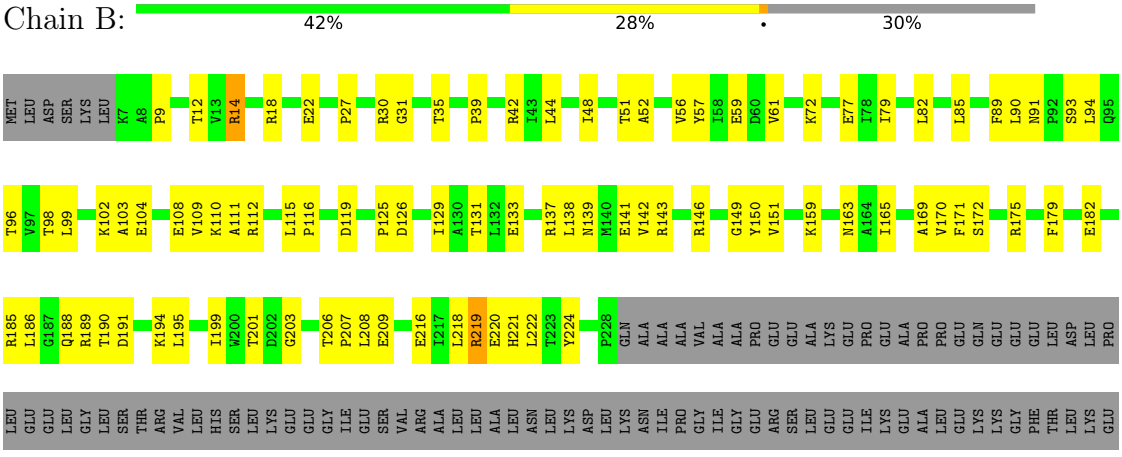
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



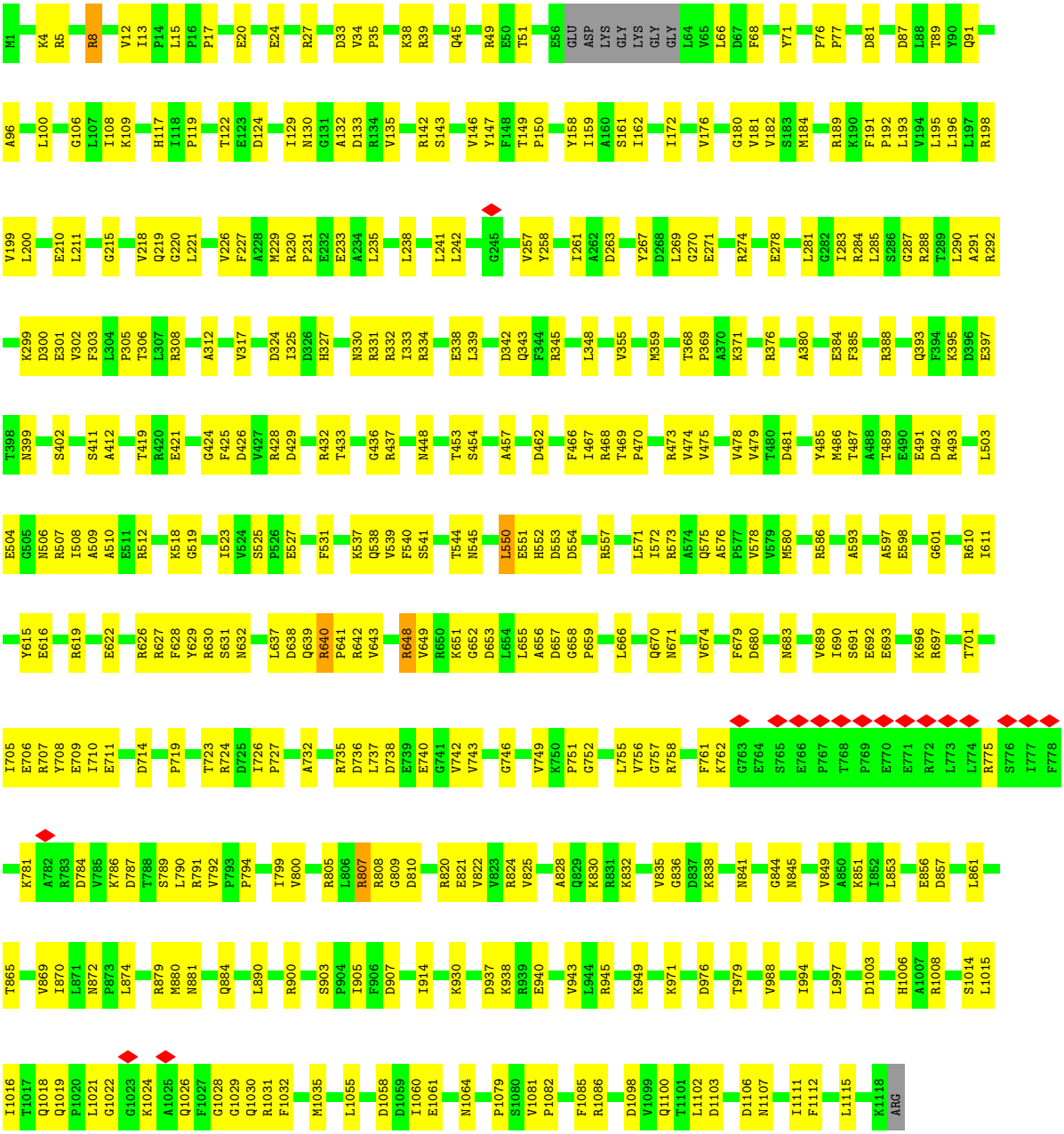
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



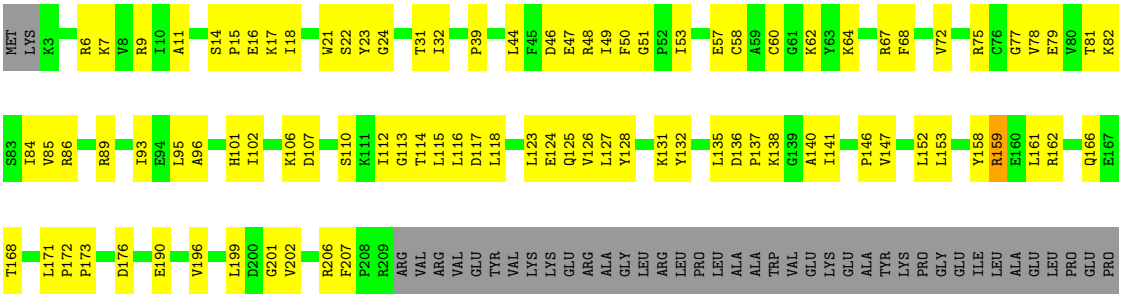
• Molecule 2: DNA-directed RNA polymerase subunit beta

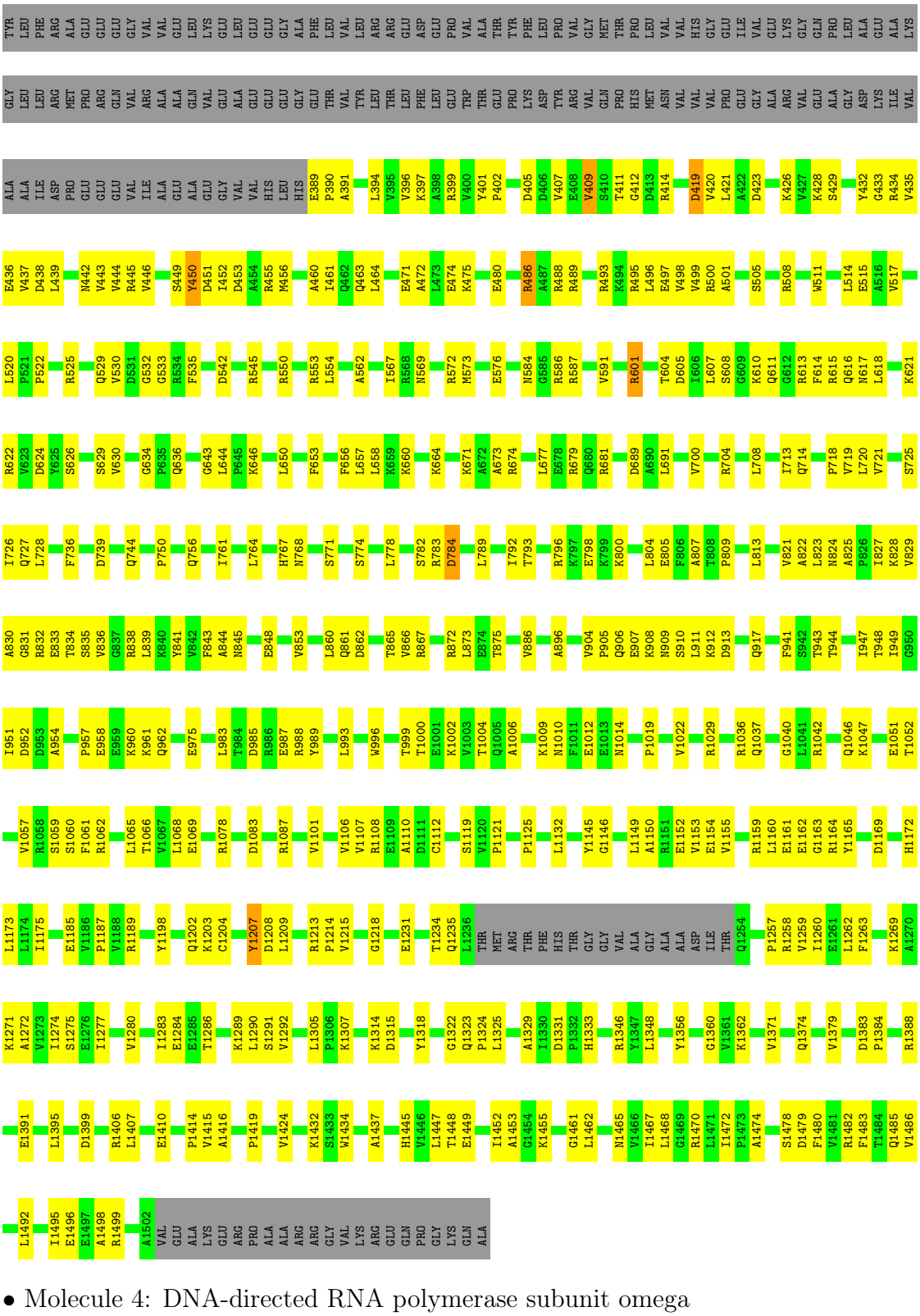
Chain C:



• Molecule 3: DNA-directed RNA polymerase subunit beta'

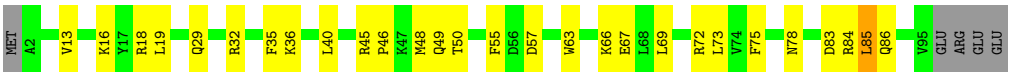
Chain D:





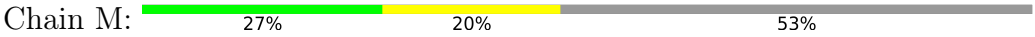
• Molecule 4: DNA-directed RNA polymerase subunit omega

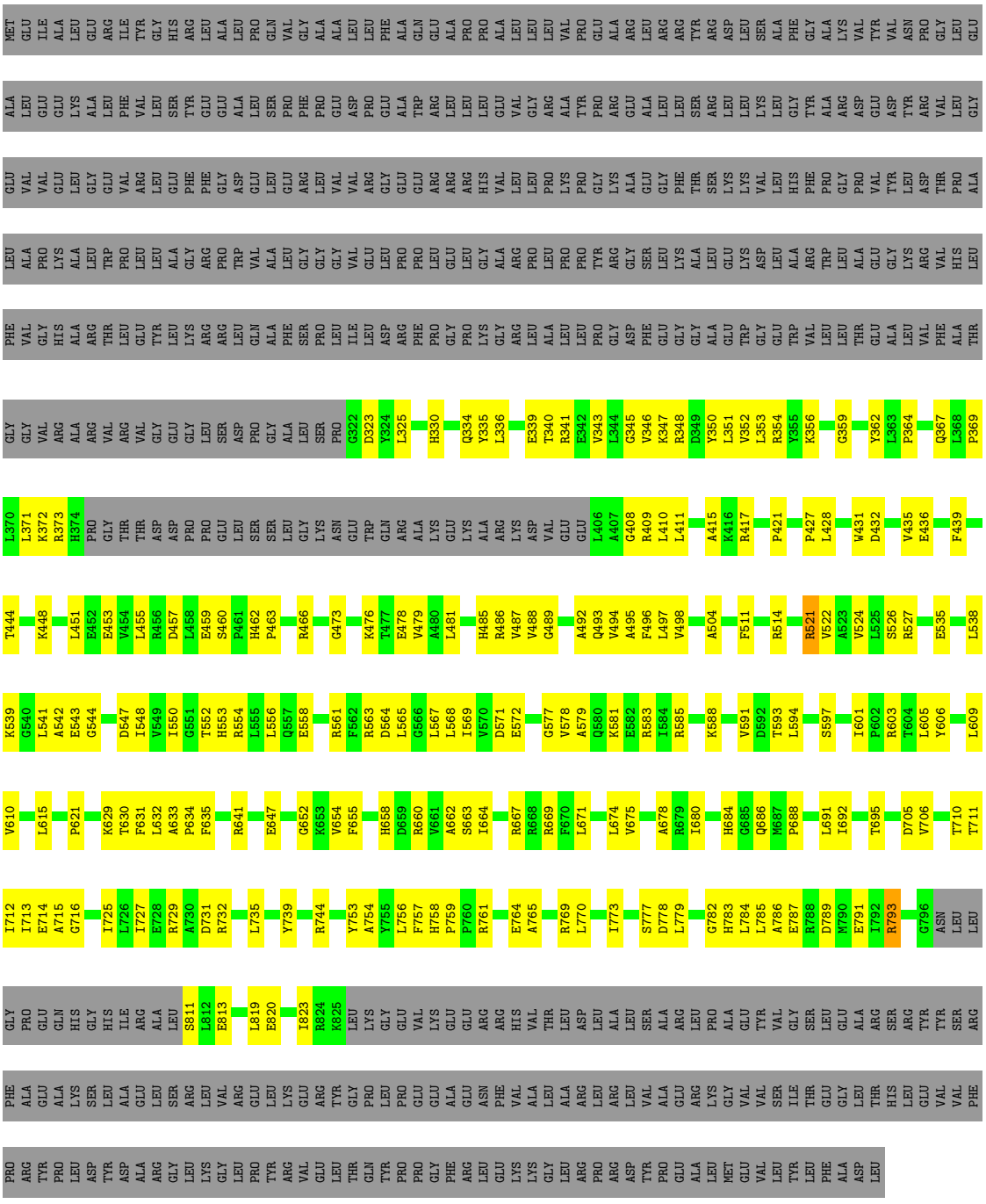
Chain E:



• Molecule 5: Transcription-repair-coupling factor

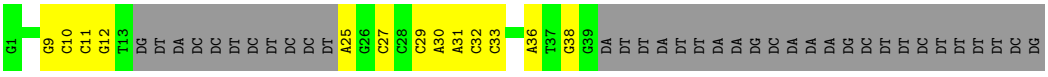
Chain M:





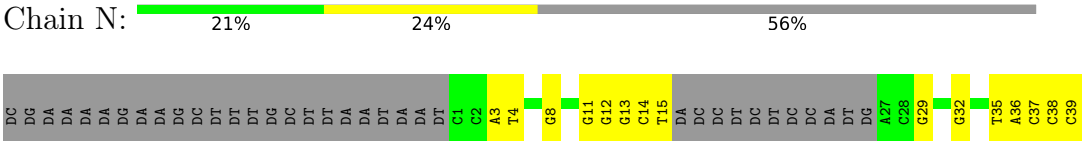
• Molecule 6: template strand DNA

Chain T:



• Molecule 7: nontemplate strand DNA

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24037	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 ($e^-/Å^2$)	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.127	Depositor
Minimum map value	-0.075	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	261.4, 261.4, 261.4	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3069999, 1.3069999, 1.3069999	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.41	0/1814	0.59	0/2466
1	B	0.40	0/1782	0.58	0/2424
2	C	0.41	0/8937	0.58	0/12087
3	D	0.41	0/10467	0.58	0/14138
4	E	0.41	0/775	0.53	0/1045
5	M	0.38	0/3706	0.63	0/5017
6	T	0.89	0/642	1.24	0/986
7	N	1.05	0/642	1.20	0/986
All	All	0.45	0/28765	0.63	0/39149

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1782	0	1834	69	0
1	B	1750	0	1797	71	0
2	C	8770	0	8874	307	0
3	D	10293	0	10521	373	0
4	E	761	0	778	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	M	3635	0	3735	156	0
6	T	574	0	316	33	0
7	N	574	0	316	32	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	28142	0	28171	997	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 18.

All (997) 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)
2:C:1086:ARG:HG2	2:C:1111:ILE:CD1	1.50	1.39
1:B:59:GLU:HG3	1:B:139:ASN:HB3	1.19	1.15
2:C:1086:ARG:CG	2:C:1111:ILE:HD12	1.79	1.12
3:D:829:VAL:HG12	3:D:832:ARG:O	1.49	1.11
2:C:1086:ARG:HG2	2:C:1111:ILE:HD12	1.07	1.02
2:C:1086:ARG:HG2	2:C:1111:ILE:HD11	1.39	1.00
5:M:554:ARG:HG2	5:M:558:GLU:HG2	1.46	0.97
2:C:257:VAL:O	2:C:261:ILE:HB	1.66	0.95
1:B:59:GLU:HG3	1:B:139:ASN:CB	1.96	0.94
3:D:1145:TYR:HE2	3:D:1207:TYR:OH	1.52	0.93
3:D:147:VAL:HG21	3:D:452:ILE:HD12	1.51	0.92
3:D:1145:TYR:CE2	3:D:1207:TYR:OH	2.23	0.92
1:B:59:GLU:CG	1:B:139:ASN:HB3	1.99	0.91
7:N:35:DT:OP2	7:N:35:DT:H3'	1.73	0.89
3:D:829:VAL:HG13	3:D:832:ARG:H	1.35	0.88
2:C:281:LEU:HD12	2:C:302:VAL:HG21	1.56	0.88
6:T:38:DG:C2	7:N:3:DA:C2	2.63	0.87
5:M:527:ARG:HA	5:M:554:ARG:HH21	1.39	0.87
6:T:29:DC:H2"	6:T:30:DA:H5'	1.57	0.86
3:D:137:PRO:HA	3:D:452:ILE:HD11	1.58	0.85
2:C:281:LEU:CD1	2:C:302:VAL:CG2	2.55	0.85
3:D:433:GLY:HA2	3:D:449:SER:O	1.76	0.85
3:D:432:TYR:CD2	3:D:450:TYR:CE1	2.67	0.82
6:T:33:DC:C2	7:N:8:DG:N2	2.47	0.82
5:M:554:ARG:HG2	5:M:558:GLU:CG	2.11	0.81
7:N:35:DT:H3'	7:N:35:DT:P	2.21	0.80
2:C:1081:VAL:HG21	2:C:1111:ILE:HB	1.61	0.80
6:T:33:DC:C2	7:N:8:DG:C2	2.72	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:LEU:CD1	2:C:302:VAL:HG21	2.14	0.78
2:C:1086:ARG:CG	2:C:1111:ILE:CD1	2.42	0.78
3:D:829:VAL:CG1	3:D:832:ARG:O	2.31	0.77
5:M:658:HIS:HE1	5:M:662:ALA:O	1.69	0.76
2:C:281:LEU:HD12	2:C:302:VAL:CG2	2.17	0.75
3:D:829:VAL:O	3:D:830:ALA:C	2.25	0.74
5:M:554:ARG:CG	5:M:558:GLU:HG2	2.17	0.74
5:M:658:HIS:CE1	5:M:662:ALA:O	2.42	0.72
3:D:1208:ASP:N	3:D:1213:ARG:O	2.22	0.72
3:D:147:VAL:HG21	3:D:452:ILE:CD1	2.20	0.72
1:A:28:LEU:HB2	1:A:193:ASP:HB2	1.73	0.70
3:D:137:PRO:O	3:D:452:ILE:HD12	1.92	0.69
3:D:828:LYS:HD2	3:D:833:GLU:HB3	1.74	0.69
3:D:414:ARG:HD3	3:D:451:ASP:OD2	1.93	0.69
2:C:292:ARG:HB2	2:C:299:LYS:HB2	1.74	0.69
2:C:710:ILE:HD12	2:C:790:LEU:HB2	1.73	0.69
5:M:658:HIS:ND1	5:M:664:ILE:HD13	2.06	0.69
3:D:1107:VAL:HB	3:D:1218:GLY:H	1.58	0.69
3:D:829:VAL:HG13	3:D:832:ARG:N	2.06	0.69
5:M:457:ASP:HB2	5:M:466:ARG:HH21	1.58	0.69
6:T:33:DC:O2	7:N:8:DG:C2	2.45	0.69
6:T:11:DC:H2"	6:T:12:DG:O5'	1.93	0.68
2:C:66:LEU:HD11	2:C:369:PRO:HG3	1.75	0.68
2:C:368:THR:H	2:C:371:LYS:HE2	1.58	0.68
5:M:498:VAL:HG13	5:M:552:THR:HG22	1.74	0.68
5:M:339:GLU:HG3	5:M:352:VAL:HG22	1.74	0.68
2:C:436:GLY:HA2	2:C:539:VAL:HA	1.76	0.68
3:D:1153:VAL:HG23	3:D:1160:LEU:HB2	1.77	0.67
6:T:11:DC:H2"	6:T:12:DG:C5'	2.24	0.67
3:D:829:VAL:N	3:D:832:ARG:O	2.23	0.67
1:B:102:LYS:HA	1:B:138:LEU:O	1.95	0.66
5:M:432:ASP:O	5:M:436:GLU:HB2	1.96	0.66
6:T:33:DC:N3	7:N:8:DG:N1	2.44	0.66
7:N:12:DG:H2"	7:N:13:DG:H5'	1.77	0.66
3:D:831:GLY:HA3	3:D:832:ARG:NH1	2.11	0.66
2:C:1035:MET:SD	2:C:1035:MET:N	2.69	0.66
3:D:51:GLY:O	3:D:86:ARG:NH2	2.29	0.66
3:D:140:ALA:HB3	3:D:452:ILE:HD12	1.77	0.65
2:C:324:ASP:O	2:C:330:ASN:ND2	2.30	0.65
1:B:179:PHE:HB2	1:B:195:LEU:HD11	1.79	0.65
3:D:1207:TYR:HA	3:D:1214:PRO:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:830:LYS:HZ3	2:C:832:LYS:HB2	1.61	0.65
5:M:634:PRO:HD3	5:M:761:ARG:HH12	1.62	0.64
3:D:831:GLY:O	3:D:832:ARG:HG3	1.96	0.64
2:C:626:ARG:HE	2:C:629:TYR:HD1	1.46	0.64
3:D:1384:PRO:HD3	3:D:1391:GLU:HB3	1.79	0.64
2:C:278:GLU:HG2	2:C:284:ARG:HA	1.80	0.64
5:M:498:VAL:HG11	5:M:504:ALA:HB2	1.78	0.64
2:C:628:PHE:H	2:C:638:ASP:HB3	1.63	0.64
3:D:190:GLU:HA	3:D:196:VAL:HA	1.79	0.64
5:M:603:ARG:HB2	5:M:791:GLU:HB3	1.80	0.64
3:D:432:TYR:HB2	3:D:450:TYR:CZ	2.33	0.63
3:D:829:VAL:O	3:D:831:GLY:N	2.31	0.63
3:D:1154:GLU:HG2	3:D:1159:ARG:HA	1.79	0.63
2:C:49:ARG:HH21	2:C:68:PHE:HD2	1.47	0.63
3:D:1010:ASN:OD1	3:D:1014:ASN:ND2	2.31	0.63
5:M:421:PRO:HA	5:M:463:PRO:HD3	1.81	0.63
2:C:841:ASN:HD21	2:C:845:ASN:HB3	1.62	0.63
6:T:38:DG:N2	7:N:3:DA:C2	2.67	0.63
2:C:195:LEU:HA	2:C:226:VAL:HG21	1.81	0.63
2:C:648:ARG:NH1	2:C:649:VAL:O	2.32	0.63
3:D:1150:ALA:HB3	3:D:1187:PRO:HB2	1.79	0.62
3:D:1155:VAL:HG22	3:D:1160:LEU:HD11	1.81	0.62
2:C:1082:PRO:HB2	2:C:1085:PHE:HB3	1.82	0.62
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.80	0.62
4:E:67:GLU:HB3	4:E:73:LEU:HD11	1.80	0.62
5:M:658:HIS:ND1	5:M:664:ILE:CD1	2.62	0.62
3:D:147:VAL:HG11	3:D:452:ILE:HD13	1.81	0.62
3:D:838:ARG:HB3	3:D:865:THR:HG23	1.81	0.62
3:D:140:ALA:HA	3:D:450:TYR:CD1	2.34	0.62
5:M:553:HIS:HD2	6:T:33:DC:H4'	1.64	0.62
2:C:20:GLU:O	2:C:24:GLU:HB3	1.99	0.62
2:C:971:LYS:HG2	2:C:988:VAL:HG13	1.82	0.62
2:C:1029:GLY:O	3:D:622:ARG:NH1	2.33	0.62
3:D:822:ALA:HB3	3:D:825:ALA:HB2	1.80	0.62
3:D:1106:VAL:H	3:D:1108:ARG:HH11	1.47	0.61
3:D:1449:GLU:HA	3:D:1452:ILE:HD12	1.80	0.61
3:D:93:ILE:HB	3:D:517:VAL:HB	1.82	0.61
3:D:82:LYS:HG3	3:D:84:ILE:H	1.66	0.61
3:D:958:GLU:O	3:D:961:LYS:NZ	2.34	0.61
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.82	0.61
3:D:951:ILE:O	3:D:1062:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:206:ARG:HD3	3:D:394:LEU:HD23	1.83	0.61
3:D:522:PRO:HA	3:D:525:ARG:HG3	1.82	0.61
2:C:629:TYR:HB3	2:C:637:LEU:HB2	1.83	0.61
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.82	0.61
3:D:1495:ILE:HD13	4:E:85:LEU:HA	1.83	0.61
6:T:33:DC:O2	7:N:8:DG:N2	2.34	0.61
3:D:660:LYS:O	3:D:660:LYS:NZ	2.34	0.61
3:D:1145:TYR:CE2	3:D:1207:TYR:CZ	2.89	0.61
6:T:38:DG:N1	7:N:3:DA:C2	2.67	0.61
2:C:598:GLU:O	2:C:651:LYS:NZ	2.33	0.60
2:C:861:LEU:HD12	2:C:865:THR:HB	1.81	0.60
2:C:576:ALA:O	2:C:671:ASN:ND2	2.34	0.60
2:C:762:LYS:HG2	2:C:786:LYS:HE3	1.82	0.60
2:C:808:ARG:HE	2:C:809:GLY:H	1.48	0.60
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.82	0.60
3:D:630:VAL:HA	3:D:744:GLN:HA	1.83	0.60
5:M:493:GLN:HG3	5:M:563:ARG:HH21	1.67	0.60
2:C:550:LEU:H	2:C:905:ILE:HD11	1.67	0.60
3:D:1101:VAL:O	3:D:1374:GLN:NE2	2.34	0.60
5:M:630:THR:HA	5:M:754:ALA:HB3	1.82	0.60
2:C:474:VAL:HA	2:C:479:VAL:HA	1.82	0.60
3:D:952:ASP:HA	3:D:1062:ARG:HH22	1.67	0.60
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.83	0.60
2:C:820:ARG:HG3	2:C:821:GLU:HG2	1.84	0.60
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.34	0.60
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.83	0.60
5:M:343:VAL:HB	5:M:346:VAL:HB	1.83	0.60
5:M:571:ASP:N	5:M:571:ASP:OD1	2.32	0.60
5:M:711:THR:HB	5:M:714:GLU:H	1.67	0.60
1:B:103:ALA:O	1:B:138:LEU:N	2.35	0.59
3:D:1057:VAL:HG22	3:D:1069:GLU:HB2	1.84	0.59
4:E:49:GLN:NE2	4:E:50:THR:O	2.35	0.59
5:M:632:LEU:HA	5:M:756:LEU:HB2	1.82	0.59
2:C:302:VAL:HG22	2:C:302:VAL:O	2.02	0.59
2:C:708:TYR:HB2	2:C:825:VAL:HB	1.84	0.59
3:D:1059:SER:OG	3:D:1060:SER:N	2.35	0.59
2:C:841:ASN:HB3	2:C:994:ILE:HG12	1.83	0.59
3:D:158:TYR:OH	3:D:162:ARG:NH1	2.35	0.59
5:M:417:ARG:NH1	5:M:591:VAL:O	2.35	0.59
2:C:4:LYS:NZ	2:C:5:ARG:O	2.35	0.59
2:C:810:ASP:N	2:C:810:ASP:OD1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:688:PRO:HG2	5:M:691:LEU:HD13	1.84	0.59
2:C:468:ARG:HH11	2:C:487:THR:HG23	1.67	0.59
2:C:736:ASP:OD1	2:C:736:ASP:N	2.35	0.59
3:D:1280:VAL:HA	3:D:1318:TYR:HA	1.84	0.59
5:M:348:ARG:NH1	5:M:350:TYR:OH	2.34	0.59
1:A:94:LEU:O	1:A:146:ARG:NH1	2.36	0.59
1:A:179:PHE:HB2	1:A:195:LEU:HD11	1.84	0.59
3:D:1112:CYS:SG	3:D:1189:ARG:NH2	2.76	0.59
2:C:15:LEU:HD13	2:C:586:ARG:HG2	1.83	0.59
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.85	0.59
5:M:323:ASP:OD2	5:M:373:ARG:NH1	2.36	0.59
2:C:269:LEU:O	2:C:288:ARG:NH1	2.33	0.58
3:D:1125:PRO:HA	3:D:1132:LEU:HA	1.85	0.58
1:B:94:LEU:O	1:B:146:ARG:NH2	2.37	0.58
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.85	0.58
3:D:957:PRO:HG3	3:D:1010:ASN:HD22	1.69	0.58
4:E:29:GLN:HA	4:E:32:ARG:HE	1.68	0.58
5:M:782:GLY:O	5:M:786:ALA:HB3	2.03	0.58
2:C:258:TYR:O	2:C:263:ASP:N	2.36	0.58
3:D:412:GLY:O	3:D:434:ARG:NH1	2.37	0.58
3:D:704:ARG:NH1	3:D:736:PHE:O	2.37	0.58
3:D:792:ILE:HA	3:D:861:GLN:HE21	1.68	0.58
3:D:1274:ILE:HA	3:D:1324:PRO:HA	1.86	0.58
3:D:1290:LEU:H	3:D:1307:LYS:HZ1	1.51	0.58
3:D:115:LEU:O	3:D:495:ARG:NH2	2.35	0.58
3:D:646:LYS:HA	3:D:720:LEU:HD11	1.84	0.58
3:D:1331:ASP:OD1	3:D:1333:HIS:ND1	2.31	0.58
1:A:151:VAL:HB	1:A:169:ALA:HB3	1.84	0.58
3:D:584:ASN:O	3:D:586:ARG:NH1	2.37	0.58
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.86	0.57
1:A:5:LYS:O	1:A:7:LYS:NZ	2.37	0.57
1:A:88:ARG:HB3	1:A:121:GLU:HB3	1.86	0.57
2:C:732:ALA:HA	2:C:735:ARG:HE	1.69	0.57
5:M:579:ALA:N	7:N:11:DG:OP1	2.34	0.57
5:M:634:PRO:HB3	5:M:761:ARG:HH22	1.69	0.57
1:B:104:GLU:HA	1:B:137:ARG:HA	1.86	0.57
2:C:327:HIS:HE1	2:C:489:THR:HG22	1.67	0.57
2:C:640:ARG:N	2:C:657:ASP:O	2.37	0.57
3:D:407:VAL:HG22	3:D:409:VAL:H	1.69	0.57
3:D:501:ALA:O	3:D:505:SER:HB3	2.05	0.57
3:D:774:SER:O	3:D:1362:LYS:NZ	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:35:PRO:HG2	2:C:38:LYS:HB2	1.87	0.57
2:C:707:ARG:NH2	2:C:709:GLU:OE1	2.37	0.57
2:C:1006:HIS:HB2	2:C:1024:LYS:HE2	1.85	0.57
3:D:6:ARG:O	3:D:6:ARG:NH1	2.36	0.57
5:M:660:ARG:HH21	5:M:729:ARG:NE	2.01	0.57
7:N:38:DC:H2"	7:N:39:DC:H5'	1.87	0.57
3:D:1395:LEU:HD12	3:D:1399:ASP:HB2	1.86	0.57
3:D:493:ARG:NH1	3:D:497:GLU:OE1	2.37	0.57
5:M:527:ARG:NH1	6:T:33:DC:OP2	2.36	0.57
2:C:274:ARG:NH2	2:C:285:LEU:O	2.37	0.57
4:E:83:ASP:OD1	4:E:83:ASP:N	2.38	0.57
5:M:453:GLU:HG2	5:M:466:ARG:HH22	1.69	0.57
1:B:18:ARG:NH2	1:B:206:THR:OG1	2.38	0.57
3:D:798:GLU:OE2	3:D:824:ASN:ND2	2.37	0.57
5:M:769:ARG:NH1	7:N:14:DC:OP1	2.37	0.57
2:C:557:ARG:HG3	2:C:844:GLY:HA3	1.86	0.57
1:B:30:ARG:HD3	1:B:191:ASP:HB2	1.87	0.56
2:C:576:ALA:O	2:C:900:ARG:NH2	2.38	0.56
7:N:36:DA:H2"	7:N:37:DC:H5'	1.87	0.56
3:D:1121:PRO:HA	3:D:1185:GLU:HG3	1.87	0.56
2:C:231:PRO:O	2:C:235:LEU:HB2	2.03	0.56
2:C:640:ARG:O	2:C:657:ASP:N	2.36	0.56
3:D:829:VAL:HG12	3:D:832:ARG:C	2.24	0.56
3:D:1202:GLN:NE2	3:D:1215:VAL:O	2.37	0.56
5:M:435:VAL:O	5:M:514:ARG:NH1	2.35	0.56
5:M:542:ALA:O	5:M:561:ARG:NH1	2.39	0.56
5:M:669:ARG:NH1	5:M:669:ARG:O	2.39	0.56
1:B:126:ASP:OD1	1:B:126:ASP:N	2.33	0.56
2:C:432:ARG:HD2	2:C:519:GLY:HA3	1.87	0.56
3:D:1472:ILE:HD12	3:D:1474:ALA:HB3	1.88	0.56
2:C:332:ARG:NH1	2:C:333:ILE:O	2.39	0.56
3:D:114:THR:HG21	3:D:498:VAL:HG21	1.87	0.56
3:D:844:ALA:HB1	3:D:867:ARG:HH11	1.70	0.56
1:B:98:THR:OG1	1:B:143:ARG:NH1	2.38	0.56
2:C:332:ARG:NH1	2:C:338:GLU:OE2	2.39	0.56
2:C:355:VAL:O	2:C:359:MET:N	2.38	0.56
2:C:397:GLU:HG3	2:C:631:SER:HB2	1.87	0.56
3:D:405:ASP:HB2	3:D:423:ASP:HA	1.87	0.56
3:D:1496:GLU:OE1	3:D:1499:ARG:NH1	2.39	0.56
4:E:13:VAL:HG21	4:E:19:LEU:HB2	1.87	0.56
2:C:453:THR:OG1	2:C:454:SER:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:739:ASP:OD1	3:D:739:ASP:N	2.37	0.56
3:D:829:VAL:O	3:D:832:ARG:N	2.38	0.56
5:M:635:PHE:H	5:M:759:PRO:HG3	1.70	0.56
2:C:189:ARG:NH1	2:C:242:LEU:O	2.39	0.56
2:C:626:ARG:HB3	2:C:639:GLN:HE22	1.71	0.56
2:C:339:LEU:O	2:C:343:GLN:NE2	2.39	0.56
2:C:426:ASP:OD1	2:C:426:ASP:N	2.39	0.56
2:C:597:ALA:HB2	2:C:655:LEU:HD21	1.88	0.56
3:D:137:PRO:O	3:D:452:ILE:CD1	2.54	0.56
1:A:175:ARG:NE	1:A:201:THR:O	2.34	0.55
1:A:199:ILE:HG21	1:A:207:PRO:HB3	1.88	0.55
2:C:33:ASP:OD1	2:C:33:ASP:N	2.38	0.55
2:C:302:VAL:HG22	2:C:306:THR:HG23	1.86	0.55
2:C:641:PRO:O	2:C:642:ARG:NH1	2.39	0.55
2:C:271:GLU:OE1	2:C:288:ARG:NE	2.39	0.55
2:C:639:GLN:HA	2:C:658:GLY:HA2	1.88	0.55
2:C:945:ARG:HG2	2:C:949:LYS:HE2	1.87	0.55
2:C:1006:HIS:NE2	2:C:1028:GLY:O	2.40	0.55
3:D:137:PRO:HA	3:D:452:ILE:CD1	2.33	0.55
3:D:829:VAL:CG1	3:D:832:ARG:H	2.12	0.55
3:D:1275:SER:OG	3:D:1277:ILE:O	2.24	0.55
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.38	0.55
2:C:732:ALA:O	2:C:735:ARG:NH2	2.40	0.55
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.88	0.55
2:C:711:GLU:O	2:C:758:ARG:NH1	2.40	0.55
3:D:48:ARG:O	3:D:89:ARG:NH2	2.36	0.55
5:M:493:GLN:NE2	5:M:541:LEU:O	2.40	0.55
7:N:12:DG:C2'	7:N:13:DG:H5'	2.36	0.55
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.89	0.55
3:D:1047:LYS:HE2	3:D:1051:GLU:HB2	1.86	0.55
5:M:569:ILE:HA	5:M:594:LEU:HB3	1.89	0.55
1:A:20:TYR:OH	1:A:198:ARG:NE	2.37	0.55
1:A:72:LYS:NZ	2:C:643:VAL:O	2.35	0.55
1:B:175:ARG:H	1:B:201:THR:HA	1.72	0.55
5:M:553:HIS:HB3	6:T:33:DC:H5'	1.88	0.55
1:B:99:LEU:HB2	1:B:142:VAL:HG13	1.89	0.55
2:C:226:VAL:HA	2:C:229:MET:HG2	1.88	0.55
3:D:141:ILE:HG13	3:D:146:PRO:HA	1.89	0.55
5:M:572:GLU:H	5:M:597:SER:HA	1.72	0.55
3:D:47:GLU:HA	3:D:86:ARG:HH22	1.70	0.55
3:D:999:THR:HA	3:D:1002:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:641:PRO:HA	2:C:656:ALA:HA	1.90	0.54
2:C:1112:PHE:HB3	2:C:1115:LEU:HB2	1.88	0.54
1:B:108:GLU:OE1	1:B:110:LYS:NZ	2.40	0.54
2:C:597:ALA:O	2:C:652:GLY:N	2.38	0.54
3:D:725:SER:OG	3:D:726:ILE:N	2.37	0.54
3:D:1101:VAL:HG21	3:D:1424:VAL:HB	1.89	0.54
5:M:606:TYR:HD1	5:M:609:LEU:HD12	1.73	0.54
1:B:96:THR:OG1	1:B:143:ARG:NE	2.32	0.54
3:D:23:TYR:HB3	3:D:89:ARG:HH21	1.72	0.54
3:D:576:GLU:OE1	3:D:587:ARG:NH2	2.41	0.54
3:D:660:LYS:HZ1	3:D:664:LYS:HG3	1.72	0.54
3:D:1479:ASP:OD1	3:D:1482:ARG:NE	2.37	0.54
1:A:42:ARG:NH1	2:C:857:ASP:OD1	2.41	0.54
3:D:168:THR:HA	3:D:394:LEU:HA	1.89	0.54
3:D:975:GLU:OE1	3:D:988:ARG:NH2	2.41	0.54
2:C:384:GLU:HA	2:C:388:ARG:HH21	1.72	0.54
2:C:448:ASN:OD1	2:C:448:ASN:N	2.37	0.54
2:C:1022:GLY:O	2:C:1026:GLN:NE2	2.38	0.54
1:A:15:THR:HA	1:A:21:GLY:HA2	1.90	0.54
1:A:176:ARG:O	1:A:200:TRP:N	2.39	0.54
1:B:188:GLN:O	3:D:646:LYS:NZ	2.41	0.54
1:B:206:THR:HG22	1:B:208:LEU:H	1.72	0.54
3:D:132:TYR:N	3:D:153:LEU:O	2.40	0.54
3:D:1453:ALA:HB1	3:D:1455:LYS:HG2	1.89	0.54
5:M:498:VAL:CG1	5:M:552:THR:HG22	2.38	0.54
5:M:782:GLY:O	5:M:786:ALA:CB	2.56	0.54
1:A:180:GLN:HE21	1:A:182:GLU:HG2	1.73	0.54
2:C:437:ARG:NH1	2:C:467:ILE:O	2.40	0.54
2:C:457:ALA:HB3	2:C:538:GLN:HA	1.90	0.54
2:C:881:ASN:O	2:C:884:GLN:NE2	2.40	0.54
3:D:1145:TYR:HE2	3:D:1207:TYR:HH	0.70	0.54
1:A:201:THR:HG23	1:A:203:GLY:H	1.71	0.53
3:D:85:VAL:HB	3:D:89:ARG:HG3	1.90	0.53
3:D:629:SER:OG	3:D:630:VAL:N	2.40	0.53
3:D:1290:LEU:HB2	3:D:1305:LEU:HB2	1.90	0.53
5:M:820:GLU:HA	5:M:823:ILE:HD12	1.89	0.53
2:C:334:ARG:NH2	2:C:342:ASP:OD2	2.41	0.53
3:D:158:TYR:O	3:D:162:ARG:HG2	2.07	0.53
3:D:1406:ARG:NH2	3:D:1410:GLU:OE1	2.42	0.53
4:E:83:ASP:HA	4:E:86:GLN:HE21	1.72	0.53
6:T:11:DC:H2"	6:T:12:DG:H5'	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:437:ARG:NH2	2:C:491:GLU:OE1	2.38	0.53
2:C:838:LYS:HB3	2:C:997:LEU:HB3	1.91	0.53
2:C:890:LEU:HD21	2:C:914:ILE:HG12	1.89	0.53
5:M:641:ARG:NH1	5:M:674:LEU:O	2.41	0.53
5:M:732:ARG:HA	7:N:14:DC:H4'	1.89	0.53
2:C:428:ARG:O	3:D:1078:ARG:NH1	2.35	0.53
3:D:414:ARG:CD	3:D:451:ASP:OD2	2.57	0.53
3:D:439:LEU:O	3:D:442:ASN:ND2	2.42	0.53
3:D:653:PHE:HB3	3:D:656:PHE:HB2	1.91	0.53
3:D:1069:GLU:OE1	3:D:1069:GLU:N	2.37	0.53
2:C:746:GLY:H	2:C:800:VAL:HG13	1.74	0.53
3:D:958:GLU:HG2	3:D:962:GLN:HE22	1.74	0.53
3:D:1283:ILE:HA	3:D:1292:VAL:HA	1.90	0.53
3:D:140:ALA:HB2	3:D:452:ILE:HB	1.91	0.53
3:D:1119:SER:O	3:D:1346:ARG:NH2	2.34	0.53
4:E:35:PHE:O	4:E:45:ARG:NH2	2.41	0.53
5:M:524:VAL:HA	5:M:550:ILE:HB	1.90	0.53
1:A:182:GLU:N	1:A:194:LYS:O	2.40	0.53
2:C:89:THR:HG22	2:C:130:ASN:H	1.72	0.53
2:C:690:ILE:O	2:C:853:LEU:N	2.42	0.53
3:D:14:SER:OG	3:D:16:GLU:OE1	2.27	0.53
3:D:15:PRO:HA	3:D:18:ILE:HD12	1.91	0.53
3:D:81:THR:OG1	3:D:82:LYS:N	2.42	0.53
3:D:985:ASP:OD1	3:D:988:ARG:NH1	2.36	0.53
4:E:57:ASP:O	4:E:63:TRP:NE1	2.39	0.53
2:C:573:ARG:O	2:C:670:GLN:NE2	2.42	0.53
2:C:640:ARG:HH22	2:C:659:PRO:HA	1.74	0.53
3:D:176:ASP:OD1	3:D:389:GLU:N	2.42	0.53
3:D:409:VAL:HB	3:D:435:VAL:HG11	1.91	0.53
5:M:494:VAL:HA	5:M:567:LEU:HB3	1.91	0.53
7:N:36:DA:H2"	7:N:37:DC:C5'	2.39	0.53
1:A:181:VAL:HA	1:A:195:LEU:HA	1.90	0.53
3:D:480:GLU:OE1	3:D:488:ARG:NH1	2.42	0.53
3:D:1291:SER:OG	3:D:1292:VAL:N	2.42	0.53
2:C:100:LEU:HB3	2:C:109:LYS:HB3	1.89	0.52
2:C:691:SER:OG	2:C:692:GLU:N	2.41	0.52
3:D:1172:HIS:HA	3:D:1175:ILE:HD12	1.90	0.52
1:A:206:THR:HG22	1:A:208:LEU:H	1.75	0.52
2:C:572:ILE:HD11	2:C:701:THR:HB	1.90	0.52
2:C:597:ALA:N	2:C:653:ASP:O	2.39	0.52
3:D:1121:PRO:HD3	3:D:1346:ARG:HH21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:HB3	1:A:141:GLU:HB2	1.90	0.52
1:B:89:PHE:HD2	1:B:146:ARG:HE	1.56	0.52
2:C:419:THR:OG1	2:C:421:GLU:OE1	2.27	0.52
2:C:1106:ASP:OD1	3:D:7:LYS:NZ	2.38	0.52
3:D:423:ASP:O	3:D:426:LYS:NZ	2.36	0.52
1:A:188:GLN:HE22	1:A:189:ARG:HE	1.58	0.52
2:C:184:MET:HB2	2:C:193:LEU:HB2	1.91	0.52
1:B:112:ARG:HB3	1:B:125:PRO:HB2	1.91	0.52
2:C:601:GLY:HA2	2:C:616:GLU:HG2	1.91	0.52
5:M:455:LEU:O	5:M:486:ARG:NH1	2.42	0.52
1:A:202:ASP:OD2	1:A:204:SER:OG	2.25	0.52
2:C:142:ARG:HA	2:C:331:ARG:HA	1.91	0.52
2:C:1055:LEU:HD21	2:C:1079:PRO:HG3	1.92	0.52
3:D:529:GLN:HE21	3:D:533:GLY:HA2	1.75	0.52
3:D:796:ARG:NH1	3:D:862:ASP:OD1	2.42	0.52
5:M:330:HIS:O	5:M:356:LYS:NZ	2.36	0.52
5:M:581:LYS:O	5:M:585:ARG:NH1	2.43	0.52
2:C:751:PRO:HB3	2:C:794:PRO:HA	1.91	0.52
3:D:450:TYR:N	3:D:450:TYR:CD2	2.77	0.52
3:D:673:ALA:O	3:D:677:LEU:HB2	2.10	0.52
3:D:1234:THR:HG23	3:D:1235:GLN:HG3	1.92	0.52
5:M:716:GLY:O	5:M:744:ARG:NH2	2.43	0.52
1:B:150:TYR:HA	1:B:170:VAL:HA	1.92	0.52
2:C:150:PRO:HA	2:C:158:TYR:HA	1.92	0.52
3:D:48:ARG:HE	3:D:77:GLY:HA3	1.73	0.52
3:D:433:GLY:CA	3:D:449:SER:O	2.54	0.52
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.92	0.52
1:B:182:GLU:HG2	1:B:194:LYS:HB3	1.92	0.52
2:C:629:TYR:HD2	2:C:637:LEU:HD12	1.74	0.52
3:D:401:TYR:HB2	3:D:444:VAL:HB	1.91	0.52
5:M:556:LEU:HD22	5:M:583:ARG:HG3	1.91	0.52
6:T:30:DA:H2'	6:T:31:DA:C8	2.44	0.52
2:C:627:ARG:NH1	2:C:638:ASP:OD2	2.44	0.51
5:M:631:PHE:N	5:M:754:ALA:O	2.43	0.51
1:A:41:ARG:HG3	1:A:177:VAL:HG23	1.93	0.51
2:C:503:LEU:HA	2:C:509:ALA:H	1.75	0.51
2:C:727:PRO:HG2	2:C:786:LYS:HA	1.92	0.51
3:D:636:GLN:NE2	3:D:727:GLN:OE1	2.41	0.51
3:D:909:ASN:HA	3:D:912:LYS:HG2	1.91	0.51
5:M:770:LEU:HA	5:M:773:ILE:HD12	1.90	0.51
2:C:399:ASN:OD1	2:C:402:SER:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:569:ASN:OD1	3:D:572:ARG:NH1	2.43	0.51
3:D:761:ILE:O	3:D:767:HIS:ND1	2.35	0.51
1:A:10:VAL:N	1:A:26:GLU:O	2.43	0.51
1:B:104:GLU:OE1	1:B:137:ARG:NH1	2.44	0.51
5:M:451:LEU:HD13	5:M:479:VAL:HA	1.91	0.51
1:B:77:GLU:HB2	3:D:872:ARG:HH11	1.76	0.51
2:C:1102:LEU:O	3:D:7:LYS:N	2.42	0.51
3:D:1161:GLU:HG2	3:D:1164:ARG:HB3	1.93	0.51
1:A:174:VAL:HA	1:A:201:THR:HA	1.92	0.51
3:D:584:ASN:ND2	3:D:591:VAL:O	2.43	0.51
2:C:512:ARG:HE	2:C:523:ILE:HG22	1.75	0.51
5:M:339:GLU:O	5:M:350:TYR:N	2.44	0.51
5:M:492:ALA:HA	5:M:564:ASP:HB3	1.93	0.51
1:B:61:VAL:O	1:B:163:ASN:ND2	2.44	0.51
2:C:638:ASP:O	2:C:640:ARG:NH1	2.43	0.51
3:D:409:VAL:HG11	3:D:435:VAL:HG21	1.92	0.51
3:D:438:ASP:HB2	3:D:445:ARG:HD3	1.93	0.51
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.44	0.51
3:D:838:ARG:O	3:D:865:THR:OG1	2.25	0.51
3:D:1083:ASP:OD2	3:D:1087:ARG:NH2	2.42	0.51
3:D:1468:LEU:HB2	3:D:1470:ARG:H	1.75	0.51
5:M:553:HIS:HD2	6:T:33:DC:C4'	2.22	0.51
3:D:112:ILE:HG23	3:D:116:LEU:HD12	1.92	0.51
3:D:135:LEU:HD21	3:D:460:ALA:HB1	1.91	0.51
6:T:25:DA:C6	7:N:15:DT:C4	2.99	0.51
1:B:150:TYR:HB2	1:B:170:VAL:HG22	1.93	0.51
2:C:238:LEU:HA	2:C:241:LEU:HB2	1.93	0.51
2:C:312:ALA:O	2:C:317:VAL:N	2.37	0.51
2:C:397:GLU:OE2	2:C:632:ASN:N	2.41	0.51
2:C:1030:GLN:NE2	3:D:626:SER:OG	2.40	0.51
5:M:495:ALA:HB3	5:M:568:LEU:HA	1.91	0.51
1:A:36:LEU:HD11	1:B:221:HIS:HD2	1.77	0.50
1:A:81:ASN:ND2	1:A:129:ILE:O	2.44	0.50
2:C:87:ASP:OD2	2:C:824:ARG:NH1	2.43	0.50
2:C:462:ASP:HB3	2:C:468:ARG:HD3	1.93	0.50
3:D:161:LEU:O	3:D:450:TYR:O	2.29	0.50
3:D:1108:ARG:NH1	3:D:1198:TYR:O	2.43	0.50
5:M:684:HIS:CE1	5:M:686:GLN:OE1	2.64	0.50
5:M:485:HIS:HA	5:M:488:VAL:HG12	1.93	0.50
3:D:117:ASP:OD2	3:D:495:ARG:NH1	2.45	0.50
3:D:843:PHE:O	3:D:867:ARG:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1483:PHE:O	3:D:1485:GLN:NE2	2.45	0.50
5:M:526:SER:C	5:M:554:ARG:HE	2.14	0.50
5:M:610:VAL:HA	5:M:615:LEU:HD11	1.94	0.50
5:M:654:VAL:HB	5:M:706:VAL:HA	1.92	0.50
1:A:124:ASN:OD1	1:A:124:ASN:N	2.44	0.50
2:C:124:ASP:OD1	2:C:124:ASP:N	2.45	0.50
2:C:740:GLU:OE1	2:C:805:ARG:NH1	2.44	0.50
5:M:758:HIS:O	5:M:761:ARG:NH2	2.43	0.50
3:D:72:VAL:HA	3:D:79:GLU:HA	1.93	0.50
3:D:199:LEU:HD13	3:D:397:LYS:HB2	1.94	0.50
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.45	0.50
5:M:568:LEU:HD13	5:M:593:THR:HG22	1.91	0.50
1:B:31:GLY:O	1:B:35:THR:OG1	2.24	0.50
2:C:191:PHE:HB2	2:C:241:LEU:HD13	1.93	0.50
2:C:468:ARG:HB3	2:C:485:TYR:HB3	1.94	0.50
2:C:710:ILE:HG21	2:C:756:VAL:HG21	1.94	0.50
3:D:472:ALA:HA	3:D:475:LYS:HD2	1.93	0.50
3:D:789:LEU:O	3:D:793:THR:OG1	2.26	0.50
5:M:493:GLN:HE22	5:M:563:ARG:H	1.60	0.50
5:M:783:HIS:HD2	5:M:784:LEU:HD23	1.76	0.50
2:C:146:VAL:HG12	2:C:162:ILE:HG12	1.93	0.50
3:D:166:GLN:HB2	3:D:396:VAL:HA	1.93	0.50
1:A:87:VAL:HG21	1:A:144:VAL:HG11	1.94	0.50
3:D:401:TYR:O	3:D:444:VAL:N	2.33	0.50
5:M:789:ASP:O	5:M:793:ARG:NE	2.34	0.50
1:A:56:VAL:HG22	1:A:142:VAL:HG23	1.94	0.49
2:C:91:GLN:HA	2:C:119:PRO:HA	1.94	0.49
2:C:198:ARG:HG2	2:C:226:VAL:HG22	1.94	0.49
2:C:303:PHE:O	2:C:306:THR:OG1	2.24	0.49
2:C:551:GLU:HB3	3:D:1065:LEU:H	1.76	0.49
2:C:630:ARG:HH21	2:C:706:GLU:HA	1.76	0.49
2:C:689:VAL:HG13	2:C:851:LYS:HB3	1.94	0.49
2:C:714:ASP:HA	2:C:719:PRO:HB3	1.93	0.49
3:D:450:TYR:N	3:D:450:TYR:HD2	2.10	0.49
5:M:351:LEU:HD23	5:M:353:LEU:HD21	1.93	0.49
5:M:460:SER:HB2	5:M:462:HIS:HD2	1.77	0.49
1:B:185:ARG:NH2	3:D:689:ASP:OD1	2.40	0.49
2:C:674:VAL:HG23	2:C:869:VAL:HB	1.94	0.49
3:D:657:LEU:HD11	3:D:691:LEU:HD13	1.94	0.49
5:M:539:LYS:O	5:M:543:GLU:N	2.43	0.49
1:A:12:THR:OG1	1:A:14:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:469:THR:H	2:C:486:MET:H	1.60	0.49
2:C:580:MET:O	2:C:903:SER:N	2.39	0.49
2:C:761:PHE:O	2:C:786:LYS:NZ	2.45	0.49
2:C:940:GLU:HA	2:C:943:VAL:HG12	1.93	0.49
3:D:771:SER:HB3	3:D:778:LEU:HD21	1.94	0.49
1:A:42:ARG:HA	2:C:856:GLU:HB2	1.94	0.49
2:C:215:GLY:O	2:C:219:GLN:N	2.41	0.49
3:D:123:LEU:HA	3:D:126:VAL:HG12	1.93	0.49
1:A:54:THR:OG1	1:A:55:SER:N	2.46	0.49
2:C:1019:GLN:HE21	3:D:622:ARG:H	1.59	0.49
3:D:112:ILE:HG22	3:D:118:LEU:HD21	1.95	0.49
3:D:399:ARG:HB3	3:D:446:VAL:HG13	1.95	0.49
3:D:907:GLU:O	3:D:910:SER:OG	2.25	0.49
1:A:180:GLN:HG3	1:A:182:GLU:HG2	1.94	0.49
1:B:216:GLU:O	1:B:219:ARG:NH1	2.46	0.49
2:C:20:GLU:O	2:C:24:GLU:CB	2.60	0.49
2:C:133:ASP:HB3	2:C:395:LYS:HB3	1.95	0.49
2:C:508:ILE:HG22	2:C:510:ALA:H	1.77	0.49
3:D:853:VAL:HG11	3:D:860:LEU:HD21	1.94	0.49
3:D:908:LYS:HA	3:D:911:LEU:HD12	1.95	0.49
5:M:782:GLY:HA2	5:M:785:LEU:HG	1.93	0.49
6:T:38:DG:N2	7:N:3:DA:N3	2.60	0.49
2:C:312:ALA:HB1	2:C:317:VAL:HB	1.94	0.49
2:C:724:ARG:NE	2:C:738:ASP:O	2.45	0.49
3:D:550:ARG:HG2	3:D:553:ARG:HH22	1.77	0.49
3:D:805:GLU:OE2	3:D:828:LYS:HG3	2.13	0.49
3:D:1149:LEU:HB2	3:D:1163:GLY:H	1.77	0.49
2:C:325:ILE:O	2:C:331:ARG:NE	2.45	0.49
2:C:693:GLU:HG3	2:C:697:ARG:HH12	1.78	0.49
2:C:711:GLU:HA	2:C:822:VAL:HA	1.94	0.49
2:C:1018:GLN:HG2	2:C:1060:ILE:HD11	1.94	0.49
3:D:835:SER:HB3	3:D:838:ARG:HG3	1.95	0.49
1:B:14:ARG:O	1:B:22:GLU:N	2.40	0.49
2:C:630:ARG:HG3	2:C:705:ILE:HB	1.95	0.49
3:D:798:GLU:HB3	3:D:822:ALA:HB1	1.95	0.49
3:D:713:ILE:O	3:D:714:GLN:NE2	2.46	0.48
3:D:782:SER:OG	3:D:783:ARG:N	2.46	0.48
3:D:750:PRO:O	3:D:756:GLN:NE2	2.46	0.48
3:D:996:TRP:O	3:D:1000:THR:OG1	2.24	0.48
4:E:48:MET:N	4:E:55:PHE:O	2.47	0.48
5:M:325:LEU:HB3	5:M:371:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:HIS:NE2	1:A:167:VAL:O	2.46	0.48
2:C:680:ASP:H	3:D:943:THR:HB	1.78	0.48
3:D:610:LYS:HD2	3:D:615:ARG:HB3	1.94	0.48
3:D:954:ALA:HB3	3:D:1062:ARG:HH11	1.78	0.48
3:D:1037:GLN:HG2	3:D:1042:ARG:HD2	1.95	0.48
3:D:1083:ASP:O	3:D:1087:ARG:HB2	2.13	0.48
5:M:585:ARG:HA	5:M:588:LYS:HB2	1.94	0.48
5:M:577:GLY:O	5:M:581:LYS:N	2.46	0.48
2:C:180:GLY:HA3	2:C:220:GLY:HA3	1.95	0.48
2:C:384:GLU:OE1	2:C:388:ARG:NE	2.47	0.48
2:C:424:GLY:O	2:C:428:ARG:NH1	2.39	0.48
3:D:1384:PRO:HA	3:D:1415:VAL:HG13	1.96	0.48
1:A:58:ILE:HA	1:A:140:MET:HA	1.96	0.48
2:C:425:PHE:HA	2:C:428:ARG:HB2	1.96	0.48
3:D:841:TYR:O	3:D:865:THR:OG1	2.32	0.48
3:D:1274:ILE:HD12	3:D:1322:GLY:HA2	1.96	0.48
3:D:1434:TRP:HA	3:D:1437:ALA:HB3	1.96	0.48
5:M:631:PHE:HE1	5:M:753:TYR:HB3	1.79	0.48
1:A:173:PRO:O	1:A:202:ASP:N	2.47	0.48
1:B:112:ARG:N	1:B:125:PRO:O	2.44	0.48
2:C:91:GLN:HB2	2:C:117:HIS:HB3	1.96	0.48
3:D:39:PRO:HG2	3:D:53:ILE:HD11	1.96	0.48
3:D:542:ASP:HA	3:D:545:ARG:HE	1.79	0.48
3:D:960:LYS:NZ	3:D:1040:GLY:O	2.47	0.48
3:D:1169:ASP:O	3:D:1173:LEU:HB2	2.14	0.48
5:M:544:GLY:O	5:M:563:ARG:NH1	2.46	0.48
6:T:36:DA:N6	7:N:4:DT:O4	2.47	0.48
1:A:53:VAL:HG21	1:A:82:LEU:HD13	1.96	0.47
1:B:149:GLY:O	1:B:171:PHE:N	2.46	0.47
2:C:51:THR:HG21	2:C:348:LEU:HD22	1.96	0.47
2:C:143:SER:N	2:C:330:ASN:O	2.40	0.47
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.94	0.47
1:A:220:GLU:O	1:A:223:THR:OG1	2.32	0.47
2:C:261:ILE:HD12	2:C:290:LEU:HD23	1.95	0.47
2:C:1008:ARG:NE	3:D:624:ASP:OD1	2.45	0.47
2:C:1058:ASP:OD1	2:C:1058:ASP:N	2.47	0.47
3:D:813:LEU:HD23	3:D:836:VAL:HG23	1.96	0.47
3:D:1275:SER:HB2	3:D:1325:LEU:HD21	1.95	0.47
3:D:1485:GLN:HE22	4:E:78:ASN:H	1.62	0.47
5:M:323:ASP:O	5:M:335:TYR:N	2.47	0.47
5:M:660:ARG:HH21	5:M:729:ARG:CZ	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:LEU:HD12	2:C:100:LEU:HD13	1.96	0.47
2:C:210:GLU:HG3	2:C:211:LEU:HD22	1.97	0.47
2:C:541:SER:O	2:C:545:ASN:ND2	2.34	0.47
2:C:692:GLU:OE1	2:C:696:LYS:NZ	2.36	0.47
3:D:125:GLN:HB3	3:D:131:LYS:HB2	1.97	0.47
3:D:611:GLN:OE1	3:D:616:GLN:NE2	2.48	0.47
3:D:613:ARG:HD3	3:D:617:ASN:HB2	1.96	0.47
7:N:36:DA:H2'	7:N:37:DC:C6	2.49	0.47
1:B:12:THR:OG1	1:B:14:ARG:NH1	2.48	0.47
2:C:1031:ARG:NH2	3:D:621:LYS:O	2.48	0.47
3:D:913:ASP:O	3:D:917:GLN:NE2	2.44	0.47
5:M:811:SER:OG	5:M:813:GLU:OE1	2.32	0.47
1:B:59:GLU:N	1:B:139:ASN:O	2.47	0.47
2:C:281:LEU:HD13	2:C:302:VAL:CG2	2.42	0.47
2:C:1100:GLN:HB3	3:D:9:ARG:HB3	1.96	0.47
3:D:866:VAL:HG23	3:D:873:LEU:HB2	1.96	0.47
6:T:10:DC:N4	7:N:29:DG:O6	2.48	0.47
2:C:292:ARG:NH2	2:C:300:ASP:O	2.48	0.47
3:D:159:ARG:NH2	3:D:159:ARG:O	2.48	0.47
3:D:1110:ALA:O	3:D:1203:LYS:N	2.45	0.47
5:M:494:VAL:HB	5:M:548:ILE:HG12	1.97	0.47
5:M:521:ARG:NH2	5:M:547:ASP:OD1	2.43	0.47
1:A:90:LEU:HD11	1:A:121:GLU:HB2	1.97	0.47
1:B:59:GLU:CB	1:B:139:ASN:HB3	2.44	0.47
1:B:151:VAL:O	1:B:169:ALA:N	2.39	0.47
2:C:147:TYR:N	2:C:161:SER:O	2.44	0.47
2:C:149:THR:HG23	2:C:159:ILE:HB	1.95	0.47
2:C:200:LEU:HD22	2:C:300:ASP:H	1.80	0.47
2:C:287:GLY:O	2:C:301:GLU:OE1	2.33	0.47
2:C:575:GLN:OE1	2:C:671:ASN:ND2	2.40	0.47
2:C:1031:ARG:NH2	2:C:1032:PHE:O	2.46	0.47
3:D:107:ASP:OD1	3:D:1445:HIS:ND1	2.48	0.47
3:D:644:LEU:N	3:D:719:VAL:O	2.48	0.47
3:D:1146:GLY:HA3	3:D:1207:TYR:CD1	2.50	0.47
5:M:408:GLY:HA2	5:M:411:LEU:HB2	1.96	0.47
2:C:525:SER:OG	2:C:527:GLU:OE1	2.33	0.47
3:D:461:ILE:HA	3:D:464:LEU:HD12	1.95	0.47
3:D:604:THR:O	3:D:608:SER:N	2.36	0.47
3:D:834:THR:OG1	3:D:835:SER:N	2.47	0.47
3:D:1356:TYR:O	3:D:1360:GLY:N	2.48	0.47
3:D:1465:ASN:HD22	3:D:1472:ILE:HG22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:336:LEU:HB2	5:M:352:VAL:HB	1.97	0.47
1:A:109:VAL:HG12	1:A:129:ILE:HD12	1.97	0.47
3:D:402:PRO:HA	3:D:443:VAL:HA	1.96	0.47
3:D:455:ARG:HH22	3:D:463:GLN:HG3	1.78	0.47
3:D:486:ARG:HA	3:D:489:ARG:HB2	1.97	0.47
6:T:30:DA:C6	7:N:11:DG:C6	3.03	0.47
1:A:35:THR:OG1	1:B:42:ARG:NE	2.40	0.47
1:B:44:LEU:HA	1:B:48:ILE:HD11	1.97	0.47
3:D:136:ASP:HB3	3:D:453:ASP:HB3	1.96	0.47
3:D:550:ARG:HE	3:D:553:ARG:HH12	1.63	0.47
3:D:886:VAL:HG23	3:D:896:ALA:HB1	1.96	0.47
5:M:711:THR:HG22	5:M:713:ILE:H	1.80	0.47
2:C:540:PHE:HB3	2:C:544:THR:HB	1.97	0.46
2:C:789:SER:HB3	2:C:791:ARG:HH21	1.80	0.46
3:D:44:LEU:O	3:D:525:ARG:NH2	2.35	0.46
3:D:679:ARG:HB3	3:D:681:ARG:HG2	1.97	0.46
3:D:843:PHE:HB2	3:D:866:VAL:HG12	1.96	0.46
3:D:1478:SER:O	3:D:1482:ARG:N	2.49	0.46
1:A:39:PRO:HG2	1:B:39:PRO:HG3	1.98	0.46
3:D:48:ARG:HB3	3:D:78:VAL:HG22	1.96	0.46
3:D:845:ASN:ND2	3:D:848:GLU:OE2	2.49	0.46
3:D:1004:THR:HG23	3:D:1036:ARG:HB3	1.97	0.46
2:C:135:VAL:HB	2:C:395:LYS:HD2	1.96	0.46
2:C:1003:ASP:OD1	2:C:1003:ASP:N	2.47	0.46
3:D:207:PHE:HD2	3:D:391:ALA:HB3	1.79	0.46
5:M:527:ARG:HA	5:M:554:ARG:NH2	2.20	0.46
3:D:101:HIS:HB2	3:D:514:LEU:HD21	1.97	0.46
3:D:1263:PHE:HE1	3:D:1371:VAL:HG11	1.80	0.46
5:M:647:GLU:O	5:M:652:GLY:N	2.43	0.46
6:T:27:DC:H42	7:N:14:DC:H42	1.63	0.46
2:C:481:ASP:OD1	2:C:506:ASN:ND2	2.48	0.46
3:D:1407:LEU:HD13	3:D:1414:PRO:HA	1.97	0.46
5:M:334:GLN:HG2	5:M:354:ARG:HH21	1.80	0.46
5:M:511:PHE:HB3	5:M:522:VAL:HG11	1.97	0.46
5:M:712:ILE:HA	5:M:715:ALA:HB3	1.98	0.46
2:C:198:ARG:HH12	2:C:230:ARG:NH1	2.14	0.46
3:D:22:SER:OG	3:D:24:GLY:O	2.34	0.46
3:D:496:LEU:HA	3:D:499:VAL:HG12	1.97	0.46
3:D:1046:GLN:HA	3:D:1052:THR:HA	1.97	0.46
5:M:334:GLN:HB3	5:M:336:LEU:HD21	1.98	0.46
5:M:711:THR:O	5:M:715:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HB3	1:B:189:ARG:HB2	1.96	0.46
3:D:152:LEU:HD23	3:D:152:LEU:HA	1.82	0.46
5:M:348:ARG:HD3	5:M:364:PRO:HB3	1.98	0.46
5:M:459:GLU:OE2	5:M:486:ARG:NH1	2.48	0.46
5:M:711:THR:HG21	6:T:30:DA:H4'	1.98	0.46
1:A:149:GLY:O	1:A:171:PHE:N	2.39	0.46
2:C:462:ASP:OD1	2:C:466:PHE:N	2.36	0.46
5:M:629:LYS:O	5:M:754:ALA:N	2.38	0.46
1:A:12:THR:HG23	1:A:24:VAL:HB	1.97	0.46
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.84	0.46
2:C:108:ILE:HB	5:M:362:TYR:HB2	1.97	0.46
2:C:305:PRO:HA	2:C:308:ARG:HE	1.81	0.46
2:C:775:ARG:HH11	2:C:781:LYS:HB3	1.80	0.46
6:T:32:DC:H2'	6:T:33:DC:C6	2.51	0.46
1:A:215:VAL:HG23	1:B:222:LEU:HD22	1.97	0.45
3:D:60:CYS:HB2	3:D:75:ARG:HD2	1.98	0.45
2:C:176:VAL:HA	2:C:182:VAL:HA	1.99	0.45
3:D:634:GLY:N	3:D:728:LEU:O	2.42	0.45
3:D:1164:ARG:NH2	3:D:1165:TYR:O	2.48	0.45
3:D:1455:LYS:HA	3:D:1455:LYS:HD3	1.72	0.45
1:A:58:ILE:HG23	1:A:140:MET:HB3	1.99	0.45
2:C:470:PRO:HA	2:C:485:TYR:HA	1.98	0.45
2:C:593:ALA:HB1	2:C:659:PRO:HD2	1.98	0.45
3:D:411:THR:HG23	3:D:436:GLU:HA	1.98	0.45
3:D:793:THR:HB	3:D:905:PRO:HA	1.97	0.45
3:D:1066:THR:N	3:D:1069:GLU:OE2	2.47	0.45
3:D:1259:VAL:HA	3:D:1262:LEU:HB2	1.98	0.45
5:M:428:LEU:HB3	5:M:431:TRP:HD1	1.80	0.45
5:M:522:VAL:HA	5:M:548:ILE:HB	1.97	0.45
1:A:112:ARG:HH11	1:A:126:ASP:HB3	1.82	0.45
2:C:45:GLN:HE21	2:C:49:ARG:HG2	1.81	0.45
2:C:1014:SER:N	2:C:1019:GLN:O	2.49	0.45
1:A:103:ALA:N	1:A:138:LEU:O	2.49	0.45
2:C:106:GLY:HA3	5:M:348:ARG:HH12	1.82	0.45
2:C:478:VAL:HA	2:C:507:ARG:HA	1.98	0.45
3:D:102:ILE:HG13	3:D:106:LYS:HG2	1.98	0.45
3:D:419:ASP:O	3:D:429:SER:N	2.40	0.45
3:D:804:LEU:H	3:D:827:ILE:HG13	1.80	0.45
6:T:38:DG:C2	7:N:3:DA:H2	2.27	0.45
2:C:578:VAL:HG23	2:C:900:ARG:HG2	1.98	0.45
2:C:723:THR:OG1	2:C:724:ARG:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:47:GLU:HG2	3:D:78:VAL:HG11	1.98	0.45
3:D:1258:ARG:HA	3:D:1258:ARG:HD2	1.70	0.45
3:D:1283:ILE:HG12	3:D:1315:ASP:HB2	1.99	0.45
6:T:25:DA:N1	7:N:15:DT:C4	2.84	0.45
1:A:110:LYS:HB2	1:A:112:ARG:HG2	1.99	0.45
2:C:302:VAL:O	2:C:306:THR:HG23	2.17	0.45
3:D:809:PRO:HB3	3:D:839:LEU:HD22	1.99	0.45
3:D:948:THR:OG1	3:D:949:ILE:N	2.50	0.45
2:C:291:ALA:HA	2:C:300:ASP:HA	1.99	0.45
3:D:904:VAL:O	3:D:906:GLN:NE2	2.49	0.45
3:D:1101:VAL:HG22	3:D:1374:GLN:HE22	1.82	0.45
5:M:621:PRO:HB3	5:M:779:LEU:HB2	1.98	0.45
6:T:9:DG:C2	7:N:32:DG:C2	3.05	0.45
1:A:108:GLU:HG3	1:A:110:LYS:HZ3	1.82	0.45
2:C:215:GLY:HA2	2:C:218:VAL:HB	1.98	0.45
2:C:552:HIS:ND1	3:D:1061:PHE:O	2.50	0.45
2:C:553:ASP:HB3	2:C:881:ASN:HD22	1.81	0.45
2:C:752:GLY:N	2:C:792:VAL:O	2.39	0.45
3:D:617:ASN:O	3:D:621:LYS:NZ	2.49	0.45
3:D:821:VAL:HG13	3:D:827:ILE:HD13	1.99	0.45
3:D:1152:GLU:N	3:D:1162:GLU:OE2	2.50	0.45
7:N:13:DG:H2'	7:N:14:DC:C6	2.52	0.45
2:C:192:PRO:HG2	2:C:195:LEU:HD22	1.99	0.44
3:D:201:GLY:HA3	3:D:397:LYS:HA	2.00	0.44
3:D:1207:TYR:CE1	3:D:1209:LEU:CD2	3.00	0.44
3:D:1272:ALA:N	3:D:1329:ALA:O	2.36	0.44
1:A:5:LYS:HD2	1:A:5:LYS:HA	1.78	0.44
1:A:123:MET:HG3	1:A:204:SER:HB3	1.99	0.44
2:C:274:ARG:NE	2:C:278:GLU:OE2	2.43	0.44
2:C:808:ARG:N	2:C:820:ARG:O	2.49	0.44
3:D:823:LEU:O	3:D:835:SER:OG	2.24	0.44
3:D:1106:VAL:N	3:D:1108:ARG:HH11	2.15	0.44
5:M:680:ILE:HG12	5:M:706:VAL:HB	1.98	0.44
2:C:300:ASP:OD2	2:C:303:PHE:N	2.50	0.44
2:C:615:TYR:HD2	2:C:619:ARG:HG3	1.81	0.44
3:D:828:LYS:HA	3:D:833:GLU:HA	2.00	0.44
1:A:49:PRO:HA	1:A:148:VAL:HA	1.99	0.44
1:B:82:LEU:HA	1:B:85:LEU:HG	2.00	0.44
3:D:114:THR:O	3:D:495:ARG:NE	2.50	0.44
3:D:421:LEU:HD21	3:D:429:SER:HB3	1.98	0.44
1:B:51:THR:HG22	1:B:146:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:133:ASP:HB3	2:C:632:ASN:HD21	1.82	0.44
2:C:693:GLU:HG3	2:C:697:ARG:NH1	2.33	0.44
2:C:1015:LEU:HG	2:C:1016:ILE:HD12	2.00	0.44
3:D:989:TYR:CZ	3:D:993:LEU:HD11	2.53	0.44
3:D:1275:SER:O	3:D:1322:GLY:N	2.39	0.44
2:C:181:VAL:HA	2:C:221:LEU:HD23	1.99	0.44
3:D:58:CYS:SG	3:D:62:LYS:N	2.90	0.44
3:D:113:GLY:HA2	3:D:118:LEU:HG	1.98	0.44
3:D:530:VAL:HG23	3:D:532:GLY:H	1.82	0.44
3:D:601:ARG:HG3	3:D:605:ASP:HB2	2.00	0.44
3:D:941:PHE:HA	3:D:944:THR:HG22	1.99	0.44
2:C:411:SER:OG	2:C:412:ALA:N	2.50	0.44
2:C:626:ARG:HA	2:C:626:ARG:HD2	1.88	0.44
2:C:738:ASP:N	2:C:742:VAL:O	2.42	0.44
3:D:158:TYR:CE1	3:D:162:ARG:HD3	2.52	0.44
5:M:497:LEU:HD23	5:M:497:LEU:HA	1.87	0.44
5:M:725:ILE:HG12	5:M:727:ILE:HD11	2.00	0.44
2:C:135:VAL:N	2:C:393:GLN:O	2.48	0.44
3:D:206:ARG:HD2	3:D:206:ARG:HA	1.79	0.44
3:D:1486:VAL:HA	4:E:75:PHE:HA	1.98	0.44
5:M:339:GLU:OE1	5:M:341:ARG:NH1	2.39	0.44
2:C:475:VAL:N	2:C:478:VAL:O	2.50	0.44
2:C:1021:LEU:O	2:C:1029:GLY:N	2.43	0.44
3:D:57:GLU:OE2	3:D:64:LYS:NZ	2.35	0.44
3:D:829:VAL:HG13	3:D:829:VAL:O	2.18	0.44
3:D:1257:PRO:HA	3:D:1260:ILE:HB	2.00	0.44
3:D:1284:GLU:O	3:D:1291:SER:N	2.51	0.44
6:T:10:DC:H2"	6:T:11:DC:O5'	2.18	0.44
2:C:836:GLY:H	2:C:849:VAL:HG13	1.83	0.43
2:C:937:ASP:OD1	2:C:938:LYS:N	2.51	0.43
3:D:449:SER:C	3:D:450:TYR:HD2	2.21	0.43
3:D:800:LYS:H	3:D:822:ALA:HB2	1.83	0.43
4:E:36:LYS:HE3	4:E:36:LYS:HB3	1.86	0.43
5:M:340:THR:HG22	5:M:347:LYS:HE3	1.99	0.43
5:M:629:LYS:HB2	5:M:753:TYR:HA	2.00	0.43
5:M:735:LEU:HD11	5:M:769:ARG:HG2	2.00	0.43
2:C:34:VAL:O	2:C:39:ARG:NE	2.44	0.43
2:C:76:PRO:HA	2:C:77:PRO:HD3	1.82	0.43
2:C:81:ASP:OD1	2:C:81:ASP:N	2.50	0.43
2:C:230:ARG:HB2	2:C:233:GLU:HG3	2.00	0.43
3:D:449:SER:C	3:D:450:TYR:CD2	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ALA:HB3	1:A:198:ARG:HB2	2.01	0.43
2:C:270:GLY:O	2:C:274:ARG:N	2.43	0.43
2:C:1102:LEU:HD13	2:C:1106:ASP:HA	1.99	0.43
3:D:6:ARG:HD2	3:D:6:ARG:HA	1.71	0.43
3:D:671:LYS:HA	3:D:674:ARG:HB3	2.00	0.43
5:M:535:GLU:HA	5:M:538:LEU:HB2	2.00	0.43
2:C:142:ARG:HD2	2:C:325:ILE:HD12	2.00	0.43
2:C:478:VAL:HG13	2:C:506:ASN:HB3	2.01	0.43
3:D:31:THR:HG22	3:D:44:LEU:HD13	1.99	0.43
3:D:171:LEU:HD12	3:D:390:PRO:HG2	2.01	0.43
3:D:1286:THR:HG1	3:D:1289:LYS:H	1.64	0.43
1:A:201:THR:OG1	1:A:202:ASP:N	2.52	0.43
2:C:283:ILE:HD12	2:C:285:LEU:HD23	2.00	0.43
2:C:872:ASN:HD21	2:C:874:LEU:HB2	1.84	0.43
3:D:123:LEU:O	3:D:127:LEU:HB2	2.18	0.43
5:M:601:ILE:HD13	5:M:605:LEU:HB2	2.00	0.43
5:M:660:ARG:NH2	5:M:729:ARG:NE	2.64	0.43
5:M:731:ASP:OD1	5:M:731:ASP:N	2.51	0.43
2:C:345:ARG:HA	2:C:348:LEU:HD12	1.98	0.43
3:D:64:LYS:H	3:D:67:ARG:HH12	1.67	0.43
3:D:131:LYS:HD2	3:D:152:LEU:HD13	2.00	0.43
3:D:419:ASP:N	3:D:429:SER:OG	2.51	0.43
3:D:784:ASP:N	3:D:784:ASP:OD1	2.52	0.43
5:M:343:VAL:O	5:M:345:GLY:N	2.51	0.43
5:M:431:TRP:O	5:M:485:HIS:ND1	2.52	0.43
5:M:487:VAL:HG21	5:M:567:LEU:HB2	2.00	0.43
2:C:473:ARG:HA	2:C:531:PHE:HA	1.99	0.43
2:C:838:LYS:HD2	2:C:838:LYS:HA	1.87	0.43
5:M:495:ALA:N	5:M:567:LEU:O	2.45	0.43
1:B:186:LEU:N	1:B:189:ARG:O	2.42	0.43
2:C:71:TYR:HA	2:C:96:ALA:HA	2.00	0.43
2:C:1103:ASP:OD2	2:C:1107:ASN:ND2	2.52	0.43
3:D:126:VAL:HG23	3:D:456:MET:HA	2.00	0.43
5:M:539:LYS:HB3	5:M:539:LYS:HE3	1.82	0.43
2:C:537:LYS:HZ2	2:C:905:ILE:HG22	1.84	0.43
2:C:1061:GLU:HA	2:C:1064:ASN:HB2	2.00	0.43
3:D:471:GLU:O	3:D:474:GLU:HG2	2.19	0.43
3:D:508:ARG:HB3	3:D:511:TRP:CD2	2.54	0.43
3:D:614:PHE:HA	3:D:618:LEU:HD12	2.01	0.43
3:D:764:LEU:O	3:D:768:ASN:ND2	2.52	0.43
3:D:807:ALA:HA	3:D:830:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1006:ALA:HA	3:D:1009:LYS:HE3	2.01	0.43
3:D:1009:LYS:HA	3:D:1012:GLU:HG3	2.01	0.43
3:D:1019:PRO:HA	3:D:1022:VAL:HG22	1.99	0.43
3:D:1269:LYS:H	3:D:1269:LYS:HG2	1.64	0.43
5:M:739:TYR:OH	5:M:787:GLU:OE2	2.37	0.43
2:C:285:LEU:HD13	2:C:285:LEU:HA	1.93	0.43
2:C:976:ASP:OD2	2:C:979:THR:N	2.52	0.43
3:D:50:PHE:HB3	3:D:86:ARG:HG3	2.00	0.43
3:D:140:ALA:CB	3:D:452:ILE:HB	2.49	0.43
2:C:626:ARG:NH1	2:C:627:ARG:O	2.52	0.42
3:D:1323:GLN:HA	3:D:1324:PRO:HD3	1.90	0.42
3:D:1498:ALA:O	4:E:84:ARG:NH2	2.51	0.42
5:M:478:GLU:HA	5:M:481:LEU:HD12	2.00	0.42
5:M:655:PHE:HB2	5:M:725:ILE:HA	2.00	0.42
1:B:72:LYS:HE3	1:B:72:LYS:HB3	1.75	0.42
1:B:109:VAL:HB	1:B:129:ILE:HB	2.01	0.42
2:C:799:ILE:O	2:C:828:ALA:N	2.52	0.42
3:D:110:SER:O	3:D:114:THR:N	2.49	0.42
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	2.00	0.42
5:M:565:LEU:HD21	5:M:568:LEU:HD21	2.01	0.42
1:B:57:TYR:O	1:B:141:GLU:N	2.35	0.42
2:C:425:PHE:O	2:C:429:ASP:N	2.48	0.42
2:C:1019:GLN:HE21	3:D:622:ARG:N	2.17	0.42
3:D:529:GLN:HA	3:D:535:PHE:HA	2.00	0.42
5:M:777:SER:OG	5:M:778:ASP:N	2.53	0.42
1:A:53:VAL:HA	1:A:144:VAL:HG22	2.00	0.42
2:C:162:ILE:N	2:C:172:ILE:O	2.41	0.42
2:C:343:GLN:HG2	2:C:385:PHE:HB2	2.02	0.42
2:C:640:ARG:HB3	2:C:642:ARG:HH12	1.83	0.42
2:C:755:LEU:HD11	2:C:790:LEU:HD23	2.01	0.42
2:C:807:ARG:HA	2:C:821:GLU:HA	2.01	0.42
3:D:106:LYS:HE2	3:D:586:ARG:HB3	2.02	0.42
3:D:138:LYS:HB2	3:D:452:ILE:HA	2.01	0.42
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.54	0.42
4:E:46:PRO:HG2	4:E:63:TRP:HA	2.01	0.42
1:B:9:PRO:HA	1:B:27:PRO:HD2	2.01	0.42
2:C:195:LEU:HD21	2:C:238:LEU:HB3	2.01	0.42
2:C:199:VAL:HA	2:C:231:PRO:HB3	2.02	0.42
2:C:492:ASP:HB3	2:C:518:LYS:HE3	2.02	0.42
5:M:410:LEU:HD23	5:M:410:LEU:HA	1.91	0.42
6:T:36:DA:N1	7:N:4:DT:N3	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HB3	1:B:203:GLY:HA2	2.01	0.42
3:D:95:LEU:HD23	3:D:95:LEU:HA	1.82	0.42
3:D:844:ALA:HA	3:D:867:ARG:HB3	2.02	0.42
5:M:427:PRO:HD3	5:M:459:GLU:HG2	2.02	0.42
5:M:658:HIS:O	5:M:710:THR:HG22	2.19	0.42
5:M:667:ARG:HA	5:M:667:ARG:HD2	1.82	0.42
1:B:110:LYS:HB3	1:B:112:ARG:HG2	2.01	0.42
1:B:185:ARG:HA	1:B:190:THR:HA	2.01	0.42
2:C:218:VAL:HG22	2:C:221:LEU:HD12	2.02	0.42
2:C:611:ILE:N	2:C:622:GLU:OE2	2.51	0.42
2:C:930:LYS:HA	2:C:930:LYS:HD2	1.84	0.42
3:D:646:LYS:O	3:D:650:LEU:HB2	2.20	0.42
3:D:1314:LYS:HE2	3:D:1314:LYS:HB2	1.85	0.42
5:M:678:ALA:HB1	5:M:705:ASP:HB2	2.01	0.42
5:M:764:GLU:N	5:M:764:GLU:OE1	2.53	0.42
1:B:18:ARG:NH1	1:B:209:GLU:OE2	2.53	0.42
1:B:112:ARG:HE	1:B:126:ASP:HA	1.85	0.42
2:C:679:PHE:N	2:C:683:ASN:OD1	2.42	0.42
3:D:572:ARG:O	3:D:576:GLU:HG2	2.20	0.42
3:D:1207:TYR:CE1	3:D:1209:LEU:HD23	2.55	0.42
3:D:1271:LYS:HB2	3:D:1271:LYS:HE3	1.83	0.42
5:M:578:VAL:N	7:N:11:DG:OP1	2.53	0.42
1:B:91:ASN:HD21	1:B:93:SER:HB2	1.85	0.42
1:B:159:LYS:HZ1	1:B:165:ILE:HA	1.85	0.42
2:C:12:VAL:HG23	2:C:13:ILE:HG23	2.02	0.42
2:C:324:ASP:OD2	2:C:327:HIS:N	2.52	0.42
2:C:469:THR:O	2:C:486:MET:N	2.51	0.42
3:D:46:ASP:HB3	3:D:49:ILE:HD12	2.02	0.42
3:D:132:TYR:O	3:D:153:LEU:N	2.52	0.42
3:D:618:LEU:HD13	3:D:1467:ILE:HG23	2.02	0.42
3:D:1445:HIS:O	3:D:1448:THR:OG1	2.28	0.42
5:M:347:LYS:HA	5:M:347:LYS:HD2	1.76	0.42
1:B:109:VAL:O	1:B:129:ILE:N	2.44	0.42
2:C:726:ILE:HD13	2:C:726:ILE:HA	1.87	0.42
2:C:737:LEU:HA	2:C:743:VAL:HA	2.02	0.42
2:C:808:ARG:HE	2:C:809:GLY:N	2.14	0.42
2:C:874:LEU:O	3:D:1029:ARG:NE	2.53	0.42
3:D:48:ARG:HA	3:D:78:VAL:HG13	2.02	0.42
4:E:40:LEU:HD23	4:E:72:ARG:HH12	1.84	0.42
5:M:369:PRO:O	5:M:372:LYS:NZ	2.51	0.42
1:B:159:LYS:HD3	1:B:163:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:762:LYS:N	2:C:784:ASP:O	2.49	0.41
1:A:76:VAL:HA	1:A:79:ILE:HD12	2.01	0.41
2:C:1103:ASP:OD1	2:C:1103:ASP:N	2.52	0.41
2:C:182:VAL:HG13	2:C:193:LEU:HB3	2.01	0.41
3:D:17:LYS:HE3	3:D:21:TRP:HZ2	1.85	0.41
3:D:140:ALA:HA	3:D:450:TYR:HD1	1.84	0.41
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.89	0.41
3:D:172:PRO:HA	3:D:173:PRO:HD3	1.84	0.41
3:D:411:THR:OG1	3:D:437:VAL:N	2.54	0.41
4:E:16:LYS:H	4:E:16:LYS:HG2	1.65	0.41
1:B:52:ALA:HB1	1:B:169:ALA:HB1	2.02	0.41
1:B:199:ILE:HG21	1:B:207:PRO:HB3	2.01	0.41
3:D:520:LEU:HA	3:D:520:LEU:HD12	1.86	0.41
5:M:660:ARG:HE	5:M:729:ARG:HD2	1.86	0.41
1:A:56:VAL:HA	1:A:142:VAL:HA	2.03	0.41
3:D:124:GLU:HA	3:D:128:TYR:HD2	1.84	0.41
3:D:835:SER:HB3	3:D:838:ARG:HE	1.85	0.41
4:E:66:LYS:HA	4:E:69:LEU:HD12	2.02	0.41
5:M:692:ILE:O	5:M:695:THR:OG1	2.33	0.41
6:T:10:DC:C2'	6:T:11:DC:C6	3.04	0.41
6:T:27:DC:N4	7:N:14:DC:H42	2.19	0.41
2:C:575:GLN:HB2	2:C:900:ARG:HH22	1.85	0.41
2:C:1086:ARG:CG	2:C:1111:ILE:HD11	2.30	0.41
3:D:95:LEU:HD12	3:D:515:GLU:HA	2.01	0.41
3:D:1406:ARG:O	3:D:1410:GLU:N	2.50	0.41
5:M:444:THR:O	5:M:448:LYS:N	2.46	0.41
1:B:115:LEU:HA	1:B:116:PRO:HD3	1.95	0.41
1:B:131:THR:OG1	1:B:133:GLU:OE2	2.35	0.41
3:D:420:VAL:HA	3:D:428:LYS:HA	2.02	0.41
3:D:1432:LYS:HE3	3:D:1432:LYS:HB3	1.88	0.41
5:M:427:PRO:HA	5:M:486:ARG:CZ	2.51	0.41
1:A:71:VAL:HA	1:A:132:LEU:HA	2.03	0.41
2:C:504:GLU:N	2:C:507:ARG:O	2.53	0.41
2:C:666:LEU:HD12	2:C:666:LEU:HA	1.94	0.41
3:D:202:VAL:HB	3:D:396:VAL:HG23	2.02	0.41
3:D:562:ALA:HB3	3:D:567:ILE:HD11	2.03	0.41
3:D:947:ILE:HD13	3:D:947:ILE:HA	1.89	0.41
5:M:415:ALA:HB1	5:M:819:LEU:HD13	2.02	0.41
1:A:143:ARG:NE	1:A:145:ASP:OD2	2.54	0.41
1:A:216:GLU:OE1	1:A:219:ARG:NH1	2.54	0.41
1:B:48:ILE:O	1:B:172:SER:OG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:8:ARG:N	2:C:907:ASP:OD2	2.53	0.41
2:C:17:PRO:HB2	2:C:20:GLU:HB3	2.02	0.41
2:C:35:PRO:O	2:C:39:ARG:N	2.53	0.41
2:C:106:GLY:HA3	5:M:348:ARG:NH1	2.36	0.41
2:C:147:TYR:O	2:C:161:SER:N	2.46	0.41
2:C:196:LEU:HA	2:C:199:VAL:HB	2.02	0.41
2:C:905:ILE:HD12	2:C:905:ILE:HA	1.96	0.41
3:D:31:THR:OG1	3:D:32:ILE:N	2.53	0.41
3:D:137:PRO:HB3	3:D:147:VAL:HG23	2.02	0.41
3:D:700:VAL:HG22	3:D:718:PRO:HD3	2.01	0.41
3:D:983:LEU:HD12	3:D:987:GLU:HG3	2.02	0.41
3:D:993:LEU:HA	3:D:996:TRP:HD1	1.86	0.41
5:M:428:LEU:HD12	5:M:486:ARG:HG3	2.03	0.41
5:M:554:ARG:CG	5:M:558:GLU:CG	2.85	0.41
1:A:49:PRO:HB3	1:A:148:VAL:HG22	2.03	0.41
1:A:214:ALA:O	1:A:218:LEU:HG	2.21	0.41
2:C:24:GLU:OE1	2:C:27:ARG:NH2	2.54	0.41
2:C:129:ILE:N	2:C:132:ALA:O	2.37	0.41
2:C:211:LEU:HB3	2:C:218:VAL:HG21	2.03	0.41
2:C:327:HIS:CD2	2:C:433:THR:HG21	2.56	0.41
3:D:550:ARG:CZ	3:D:573:MET:HB3	2.51	0.41
3:D:708:LEU:HD21	3:D:1231:GLU:HB2	2.03	0.41
3:D:1068:LEU:HA	3:D:1068:LEU:HD12	1.86	0.41
5:M:364:PRO:HB2	5:M:367:GLN:HE22	1.85	0.41
2:C:285:LEU:HG	2:C:301:GLU:O	2.22	0.40
2:C:757:GLY:HA2	2:C:789:SER:HB2	2.02	0.40
3:D:658:LEU:HD13	3:D:673:ALA:HB3	2.02	0.40
5:M:765:ALA:O	5:M:769:ARG:HB2	2.21	0.40
1:A:108:GLU:HG3	1:A:110:LYS:NZ	2.36	0.40
1:B:220:GLU:OE2	1:B:224:TYR:OH	2.31	0.40
2:C:683:ASN:HD21	2:C:870:ILE:HG22	1.86	0.40
2:C:755:LEU:HD21	2:C:790:LEU:HG	2.04	0.40
2:C:890:LEU:HA	2:C:890:LEU:HD23	1.86	0.40
3:D:96:ALA:HB3	3:D:554:LEU:HD23	2.02	0.40
3:D:644:LEU:O	3:D:721:VAL:N	2.38	0.40
5:M:325:LEU:HD11	5:M:353:LEU:HD22	2.03	0.40
5:M:439:PHE:HB2	5:M:514:ARG:NH2	2.36	0.40
5:M:453:GLU:OE2	5:M:466:ARG:NH1	2.45	0.40
5:M:496:PHE:HA	5:M:569:ILE:HB	2.03	0.40
5:M:633:ALA:O	5:M:758:HIS:N	2.40	0.40
5:M:671:LEU:O	5:M:675:VAL:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LEU:N	1:B:119:ASP:O	2.38	0.40
2:C:263:ASP:O	2:C:267:TYR:N	2.53	0.40
2:C:749:VAL:HB	2:C:792:VAL:HG21	2.03	0.40
3:D:67:ARG:HH11	3:D:68:PHE:HD2	1.68	0.40
3:D:607:LEU:HA	3:D:607:LEU:HD13	1.91	0.40
3:D:1348:LEU:HD23	3:D:1348:LEU:HA	1.92	0.40
5:M:473:GLY:N	5:M:476:LYS:HD3	2.37	0.40
5:M:635:PHE:HA	5:M:757:PHE:HD2	1.87	0.40
1:A:14:ARG:O	1:A:22:GLU:N	2.47	0.40
1:A:153:ALA:HA	1:A:156:HIS:HE2	1.86	0.40
1:B:14:ARG:HB2	1:B:22:GLU:HB2	2.04	0.40
2:C:109:LYS:HZ1	5:M:359:GLY:HA2	1.86	0.40
2:C:122:THR:OG1	2:C:124:ASP:OD1	2.30	0.40
2:C:198:ARG:NH1	2:C:227:PHE:O	2.55	0.40
2:C:554:ASP:N	2:C:880:MET:O	2.53	0.40
2:C:571:LEU:HD23	2:C:571:LEU:HA	1.90	0.40
2:C:807:ARG:N	2:C:810:ASP:OD2	2.54	0.40
3:D:646:LYS:HG2	3:D:720:LEU:HD21	2.02	0.40
5:M:428:LEU:HD13	5:M:489:GLY:HA3	2.04	0.40
1:A:185:ARG:NH2	1:A:187:GLY:O	2.54	0.40
1:B:91:ASN:ND2	1:B:94:LEU:H	2.18	0.40
2:C:376:ARG:O	2:C:380:ALA:CB	2.69	0.40
2:C:835:VAL:HG22	2:C:849:VAL:HG22	2.04	0.40
2:C:1098:ASP:O	3:D:11:ALA:N	2.43	0.40
5:M:603:ARG:N	5:M:791:GLU:OE1	2.54	0.40
6:T:11:DC:H2'	6:T:12:DG:H8	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	224/315 (71%)	214 (96%)	10 (4%)	0	100	100
1	B	220/315 (70%)	202 (92%)	18 (8%)	0	100	100
2	C	1107/1119 (99%)	1041 (94%)	66 (6%)	0	100	100
3	D	1298/1524 (85%)	1221 (94%)	77 (6%)	0	100	100
4	E	92/99 (93%)	87 (95%)	5 (5%)	0	100	100
5	M	453/978 (46%)	399 (88%)	53 (12%)	1 (0%)	47	81
All	All	3394/4350 (78%)	3164 (93%)	229 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	M	663	SER

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	199/273 (73%)	197 (99%)	2 (1%)	76	86
1	B	195/273 (71%)	193 (99%)	2 (1%)	76	86
2	C	936/941 (100%)	928 (99%)	8 (1%)	78	88
3	D	1102/1279 (86%)	1091 (99%)	11 (1%)	76	86
4	E	83/88 (94%)	82 (99%)	1 (1%)	71	84
5	M	383/805 (48%)	380 (99%)	3 (1%)	81	89
All	All	2898/3659 (79%)	2871 (99%)	27 (1%)	79	88

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	87	VAL
1	B	14	ARG
1	B	219	ARG

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Mol	Chain	Res	Type
2	C	8	ARG
2	C	493	ARG
2	C	550	LEU
2	C	610	ARG
2	C	640	ARG
2	C	648	ARG
2	C	807	ARG
2	C	879	ARG
3	D	159	ARG
3	D	409	VAL
3	D	419	ASP
3	D	450	TYR
3	D	486	ARG
3	D	601	ARG
3	D	784	ASP
3	D	875	THR
3	D	1207	TYR
3	D	1447	LEU
3	D	1492	LEU
4	E	85	LEU
5	M	409	ARG
5	M	521	ARG
5	M	793	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	GLN
1	A	188	GLN
1	B	38	ASN
1	B	91	ASN
2	C	45	GLN
2	C	204	GLN
2	C	327	HIS
2	C	330	ASN
2	C	343	GLN
2	C	498	GLN
2	C	663	ASN
2	C	704	HIS
2	C	829	GLN
2	C	881	ASN
2	C	1030	GLN

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Mol	Chain	Res	Type
2	C	1100	GLN
2	C	1107	ASN
3	D	442	ASN
3	D	529	GLN
3	D	575	GLN
3	D	714	GLN
3	D	768	ASN
3	D	861	GLN
3	D	962	GLN
3	D	1010	ASN
3	D	1014	ASN
3	D	1184	GLN
3	D	1442	ASN
3	D	1465	ASN
4	E	86	GLN
5	M	367	GLN
5	M	462	HIS
5	M	490	HIS
5	M	553	HIS
5	M	658	HIS
5	M	684	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

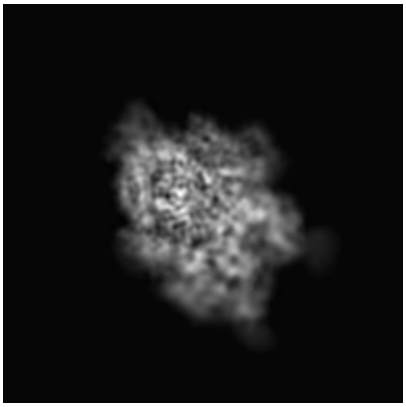
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30117. These allow visual inspection of the internal detail of the map and identification of artifacts.

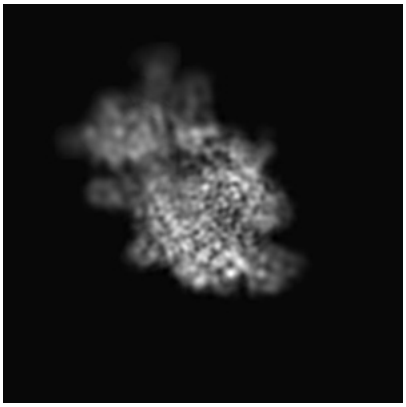
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

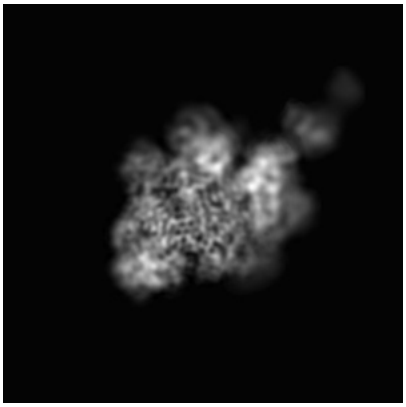
6.1.1 Primary map



X



Y

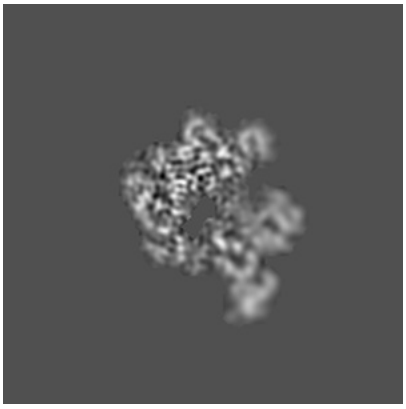


Z

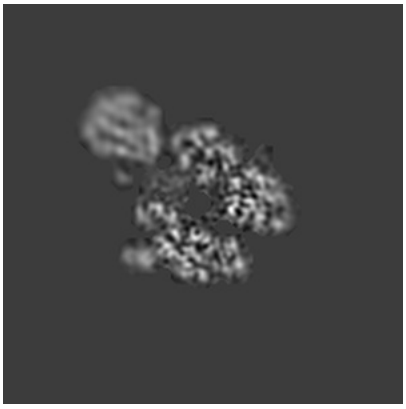
The images above show the map projected in three orthogonal directions.

6.2 Central slices

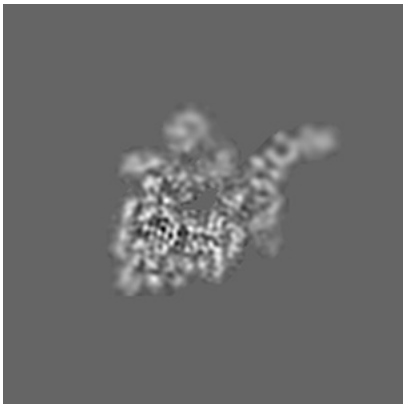
6.2.1 Primary map



X Index: 100



Y Index: 100

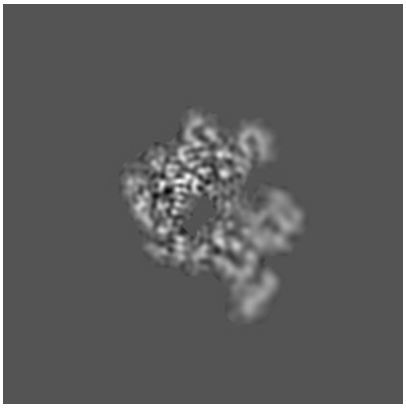


Z Index: 100

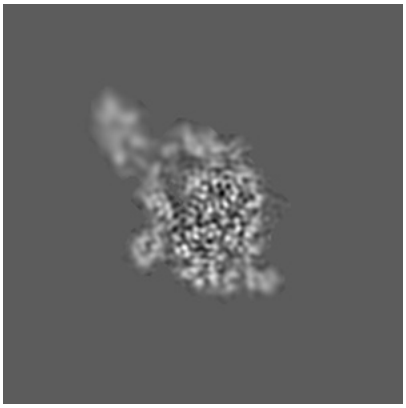
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

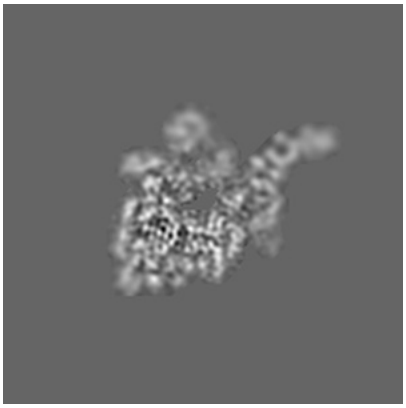
6.3.1 Primary map



X Index: 99



Y Index: 89

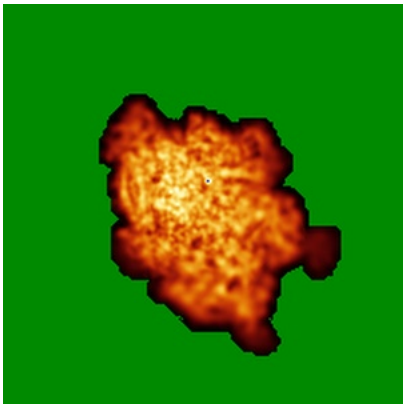


Z Index: 100

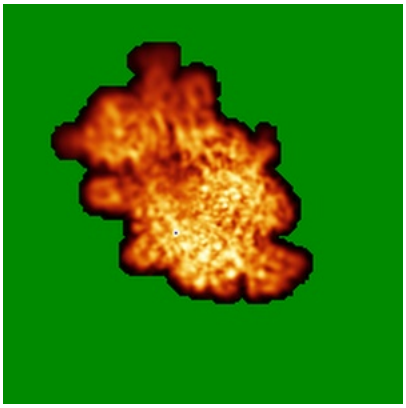
The images above show the largest variance slices of the map in three orthogonal directions.

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

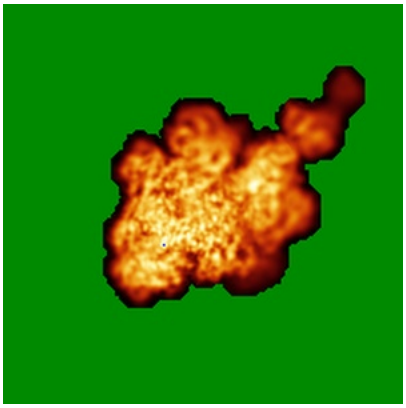
6.4.1 Primary map



X



Y

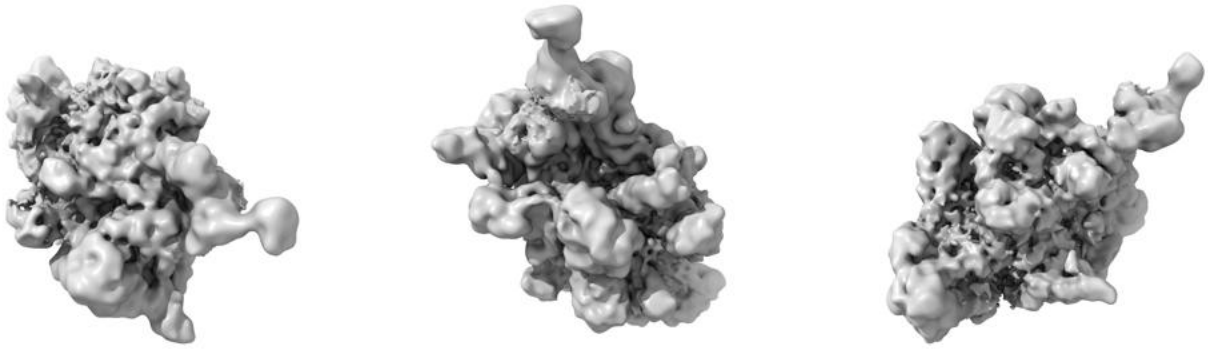


Z

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

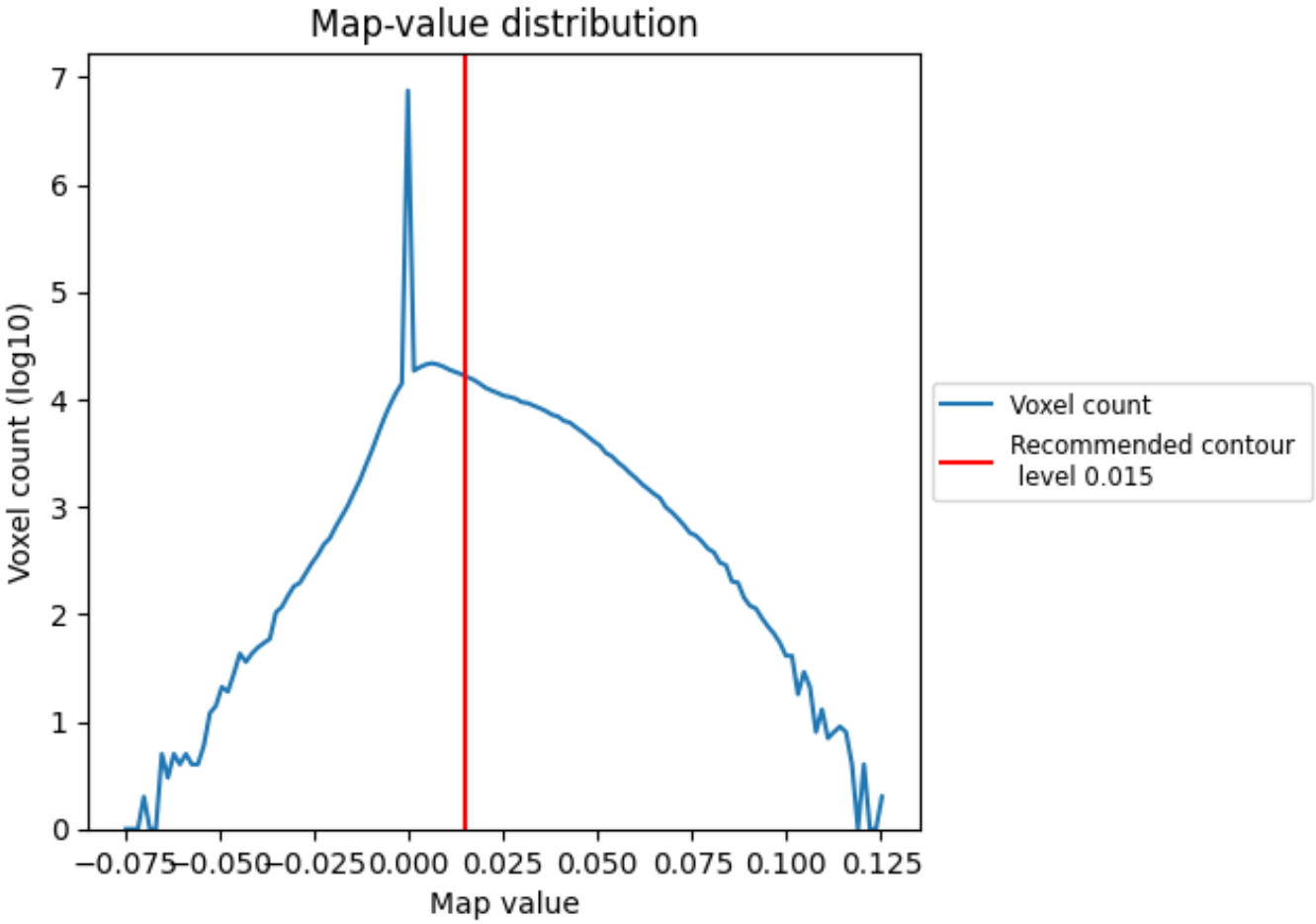
6.6 Mask visualisation (i)

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

7 Map analysis

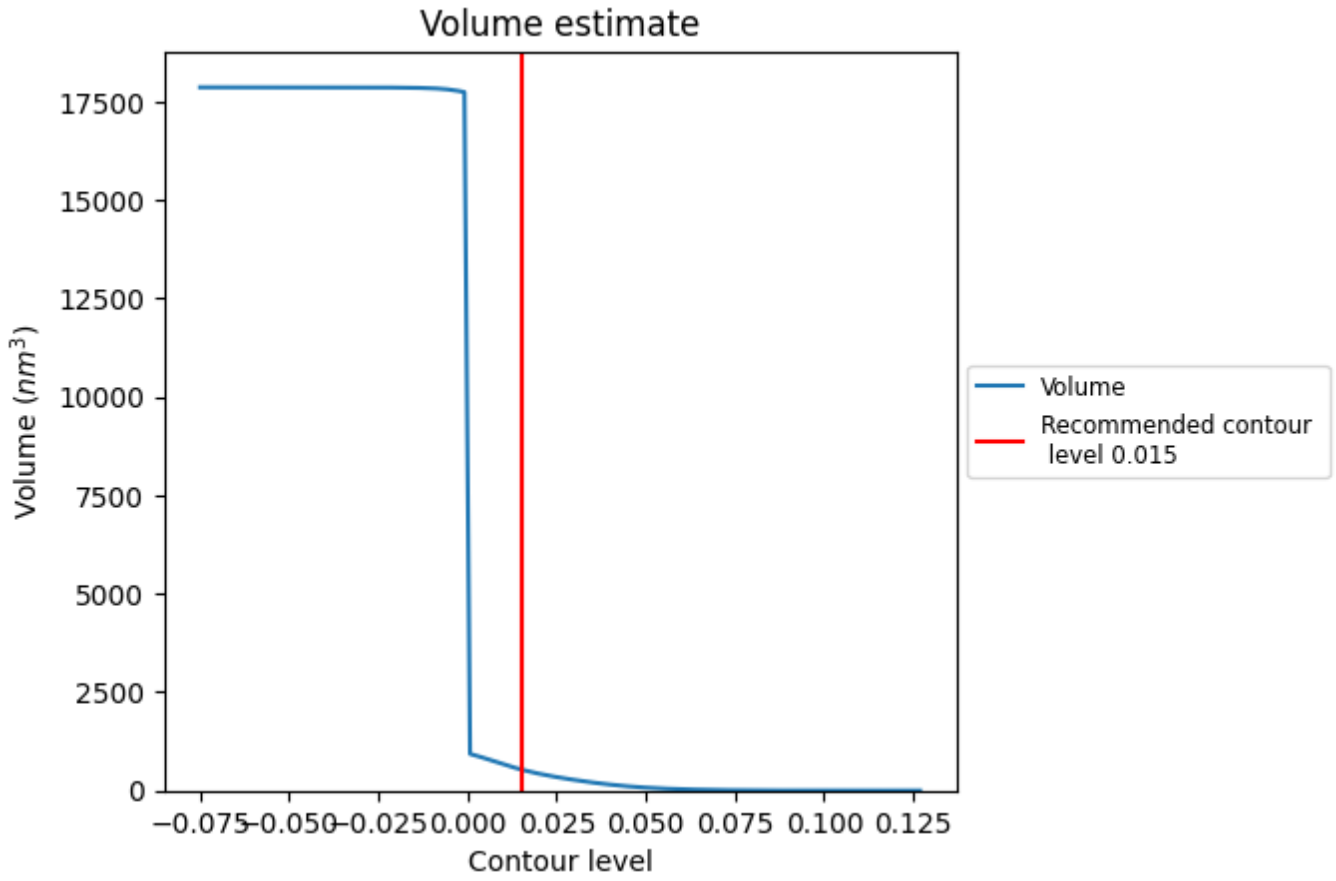
This section contains the results of statistical analysis of the map.

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.

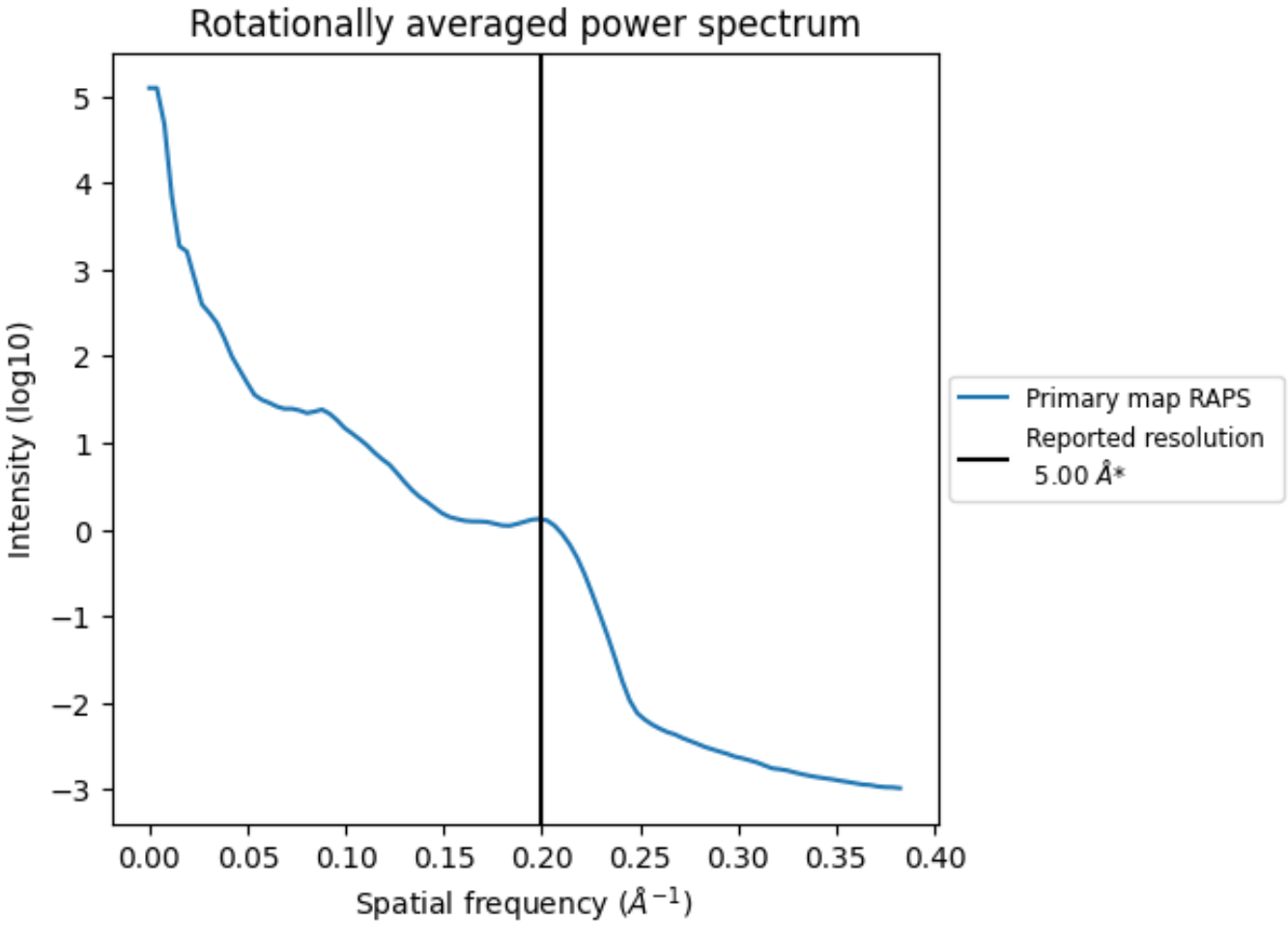
7.2 Volume estimate



The volume at the recommended contour level is 537 nm^3; this corresponds to an approximate mass of 486 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 0.200 Å^{-1}

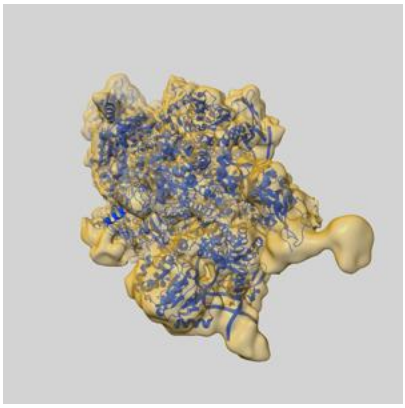
8 Fourier-Shell correlation

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

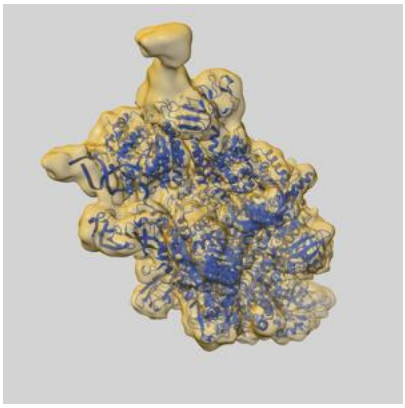
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30117 and PDB model 6M6A. Per-residue inclusion information can be found in section 3 on page 5.

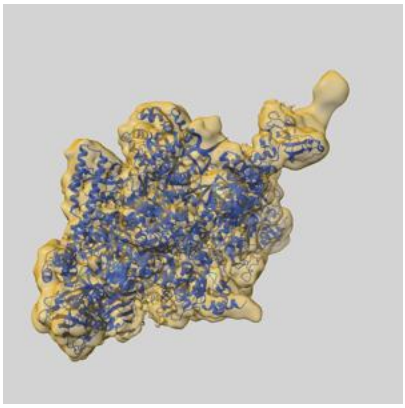
9.1 Map-model overlay



X



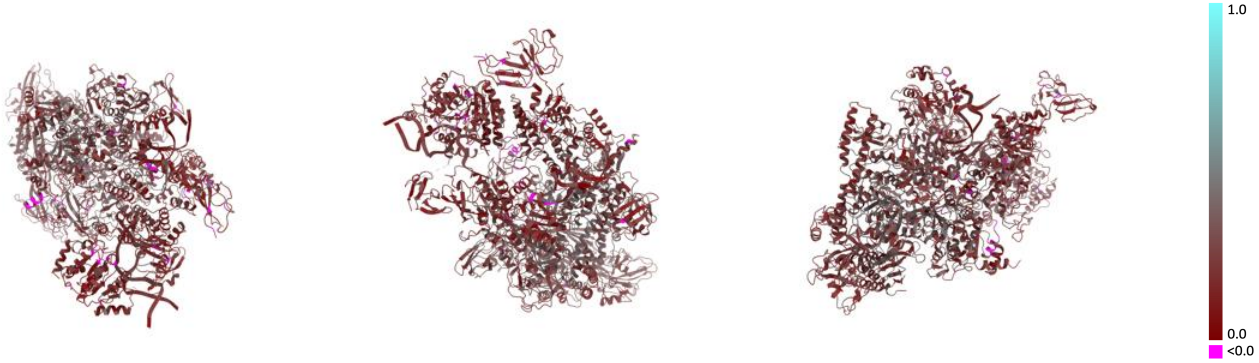
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

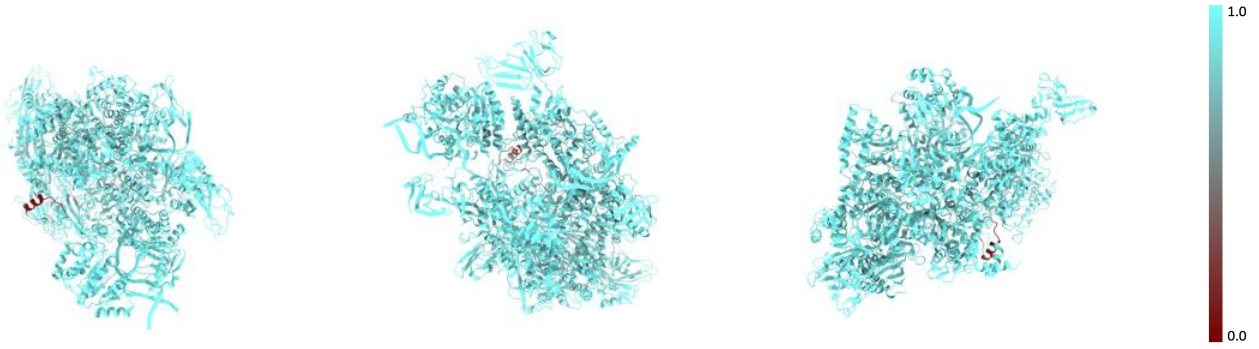
9.2 Q-score mapped to coordinate model (i)



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.

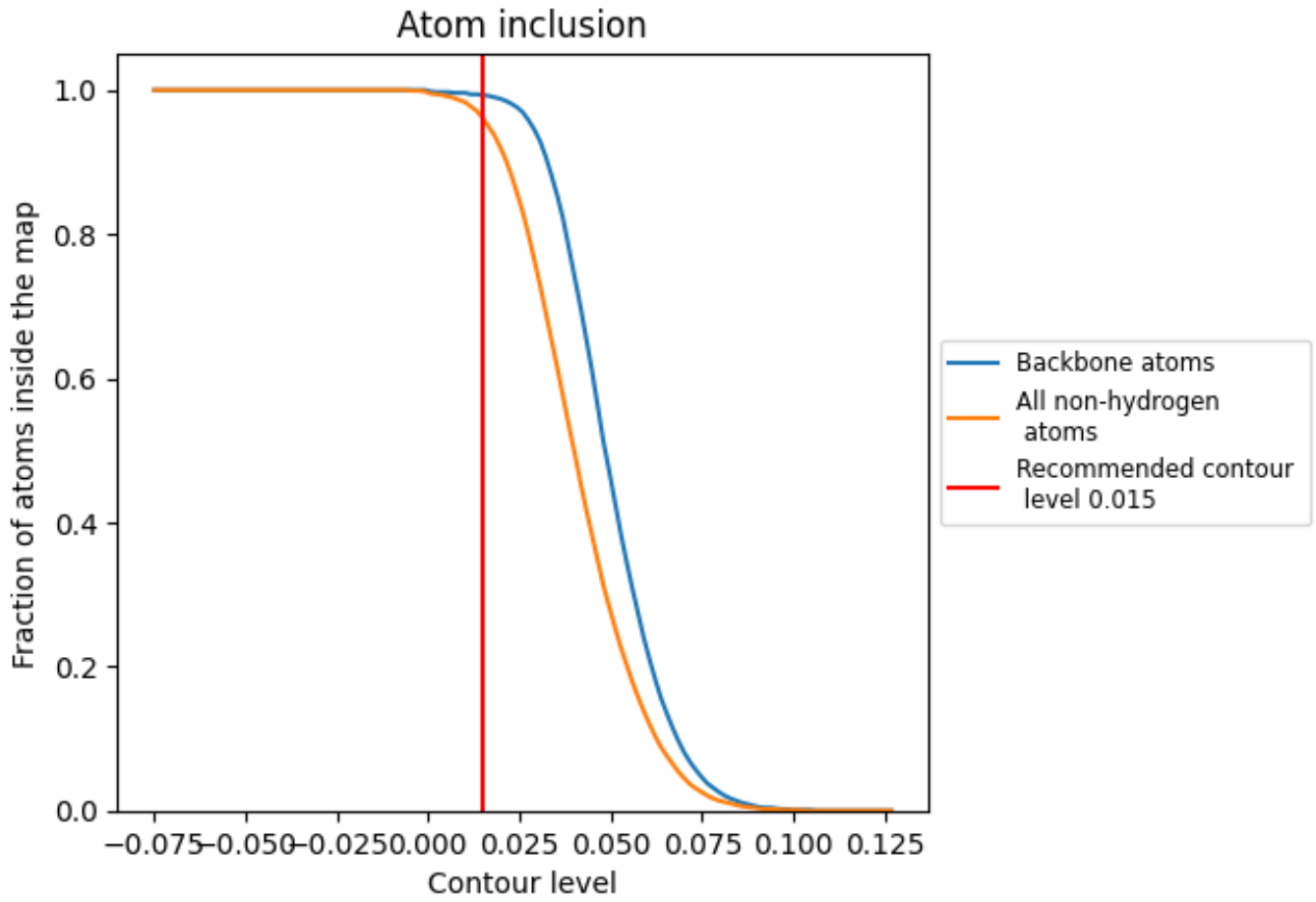
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.2560
A	0.9740	0.2790
B	0.9730	0.2600
C	0.9470	0.2700
D	0.9620	0.2660
E	0.9810	0.2910
M	0.9700	0.1860
N	0.9900	0.2090
T	0.9840	0.2100