Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 03:20 pm GMT

PDB ID	:	6YUF
EMDB ID	:	EMD-10930
Title	:	Cohesin complex with loader gripping DNA
Authors	:	Higashi, T.L.; Eickhoff, P.; Sousa, J.S.; Costa, A.; Uhlmann, F.
Deposited on	:	2020-04-27
Resolution	:	3.94 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:

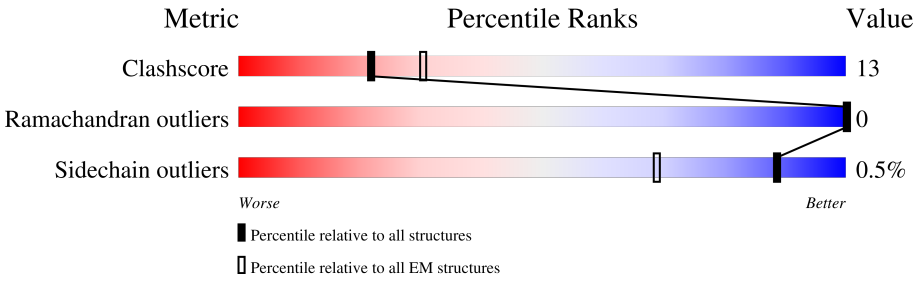
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.94 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	B	628	17% 6% 76%
2	D	1587	7% 54% 25% 20%
3	A	1228	23% 7% 69%
4	C	1194	27% 10% 62%
5	X	32	75% 22%
6	Y	32	84% 12%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19528 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 Cohesin subunit rad21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	152	1195	758	206	225	6	0	0

- Molecule 2 is a protein called Sister chromatid cohesion protein mis4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	1272	10247	6604	1687	1910	46	0	0

- Molecule 3 is a protein called Structural maintenance of chromosomes protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	384	3047	1932	521	587	7	0	0

- Molecule 4 is a protein called Structural maintenance of chromosomes protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	456	3665	2294	644	714	13	0	0

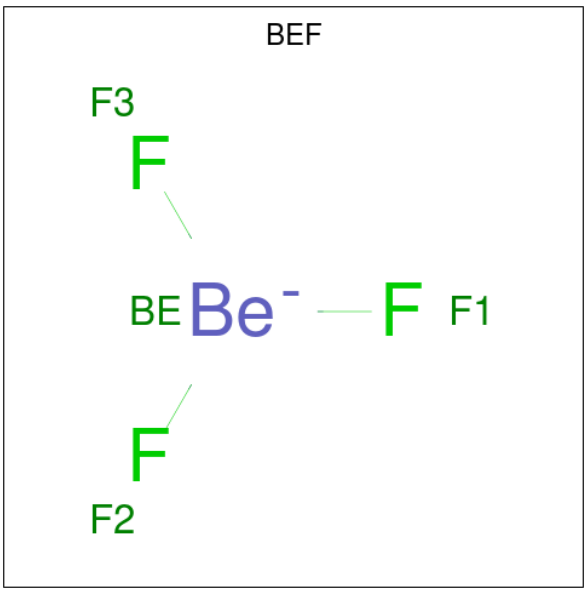
- Molecule 5 is a DNA chain called DNA (32-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	X	32	658	312	129	185	32	0	0

- Molecule 6 is a DNA chain called DNA (32-MER).

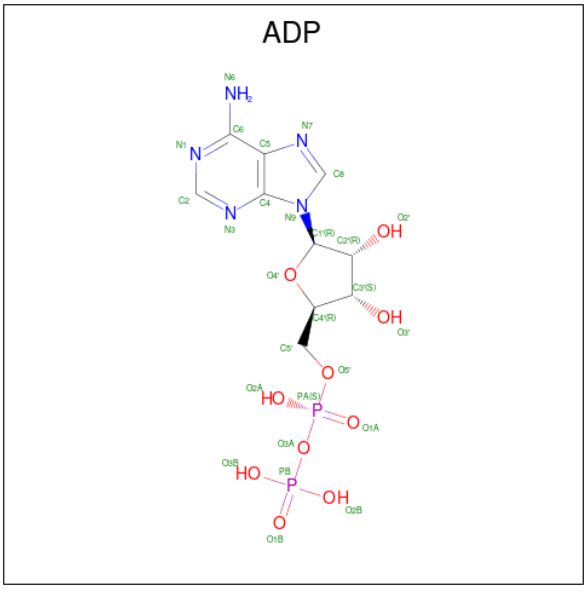
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	Y	32	654	313	110	199	32	0	0

- Molecule 7 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
7	A	1	Total	Be	F	0
			4	1	3	
7	C	1	Total	Be	F	0
			4	1	3	

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



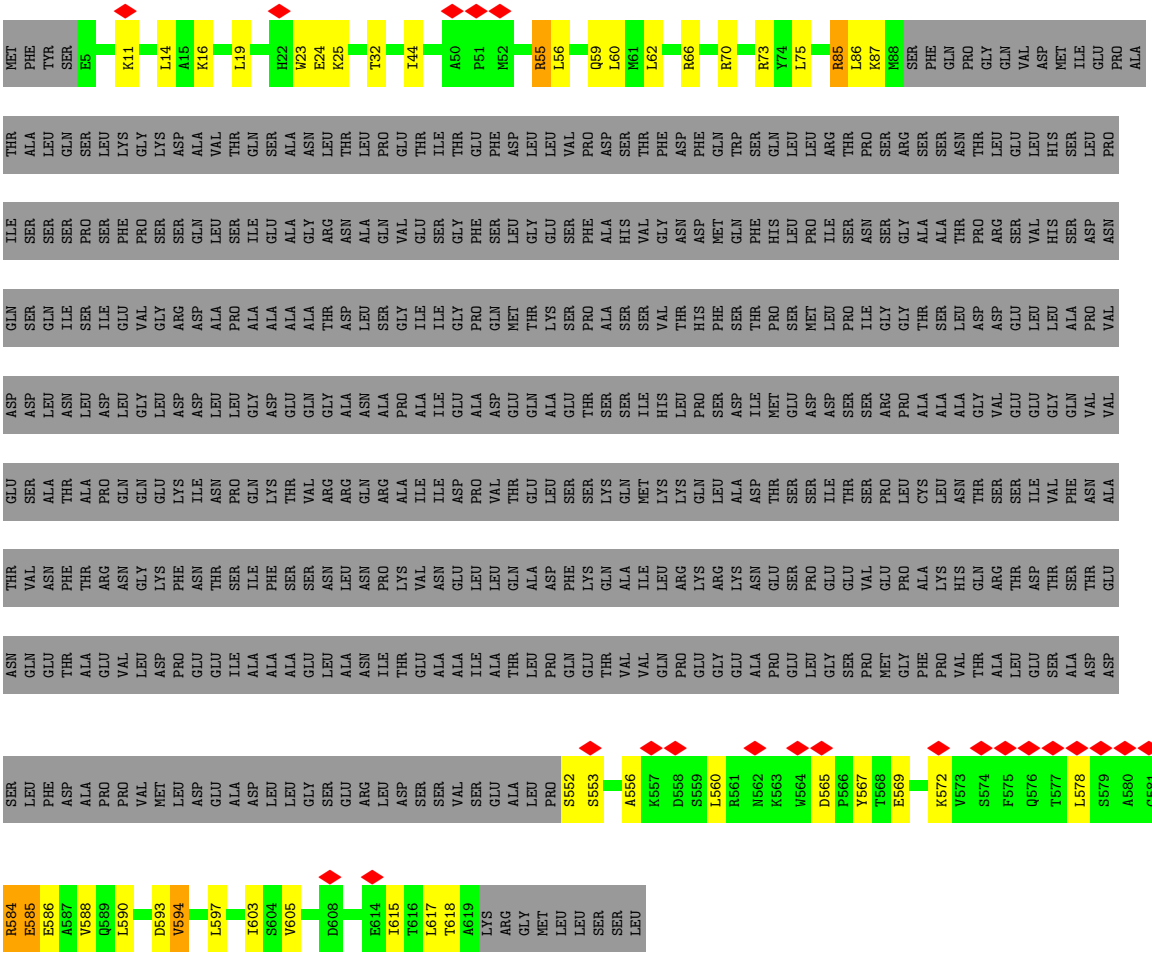
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	C	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

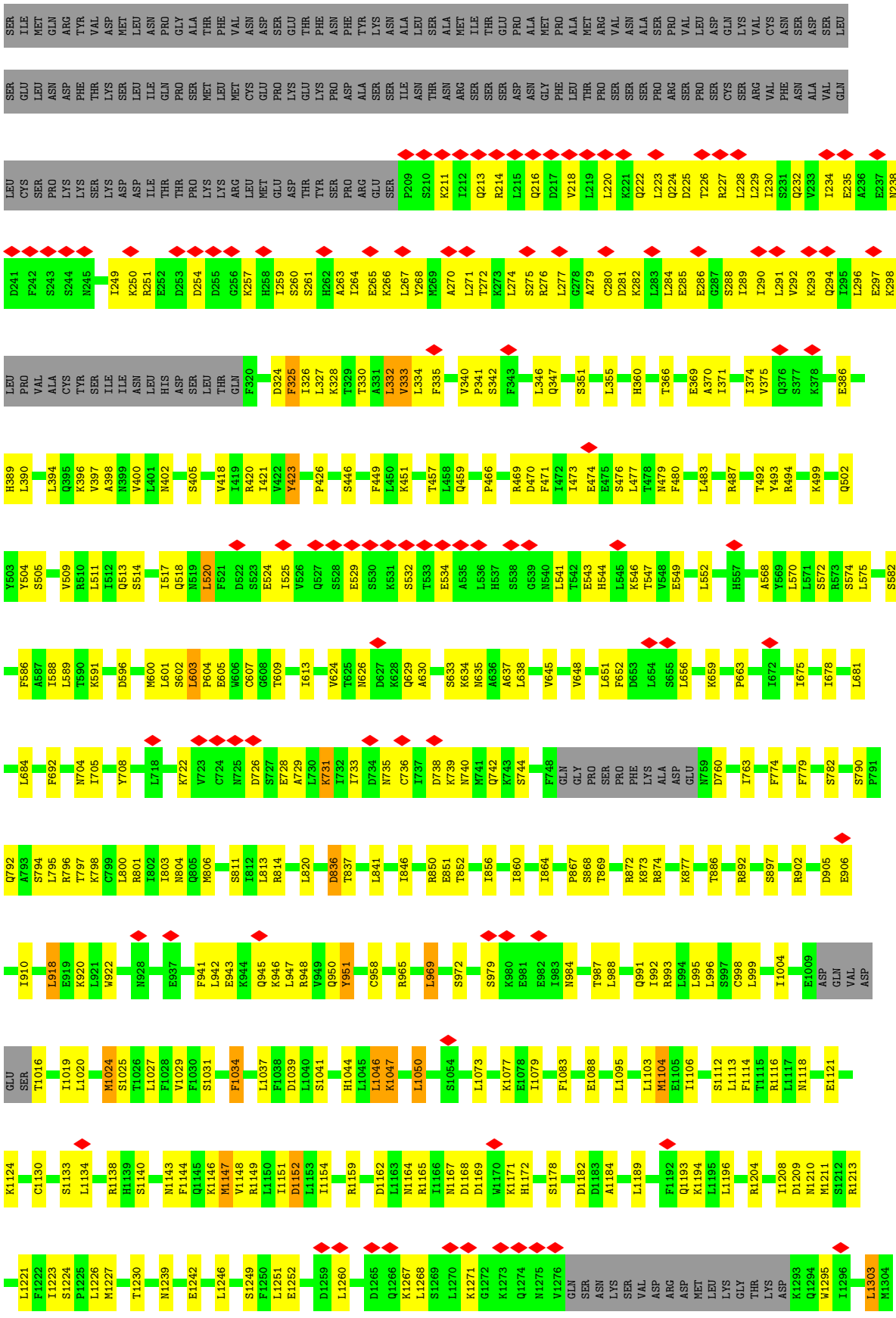
• Molecule 1: Cohesin subunit rad21

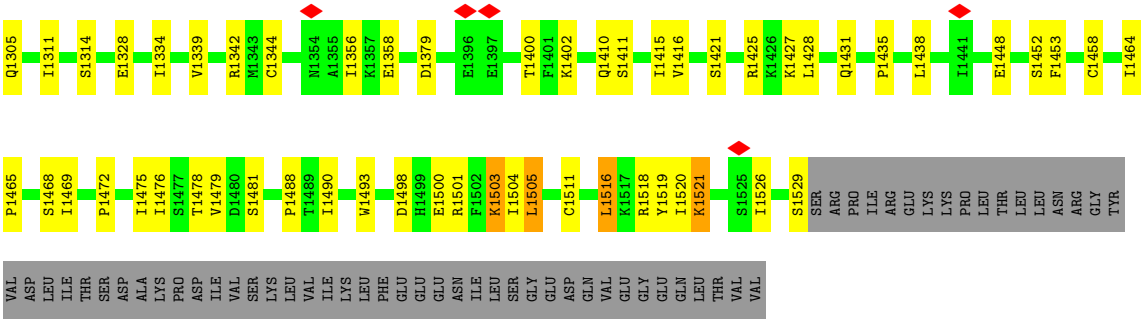
Chain B:



• Molecule 2: Sister chromatid cohesion protein mis4

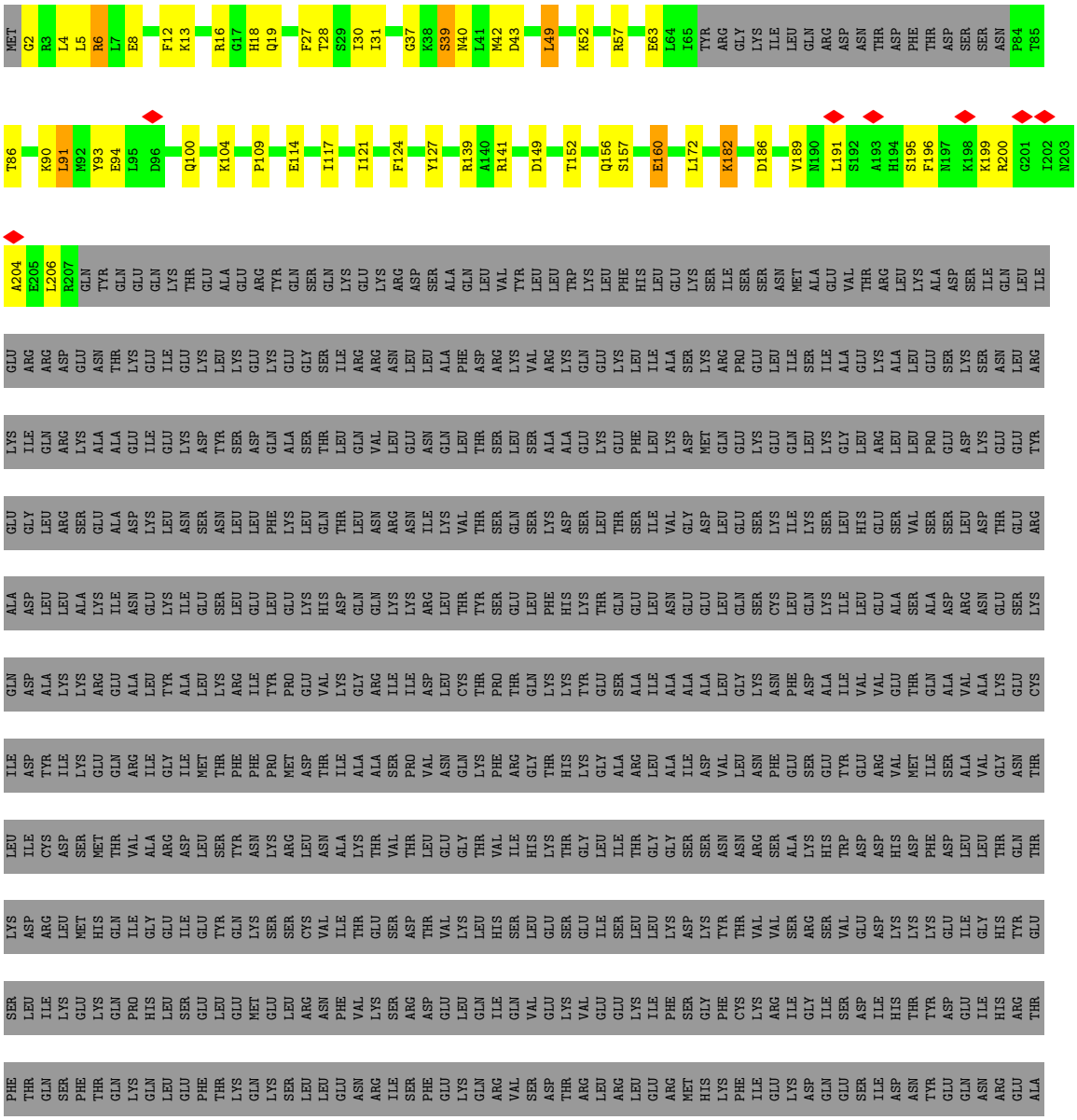
Chain D:

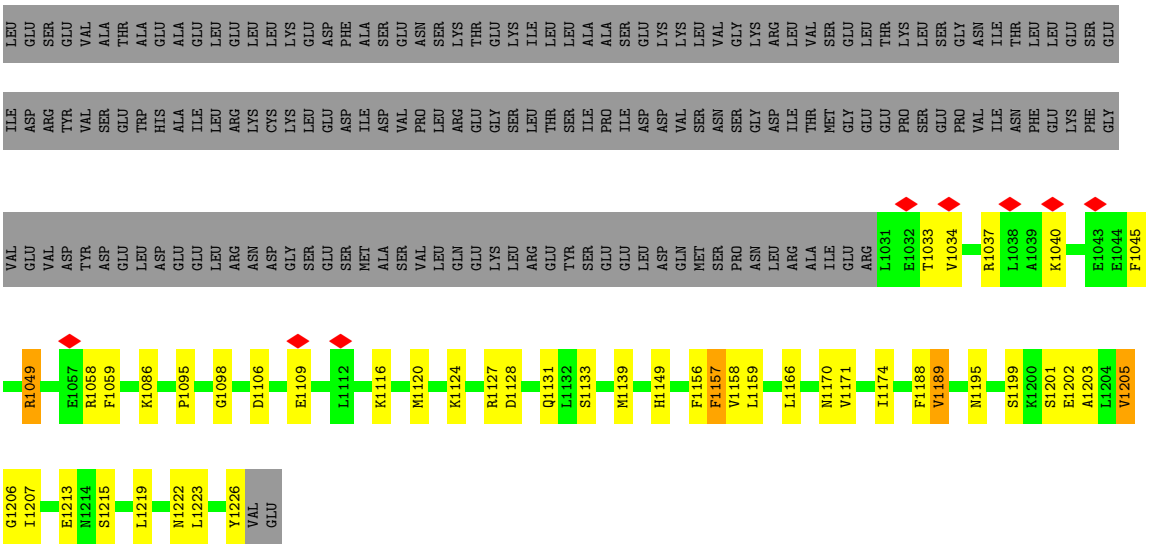

SER ILE MET GLN ARG TYR VAL ASP MET LEU ASN PRO GLY ALA THR PHE VAL ASN ASP SER GLU THR PHE ASN PHE TYR LYS ASN ALA LEU SER ALA MET ILE THR GLU PRO ALA MET PRO ALA MET ARG VAL ASN ALA SER PRO VAL LEU ASP GLN LYS VAL CYS ASN SER ASP SER LEU
SER GLU LEU ASN ASP PHE THR LYS SER LEU ILE GLN PRO SER MET LEU MET CYS GLU PRO LYS GLU LYS PRO ASP SER SER ILE ASN THR ASN ARG SER SER SER ASP ASN GLY PHE LEU THR PRO SER SER SER PRO PRO ARG SER PRO SER CYS SER ARG VAL PHE ASN ALA VAL GLN
LEU CYS SER PRO LYS LYS SER LYS ASP ASP ILE THR THR PRO LYS LYS ARG LEU MET GLU ASP THR TYR SER PRO ARG GLU SER P209 S210 K211 T212 Q213 R214 L215 Q216 D217 V218 L219 L220 K221 Q222 L223 Q224 D225 T226 R227 L228 L229 I230 S231 Q232 Y233 I234 E235 A236 E237 N238 S239 E240
D241 P242 S243 S244 N245 I249 K250 R251 E252 D253 D254 D255 G256 K257 H258 I259 S260 S261 H262 A263 I264 E265 K266 L267 Y268 M269 A270 L271 T272 K273 L274 S275 R276 L277 G278 A279 C280 D281 K282 L283 L284 E285 E286 G287 S288 I289 I290 L291 V292 K293 Q294 I295 L296 E297 K298 E299 L300 K301 E302
LEU PRO VAL ALA CYS TYR SER ILE ILE ASN LEU HIS ASP SER LEU THR GLN F320 D324 F325 I326 L327 K328 T329 T330 A331 L332 V333 L334 F335 V340 P341 S342 F343 L346 Q347 S351 L355 H360 T366 E369 A370 I371 I374 V375 Q376 S377 K378 E386
H389 L390 L394 Q395 K396 V397 A398 N399 V400 L401 N402 S405 V418 I419 R420 I421 V422 Y423 P426 S446 F449 L450 K451 T457 L458 Q459 P466 R469 D470 F471 I472 I473 E474 E475 S476 L477 T478 N479 F480 L483 R487 T492 Y493 R494 K499 Q502
Y503 Y504 S505 V509 R510 L511 I512 Q513 S514 I517 Q518 N519 L520 F521 D522 S523 E524 I525 V526 Q527 S528 E529 S530 K531 S532 T533 E534 A535 L536 H537 S538 G539 N540 L541 T542 E543 H544 L545 K546 T547 V548 E549 L552 H557 A568 Y569 L570 L571 S572 R573 S574 L575 S582 D583
F586 A587 I588 L589 T590 K591 D596 M600 L601 S602 L603 P604 E605 W606 C607 G608 T609 I613 V624 T625 N626 D627 K628 Q629 A630 S633 K634 M635 A636 A637 L638 V645 V648 L651 F652 D653 L654 S655 L656 K659 P663 I672 I675 I678 L681
L684 F692 N704 I705 Y708 L718 K722 V723 C724 N725 D726 S727 E728 A729 L730 K731 I732 I733 D734 N735 C736 I737 D738 K739 N740 M741 Q742 K743 S744 F748 GLN GLY PRO SER PRO PHE LYS ALA ASP GLU N759 D760 I763 F774 F779 S782 S790 P791
Q792 A793 S794 L795 R796 T797 K798 C799 L800 R801 I802 I803 N804 Q805 M806 S811 I812 L813 R814 L820 D836 T837 L841 I846 R850 E851 T852 I856 I860 I864 P867 S868 T869 R872 K873 R874 K877 T886 R892 S897 R902 D905 E906
I910 L918 E919 K920 L921 W922 N928 E937 F941 L942 E943 K944 Q945 K946 L947 R948 V949 Q950 Y951 C958 R965 L969 S972 S979 K980 E981 E982 I983 N984 T987 L988 Q991 I992 R993 L994 L995 L996 S997 C998 L999 I1004 E1009 ASP GLN VAL ASP
GLU SER T1016 I1019 L1020 M1024 S1025 T1026 L1027 F1028 V1029 F1030 S1031 F1034 L1037 F1038 D1039 L1040 S1041 H1044 L1045 L1046 K1047 L1050 S1054 L1073 K1077 E1078 I1079 F1083 E1088 L1095 L1103 M1104 E1105 I1106 S1112 L1113 F1114 T1115 R1116 L1117 N1118 E1121
K1124 C1130 S1133 L1134 R1138 H1139 S1140 N1143 F1144 Q1145 K1146 M1147 V1148 R1149 L1150 I1151 D1152 L1153 I1154 R1159 D1162 L1163 N1164 R1165 I1166 N1167 D1168 D1169 W1170 K1171 H1172 S1178 D1182 D1183 A1184 L1189 F1192 Q1193 K1194 L1195 L1196 R1204 I1208 D1209 N1210 M1211 S1212 R1213
L1221 F1222 I1223 S1224 P1225 L1226 M1227 T1230 N1239 E1242 L1246 S1249 F1250 L1251 E1252 D1259 L1260 D1265 Q1266 K1267 L1268 S1269 L1270 K1271 G1272 K1273 Q1274 N1275 V1276 GLN SER ASN LYS SER VAL ASP ARG ASP MET LEU LYS GLY THR LYS ASP K1293 Q1294 W1295 I1296 L1303 M1304



• Molecule 3: Structural maintenance of chromosomes protein 1

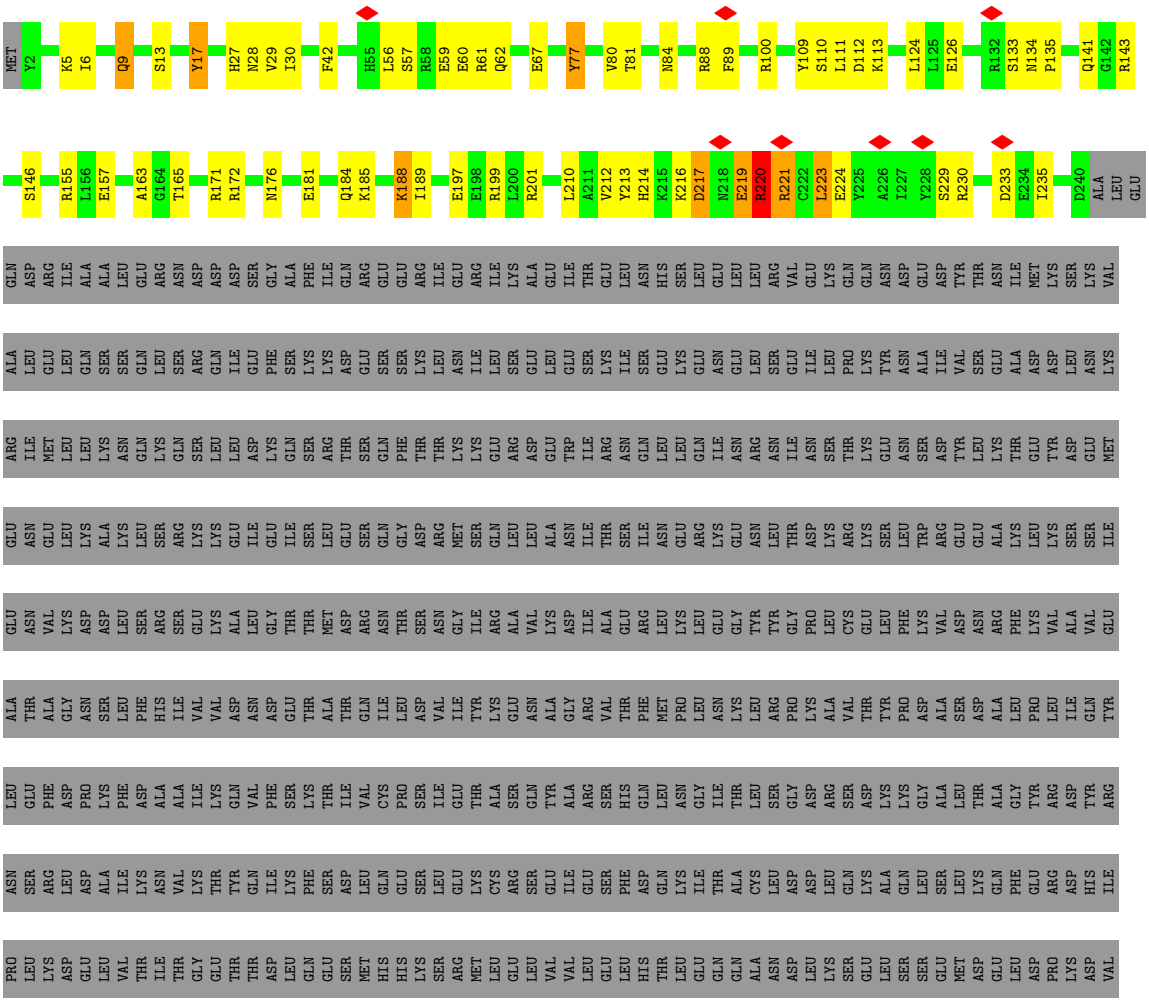
Chain A:

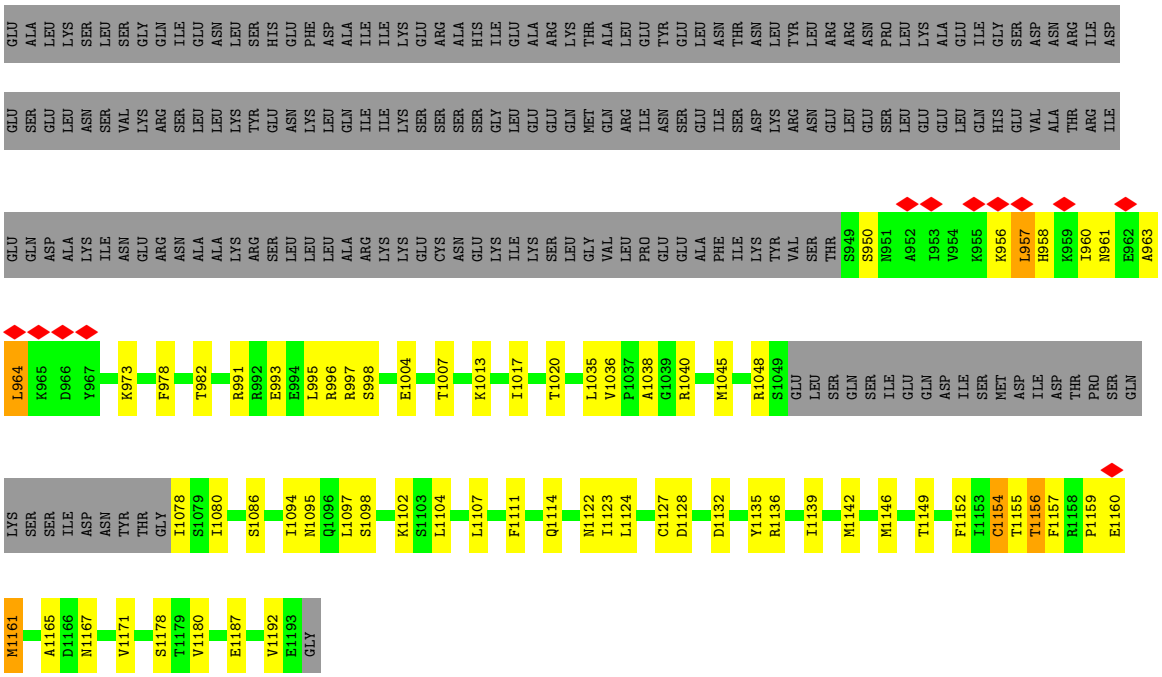




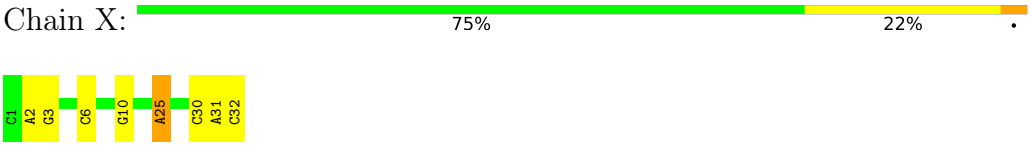
• Molecule 4: Structural maintenance of chromosomes protein 3

Chain C:

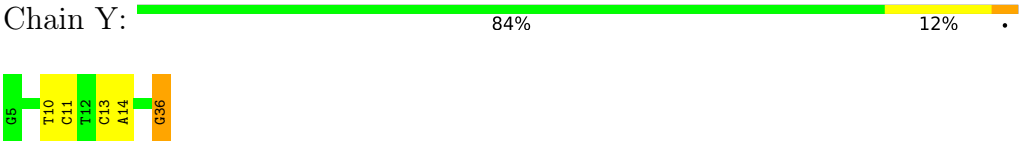




• Molecule 5: DNA (32-MER)



• Molecule 6: DNA (32-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	255148	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 ($e^-/Å^2$)	33.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.069	Depositor
Minimum map value	-1.652	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	392.40002, 392.40002, 392.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	B	0.70	3/1211 (0.2%)	1.06	6/1634 (0.4%)
2	D	0.67	26/10425 (0.2%)	0.87	40/14086 (0.3%)
3	A	0.76	8/3100 (0.3%)	0.91	14/4170 (0.3%)
4	C	1.02	24/3717 (0.6%)	1.22	37/4996 (0.7%)
5	X	0.88	0/740	0.99	1/1139 (0.1%)
6	Y	0.87	0/730	1.15	1/1125 (0.1%)
All	All	0.78	61/19923 (0.3%)	0.98	99/27150 (0.4%)

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	B	0	1
2	D	0	3
4	C	0	2
All	All	0	6

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	9	GLN	CD-NE2	-20.98	0.80	1.32
4	C	9	GLN	CB-CG	-15.87	1.09	1.52
4	C	17	TYR	CE1-CZ	-14.38	1.19	1.38
2	D	325	PHE	CD2-CE2	-13.93	1.11	1.39
4	C	17	TYR	CG-CD1	13.48	1.56	1.39
4	C	17	TYR	CB-CG	13.21	1.71	1.51
3	A	160	GLU	CD-OE2	-12.61	1.11	1.25
4	C	9	GLN	CG-CD	-11.49	1.24	1.51
3	A	152	THR	CB-CG2	-11.30	1.15	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1029	VAL	CB-CG1	-11.17	1.29	1.52
4	C	77	TYR	CD1-CE1	-10.44	1.23	1.39
3	A	160	GLU	CB-CG	-9.55	1.34	1.52
2	D	325	PHE	CB-CG	-9.47	1.35	1.51
2	D	423	TYR	CD1-CE1	-9.07	1.25	1.39
4	C	220	ARG	CG-CD	8.62	1.73	1.51
4	C	220	ARG	CD-NE	-8.60	1.31	1.46
2	D	951	TYR	CD1-CE1	-8.57	1.26	1.39
2	D	998	CYS	CB-SG	-8.46	1.67	1.82
4	C	17	TYR	CD2-CE2	-8.07	1.27	1.39
4	C	1152	PHE	CB-CG	-8.03	1.37	1.51
4	C	1152	PHE	CE1-CZ	-7.43	1.23	1.37
4	C	219	GLU	CG-CD	-7.33	1.41	1.51
2	D	1520	ILE	CG1-CD1	-7.27	1.00	1.50
4	C	1152	PHE	CE2-CZ	-7.13	1.23	1.37
3	A	1205	VAL	CB-CG2	-7.10	1.38	1.52
4	C	1152	PHE	CG-CD2	-7.00	1.28	1.38
2	D	332	LEU	CG-CD2	-6.84	1.26	1.51
2	D	1511	CYS	CB-SG	-6.83	1.70	1.82
3	A	182	LYS	CE-NZ	-6.80	1.32	1.49
4	C	1154	CYS	CB-SG	-6.67	1.71	1.82
2	D	325	PHE	CD1-CE1	-6.55	1.26	1.39
4	C	17	TYR	CE2-CZ	6.44	1.47	1.38
2	D	1140	SER	CB-OG	-6.34	1.34	1.42
4	C	217	ASP	CB-CG	6.34	1.65	1.51
2	D	1050	LEU	CG-CD1	-6.11	1.29	1.51
3	A	1157	PHE	CE1-CZ	-6.09	1.25	1.37
2	D	852	THR	CB-CG2	-6.05	1.32	1.52
2	D	1088	GLU	CD-OE1	-5.92	1.19	1.25
2	D	602	SER	C-N	-5.91	1.20	1.34
2	D	969	LEU	CG-CD2	-5.89	1.30	1.51
4	C	964	LEU	CG-CD1	5.88	1.73	1.51
4	C	1152	PHE	CD2-CE2	-5.83	1.27	1.39
2	D	1503	LYS	CG-CD	-5.82	1.32	1.52
1	B	594	VAL	CB-CG1	-5.80	1.40	1.52
2	D	333	VAL	CB-CG1	-5.79	1.40	1.52
2	D	1034	PHE	CB-CG	-5.70	1.41	1.51
2	D	1503	LYS	CE-NZ	-5.68	1.34	1.49
2	D	1211	MET	CB-CG	-5.65	1.33	1.51
4	C	17	TYR	CZ-OH	-5.57	1.28	1.37
4	C	126	GLU	CG-CD	5.51	1.60	1.51
1	B	55	ARG	CG-CD	-5.45	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1034	PHE	CD1-CE1	-5.45	1.28	1.39
2	D	951	TYR	CG-CD1	-5.43	1.32	1.39
2	D	731	LYS	CD-CE	-5.40	1.37	1.51
3	A	1059	PHE	CB-CG	-5.40	1.42	1.51
2	D	860	ILE	CG1-CD1	-5.38	1.13	1.50
2	D	624	VAL	CB-CG1	-5.21	1.42	1.52
1	B	597	LEU	CG-CD1	-5.18	1.32	1.51
4	C	219	GLU	CD-OE1	-5.15	1.20	1.25
4	C	9	GLN	CD-OE1	-5.12	1.12	1.24
3	A	1157	PHE	CE2-CZ	-5.02	1.27	1.37

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	220	ARG	NE-CZ-NH1	-28.91	105.84	120.30
4	C	220	ARG	NE-CZ-NH2	27.54	134.07	120.30
2	D	1211	MET	CG-SD-CE	-19.59	68.85	100.20
2	D	332	LEU	CB-CG-CD1	-16.68	82.64	111.00
1	B	617	LEU	CA-CB-CG	15.22	150.31	115.30
3	A	149	ASP	CB-CG-OD2	15.13	131.92	118.30
4	C	17	TYR	CD1-CE1-CZ	-15.04	106.26	119.80
4	C	17	TYR	CB-CG-CD1	14.99	130.00	121.00
3	A	1120	MET	CG-SD-CE	-13.89	77.98	100.20
2	D	1189	LEU	CB-CG-CD2	13.85	134.54	111.00
2	D	1503	LYS	CD-CE-NZ	-13.31	81.09	111.70
4	C	964	LEU	CB-CG-CD1	12.61	132.44	111.00
4	C	957	LEU	CB-CG-CD2	-12.28	90.13	111.00
4	C	957	LEU	CB-CG-CD1	-12.23	90.21	111.00
4	C	17	TYR	CG-CD1-CE1	11.85	130.78	121.30
2	D	1227	MET	CG-SD-CE	-11.80	81.33	100.20
3	A	149	ASP	OD1-CG-OD2	-11.14	102.13	123.30
4	C	964	LEU	CB-CG-CD2	-10.82	92.60	111.00
4	C	9	GLN	CG-CD-OE1	10.57	142.74	121.60
3	A	1205	VAL	CG1-CB-CG2	-10.52	94.08	110.90
1	B	85	ARG	NE-CZ-NH2	9.94	125.27	120.30
4	C	217	ASP	CB-CG-OD1	9.53	126.87	118.30
4	C	9	GLN	CG-CD-NE2	-9.48	93.95	116.70
4	C	1142	MET	CG-SD-CE	-9.30	85.33	100.20
2	D	918	LEU	CB-CG-CD1	-8.92	95.84	111.00
2	D	999	LEU	CB-CG-CD2	8.78	125.93	111.00
4	C	17	TYR	N-CA-CB	8.77	126.39	110.60
3	A	149	ASP	CB-CG-OD1	8.48	125.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1024	MET	CG-SD-CE	-8.25	87.00	100.20
2	D	332	LEU	CB-CG-CD2	-8.24	97.00	111.00
3	A	49	LEU	CB-CG-CD1	-8.24	97.00	111.00
4	C	1154	CYS	CA-CB-SG	-8.18	99.28	114.00
2	D	1303	LEU	CA-CB-CG	-8.17	96.50	115.30
4	C	17	TYR	CD1-CG-CD2	-8.11	108.97	117.90
4	C	188	LYS	CD-CE-NZ	-7.92	93.49	111.70
4	C	126	GLU	OE1-CD-OE2	-7.86	113.86	123.30
2	D	1516	LEU	CD1-CG-CD2	-7.73	87.31	110.50
3	A	1139	MET	CG-SD-CE	-7.64	87.97	100.20
2	D	520	LEU	CA-CB-CG	7.59	132.76	115.30
1	B	85	ARG	NE-CZ-NH1	-7.58	116.51	120.30
2	D	1046	LEU	CB-CG-CD1	7.55	123.84	111.00
2	D	1088	GLU	OE1-CD-OE2	-7.54	114.25	123.30
2	D	1520	ILE	CG1-CB-CG2	-7.54	94.82	111.40
4	C	17	TYR	CE1-CZ-OH	-7.53	99.77	120.10
2	D	836	ASP	CB-CG-OD1	7.52	125.07	118.30
4	C	217	ASP	OD1-CG-OD2	-7.48	109.08	123.30
2	D	1050	LEU	CB-CG-CD1	-7.42	98.38	111.00
2	D	999	LEU	CA-CB-CG	7.24	131.95	115.30
1	B	85	ARG	NH1-CZ-NH2	-7.23	111.45	119.40
2	D	1104	MET	CG-SD-CE	-7.18	88.72	100.20
2	D	1498	ASP	CB-CG-OD1	7.17	124.75	118.30
2	D	603	LEU	CA-CB-CG	7.08	131.59	115.30
4	C	17	TYR	CE1-CZ-CE2	7.07	131.11	119.80
2	D	999	LEU	CB-CA-C	-6.95	96.99	110.20
4	C	221	ARG	NE-CZ-NH1	6.81	123.71	120.30
2	D	1521	LYS	CD-CE-NZ	6.76	127.24	111.70
2	D	996	LEU	CB-CG-CD2	6.73	122.43	111.00
4	C	1156	THR	CB-CA-C	-6.68	93.56	111.60
4	C	157	GLU	OE1-CD-OE2	-6.66	115.31	123.30
2	D	1147	MET	CG-SD-CE	-6.55	89.71	100.20
4	C	1161	MET	CB-CG-SD	6.49	131.87	112.40
3	A	156	GLN	CB-CA-C	6.47	123.33	110.40
3	A	124	PHE	CB-CG-CD2	6.40	125.28	120.80
6	Y	36	DG	OP1-P-OP2	-6.37	110.05	119.60
2	D	951	TYR	CB-CG-CD1	-6.31	117.22	121.00
1	B	24	GLU	OE1-CD-OE2	-6.30	115.73	123.30
2	D	951	TYR	CB-CG-CD2	6.24	124.74	121.00
2	D	841	LEU	CB-CG-CD1	6.06	121.30	111.00
2	D	1211	MET	CA-CB-CG	6.02	123.53	113.30
2	D	1020	LEU	CA-CB-CG	5.86	128.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1152	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	85	ARG	CD-NE-CZ	5.76	131.67	123.60
3	A	91	LEU	CB-CG-CD1	-5.71	101.29	111.00
3	A	1058	ARG	CG-CD-NE	5.70	123.78	111.80
4	C	9	GLN	CB-CA-C	-5.61	99.18	110.40
2	D	731	LYS	CG-CD-CE	5.58	128.66	111.90
4	C	1152	PHE	CG-CD1-CE1	-5.57	114.67	120.80
4	C	1152	PHE	CB-CG-CD2	-5.57	116.90	120.80
2	D	1379	ASP	CB-CG-OD1	5.54	123.28	118.30
2	D	1505	LEU	CB-CG-CD2	5.47	120.30	111.00
2	D	1260	LEU	CA-CB-CG	5.42	127.77	115.30
4	C	1132	ASP	CB-CG-OD1	5.33	123.10	118.30
2	D	1047	LYS	CD-CE-NZ	5.33	123.95	111.70
4	C	220	ARG	N-CA-CB	5.32	120.17	110.60
2	D	624	VAL	CA-CB-CG1	-5.29	102.97	110.90
4	C	223	LEU	CB-CG-CD1	-5.28	102.02	111.00
4	C	1152	PHE	CB-CG-CD1	5.26	124.49	120.80
4	C	219	GLU	CB-CA-C	5.25	120.90	110.40
3	A	39	SER	CB-CA-C	-5.23	100.16	110.10
4	C	217	ASP	CB-CG-OD2	5.21	122.99	118.30
3	A	1189	VAL	CG1-CB-CG2	-5.19	102.59	110.90
4	C	963	ALA	C-N-CA	-5.19	108.73	121.70
4	C	219	GLU	OE1-CD-OE2	5.18	129.52	123.30
4	C	77	TYR	CD1-CE1-CZ	5.17	124.45	119.80
2	D	1047	LYS	CB-CG-CD	5.13	124.93	111.60
2	D	1046	LEU	CA-CB-CG	5.07	126.96	115.30
5	X	25	DA	O4'-C1'-N9	5.05	111.53	108.00
3	A	1049	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	D	1260	LEU	CB-CG-CD2	5.00	119.50	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	85	ARG	Sidechain
4	C	220	ARG	Sidechain
4	C	235	ILE	Peptide
2	D	1178	SER	Peptide
2	D	722	LYS	Peptide
2	D	744	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1195	0	1238	47	0
2	D	10247	0	10549	303	0
3	A	3047	0	3045	64	0
4	C	3665	0	3668	90	0
5	X	658	0	358	7	0
6	Y	654	0	365	4	0
7	A	4	0	0	0	0
7	C	4	0	0	1	0
8	A	27	0	11	4	0
8	C	27	0	11	1	0
All	All	19528	0	19245	498	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 13.

All (498) 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:D:290:ILE:HD11	2:D:346:LEU:CD1	1.66	1.25
2:D:268:TYR:HB2	2:D:332:LEU:CD2	1.73	1.18
2:D:290:ILE:CD1	2:D:346:LEU:HD12	1.73	1.16
2:D:290:ILE:HD11	2:D:346:LEU:HD12	1.01	1.00
2:D:268:TYR:HB2	2:D:332:LEU:HD21	0.99	0.96
2:D:268:TYR:CB	2:D:332:LEU:HD21	1.94	0.96
2:D:286:GLU:HG3	2:D:346:LEU:HD21	1.50	0.92
1:B:556:ALA:HB3	1:B:593:ASP:OD1	1.69	0.91
4:C:220:ARG:O	4:C:224:GLU:HB2	1.73	0.88
1:B:572:LYS:NZ	1:B:594:VAL:CG1	2.38	0.87
2:D:264:ILE:HG23	2:D:332:LEU:CD1	2.05	0.86
1:B:565:ASP:OD1	1:B:618:THR:HG22	1.76	0.85
2:D:280:CYS:HB2	2:D:340:VAL:HA	1.59	0.84
1:B:572:LYS:HZ3	1:B:594:VAL:CG1	1.89	0.84
1:B:556:ALA:CB	1:B:593:ASP:OD1	2.26	0.83
1:B:572:LYS:HZ3	1:B:594:VAL:HG13	1.44	0.81
2:D:280:CYS:SG	2:D:341:PRO:CD	2.69	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:296:LEU:HD13	2:D:333:VAL:HG11	1.62	0.81
2:D:1223:ILE:HG22	2:D:1303:LEU:HD11	1.63	0.79
2:D:280:CYS:SG	2:D:341:PRO:HD2	2.22	0.79
2:D:1024:MET:HG3	2:D:1027:LEU:HD12	1.66	0.78
3:A:1195:ASN:O	3:A:1199:SER:HB3	1.82	0.78
1:B:553:SER:HA	1:B:593:ASP:OD2	1.84	0.77
2:D:285:GLU:HG2	2:D:346:LEU:HG	1.65	0.77
2:D:801:ARG:NH1	2:D:804:ASN:OD1	2.18	0.77
2:D:477:LEU:O	2:D:480:PHE:HB3	1.85	0.76
2:D:272:THR:HG22	2:D:276:ARG:HH22	1.52	0.75
2:D:264:ILE:HG23	2:D:332:LEU:HD12	1.69	0.75
3:A:37:GLY:HA3	3:A:1207:ILE:HG21	1.69	0.74
2:D:1044:HIS:HA	2:D:1047:LYS:HE2	1.70	0.73
2:D:1143:ASN:HB3	2:D:1146:LYS:HB2	1.71	0.73
4:C:27:HIS:NE2	4:C:1154:CYS:SG	2.61	0.73
2:D:280:CYS:SG	2:D:341:PRO:HD3	2.29	0.73
2:D:1103:LEU:HG	2:D:1149:ARG:HH22	1.53	0.72
2:D:659:LYS:HB3	2:D:663:PRO:HB3	1.71	0.71
2:D:264:ILE:HG23	2:D:332:LEU:HD11	1.73	0.71
1:B:585:GLU:CD	1:B:585:GLU:H	1.95	0.70
2:D:1151:ILE:O	2:D:1210:ASN:ND2	2.24	0.70
2:D:264:ILE:CG2	2:D:332:LEU:HD11	2.22	0.69
4:C:56:LEU:HD13	4:C:61:ARG:HB2	1.72	0.69
2:D:290:ILE:HD11	2:D:346:LEU:HD11	1.71	0.69
2:D:251:ARG:NH1	2:D:257:LYS:O	2.25	0.69
4:C:143:ARG:O	4:C:146:SER:OG	2.11	0.69
2:D:1196:LEU:HB3	2:D:1204:ARG:HH21	1.58	0.69
2:D:987:THR:O	2:D:991:GLN:NE2	2.25	0.69
4:C:213:TYR:O	4:C:217:ASP:N	2.24	0.69
4:C:1114:GLN:OE1	4:C:1122:ASN:ND2	2.27	0.68
2:D:1134:LEU:HD22	2:D:1154:ILE:HG13	1.76	0.68
4:C:30:ILE:HB	4:C:1155:THR:HG22	1.75	0.68
1:B:553:SER:HA	1:B:593:ASP:CG	2.14	0.68
2:D:811:SER:HA	2:D:814:ARG:HD3	1.76	0.68
2:D:541:LEU:HG	2:D:544:HIS:H	1.58	0.68
4:C:213:TYR:HE1	4:C:964:LEU:HD13	1.59	0.68
1:B:87:LYS:HA	4:C:199:ARG:HH22	1.59	0.67
3:A:42:MET:HG3	3:A:1158:VAL:HG11	1.77	0.67
4:C:219:GLU:HG3	4:C:220:ARG:HH12	1.60	0.67
4:C:141:GLN:OE1	7:C:1201:BEF:F3	2.03	0.66
4:C:213:TYR:HA	4:C:216:LYS:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1152:ASP:HA	2:D:1210:ASN:HD22	1.61	0.66
3:A:2:GLY:N	3:A:93:TYR:HH	1.94	0.66
2:D:1148:VAL:HA	2:D:1151:ILE:HG22	1.76	0.66
2:D:347:GLN:NE2	2:D:351:SER:OG	2.29	0.66
2:D:728:GLU:HA	2:D:731:LYS:HD2	1.79	0.65
2:D:790:SER:O	2:D:796:ARG:NH2	2.29	0.65
2:D:296:LEU:O	2:D:300:LEU:HG	1.96	0.65
2:D:286:GLU:CG	2:D:346:LEU:HD21	2.26	0.65
2:D:1095:LEU:HD21	2:D:1106:ILE:HG21	1.78	0.65
2:D:279:ALA:HA	2:D:282:LYS:HD3	1.78	0.65
2:D:466:PRO:HA	2:D:469:ARG:HB2	1.77	0.65
2:D:525:ILE:HG12	2:D:544:HIS:HB3	1.80	0.64
2:D:1501:ARG:HA	2:D:1504:ILE:HG12	1.79	0.64
2:D:296:LEU:CD1	2:D:333:VAL:HG11	2.28	0.64
2:D:1469:ILE:HD11	2:D:1526:ILE:HG21	1.80	0.64
3:A:16:ARG:HD3	3:A:1213:GLU:HB3	1.79	0.63
4:C:62:GLN:NE2	4:C:67:GLU:OE2	2.30	0.63
3:A:199:LYS:HB2	3:A:1045:PHE:HE2	1.64	0.63
4:C:172:ARG:O	4:C:176:ASN:ND2	2.29	0.63
2:D:1167:ASN:ND2	2:D:1182:ASP:OD1	2.32	0.62
2:D:261:SER:HA	2:D:264:ILE:HD12	1.80	0.62
3:A:16:ARG:O	3:A:19:GLN:NE2	2.31	0.62
2:D:1130:CYS:HA	2:D:1133:SER:HB2	1.81	0.62
2:D:213:GLN:HE21	2:D:214:ARG:HH22	1.48	0.62
2:D:272:THR:O	2:D:275:SER:OG	2.16	0.62
4:C:223:LEU:HD12	4:C:957:LEU:HD22	1.82	0.62
2:D:263:ALA:HA	2:D:266:LYS:HE2	1.82	0.61
2:D:1121:GLU:HA	2:D:1124:LYS:HE3	1.82	0.61
1:B:556:ALA:HB3	1:B:593:ASP:CG	2.21	0.61
2:D:292:VAL:O	2:D:296:LEU:HG	2.00	0.61
2:D:902:ARG:NH2	2:D:905:ASP:OD2	2.33	0.61
2:D:1305:GLN:HG2	2:D:1339:VAL:HG22	1.82	0.61
2:D:226:THR:HG22	2:D:270:ALA:HB1	1.82	0.61
2:D:285:GLU:N	2:D:285:GLU:OE1	2.32	0.61
3:A:157:SER:N	3:A:160:GLU:OE2	2.34	0.61
2:D:264:ILE:CG2	2:D:332:LEU:CD1	2.77	0.61
2:D:864:ILE:O	2:D:902:ARG:NH1	2.34	0.61
1:B:578:LEU:HB2	1:B:586:GLU:HB3	1.82	0.61
2:D:398:ALA:O	2:D:402:ASN:ND2	2.34	0.61
2:D:1268:LEU:HA	2:D:1271:LYS:HB2	1.83	0.61
2:D:1516:LEU:O	2:D:1519:TYR:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:1128:ASP:OD1	4:C:1128:ASP:N	2.29	0.60
3:A:1086:LYS:NZ	3:A:1098:GLY:O	2.34	0.60
2:D:1164:ASN:O	2:D:1165:ARG:NH2	2.30	0.60
2:D:1073:LEU:HD13	2:D:1113:LEU:HD21	1.82	0.60
3:A:206:LEU:HD13	3:A:1034:VAL:HG21	1.83	0.60
1:B:584:ARG:HH21	1:B:584:ARG:HG3	1.67	0.60
1:B:62:LEU:HD21	1:B:66:ARG:HH21	1.67	0.60
2:D:249:ILE:O	2:D:257:LYS:HA	2.01	0.60
1:B:16:LYS:NZ	1:B:32:THR:OG1	2.33	0.59
2:D:1295:TRP:HE1	3:A:1095:PRO:HD2	1.66	0.59
3:A:43:ASP:OD2	3:A:57:ARG:NH2	2.35	0.59
4:C:993:GLU:OE1	4:C:996:ARG:NH1	2.35	0.59
3:A:1157:PHE:HE2	3:A:1159:LEU:HD21	1.67	0.59
3:A:1201:SER:OG	3:A:1202:GLU:N	2.34	0.59
1:B:585:GLU:CD	1:B:585:GLU:N	2.56	0.59
2:D:1047:LYS:HA	2:D:1050:LEU:HD13	1.85	0.59
3:A:2:GLY:N	3:A:94:GLU:O	2.35	0.59
2:D:1342:ARG:HH22	3:A:1116:LYS:HD2	1.67	0.58
2:D:603:LEU:HB3	2:D:605:GLU:OE1	2.03	0.58
1:B:25:LYS:O	1:B:70:ARG:NH2	2.37	0.58
2:D:492:THR:HG22	2:D:493:TYR:H	1.69	0.58
3:A:49:LEU:HD11	3:A:1156:PHE:HZ	1.68	0.58
2:D:1114:PHE:O	2:D:1118:ASN:N	2.37	0.58
2:D:524:GLU:HG3	2:D:525:ILE:HG13	1.86	0.58
3:A:4:LEU:HD12	3:A:91:LEU:HD11	1.86	0.58
4:C:13:SER:O	4:C:1178:SER:OG	2.21	0.58
2:D:300:LEU:CD2	2:D:326:ILE:HD11	2.33	0.58
2:D:529:GLU:OE2	2:D:742:GLN:N	2.37	0.58
2:D:681:LEU:HA	2:D:684:LEU:HD12	1.85	0.57
2:D:300:LEU:HD23	2:D:326:ILE:HD11	1.85	0.57
2:D:218:VAL:O	2:D:222:GLN:HG2	2.05	0.57
2:D:634:LYS:HD2	2:D:795:LEU:HD21	1.86	0.57
2:D:397:VAL:HA	2:D:400:VAL:HG22	1.86	0.57
2:D:225:ASP:O	2:D:229:LEU:HG	2.05	0.57
2:D:471:PHE:O	2:D:474:GLU:HB3	2.05	0.57
2:D:836:ASP:HB2	2:D:874:ARG:HD2	1.87	0.56
4:C:1036:VAL:HG12	4:C:1038:ALA:H	1.70	0.56
2:D:290:ILE:HA	2:D:293:LYS:HE2	1.86	0.56
2:D:897:SER:OG	2:D:965:ARG:NH1	2.38	0.56
2:D:942:LEU:HB2	2:D:946:LYS:HE3	1.86	0.56
2:D:1016:THR:HG23	2:D:1019:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:139:ARG:NH1	5:X:6:DC:OP1	2.37	0.56
1:B:603:ILE:HG23	1:B:618:THR:H	1.70	0.56
2:D:274:LEU:HD13	2:D:277:LEU:HD11	1.88	0.56
2:D:324:ASP:O	2:D:328:LYS:NZ	2.33	0.56
3:A:52:LYS:HE2	5:X:6:DC:H5"	1.86	0.56
4:C:1159:PRO:HB3	4:C:1192:VAL:HG11	1.87	0.56
1:B:86:LEU:O	4:C:199:ARG:NH1	2.38	0.56
3:A:28:THR:HG22	3:A:1203:ALA:HB3	1.88	0.56
2:D:635:ASN:HD22	2:D:798:LYS:HG3	1.71	0.56
3:A:1158:VAL:HG13	3:A:1189:VAL:HG23	1.88	0.56
4:C:112:ASP:OD1	4:C:113:LYS:NZ	2.38	0.56
2:D:502:GLN:O	2:D:505:SER:OG	2.16	0.56
2:D:846:ILE:HD11	2:D:856:ILE:HG21	1.87	0.56
2:D:867:PRO:O	2:D:872:ARG:NH2	2.39	0.56
2:D:1500:GLU:HG2	2:D:1503:LYS:HE3	1.88	0.56
1:B:572:LYS:NZ	1:B:594:VAL:HG12	2.21	0.55
2:D:544:HIS:O	2:D:547:THR:OG1	2.23	0.55
2:D:1246:LEU:O	2:D:1249:SER:OG	2.20	0.55
4:C:28:ASN:ND2	4:C:1167:ASN:OD1	2.39	0.55
2:D:1193:GLN:NE2	2:D:1226:LEU:O	2.39	0.55
2:D:224:GLN:N	2:D:227:ARG:HH11	2.04	0.55
2:D:286:GLU:HG3	2:D:346:LEU:HD11	1.88	0.55
1:B:553:SER:HA	1:B:593:ASP:OD1	2.07	0.55
2:D:264:ILE:O	2:D:332:LEU:HD11	2.06	0.55
2:D:284:LEU:HD12	2:D:286:GLU:OE1	2.07	0.55
3:A:8:GLU:OE1	3:A:18:HIS:NE2	2.40	0.55
4:C:1136:ARG:NH1	4:C:1160:GLU:OE2	2.40	0.55
2:D:264:ILE:HD11	2:D:325:PHE:CZ	2.41	0.55
4:C:163:ALA:HB2	4:C:1020:THR:HG21	1.87	0.55
2:D:285:GLU:CG	2:D:346:LEU:HG	2.36	0.55
2:D:675:ILE:HD13	2:D:678:ILE:HD13	1.86	0.55
4:C:1040:ARG:NH1	4:C:1086:SER:OG	2.40	0.55
2:D:366:THR:O	2:D:369:GLU:HG3	2.07	0.55
3:A:8:GLU:HB2	3:A:18:HIS:HE2	1.72	0.55
2:D:324:ASP:HA	2:D:327:LEU:HD12	1.89	0.55
2:D:601:LEU:HA	2:D:609:THR:HG21	1.89	0.55
2:D:1167:ASN:O	2:D:1171:LYS:N	2.31	0.55
4:C:133:SER:OG	4:C:134:ASN:N	2.39	0.54
2:D:351:SER:O	2:D:355:LEU:HD12	2.07	0.54
2:D:1034:PHE:HZ	2:D:1037:LEU:HD22	1.72	0.54
2:D:1143:ASN:O	2:D:1147:MET:N	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:9:GLN:NE2	4:C:17:TYR:HA	2.22	0.54
1:B:582:CYS:O	1:B:586:GLU:HG2	2.05	0.54
2:D:979:SER:OG	2:D:984:ASN:OD1	2.22	0.54
2:D:1159:ARG:HD2	2:D:1213:ARG:HB3	1.89	0.54
4:C:9:GLN:HE21	4:C:17:TYR:HA	1.73	0.54
2:D:297:GLU:O	2:D:301:LYS:HG3	2.08	0.54
2:D:1490:ILE:HA	2:D:1493:TRP:CD2	2.43	0.54
4:C:229:SER:O	4:C:233:ASP:HB2	2.08	0.53
3:A:1128:ASP:OD1	3:A:1128:ASP:N	2.41	0.53
3:A:39:SER:OG	8:A:1302:ADP:O1B	2.25	0.53
3:A:6:ARG:NH1	3:A:100:GLN:OE1	2.42	0.53
2:D:850:ARG:NH1	2:D:851:GLU:OE2	2.41	0.53
2:D:874:ARG:NH2	5:X:25:DA:OP1	2.42	0.53
3:A:63:GLU:N	3:A:63:GLU:OE1	2.42	0.53
1:B:578:LEU:CB	1:B:586:GLU:HB3	2.38	0.53
2:D:813:LEU:HD22	2:D:820:LEU:HB2	1.91	0.53
2:D:360:HIS:CG	2:D:420:ARG:HH22	2.27	0.53
2:D:483:LEU:HB2	2:D:589:LEU:HD13	1.91	0.52
3:A:12:PHE:HE2	3:A:40:ASN:HB3	1.74	0.52
3:A:182:LYS:HE3	3:A:182:LYS:HA	1.91	0.52
4:C:210:LEU:HA	4:C:213:TYR:HB3	1.90	0.52
2:D:235:GLU:O	2:D:239:SER:OG	2.21	0.52
2:D:950:GLN:HE22	2:D:995:LEU:HB2	1.73	0.52
2:D:251:ARG:HH11	2:D:257:LYS:H	1.55	0.52
2:D:1034:PHE:HE1	2:D:1037:LEU:HD13	1.75	0.52
4:C:57:SER:H	4:C:60:GLU:HB2	1.74	0.52
2:D:470:ASP:OD1	2:D:470:ASP:N	2.42	0.52
2:D:630:ALA:O	2:D:634:LYS:NZ	2.43	0.52
1:B:585:GLU:HA	1:B:588:VAL:HG12	1.91	0.52
2:D:347:GLN:HE22	2:D:351:SER:HG	1.54	0.52
2:D:250:LYS:HD2	2:D:254:ASP:HB3	1.92	0.52
2:D:873:LYS:O	2:D:877:LYS:NZ	2.41	0.52
4:C:214:HIS:O	4:C:221:ARG:NH1	2.43	0.52
2:D:534:GLU:OE1	2:D:735:ASN:ND2	2.42	0.51
4:C:197:GLU:OE1	4:C:201:ARG:NH2	2.37	0.51
2:D:524:GLU:OE1	2:D:547:THR:OG1	2.29	0.51
3:A:27:PHE:HA	3:A:1188:PHE:O	2.10	0.51
3:A:1149:HIS:CE1	3:A:1157:PHE:HE1	2.28	0.51
2:D:271:LEU:HD13	2:D:335:PHE:HB3	1.91	0.51
2:D:868:SER:O	2:D:872:ARG:NE	2.39	0.51
2:D:918:LEU:O	2:D:922:TRP:HD1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:ASP:OD1	1:B:618:THR:CG2	2.55	0.51
2:D:582:SER:HA	2:D:586:PHE:HB3	1.91	0.51
4:C:213:TYR:CE1	4:C:964:LEU:HD13	2.42	0.51
4:C:957:LEU:O	4:C:961:ASN:HB2	2.11	0.51
2:D:296:LEU:HA	2:D:299:GLU:OE1	2.11	0.51
2:D:792:GLN:O	2:D:796:ARG:NH1	2.43	0.50
2:D:1468:SER:OG	2:D:1469:ILE:N	2.44	0.50
1:B:19:LEU:HG	1:B:23:TRP:CD1	2.45	0.50
4:C:230:ARG:NH2	4:C:950:SER:OG	2.44	0.50
2:D:943:GLU:HA	2:D:947:LEU:HD21	1.93	0.50
2:D:1162:ASP:OD2	2:D:1165:ARG:NH2	2.45	0.50
1:B:556:ALA:HB2	1:B:593:ASP:OD1	2.07	0.50
2:D:1168:ASP:O	2:D:1172:HIS:N	2.45	0.50
2:D:733:ILE:HD12	2:D:736:CYS:HB2	1.92	0.50
2:D:1295:TRP:NE1	3:A:1095:PRO:HD2	2.27	0.50
2:D:518:GLN:HE21	2:D:520:LEU:H	1.58	0.50
2:D:1077:LYS:HG2	2:D:1079:ILE:H	1.76	0.50
2:D:836:ASP:OD1	2:D:837:THR:N	2.45	0.50
1:B:75:LEU:HD13	4:C:991:ARG:HD2	1.92	0.50
1:B:572:LYS:HZ2	1:B:594:VAL:CG1	2.24	0.50
4:C:1035:LEU:HD13	4:C:1104:LEU:HD11	1.94	0.50
2:D:371:ILE:O	2:D:375:VAL:HG22	2.12	0.49
2:D:605:GLU:OE1	2:D:605:GLU:N	2.44	0.49
3:A:5:LEU:HD11	3:A:94:GLU:HB2	1.94	0.49
1:B:44:ILE:HD13	1:B:60:LEU:HD12	1.94	0.49
2:D:459:GLN:HE21	2:D:514:SER:HB3	1.77	0.49
1:B:583:ASN:HB3	3:A:1226:TYR:HB3	1.95	0.49
2:D:268:TYR:O	2:D:271:LEU:HG	2.12	0.49
2:D:634:LYS:O	2:D:638:LEU:HD23	2.12	0.49
4:C:27:HIS:HB3	4:C:1165:ALA:HA	1.93	0.49
2:D:726:ASP:HB3	2:D:729:ALA:HB3	1.94	0.49
2:D:596:ASP:O	2:D:600:MET:HG2	2.11	0.49
4:C:1124:LEU:O	4:C:1154:CYS:HA	2.13	0.49
2:D:1027:LEU:O	2:D:1031:SER:OG	2.22	0.49
2:D:1421:SER:O	2:D:1425:ARG:NE	2.46	0.49
3:A:16:ARG:HG2	3:A:1215:SER:HB3	1.93	0.49
3:A:1124:LYS:HE3	3:A:1127:ARG:HE	1.77	0.49
3:A:1222:ASN:OD1	3:A:1223:LEU:N	2.46	0.49
2:D:651:LEU:HD23	2:D:774:PHE:HZ	1.76	0.49
3:A:90:LYS:HE2	3:A:104:LYS:HB2	1.93	0.49
1:B:582:CYS:C	1:B:584:ARG:H	2.16	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1033:THR:HB	3:A:1037:ARG:HH21	1.76	0.49
2:D:675:ILE:HB	2:D:678:ILE:HB	1.94	0.49
4:C:1095:ASN:OD1	4:C:1102:LYS:NZ	2.28	0.49
2:D:235:GLU:HA	2:D:238:ASN:HD22	1.78	0.48
2:D:513:GLN:HE22	2:D:704:ASN:HB2	1.77	0.48
2:D:513:GLN:NE2	2:D:704:ASN:HB2	2.28	0.48
6:Y:10:DT:H2"	6:Y:11:DC:H5"	1.95	0.48
3:A:195:SER:HB2	3:A:1045:PHE:CE1	2.49	0.48
2:D:268:TYR:CB	2:D:332:LEU:CD2	2.67	0.48
2:D:271:LEU:CD1	2:D:335:PHE:HB3	2.42	0.48
2:D:633:SER:OG	2:D:634:LYS:N	2.46	0.48
2:D:760:ASP:HA	2:D:763:ILE:HD13	1.96	0.48
4:C:100:ARG:NH1	4:C:109:TYR:OH	2.46	0.48
1:B:14:LEU:HD11	1:B:60:LEU:HD13	1.96	0.48
2:D:374:ILE:HG22	2:D:386:GLU:HB3	1.95	0.48
2:D:634:LYS:HE2	2:D:795:LEU:HD11	1.95	0.48
2:D:1311:ILE:O	2:D:1314:SER:OG	2.31	0.48
2:D:1427:LYS:HD2	2:D:1431:GLN:HE22	1.79	0.48
2:D:1112:SER:O	2:D:1116:ARG:NH1	2.47	0.48
2:D:1079:ILE:HG23	2:D:1083:PHE:HD2	1.77	0.48
4:C:1048:ARG:HH11	4:C:1078:ILE:HG21	1.79	0.48
2:D:1034:PHE:CE1	2:D:1037:LEU:HD13	2.49	0.47
2:D:1529:SER:O	2:D:1529:SER:OG	2.32	0.47
4:C:993:GLU:HG3	4:C:997:ARG:HH21	1.78	0.47
2:D:330:THR:O	2:D:334:LEU:HD23	2.15	0.47
2:D:251:ARG:NH1	2:D:257:LYS:H	2.13	0.47
2:D:301:LYS:HB2	2:D:302:GLU:OE2	2.14	0.47
2:D:1501:ARG:HB3	2:D:1505:LEU:HD23	1.95	0.47
3:A:1124:LYS:CE	3:A:1127:ARG:HE	2.27	0.47
2:D:394:LEU:HA	2:D:397:VAL:HG22	1.96	0.47
3:A:31:ILE:O	3:A:1206:GLY:HA2	2.15	0.47
4:C:27:HIS:HE2	4:C:1154:CYS:HG	1.59	0.47
1:B:560:LEU:HD22	1:B:567:TYR:CE2	2.50	0.47
2:D:264:ILE:CD1	2:D:325:PHE:CZ	2.97	0.47
2:D:1159:ARG:NH1	2:D:1252:GLU:OE2	2.47	0.47
2:D:1476:ILE:HA	2:D:1479:VAL:HG22	1.97	0.47
2:D:294:GLN:HA	2:D:297:GLU:OE1	2.14	0.47
2:D:386:GLU:OE2	2:D:389:HIS:ND1	2.35	0.47
2:D:509:VAL:HG11	2:D:600:MET:HE1	1.97	0.47
2:D:1169:ASP:OD1	2:D:1169:ASP:N	2.47	0.47
2:D:1464:ILE:HD12	2:D:1465:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1106:ASP:OD1	3:A:1109:GLU:N	2.40	0.47
4:C:217:ASP:O	4:C:220:ARG:N	2.45	0.47
2:D:1268:LEU:HD12	2:D:1271:LYS:HB2	1.96	0.47
2:D:1410:GLN:HA	2:D:1464:ILE:HD13	1.97	0.47
1:B:590:LEU:HA	1:B:590:LEU:HD23	1.77	0.47
2:D:268:TYR:HE2	2:D:335:PHE:CE1	2.32	0.47
2:D:1435:PRO:HG3	2:D:1453:PHE:HE2	1.80	0.47
1:B:585:GLU:N	1:B:585:GLU:OE2	2.48	0.47
2:D:476:SER:O	2:D:504:TYR:OH	2.33	0.47
2:D:211:LYS:HB2	2:D:214:ARG:O	2.15	0.46
2:D:790:SER:OG	2:D:792:GLN:O	2.30	0.46
2:D:1143:ASN:O	2:D:1146:LYS:N	2.44	0.46
4:C:220:ARG:O	4:C:224:GLU:CB	2.54	0.46
2:D:869:THR:HG23	2:D:910:ILE:HD11	1.97	0.46
3:A:1166:LEU:HD22	3:A:1170:ASN:HD21	1.80	0.46
8:A:1302:ADP:H5'1	4:C:1097:LEU:O	2.14	0.46
2:D:374:ILE:HG13	2:D:375:VAL:HG13	1.97	0.46
2:D:626:ASN:HD21	2:D:629:GLN:HE22	1.64	0.46
1:B:19:LEU:HG	1:B:23:TRP:HD1	1.81	0.46
2:D:285:GLU:HA	2:D:288:SER:HB3	1.97	0.46
2:D:1104:MET:SD	2:D:1104:MET:N	2.88	0.46
1:B:572:LYS:NZ	1:B:594:VAL:HG13	2.14	0.46
4:C:220:ARG:NH1	4:C:957:LEU:HD21	2.30	0.46
3:A:49:LEU:HD11	3:A:1156:PHE:CZ	2.49	0.46
4:C:212:VAL:O	4:C:216:LYS:N	2.49	0.46
2:D:607:CYS:HB2	2:D:708:TYR:HD2	1.81	0.46
2:D:951:TYR:HD1	2:D:995:LEU:HD11	1.81	0.46
2:D:1039:ASP:OD1	2:D:1041:SER:N	2.44	0.46
1:B:55:ARG:HG3	1:B:56:LEU:HD12	1.97	0.45
2:D:216:GLN:O	2:D:220:LEU:HG	2.16	0.45
2:D:270:ALA:O	2:D:274:LEU:HD23	2.15	0.45
2:D:509:VAL:O	2:D:513:GLN:N	2.48	0.45
2:D:1182:ASP:O	2:D:1184:ALA:N	2.49	0.45
2:D:1267:LYS:HG3	2:D:1271:LYS:HG3	1.98	0.45
4:C:978:PHE:O	4:C:982:THR:OG1	2.21	0.45
2:D:280:CYS:SG	2:D:281:ASP:N	2.89	0.45
2:D:518:GLN:NE2	2:D:520:LEU:HB3	2.31	0.45
1:B:75:LEU:HD23	4:C:189:ILE:HD13	1.98	0.45
1:B:552:SER:O	1:B:593:ASP:OD1	2.35	0.45
2:D:259:ILE:HG22	2:D:260:SER:O	2.17	0.45
2:D:1209:ASP:OD1	2:D:1209:ASP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:42:PHE:CD1	4:C:1123:ILE:HD11	2.52	0.45
2:D:446:SER:HA	2:D:449:PHE:CD2	2.51	0.45
2:D:905:ASP:OD1	2:D:906:GLU:N	2.48	0.45
2:D:1193:GLN:NE2	2:D:1230:THR:OG1	2.50	0.45
4:C:29:VAL:HG12	4:C:1161:MET:HE3	1.98	0.45
2:D:856:ILE:HD13	2:D:856:ILE:HA	1.86	0.45
4:C:181:GLU:O	4:C:184:GLN:HG3	2.16	0.45
1:B:560:LEU:HD11	1:B:572:LYS:NZ	2.32	0.45
2:D:487:ARG:HB2	6:Y:10:DT:H3'	1.99	0.45
2:D:1144:PHE:HA	2:D:1147:MET:HG3	1.99	0.45
2:D:291:LEU:HD12	2:D:292:VAL:N	2.33	0.44
2:D:1448:GLU:O	2:D:1452:SER:OG	2.21	0.44
4:C:89:PHE:HE1	4:C:124:LEU:HA	1.82	0.44
4:C:957:LEU:C	4:C:957:LEU:HD23	2.38	0.44
2:D:794:SER:O	2:D:797:THR:OG1	2.26	0.44
2:D:1411:SER:O	2:D:1415:ILE:HG12	2.18	0.44
2:D:1488:PRO:HB2	3:A:1049:ARG:HH12	1.81	0.44
2:D:1518:ARG:HD3	2:D:1521:LYS:HD2	1.98	0.44
4:C:9:GLN:OE1	4:C:77:TYR:CE1	2.71	0.44
4:C:1187:GLU:OE2	4:C:1187:GLU:N	2.48	0.44
2:D:1478:THR:O	2:D:1481:SER:OG	2.21	0.44
3:A:186:ASP:HA	3:A:189:VAL:HG12	1.98	0.44
4:C:1124:LEU:HB3	4:C:1127:CYS:SG	2.58	0.44
6:Y:13:DC:H2"	6:Y:14:DA:H8	1.83	0.44
2:D:969:LEU:O	2:D:972:SER:OG	2.23	0.44
2:D:988:LEU:O	2:D:992:ILE:HG12	2.17	0.44
8:A:1302:ADP:O2B	4:C:1098:SER:HB2	2.17	0.44
4:C:110:SER:OG	4:C:111:LEU:N	2.50	0.44
4:C:165:THR:O	4:C:165:THR:OG1	2.33	0.44
2:D:423:TYR:OH	4:C:973:LYS:HG2	2.17	0.44
2:D:779:PHE:O	2:D:782:SER:OG	2.34	0.44
2:D:1334:ILE:HD11	2:D:1344:CYS:SG	2.57	0.44
3:A:114:GLU:HB3	3:A:121:ILE:HD11	1.99	0.44
4:C:110:SER:OG	4:C:111:LEU:O	2.33	0.44
2:D:532:SER:O	2:D:532:SER:OG	2.36	0.44
2:D:601:LEU:HD12	2:D:613:ILE:HD12	1.99	0.44
2:D:958:CYS:O	2:D:1025:SER:OG	2.35	0.44
2:D:1046:LEU:HD13	2:D:1050:LEU:HD11	1.98	0.44
4:C:217:ASP:OD1	4:C:220:ARG:HB2	2.17	0.44
2:D:1239:ASN:OD1	2:D:1242:GLU:N	2.48	0.44
2:D:280:CYS:HB2	2:D:340:VAL:CA	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:GLU:HA	2:D:289:ILE:HG13	2.00	0.44
2:D:1251:LEU:HD21	2:D:1328:GLU:HG2	1.99	0.44
4:C:1107:LEU:HD12	4:C:1111:PHE:CZ	2.53	0.44
2:D:328:LYS:HZ2	2:D:396:LYS:HE3	1.83	0.43
2:D:511:LEU:O	2:D:514:SER:OG	2.30	0.43
2:D:652:PHE:CZ	2:D:656:LEU:HB3	2.53	0.43
3:A:13:LYS:HB2	8:A:1302:ADP:C5	2.53	0.43
3:A:86:THR:HG21	3:A:109:PRO:HD3	1.99	0.43
4:C:1146:MET:HA	4:C:1149:THR:HG22	2.00	0.43
2:D:735:ASN:HA	2:D:738:ASP:HB3	2.00	0.43
2:D:1138:ARG:HH22	2:D:1194:LYS:HZ3	1.64	0.43
3:A:191:LEU:O	3:A:195:SER:HB3	2.18	0.43
4:C:134:ASN:HA	4:C:135:PRO:HD3	1.87	0.43
4:C:1045:MET:HA	4:C:1078:ILE:HG12	2.00	0.43
1:B:583:ASN:N	1:B:583:ASN:HD22	2.16	0.43
2:D:293:LYS:HA	2:D:296:LEU:HD12	1.98	0.43
3:A:172:LEU:HD23	3:A:172:LEU:HA	1.90	0.43
2:D:213:GLN:HE21	2:D:214:ARG:NH2	2.14	0.43
4:C:1013:LYS:O	4:C:1017:ILE:HG12	2.18	0.43
4:C:1094:ILE:HD12	4:C:1097:LEU:HD12	2.00	0.43
2:D:332:LEU:HA	2:D:332:LEU:HD23	1.64	0.43
2:D:470:ASP:HA	2:D:473:ILE:HD12	2.00	0.43
2:D:604:PRO:HB2	2:D:692:PHE:HZ	1.83	0.43
3:A:1159:LEU:HD23	3:A:1159:LEU:HA	1.73	0.43
2:D:234:ILE:O	2:D:238:ASN:ND2	2.52	0.43
2:D:568:ALA:O	2:D:572:SER:HB3	2.19	0.43
3:A:117:ILE:HD11	3:A:127:TYR:HA	2.01	0.43
4:C:59:GLU:HG2	4:C:60:GLU:OE2	2.19	0.43
1:B:569:GLU:HB2	1:B:615:ILE:HD11	2.01	0.43
2:D:549:GLU:HA	2:D:552:LEU:HD12	2.01	0.43
2:D:280:CYS:CB	2:D:340:VAL:HA	2.41	0.43
2:D:282:LYS:HD2	2:D:282:LYS:N	2.34	0.43
3:A:30:ILE:HA	3:A:1205:VAL:HG23	2.01	0.43
4:C:165:THR:OG1	4:C:1013:LYS:HE3	2.19	0.43
4:C:185:LYS:HA	4:C:188:LYS:HE2	2.01	0.43
6:Y:36:DG:H8	6:Y:36:DG:OP2	2.02	0.43
2:D:987:THR:HG23	2:D:988:LEU:HD22	2.01	0.42
2:D:517:ILE:HG12	2:D:708:TYR:HD1	1.84	0.42
2:D:543:GLU:HA	2:D:546:LYS:HB2	2.01	0.42
2:D:1472:PRO:HA	2:D:1475:ILE:HG12	2.01	0.42
4:C:84:ASN:HD22	4:C:88:ARG:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:541:LEU:HD23	2:D:544:HIS:CD2	2.54	0.42
2:D:886:THR:O	2:D:892:ARG:NH2	2.53	0.42
4:C:1171:VAL:HG12	4:C:1180:VAL:HG12	1.99	0.42
1:B:59:GLN:HE22	4:C:171:ARG:NH1	2.18	0.42
2:D:370:ALA:HB1	2:D:390:LEU:HD11	2.01	0.42
3:A:1133:SER:HB3	8:C:1202:ADP:H5'1	2.02	0.42
1:B:605:VAL:HG21	3:A:1219:LEU:HD11	2.02	0.42
2:D:418:VAL:HA	2:D:421:ILE:HG12	2.02	0.42
2:D:1438:LEU:HD12	2:D:1438:LEU:HA	1.83	0.42
3:A:42:MET:HG3	3:A:1158:VAL:CG1	2.48	0.42
1:B:584:ARG:HH21	1:B:584:ARG:CG	2.30	0.42
2:D:229:LEU:HA	2:D:232:GLN:OE1	2.20	0.42
2:D:1143:ASN:O	2:D:1147:MET:HG3	2.19	0.42
4:C:29:VAL:HG13	4:C:1165:ALA:HB2	2.01	0.42
5:X:30:DC:H2'	5:X:31:DA:C8	2.55	0.42
2:D:1356:ILE:HG13	2:D:1358:GLU:H	1.83	0.42
2:D:518:GLN:HE21	2:D:520:LEU:HB3	1.83	0.42
4:C:1156:THR:HB	4:C:1157:PHE:H	1.34	0.42
2:D:426:PRO:HB3	2:D:479:ASN:HD21	1.85	0.42
2:D:1208:ILE:HD12	2:D:1208:ILE:HA	1.90	0.42
4:C:6:ILE:HG23	4:C:80:VAL:HG12	2.02	0.42
4:C:155:ARG:CD	4:C:1080:ILE:HD11	2.50	0.42
2:D:1004:ILE:HD13	2:D:1004:ILE:HG21	1.87	0.41
2:D:1221:LEU:O	2:D:1224:SER:N	2.43	0.41
4:C:1135:TYR:O	4:C:1139:ILE:HG12	2.20	0.41
2:D:281:ASP:OD1	2:D:342:SER:OG	2.37	0.41
2:D:1458:CYS:HB3	2:D:1516:LEU:HD12	2.02	0.41
5:X:10:DG:H5'	5:X:10:DG:C8	2.55	0.41
2:D:265:GLU:OE2	2:D:268:TYR:HD1	2.03	0.41
2:D:240:GLU:OE2	2:D:257:LYS:HD2	2.21	0.41
3:A:1127:ARG:HB3	3:A:1131:GLN:HE21	1.86	0.41
4:C:134:ASN:N	4:C:134:ASN:OD1	2.52	0.41
2:D:264:ILE:HA	2:D:267:LEU:HD12	2.03	0.41
2:D:803:ILE:HA	2:D:806:MET:HB3	2.01	0.41
2:D:225:ASP:O	2:D:228:LEU:HB3	2.21	0.41
2:D:227:ARG:O	2:D:230:ILE:HB	2.21	0.41
2:D:948:ARG:HD3	2:D:948:ARG:HA	1.84	0.41
2:D:1221:LEU:O	2:D:1223:ILE:N	2.54	0.41
4:C:958:HIS:O	4:C:961:ASN:HB3	2.20	0.41
5:X:2:DA:H2"	5:X:3:DG:C8	2.56	0.41
2:D:223:LEU:HG	2:D:227:ARG:CZ	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:405:SER:HA	2:D:457:THR:HG22	2.03	0.41
2:D:570:LEU:O	2:D:574:SER:OG	2.24	0.41
4:C:1004:GLU:O	4:C:1007:THR:OG1	2.34	0.41
2:D:297:GLU:HA	2:D:300:LEU:HD12	2.03	0.41
2:D:451:LYS:HE3	2:D:451:LYS:HB2	1.80	0.41
2:D:494:ARG:HH22	5:X:32:DC:H4'	1.85	0.41
2:D:499:LYS:HA	2:D:499:LYS:HD3	1.89	0.41
2:D:575:LEU:HD21	2:D:637:ALA:HB2	2.02	0.41
2:D:588:ILE:O	2:D:591:LYS:HG2	2.20	0.41
4:C:956:LYS:O	4:C:960:ILE:HG12	2.19	0.41
2:D:1165:ARG:HD3	2:D:1165:ARG:HA	1.82	0.41
3:A:195:SER:OG	3:A:196:PHE:N	2.53	0.41
4:C:995:LEU:O	4:C:998:SER:OG	2.31	0.41
2:D:286:GLU:HG3	2:D:346:LEU:CD2	2.35	0.40
2:D:645:VAL:HA	2:D:648:VAL:HG12	2.01	0.40
2:D:705:ILE:HD12	2:D:705:ILE:HA	1.89	0.40
2:D:800:LEU:HD23	2:D:800:LEU:HA	1.83	0.40
4:C:5:LYS:O	4:C:81:THR:OG1	2.32	0.40
2:D:941:PHE:O	2:D:945:GLN:HB2	2.21	0.40
2:D:298:LYS:HA	2:D:301:LYS:HE3	2.03	0.40
2:D:920:LYS:HD3	2:D:920:LYS:HA	1.94	0.40
2:D:1416:VAL:HG21	2:D:1428:LEU:HD21	2.03	0.40
3:A:200:ARG:O	3:A:204:ALA:HB2	2.21	0.40
2:D:286:GLU:OE1	2:D:286:GLU:N	2.41	0.40
2:D:402:ASN:O	2:D:405:SER:OG	2.28	0.40
2:D:739:LYS:HD3	2:D:739:LYS:HA	1.89	0.40
2:D:993:ARG:HD3	2:D:1037:LEU:HD23	2.04	0.40
2:D:1400:THR:O	2:D:1402:LYS:N	2.52	0.40
3:A:31:ILE:HD12	3:A:31:ILE:HA	1.86	0.40
3:A:1171:VAL:HA	3:A:1174:ILE:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	148/628 (24%)	137 (93%)	11 (7%)	0	100	100
2	D	1262/1587 (80%)	1148 (91%)	114 (9%)	0	100	100
3	A	378/1228 (31%)	351 (93%)	27 (7%)	0	100	100
4	C	450/1194 (38%)	402 (89%)	48 (11%)	0	100	100
All	All	2238/4637 (48%)	2038 (91%)	200 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	132/539 (24%)	126 (96%)	6 (4%)	27	54
2	D	1186/1480 (80%)	1184 (100%)	2 (0%)	93	96
3	A	330/1102 (30%)	327 (99%)	3 (1%)	78	87
4	C	407/1082 (38%)	407 (100%)	0	100	100
All	All	2055/4203 (49%)	2044 (100%)	11 (0%)	89	93

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	11	LYS
1	B	73	ARG
1	B	582	CYS
1	B	583	ASN
1	B	584	ARG
1	B	585	GLU
2	D	299	GLU
2	D	740	ASN
3	A	6	ARG
3	A	141	ARG

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Mol	Chain	Res	Type
3	A	1040	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	583	ASN
2	D	238	ASN
2	D	258	HIS
2	D	402	ASN
2	D	459	GLN
2	D	513	GLN
2	D	518	GLN
2	D	626	ASN
2	D	682	ASN
2	D	1167	ASN
4	C	28	ASN
4	C	34	ASN
4	C	1114	GLN
4	C	1122	ASN
4	C	1167	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	BEF	C	1201	8	0,3,3	-	-	-		
8	ADP	C	1202	7	24,29,29	2.04	4 (16%)	29,45,45	1.90	8 (27%)
8	ADP	A	1302	7	24,29,29	2.03	4 (16%)	29,45,45	1.91	8 (27%)
7	BEF	A	1301	8	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ADP	C	1202	7	-	7/12/32/32	0/3/3/3
8	ADP	A	1302	7	-	7/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1202	ADP	PA-O5'	7.57	1.89	1.59
8	A	1302	ADP	PA-O5'	7.54	1.89	1.59
8	A	1302	ADP	O2'-C2'	-3.42	1.34	1.43
8	C	1202	ADP	O2'-C2'	-3.41	1.34	1.43
8	C	1202	ADP	O5'-C5'	-2.37	1.35	1.44
8	A	1302	ADP	O5'-C5'	-2.34	1.35	1.44
8	C	1202	ADP	O4'-C1'	-2.32	1.37	1.41
8	A	1302	ADP	O4'-C1'	-2.20	1.38	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	1202	ADP	PA-O3A-PB	-5.80	112.92	132.83
8	A	1302	ADP	PA-O3A-PB	-5.79	112.97	132.83
8	C	1202	ADP	O5'-PA-O1A	-4.11	93.02	109.07
8	A	1302	ADP	O2A-PA-O5'	-3.16	93.06	107.75
8	A	1302	ADP	O4'-C1'-C2'	-3.04	102.48	106.93
8	C	1202	ADP	O4'-C1'-C2'	-3.00	102.54	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1302	ADP	O5'-PA-O1A	-2.89	97.77	109.07
8	C	1202	ADP	O3B-PB-O3A	-2.76	95.38	104.64
8	A	1302	ADP	O3B-PB-O3A	-2.75	95.40	104.64
8	A	1302	ADP	O2B-PB-O1B	2.37	119.97	110.68
8	C	1202	ADP	O2B-PB-O1B	2.37	119.97	110.68
8	C	1202	ADP	C3'-C2'-C1'	-2.30	97.52	100.98
8	C	1202	ADP	C2-N1-C6	-2.28	114.85	118.75
8	A	1302	ADP	C2-N1-C6	-2.27	114.88	118.75
8	A	1302	ADP	C3'-C2'-C1'	-2.26	97.58	100.98
8	C	1202	ADP	O2A-PA-O5'	-2.14	97.80	107.75

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1302	ADP	PA-O3A-PB-O2B
8	A	1302	ADP	C5'-O5'-PA-O1A
8	A	1302	ADP	C5'-O5'-PA-O2A
8	A	1302	ADP	C3'-C4'-C5'-O5'
8	C	1202	ADP	PA-O3A-PB-O2B
8	C	1202	ADP	C5'-O5'-PA-O1A
8	C	1202	ADP	C3'-C4'-C5'-O5'
8	A	1302	ADP	O4'-C4'-C5'-O5'
8	C	1202	ADP	O4'-C4'-C5'-O5'
8	A	1302	ADP	PA-O3A-PB-O1B
8	A	1302	ADP	C5'-O5'-PA-O3A
8	C	1202	ADP	C5'-O5'-PA-O3A
8	C	1202	ADP	C5'-O5'-PA-O2A
8	C	1202	ADP	PA-O3A-PB-O1B

There are no ring outliers.

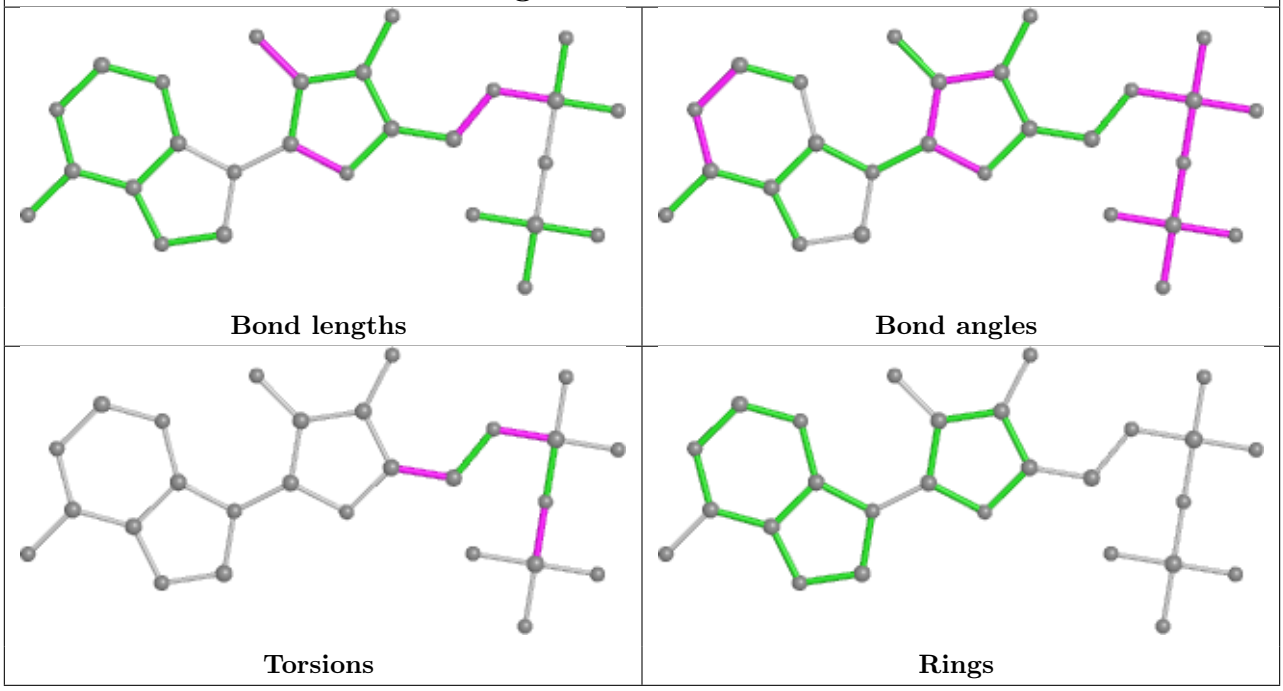
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1201	BEF	1	0
8	C	1202	ADP	1	0
8	A	1302	ADP	4	0

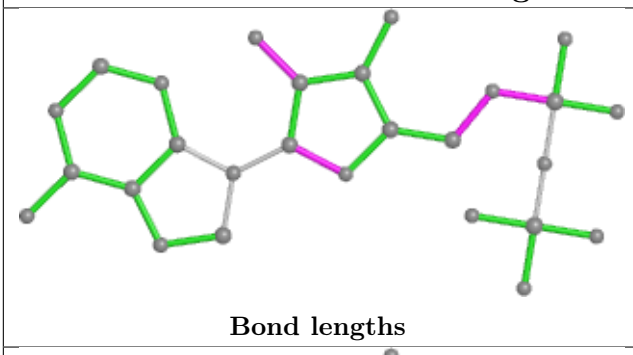
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

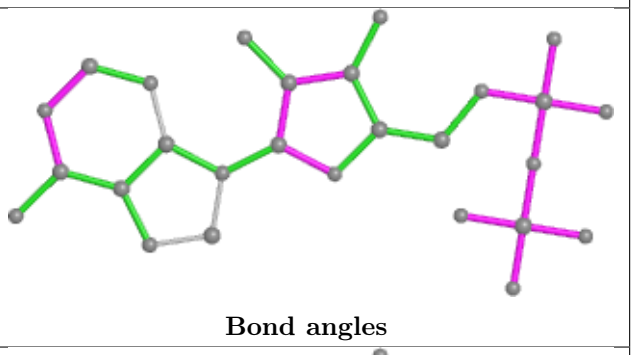
Ligand ADP C 1202



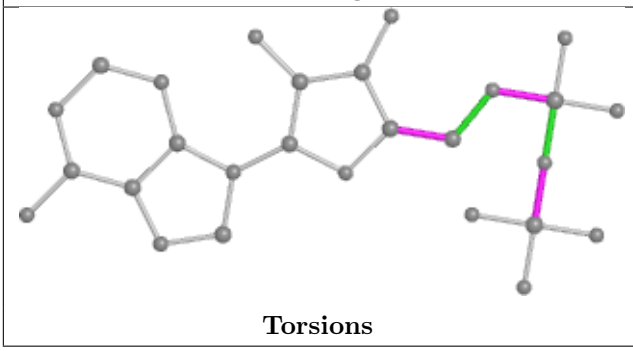
Ligand ADP A 1302



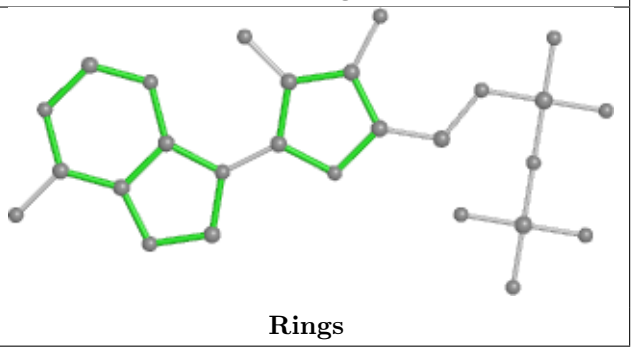
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	602:SER	C	603:LEU	N	1.20

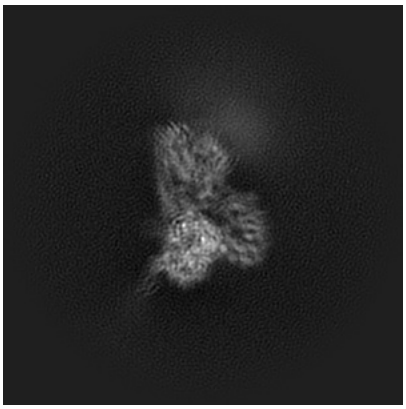
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10930. These allow visual inspection of the internal detail of the map and identification of artifacts.

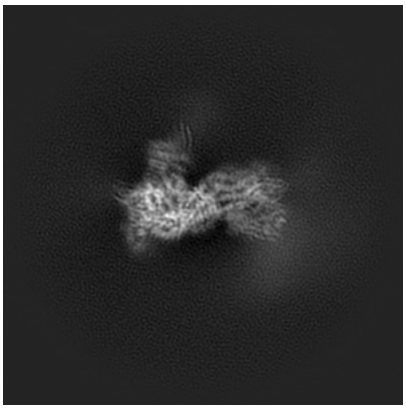
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

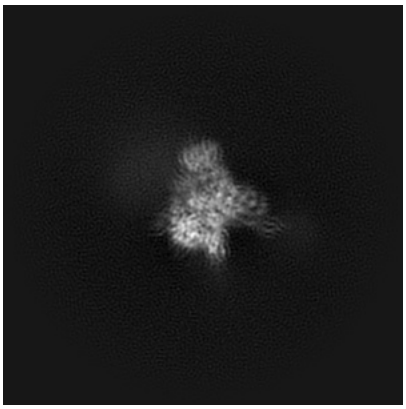
6.1.1 Primary map



X

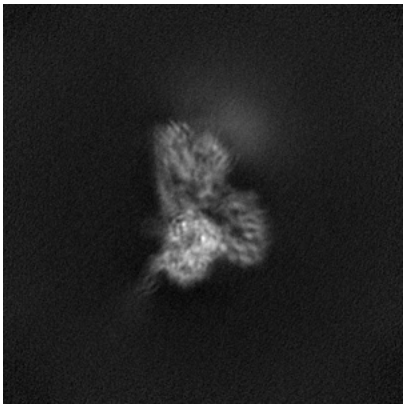


Y

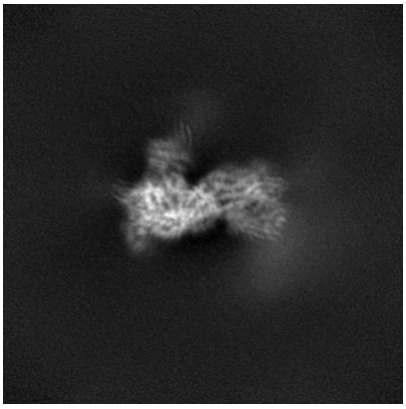


Z

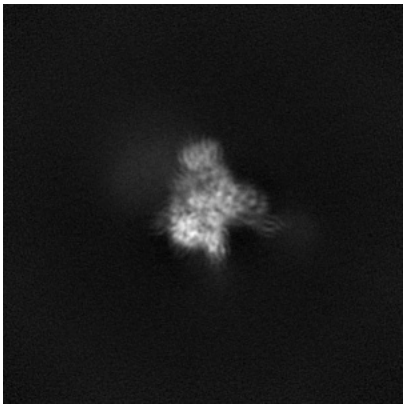
6.1.2 Raw map



X



Y

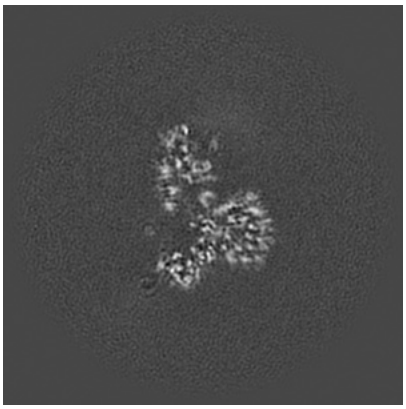


Z

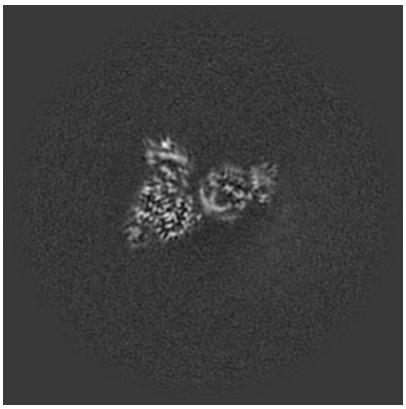
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

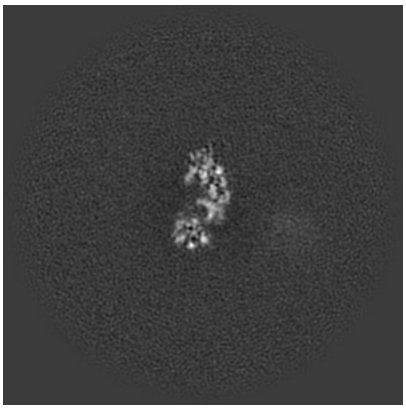
6.2.1 Primary map



X Index: 180

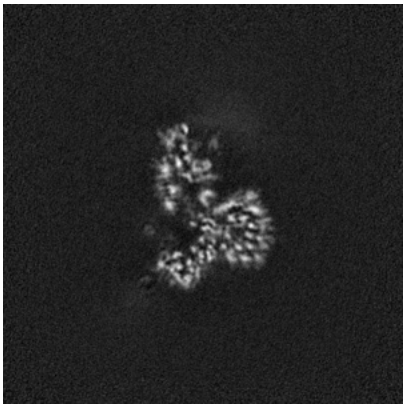


Y Index: 180

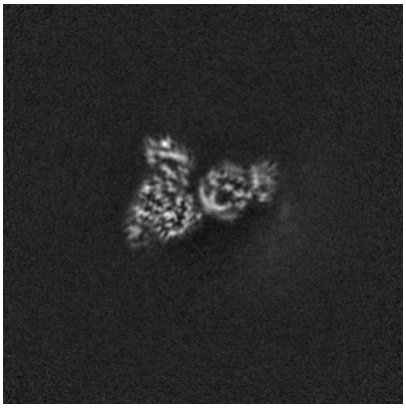


Z Index: 180

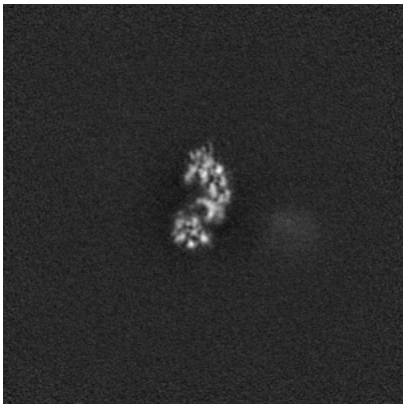
6.2.2 Raw map



X Index: 180



Y Index: 180

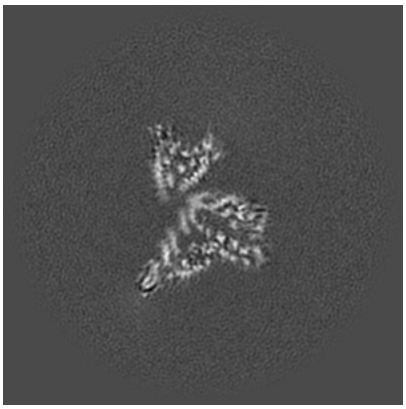


Z Index: 180

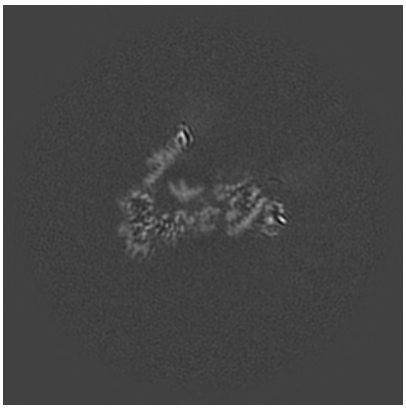
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

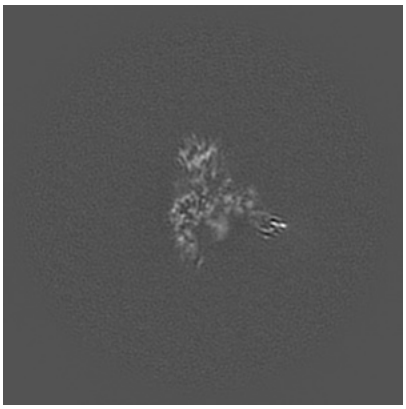
6.3.1 Primary map



X Index: 188

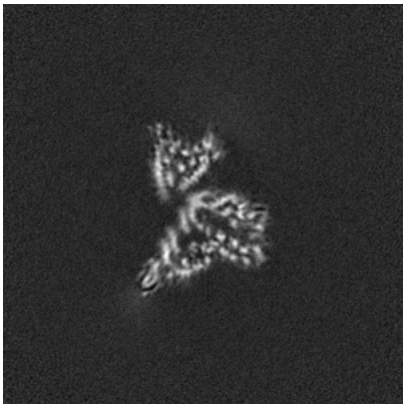


Y Index: 163

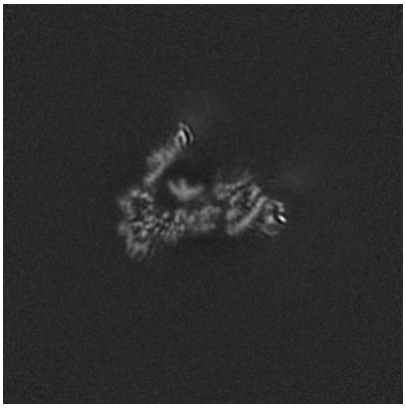


Z Index: 160

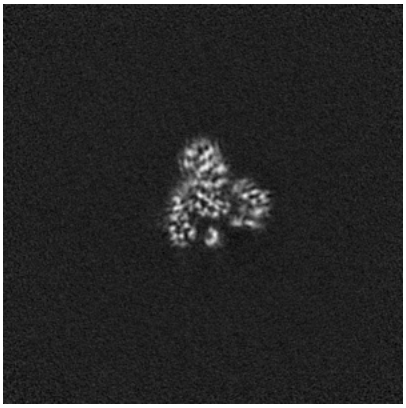
6.3.2 Raw map



X Index: 188



Y Index: 163



Z Index: 140

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

6.4.2 Raw map

X Y Z

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

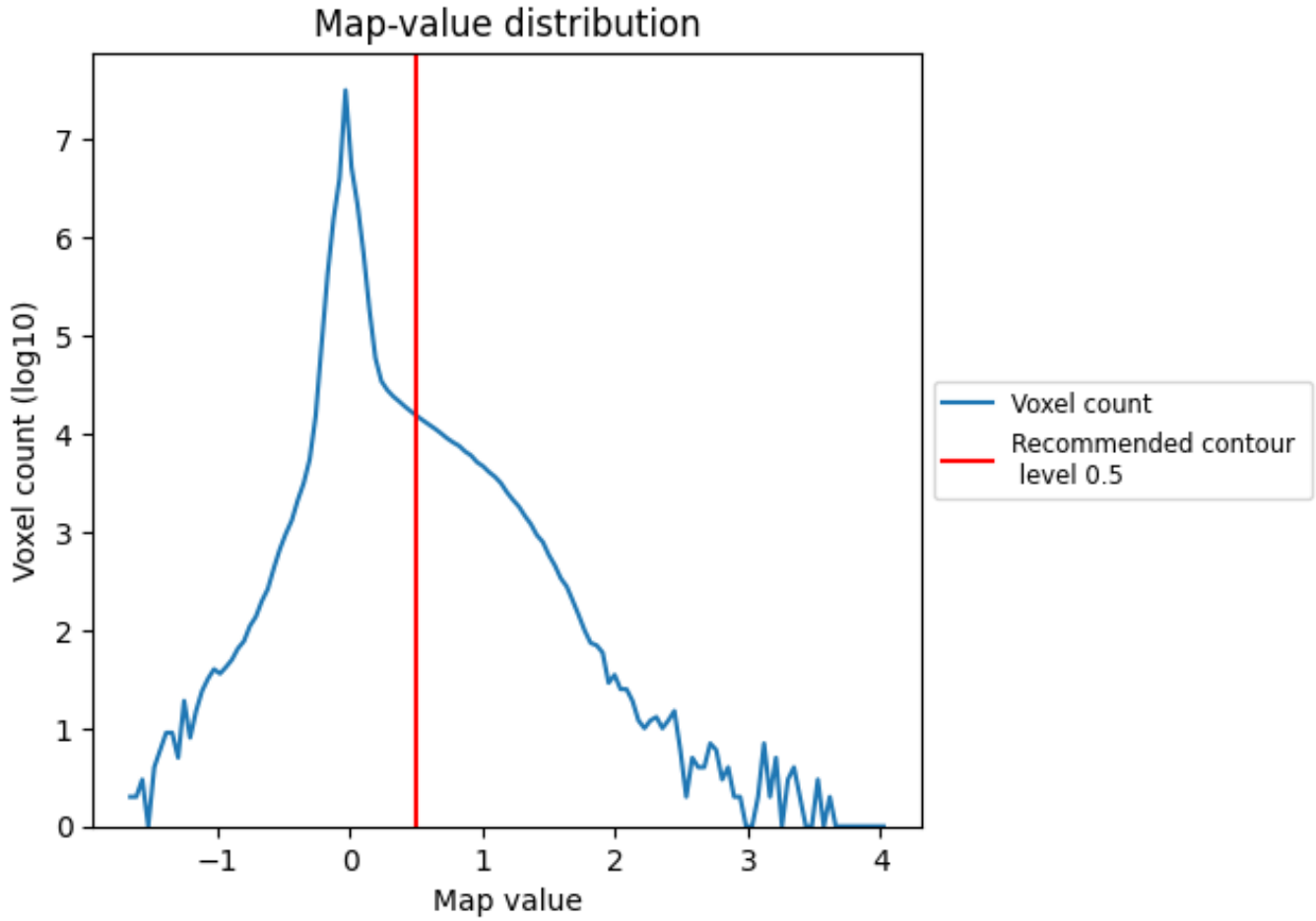
6.5 Mask visualisation (i)

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

7 Map analysis

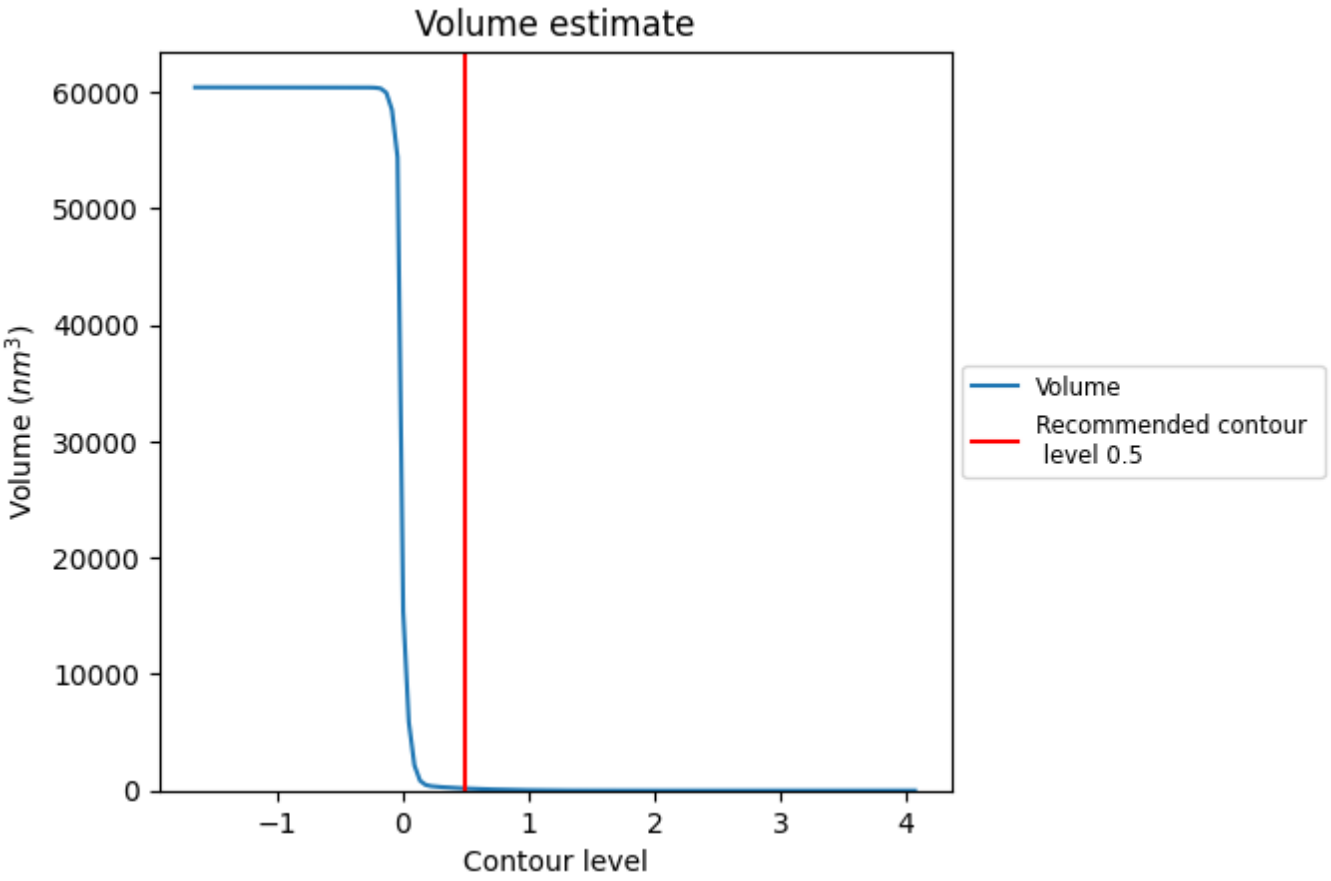
This section contains the results of statistical analysis of the map.

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.

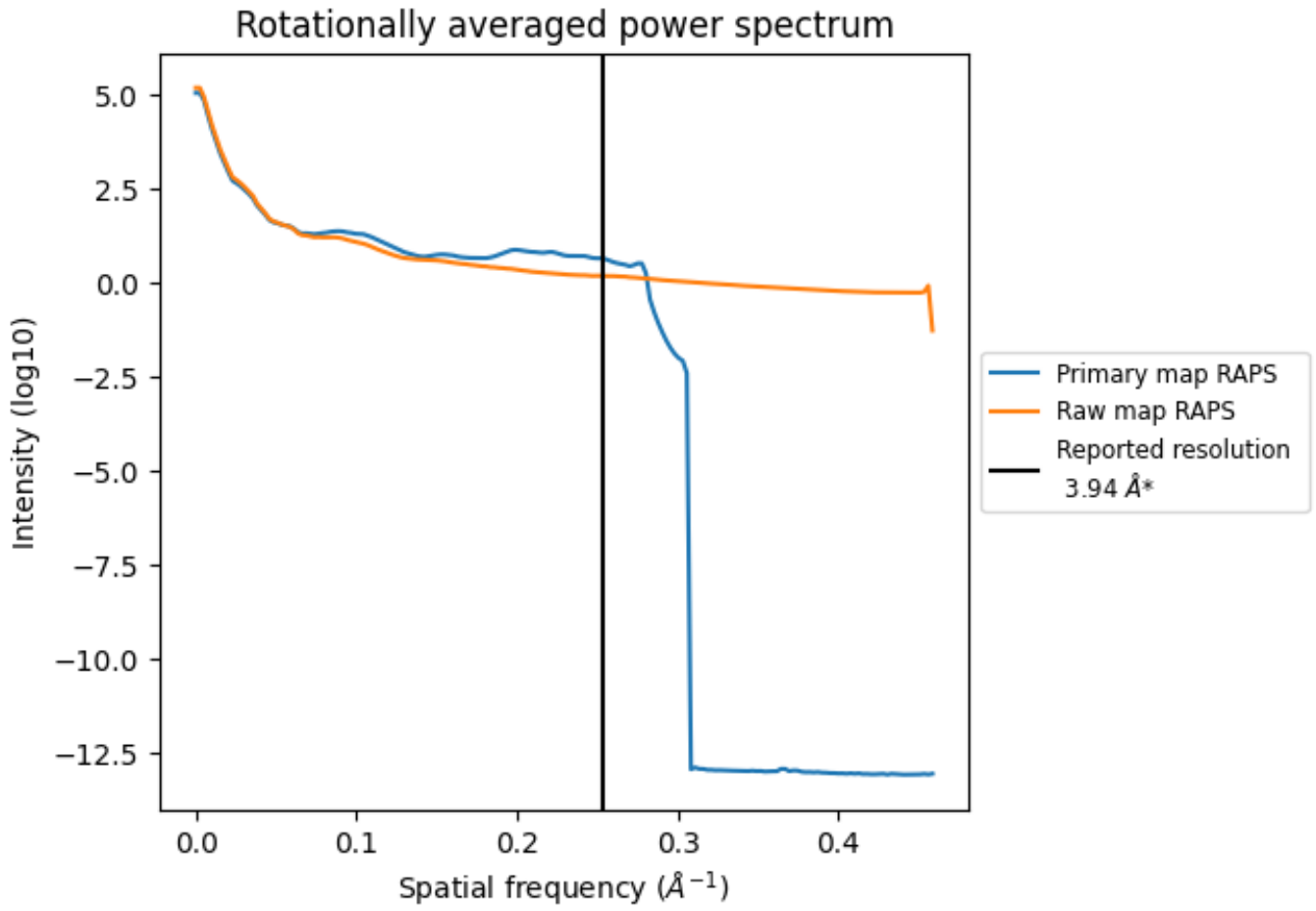
7.2 Volume estimate



The volume at the recommended contour level is 179 nm^3; this corresponds to an approximate mass of 161 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)

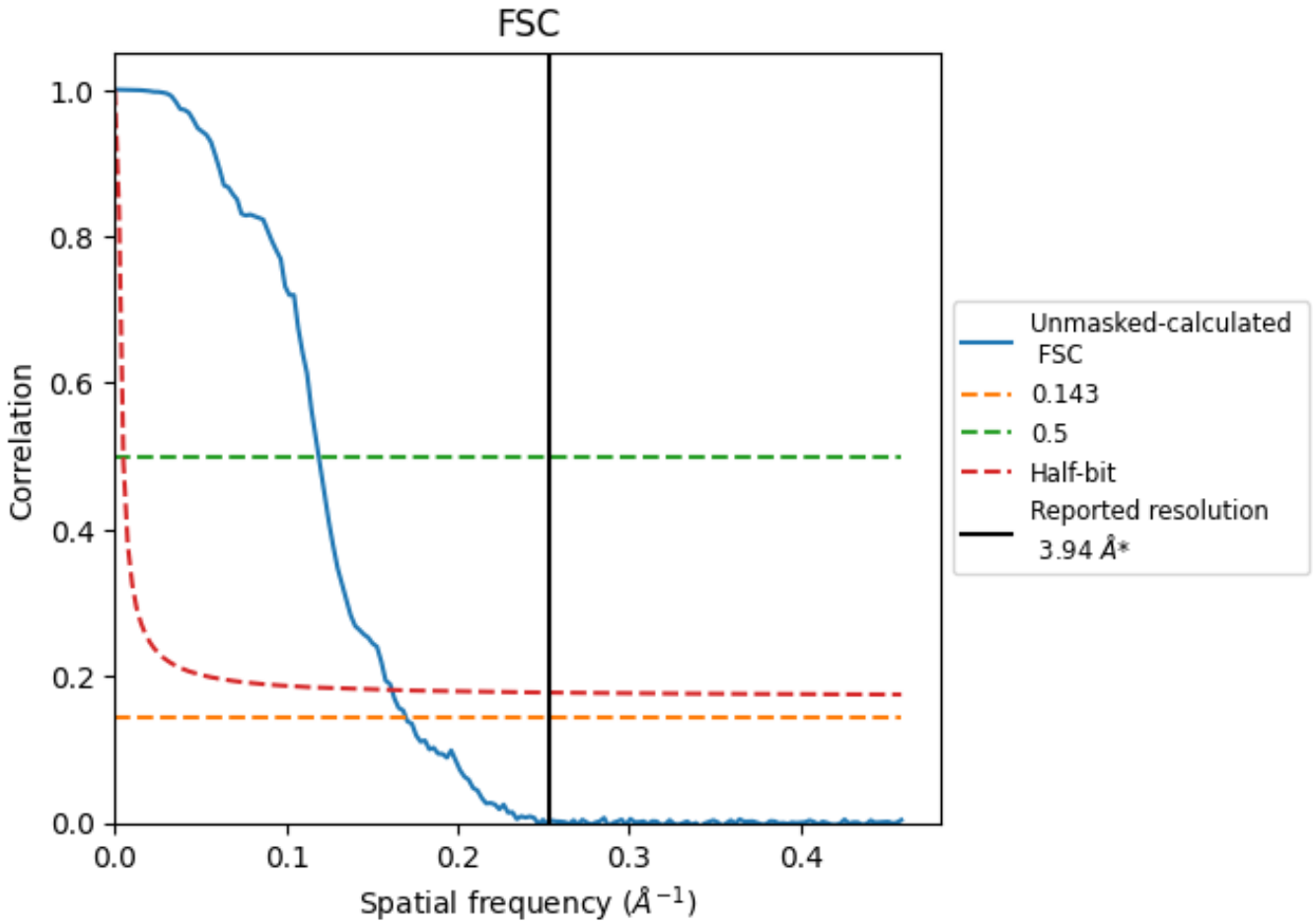


*Reported resolution corresponds to spatial frequency of 0.254 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.254 Å^{-1}

8.2 Resolution estimates (i)

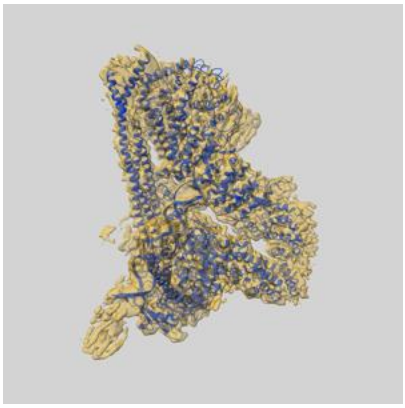
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.94	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.89	8.41	6.19

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.89 differs from the reported value 3.94 by more than 10 %

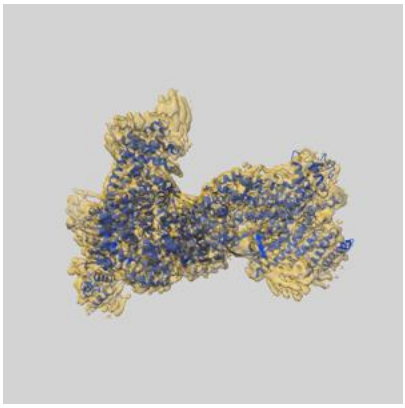
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10930 and PDB model 6YUF. Per-residue inclusion information can be found in section 3 on page 6.

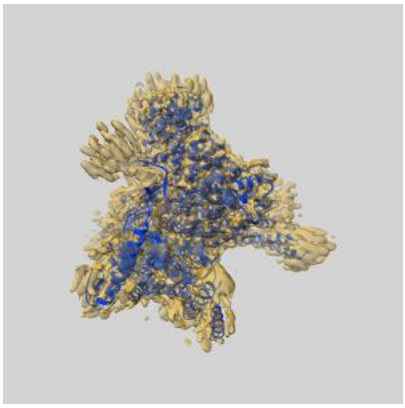
9.1 Map-model overlay



X



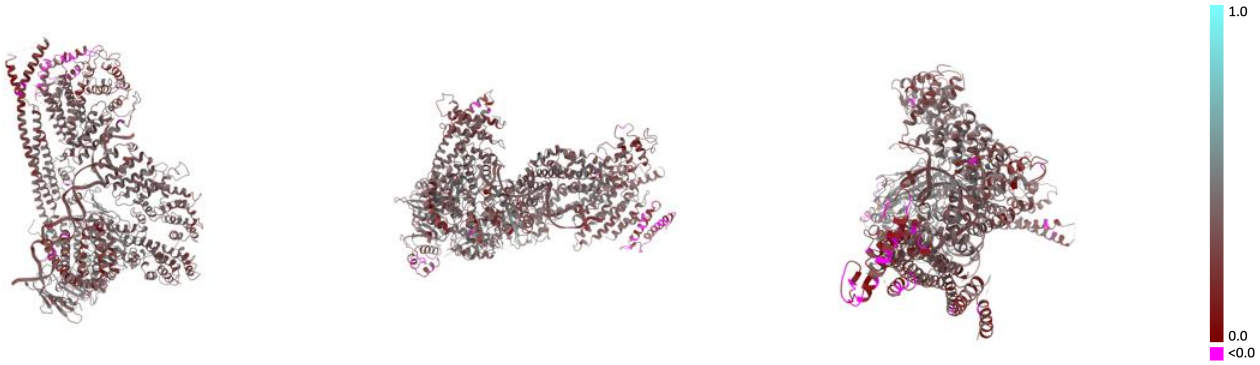
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

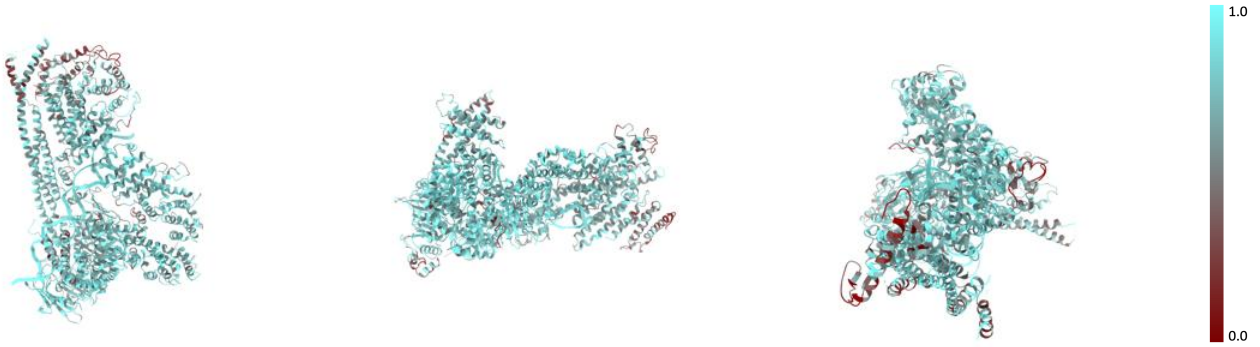
9.2 Q-score mapped to coordinate model (i)



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.

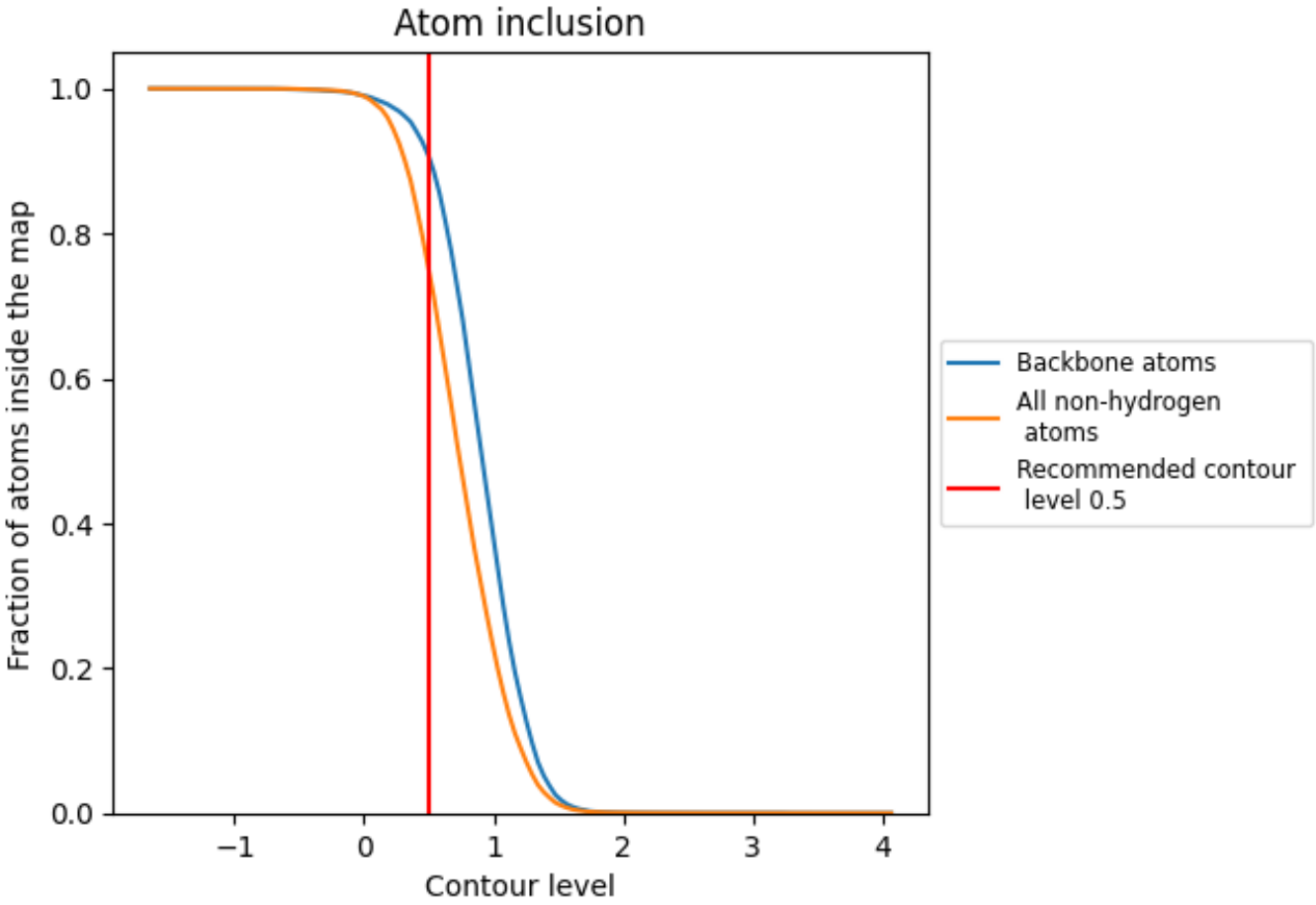
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 75% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7499	0.3480
A	0.7997	0.3990
B	0.6826	0.3130
C	0.7816	0.3820
D	0.7100	0.3290
X	0.9088	0.3100
Y	0.9220	0.3230