



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:33 AM UTC

PDB ID : 7VWZ / pdb_00007vwz
EMDB ID : EMD-32166
Title : Cryo-EM structure of Rob-dependent transcription activation complex in a unique conformation
Authors : Lin, W.; Feng, Y.; Shi, J.
Deposited on : 2021-11-12
Resolution : 4.00 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:

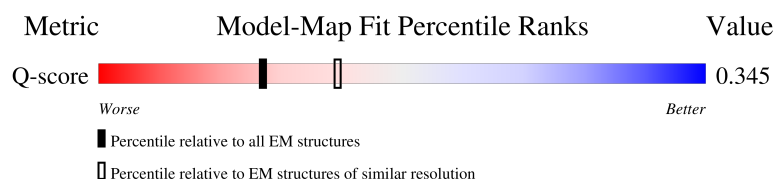
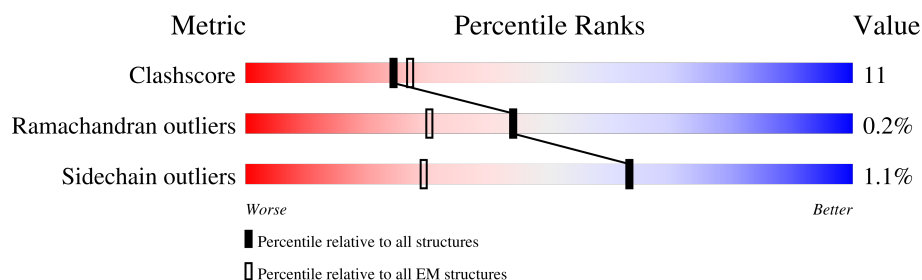
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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 $\leq 5\%$. 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	329	
1	B	329	
2	C	1342	
3	D	1407	

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Mol	Chain	Length	Quality of chain
4	E	91	
5	F	613	
6	1	70	
7	2	70	
8	G	289	
8	I	289	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 34509 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	311	Total	C	N	O	S	0	0
			2418	1512	425	473	8		
1	B	228	Total	C	N	O	S	0	0
			1767	1100	312	349	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1339	Total	C	N	O	S	0	0
			10550	6621	1834	2052	43		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1332	Total	C	N	O	S	0	0
			10361	6508	1848	1955	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	478	Total	C	N	O	S	0	0
			3879	2425	693	738	23		

- Molecule 6 is a DNA chain called micF promoter DNA forward strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	65	Total	C	N	O	P	0	0
			1330	634	254	378	64		

- Molecule 7 is a DNA chain called micF promoter DNA reverse strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	2	64	Total	C	N	O	P	0	0
			1324	631	236	393	64		

- Molecule 8 is a protein called Right origin-binding protein.

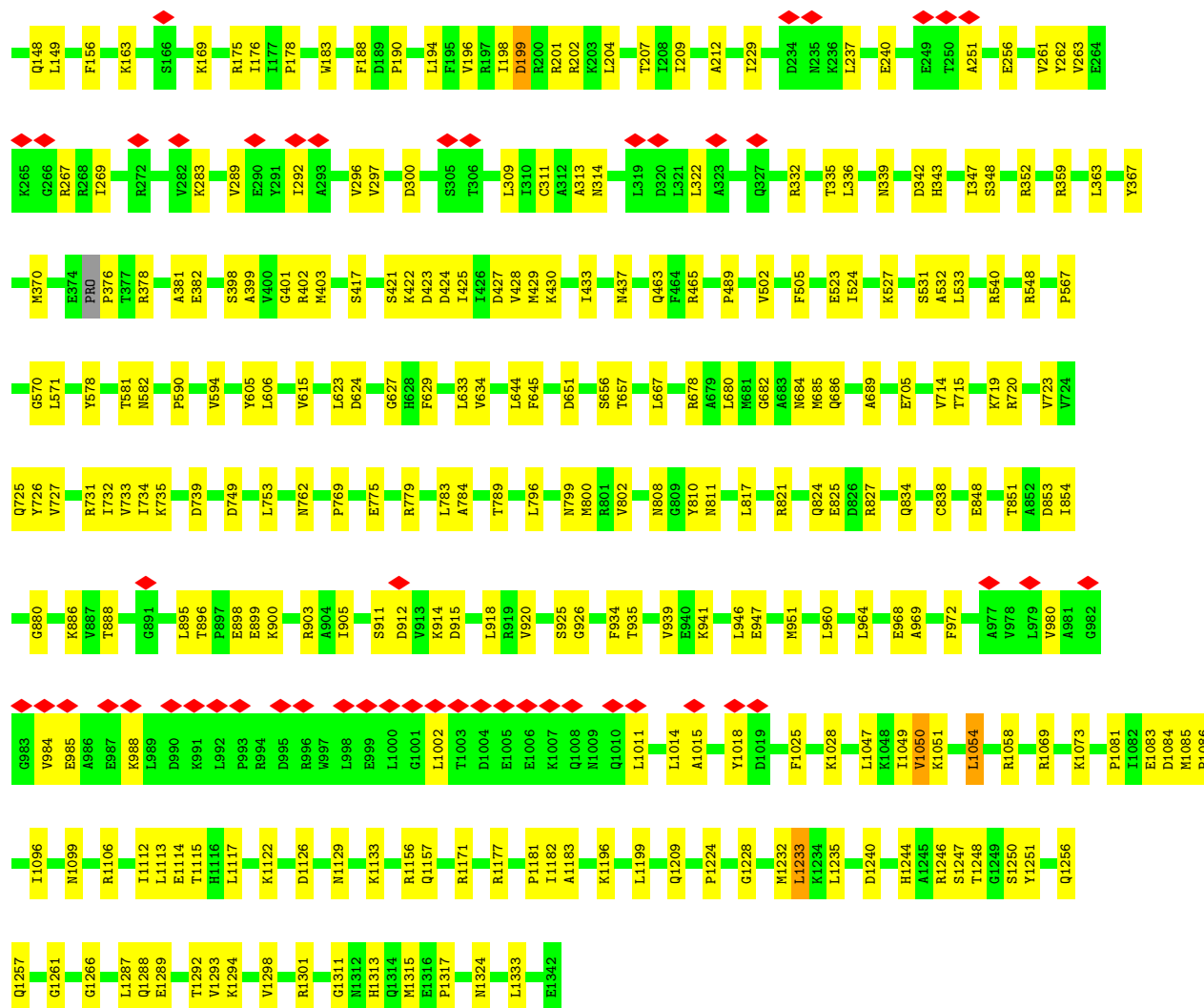
Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	114	Total	C	N	O	S	0	0
			923	596	173	153	1		
8	I	164	Total	C	N	O	S	0	0
			1327	842	220	256	9		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

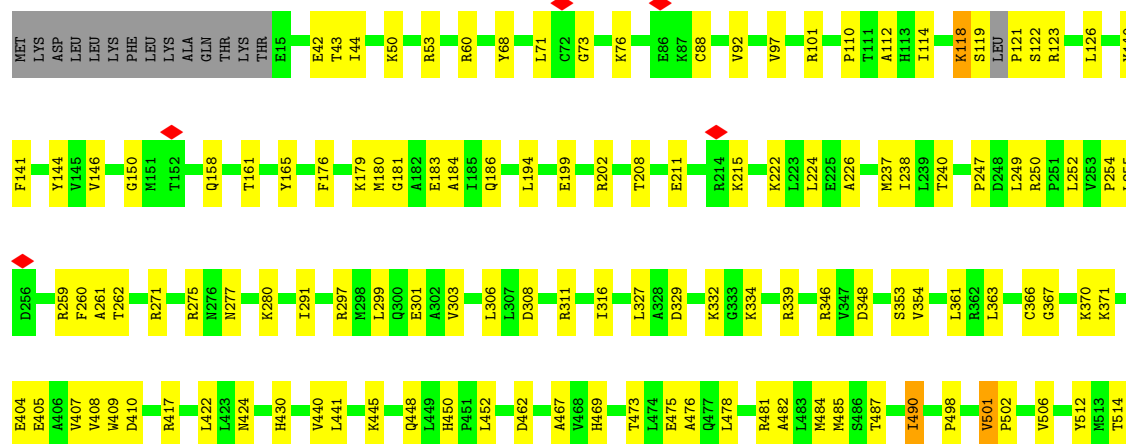
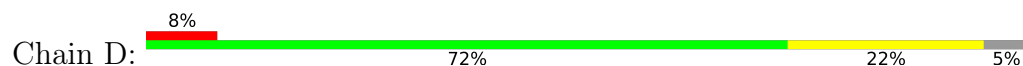
Mol	Chain	Residues	Atoms		AltConf
9	D	2	Total	Zn	0
			2	2	

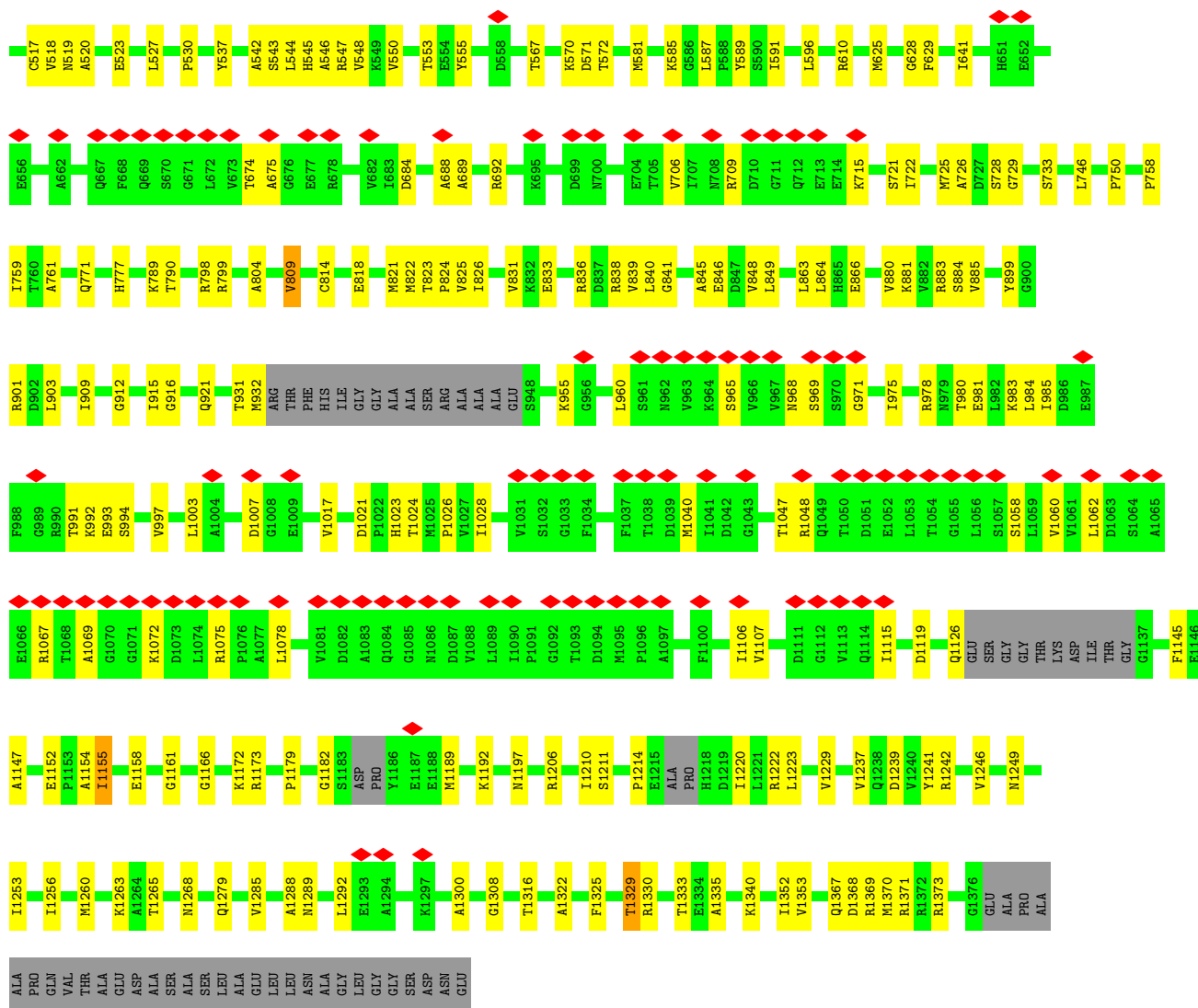
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

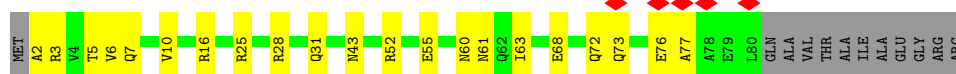


• Molecule 3: DNA-directed RNA polymerase subunit beta'

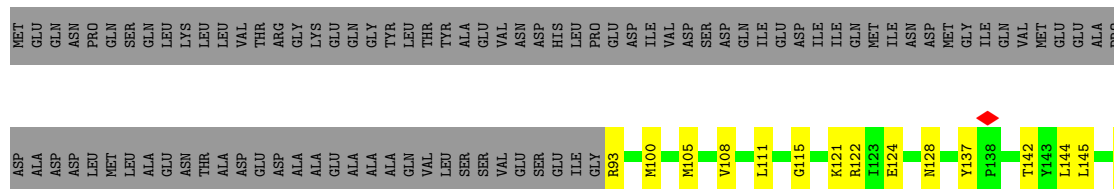




• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD





MET ASP GLN ALA GLY ILE ILE ARG ASP LEU LEU ILE TRP LEU LEU GLY HIS LEU ASP GLN PRO LEU SER LEU ASP ASN VAL ALA LYS ALA GLY TYR SER LYS TRP HIS LEU GLN ARG MET PHE LYS ASP VAL THR HIS ALA ILE GLY TYR ILE ARG ARG ARG LEU SER

LYS SER VAL ALA LEU ARG LEU THR ARG PRO ILE LEU ASP ILE ALA LEU GLN TYR ARG PHE ASP SER GLN GLN THR PHE THR ARG ALA PHE LYS LYS PHE ALA GLN THR PRO ALA LEU TVR ARG ARG SER PRO GLU TRP SER ALA PHE GLY ILE ARG PRO PRO ARG LEU ARG LEU

GLY E122 P126 E127 H128 K129 F130 V131 T132 L133 E134 D136 T136 F137 L138 I139 G140 V141 T142 Q143 S144 Y146 C147 S148 L149 E150 Q151 I152 S153 D154 F155 R156 H157 E158 M159 R160 Y161 Q162 F163 W164 H165 D166 F167 L168 G169 M170 A171 P172 T173 I174 P176 V177 L178 Y179 G180 L181 N182

E183 T184 R185 P186 S187 Q188 D191 Q194 E195 V196 F197 Y198 T199 T200 A201 L202 A203 Q204 D205 Q206 A207 D208 G209 Y210 V211 L212 T213 G214 H215 P216 V217 M218 L219 Q220 C221 G222 E223 Y224 V225 M226 F227 T228 Y229 E230 G231 L232 G233 T234 G235 V236 Q237 E238 F239 I240 L241 T242 V243 Y244

G245 T246 C247 M248 P249 M250 L251 N252 L253 T254 R255 R256 K257 G258 Q259 D260 I261 E262 R263 Y264 Y265 P266 A267 E268 D269 ALA LYS ALA GLY D274 R275 P276 I277 N278 L279 R280 C281 E282 L283 L284 I285 P286 I287 R288 R289

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	335021	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size ($\text{\AA}$)	264.0, 264.0, 264.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	0.25	0/2449	0.56	0/3318
1	B	0.26	0/1789	0.58	0/2425
2	C	0.28	0/10717	0.61	4/14458 (0.0%)
3	D	0.29	0/10513	0.63	1/14185 (0.0%)
4	E	0.24	0/629	0.56	0/847
5	F	0.26	0/3929	0.67	5/5277 (0.1%)
6	1	0.30	0/1495	0.51	0/2304
7	2	0.31	0/1484	0.52	0/2293
8	G	0.26	0/944	0.69	1/1273 (0.1%)
8	I	0.25	0/1359	0.59	1/1845 (0.1%)
All	All	0.28	0/35308	0.61	12/48225 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	G	18	LEU	N-CA-C	-8.03	103.05	113.17
5	F	505	ILE	N-CA-C	6.96	117.72	110.62
3	D	490	ILE	N-CA-C	-6.95	106.01	112.96
2	C	347	ILE	N-CA-C	-6.92	107.13	113.71
5	F	500	ILE	N-CA-C	-6.65	107.01	113.53
2	C	1261	GLY	N-CA-C	6.15	118.31	112.04
8	I	244	TYR	N-CA-C	5.94	120.66	113.17
5	F	295	CYS	N-CA-C	5.18	116.62	111.07
2	C	825	GLU	CA-C-N	5.10	131.28	121.54
2	C	825	GLU	C-N-CA	5.10	131.28	121.54
5	F	529	GLU	CA-C-N	-5.02	113.36	120.49
5	F	529	GLU	C-N-CA	-5.02	113.36	120.49

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	2418	0	2467	45	0
1	B	1767	0	1789	37	0
2	C	10550	0	10558	196	0
3	D	10361	0	10580	235	0
4	E	627	0	634	16	0
5	F	3879	0	3931	74	0
6	1	1330	0	730	60	0
7	2	1324	0	727	31	0
8	G	923	0	944	68	0
8	I	1327	0	1267	35	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	34509	0	33627	724	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 11.

All (724) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:VAL:HB	1:B:195:ARG:O	1.37	1.18
8:G:18:LEU:HD11	8:G:57:ARG:CB	1.74	1.17
2:C:796:LEU:HD11	2:C:1233:LEU:HD23	1.32	1.10
6:1:55:DC:H2''	6:1:56:DA:O5'	1.46	1.08
2:C:796:LEU:CD1	2:C:1233:LEU:HD23	1.85	1.07
3:D:537:TYR:HA	3:D:542:ALA:HB3	1.10	1.07
3:D:520:ALA:HB1	3:D:543:SER:HB3	1.11	1.06
3:D:537:TYR:CA	3:D:542:ALA:HB3	1.85	1.05
3:D:1155:ILE:HG23	3:D:1210:ILE:HG13	1.36	1.05
8:G:6:ILE:HD12	8:I:246:THR:HG21	1.34	1.05
3:D:520:ALA:CB	3:D:543:SER:HB3	1.88	1.03
3:D:121:PRO:CB	3:D:126:LEU:HD22	1.88	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:18:LEU:HD11	8:G:57:ARG:HB2	1.02	0.99
6:1:84:DG:H2''	6:1:85:DA:H5'	1.43	0.99
3:D:1155:ILE:CG2	3:D:1210:ILE:HG13	1.94	0.98
5:F:330:LEU:HD11	5:F:333:VAL:CG1	1.92	0.98
3:D:520:ALA:HB1	3:D:543:SER:CB	1.94	0.97
8:G:42:PHE:CZ	8:G:50:ILE:HD13	1.99	0.97
8:G:57:ARG:O	8:G:61:LYS:HB2	1.64	0.96
8:G:18:LEU:CD1	8:G:57:ARG:HB2	1.97	0.93
2:C:796:LEU:HD11	2:C:1233:LEU:CD2	1.98	0.92
2:C:367:TYR:CE2	2:C:376:PRO:HB3	2.04	0.92
8:G:56:ALA:HB1	8:G:115:ARG:HB3	1.51	0.91
5:F:330:LEU:HD11	5:F:333:VAL:HG11	1.53	0.89
2:C:633:LEU:HD23	2:C:633:LEU:H	1.36	0.88
3:D:1155:ILE:HG12	3:D:1210:ILE:HD11	1.54	0.86
8:G:56:ALA:CB	8:G:115:ARG:HG2	2.05	0.86
8:G:18:LEU:HD12	8:G:61:LYS:HG3	1.57	0.85
3:D:121:PRO:HB3	3:D:126:LEU:HD22	1.58	0.85
8:G:57:ARG:O	8:G:61:LYS:CB	2.24	0.85
5:F:330:LEU:CD1	5:F:333:VAL:HG11	2.07	0.85
5:F:330:LEU:CD1	5:F:333:VAL:CG1	2.55	0.84
2:C:198:ILE:H	2:C:201:ARG:HB2	1.43	0.83
3:D:520:ALA:CB	3:D:543:SER:CB	2.54	0.82
3:D:517:CYS:SG	3:D:519:ASN:ND2	2.53	0.82
3:D:121:PRO:HB2	3:D:126:LEU:HD22	1.59	0.81
3:D:1155:ILE:HG23	3:D:1210:ILE:CG1	2.10	0.81
3:D:520:ALA:HB3	3:D:546:ALA:HB2	1.63	0.80
7:2:16:DG:O6	7:2:17:DA:N6	2.15	0.80
5:F:474:MET:HG3	5:F:476:ARG:O	1.81	0.80
2:C:834:GLN:HB3	2:C:1054:LEU:CD2	2.13	0.79
3:D:518:VAL:CG2	3:D:709:ARG:HG2	2.13	0.78
8:G:56:ALA:HB1	8:G:115:ARG:CB	2.13	0.78
6:1:85:DA:H2''	6:1:86:DT:O4'	1.84	0.77
3:D:537:TYR:HA	3:D:542:ALA:CB	2.05	0.76
8:G:50:ILE:O	8:G:54:ILE:HG13	1.86	0.76
5:F:505:ILE:HD12	5:F:505:ILE:H	1.50	0.75
3:D:119:SER:O	3:D:122:SER:HA	1.87	0.75
8:G:18:LEU:CD1	8:G:57:ARG:CB	2.59	0.75
8:G:53:TYR:O	8:G:57:ARG:HG2	1.86	0.75
1:B:192:VAL:HB	1:B:195:ARG:C	2.11	0.74
2:C:834:GLN:HB3	2:C:1054:LEU:HD21	1.70	0.74
6:1:30:DG:H1	7:2:61:DC:H42	1.33	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:31:DC:O2	6:1:32:DA:C8	2.41	0.73
6:1:80:DC:N3	6:1:81:DA:C6	2.56	0.73
2:C:1233:LEU:N	2:C:1233:LEU:HD12	2.01	0.73
6:1:31:DC:H41	8:G:36:TRP:CB	2.01	0.73
3:D:512:TYR:CE2	3:D:544:LEU:HD23	2.24	0.72
3:D:520:ALA:CB	3:D:546:ALA:HB2	2.19	0.72
2:C:131:THR:HG23	2:C:133:ASN:H	1.54	0.72
8:G:6:ILE:HD12	8:I:246:THR:CG2	2.17	0.72
5:F:488:LEU:HD12	5:F:488:LEU:O	1.88	0.71
8:G:57:ARG:HA	8:G:60:SER:OG	1.90	0.71
1:B:192:VAL:CB	1:B:195:ARG:O	2.28	0.71
8:G:57:ARG:O	8:G:61:LYS:N	2.22	0.71
5:F:470:MET:O	5:F:474:MET:HG2	1.92	0.70
1:B:194:GLN:O	1:B:195:ARG:HG3	1.93	0.69
2:C:198:ILE:HB	2:C:201:ARG:HG3	1.73	0.69
3:D:809:VAL:HG13	3:D:915:ILE:HD11	1.75	0.68
3:D:841:GLY:HA2	3:D:901:ARG:HD3	1.74	0.68
8:G:18:LEU:CD1	8:G:57:ARG:C	2.67	0.67
2:C:367:TYR:CD2	2:C:376:PRO:HB3	2.30	0.67
6:1:55:DC:H2''	6:1:56:DA:C5'	2.24	0.67
8:G:6:ILE:HB	8:I:246:THR:HG23	1.77	0.67
7:2:35:DT:H2''	7:2:36:DG:O5'	1.95	0.66
2:C:1069:ARG:NH2	2:C:1114:GLU:OE2	2.29	0.66
6:1:51:DC:H2''	6:1:52:DC:O5'	1.95	0.66
8:G:56:ALA:HB1	8:G:115:ARG:CG	2.24	0.66
3:D:53:ARG:HH21	3:D:88:CYS:HA	1.60	0.66
6:1:80:DC:C4	6:1:81:DA:N6	2.64	0.65
2:C:198:ILE:O	2:C:201:ARG:HG2	1.95	0.65
2:C:633:LEU:H	2:C:633:LEU:CD2	2.09	0.65
8:G:56:ALA:HB1	8:G:115:ARG:HG2	1.77	0.65
6:1:85:DA:N6	7:2:5:DA:N6	2.45	0.65
6:1:80:DC:C2'	6:1:81:DA:C8	2.80	0.64
7:2:16:DG:C6	7:2:17:DA:N6	2.66	0.64
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.71	0.64
8:G:5:GLY:C	8:I:245:GLY:H	2.06	0.64
2:C:178:PRO:HD2	2:C:183:TRP:HD1	1.61	0.64
3:D:518:VAL:HG21	3:D:709:ARG:HG2	1.78	0.64
3:D:1154:ALA:CB	3:D:1214:PRO:O	2.45	0.64
8:G:45:VAL:HG21	8:I:244:TYR:O	1.98	0.64
7:2:17:DA:H1'	7:2:18:DG:C2	2.32	0.64
2:C:156:PHE:HB3	2:C:175:ARG:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:SER:O	3:D:123:ARG:HB2	1.96	0.63
6:1:85:DA:C5	6:1:86:DT:C4	2.86	0.63
8:G:7:ILE:H	8:I:245:GLY:HA3	1.62	0.63
1:B:61:ILE:HG23	1:B:142:MET:HB3	1.81	0.63
3:D:1161:GLY:HA3	3:D:1179:PRO:HA	1.80	0.62
8:G:58:ARG:HG2	8:G:80:TYR:O	2.00	0.62
2:C:196:VAL:HG11	2:C:209:ILE:HD11	1.81	0.62
1:B:131:CYS:SG	1:B:132:HIS:N	2.72	0.62
2:C:1115:THR:HG23	2:C:1228:GLY:HA3	1.82	0.62
3:D:194:LEU:HD22	3:D:224:LEU:HD22	1.82	0.62
3:D:520:ALA:HB2	3:D:543:SER:OG	2.00	0.62
3:D:1155:ILE:HG12	3:D:1210:ILE:CD1	2.28	0.61
3:D:110:PRO:HB3	3:D:240:THR:HG22	1.81	0.61
6:1:80:DC:H2''	6:1:81:DA:C8	2.36	0.61
6:1:80:DC:C2	6:1:81:DA:C5	2.87	0.61
6:1:84:DG:C2'	6:1:85:DA:H5'	2.25	0.61
2:C:834:GLN:HG2	2:C:1054:LEU:HD21	1.82	0.61
3:D:271:ARG:HH12	3:D:316:ILE:HG21	1.66	0.61
1:A:190:ALA:H	1:A:199:ASP:HA	1.67	0.60
2:C:1313:HIS:O	4:E:28:ARG:NH2	2.34	0.60
5:F:465:ARG:HA	5:F:468:ARG:HH21	1.66	0.60
7:2:45:DG:H2''	7:2:46:DT:O5'	2.02	0.60
2:C:633:LEU:HD23	2:C:633:LEU:N	2.15	0.60
2:C:1298:VAL:HA	2:C:1301:ARG:HG2	1.84	0.60
5:F:161:LEU:HD11	5:F:265:GLN:HB2	1.84	0.60
6:1:80:DC:H2'	6:1:81:DA:C8	2.37	0.60
5:F:142:THR:HG21	5:F:232:ARG:HH22	1.68	0.59
2:C:726:TYR:HB3	2:C:733:VAL:HB	1.83	0.59
5:F:166:VAL:HG23	5:F:259:PHE:HA	1.84	0.59
1:B:81:ILE:HG12	1:B:131:CYS:HB2	1.84	0.59
2:C:719:LYS:O	2:C:779:ARG:NH1	2.36	0.59
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.36	0.59
6:1:85:DA:N7	6:1:86:DT:C4	2.71	0.59
2:C:1113:LEU:HD11	3:D:641:ILE:HD12	1.84	0.59
3:D:371:LYS:HE3	3:D:445:LYS:HE2	1.85	0.59
3:D:822:MET:SD	3:D:838:ARG:NH2	2.75	0.59
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.36	0.59
3:D:518:VAL:HG22	3:D:709:ARG:HG2	1.85	0.58
7:2:16:DG:H2'	7:2:17:DA:H5'	1.84	0.58
8:I:237:GLN:O	8:I:241:LEU:N	2.36	0.58
6:1:31:DC:C2	6:1:32:DA:C8	2.92	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:899:TYR:HB3	3:D:909:ILE:HG21	1.86	0.58
1:A:28:LEU:HD23	1:A:201:LEU:HD23	1.84	0.58
3:D:261:ALA:HB2	5:F:505:ILE:HD13	1.86	0.58
3:D:1206:ARG:NH2	3:D:1223:LEU:O	2.36	0.58
5:F:124:GLU:O	5:F:128:ASN:N	2.31	0.58
1:B:96:ASP:OD1	1:B:148:ARG:NH1	2.37	0.58
3:D:1173:ARG:HB2	3:D:1192:LYS:HD2	1.85	0.58
5:F:270:VAL:O	5:F:274:ARG:N	2.32	0.58
3:D:506:VAL:HG12	3:D:628:GLY:HA3	1.85	0.58
1:A:592:THR:OG1	1:A:593:VAL:N	2.37	0.57
5:F:145:LEU:HD21	5:F:225:ARG:HG2	1.84	0.57
2:C:834:GLN:CG	2:C:1054:LEU:HD21	2.34	0.57
2:C:821:ARG:NH1	2:C:824:GLN:OE1	2.37	0.57
3:D:475:GLU:OE2	4:E:28:ARG:NH1	2.37	0.57
6:1:38:DT:O4	7:2:52:DC:N4	2.36	0.57
3:D:1179:PRO:HB2	3:D:1182:GLY:H	1.70	0.57
6:1:85:DA:H2''	6:1:86:DT:C5'	2.33	0.57
3:D:839:VAL:HG13	3:D:864:LEU:HD13	1.85	0.57
8:G:12:ILE:H	8:I:149:LEU:HD22	1.70	0.57
8:G:57:ARG:HG3	8:G:57:ARG:HH11	1.70	0.57
1:A:604:ILE:HG23	1:A:609:ASP:HB3	1.87	0.57
2:C:402:ARG:NH1	2:C:417:SER:O	2.38	0.57
3:D:520:ALA:HB2	3:D:543:SER:CB	2.35	0.57
3:D:824:PRO:HB2	3:D:826:ILE:HG23	1.86	0.57
6:1:30:DG:H1'	6:1:31:DC:C5	2.40	0.57
5:F:227:GLN:HB3	5:F:252:LEU:HD13	1.87	0.57
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.87	0.56
6:1:30:DG:N2	7:2:62:DT:O2	2.37	0.56
1:A:101:THR:HG1	1:A:116:THR:HG1	1.45	0.56
3:D:836:ARG:NH2	3:D:866:GLU:OE2	2.38	0.56
8:G:5:GLY:N	8:I:246:THR:H	2.03	0.56
2:C:848:GLU:OE1	2:C:886:LYS:NZ	2.37	0.56
6:1:85:DA:C8	6:1:86:DT:C5	2.93	0.56
3:D:252:LEU:HG	3:D:262:THR:HG22	1.87	0.56
3:D:519:ASN:OD1	3:D:520:ALA:N	2.39	0.56
2:C:256:GLU:HA	2:C:261:VAL:HA	1.87	0.56
2:C:725:GLN:HG3	2:C:735:LYS:HB2	1.87	0.56
2:C:834:GLN:CB	2:C:1054:LEU:HD21	2.36	0.56
3:D:306:LEU:HB3	3:D:327:LEU:HD12	1.87	0.56
5:F:93:ARG:NH1	7:2:7:DC:OP1	2.39	0.56
5:F:596:ARG:NH2	8:G:75:ASP:OD1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HB2	1:B:144:ILE:HB	1.88	0.55
3:D:146:VAL:HG12	3:D:158:GLN:H	1.71	0.55
3:D:1220:ILE:HG23	3:D:1229:VAL:HG22	1.88	0.55
6:1:31:DC:H41	8:G:36:TRP:HB2	1.72	0.55
8:G:5:GLY:N	8:I:246:THR:N	2.54	0.55
3:D:407:VAL:HA	3:D:410:ASP:HB2	1.86	0.55
3:D:750:PRO:HD3	3:D:777:HIS:HB3	1.88	0.55
3:D:983:LYS:HA	3:D:994:SER:HA	1.87	0.55
8:G:20:GLN:O	8:G:81:ARG:NH2	2.40	0.55
2:C:985:GLU:HB2	2:C:988:LYS:HB2	1.89	0.55
6:1:74:DA:OP1	6:1:75:DG:N2	2.40	0.55
2:C:727:VAL:HA	2:C:732:ILE:HG22	1.88	0.55
3:D:334:LYS:HB3	3:D:339:ARG:HD2	1.88	0.55
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.89	0.55
3:D:523:GLU:OE2	3:D:547:ARG:NH1	2.39	0.55
3:D:1155:ILE:HG21	3:D:1210:ILE:HG13	1.82	0.55
6:1:33:DC:H42	7:2:57:DA:H61	1.54	0.55
1:A:225:ALA:HA	1:A:228:LEU:HB2	1.89	0.55
2:C:339:ASN:O	2:C:343:HIS:N	2.40	0.55
2:C:838:CYS:HB2	2:C:918:LEU:HD22	1.89	0.55
2:C:980:VAL:HA	2:C:984:VAL:HB	1.88	0.55
2:C:229:ILE:HG23	2:C:332:ARG:HG3	1.88	0.55
7:2:16:DG:C2'	7:2:17:DA:H5'	2.37	0.55
3:D:684:ASP:O	3:D:688:ALA:N	2.37	0.55
5:F:333:VAL:O	5:F:337:VAL:HG23	2.07	0.55
8:G:42:PHE:CD2	8:G:50:ILE:HB	2.42	0.55
8:G:5:GLY:O	8:I:243:VAL:N	2.39	0.54
2:C:1117:LEU:HD11	2:C:1182:ILE:HG21	1.89	0.54
3:D:353:SER:OG	3:D:354:VAL:N	2.40	0.54
1:A:626:LYS:NZ	6:1:28:DC:H5''	2.23	0.54
2:C:581:THR:OG1	2:C:582:ASN:N	2.40	0.54
3:D:482:ALA:HA	4:E:6:VAL:HG21	1.89	0.54
3:D:823:THR:O	3:D:838:ARG:NH1	2.40	0.54
8:G:42:PHE:CE1	8:G:50:ILE:HD13	2.43	0.54
1:B:158:ARG:HB3	1:B:172:LEU:HD21	1.89	0.54
2:C:531:SER:OG	2:C:532:ALA:N	2.40	0.54
3:D:473:THR:HG23	3:D:476:ALA:H	1.72	0.54
2:C:422:LYS:HA	2:C:425:ILE:HD12	1.90	0.54
2:C:1196:LYS:HA	2:C:1199:LEU:HB2	1.90	0.54
3:D:277:ASN:HA	3:D:280:LYS:HZ3	1.73	0.54
8:G:34:SER:OG	8:G:35:LYS:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:97:ARG:HG2	2:C:123:TYR:HB2	1.90	0.54
2:C:202:ARG:O	2:C:204:LEU:HG	2.08	0.54
3:D:1155:ILE:CG2	3:D:1210:ILE:CG1	2.77	0.54
3:D:1268:ASN:HB2	3:D:1300:ALA:HA	1.90	0.54
2:C:1288:GLN:O	2:C:1292:THR:OG1	2.25	0.53
2:C:58:PRO:HB3	2:C:69:GLN:HG2	1.90	0.53
3:D:981:GLU:HA	3:D:997:VAL:HG22	1.90	0.53
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	1.89	0.53
5:F:144:LEU:O	5:F:148:TYR:N	2.38	0.53
2:C:1247:SER:OG	2:C:1248:THR:N	2.41	0.53
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.89	0.53
3:D:932:MET:SD	3:D:932:MET:N	2.81	0.53
1:A:157:THR:O	1:A:161:SER:N	2.39	0.53
2:C:1246:ARG:NH2	2:C:1250:SER:O	2.41	0.53
3:D:519:ASN:HD21	3:D:545:HIS:CE1	2.27	0.53
2:C:1129:ASN:O	2:C:1133:LYS:NZ	2.41	0.53
8:G:115:ARG:NH1	8:G:116:PRO:O	2.41	0.53
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.91	0.53
2:C:802:VAL:N	2:C:1228:GLY:O	2.42	0.53
8:G:119:ARG:NH2	8:I:194:GLN:O	2.41	0.53
2:C:237:LEU:HD22	2:C:289:VAL:HA	1.89	0.53
8:I:256:ARG:HB3	8:I:288:ARG:HB3	1.91	0.53
1:A:32:GLU:HA	1:A:198:LEU:HD22	1.90	0.52
2:C:775:GLU:OE1	2:C:1171:ARG:NH2	2.43	0.52
3:D:1172:LYS:HD2	3:D:1189:MET:HB2	1.91	0.52
5:F:330:LEU:HD11	5:F:333:VAL:HG13	1.86	0.52
1:A:59:VAL:HG12	1:A:144:ILE:HG22	1.91	0.52
3:D:1241:TYR:HB3	3:D:1246:VAL:HB	1.92	0.52
6:1:31:DC:N4	8:G:36:TRP:CB	2.70	0.52
7:2:17:DA:OP2	7:2:17:DA:H3'	2.09	0.52
8:G:18:LEU:HD12	8:G:61:LYS:CG	2.34	0.52
1:A:100:LEU:HD21	1:A:121:VAL:HG21	1.90	0.52
3:D:722:ILE:HA	3:D:725:MET:HE2	1.90	0.52
8:G:99:THR:HG22	8:G:101:ALA:H	1.75	0.52
1:B:51:MET:HE3	1:B:52:PRO:HD2	1.91	0.52
2:C:14:ASP:HB3	2:C:1157:GLN:HG2	1.90	0.52
5:F:240:ARG:HH22	5:F:353:LEU:HA	1.75	0.52
5:F:254:GLU:HA	5:F:257:LYS:HB2	1.90	0.52
2:C:149:LEU:N	2:C:531:SER:O	2.41	0.52
2:C:424:ASP:HA	2:C:427:ASP:HB2	1.91	0.52
3:D:43:THR:OG1	3:D:44:ILE:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:404:GLU:OE2	3:D:409:TRP:NE1	2.34	0.52
3:D:424:ASN:HB3	3:D:467:ALA:HB3	1.91	0.52
8:I:183:GLU:HB3	8:I:197:PHE:HB2	1.92	0.52
2:C:97:ARG:HA	2:C:123:TYR:HA	1.91	0.52
3:D:367:GLY:HA3	3:D:448:GLN:HB3	1.92	0.52
1:B:189:ALA:O	1:B:200:LYS:NZ	2.42	0.52
3:D:1023:HIS:HB3	3:D:1126:GLN:H	1.74	0.52
2:C:734:ILE:HG22	2:C:749:ASP:HB2	1.91	0.52
6:1:85:DA:N6	7:2:5:DA:C6	2.78	0.52
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.92	0.52
3:D:114:ILE:HD11	3:D:118:LYS:HG2	1.92	0.52
3:D:571:ASP:OD1	3:D:571:ASP:N	2.38	0.52
3:D:1147:ALA:HB3	3:D:1308:GLY:HA2	1.91	0.52
3:D:140:TYR:HD1	5:F:100:MET:HE1	1.75	0.51
5:F:105:MET:HE1	5:F:388:ILE:HG13	1.92	0.51
6:1:31:DC:N4	8:G:36:TRP:HB3	2.24	0.51
8:G:42:PHE:CE2	8:G:50:ILE:HD13	2.43	0.51
1:A:215:GLU:OE2	1:A:219:ARG:NH2	2.43	0.51
2:C:1256:GLN:O	2:C:1301:ARG:NH2	2.42	0.51
3:D:809:VAL:HG23	3:D:912:GLY:H	1.75	0.51
5:F:238:LYS:NZ	5:F:241:SER:O	2.40	0.51
2:C:723:VAL:HB	2:C:735:LYS:HB3	1.92	0.51
2:C:851:THR:HG22	2:C:853:ASP:H	1.75	0.51
3:D:481:ARG:HA	3:D:485:MET:HE2	1.93	0.51
6:1:31:DC:O2	6:1:32:DA:H8	1.89	0.51
1:A:37:HIS:HB2	1:B:45:ARG:HH22	1.76	0.51
2:C:769:PRO:HA	2:C:784:ALA:HA	1.92	0.51
2:C:1122:LYS:O	2:C:1126:ASP:N	2.44	0.51
3:D:417:ARG:NH2	4:E:43:ASN:OD1	2.43	0.51
3:D:1368:ASP:HA	3:D:1371:ARG:HG2	1.91	0.51
8:G:57:ARG:O	8:G:61:LYS:CG	2.58	0.51
3:D:674:THR:OG1	3:D:675:ALA:N	2.43	0.51
3:D:548:VAL:N	3:D:572:THR:O	2.41	0.51
3:D:1154:ALA:HB2	3:D:1214:PRO:O	2.10	0.51
2:C:212:ALA:HA	2:C:359:ARG:HG3	1.91	0.51
8:I:182:ASN:HB3	8:I:260:ASP:HB2	1.93	0.51
3:D:422:LEU:HB2	3:D:469:HIS:HB2	1.93	0.51
8:G:58:ARG:HB3	8:G:82:PHE:CZ	2.45	0.51
8:I:261:ILE:HD12	8:I:284:LEU:HD23	1.93	0.51
3:D:68:TYR:HD1	3:D:92:VAL:HG12	1.76	0.51
3:D:1060:VAL:HG13	3:D:1106:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:257:LYS:O	5:F:260:ARG:NH2	2.42	0.51
8:I:255:ARG:HE	8:I:286:PRO:HD2	1.76	0.51
2:C:31:GLN:NE2	2:C:527:LYS:O	2.44	0.51
2:C:339:ASN:HB3	2:C:343:HIS:H	1.76	0.51
3:D:141:PHE:O	3:D:297:ARG:NH2	2.45	0.50
3:D:183:GLU:HA	3:D:186:GLN:HB2	1.94	0.50
3:D:1154:ALA:N	3:D:1214:PRO:O	2.45	0.50
1:A:15:ASP:OD1	1:A:27:THR:OG1	2.29	0.50
1:A:133:LEU:HD21	1:A:140:ILE:HD11	1.92	0.50
1:B:86:LYS:HZ3	1:B:174:ASP:H	1.57	0.50
1:B:194:GLN:O	1:B:195:ARG:CG	2.59	0.50
2:C:148:GLN:NE2	2:C:533:LEU:O	2.44	0.50
2:C:656:SER:OG	2:C:657:THR:N	2.43	0.50
6:1:80:DC:C4	6:1:81:DA:C6	3.00	0.50
3:D:689:ALA:HA	3:D:692:ARG:HD3	1.92	0.50
5:F:261:LEU:HD12	5:F:266:PHE:HD1	1.76	0.50
6:1:82:DC:N3	7:2:9:DG:N2	2.59	0.50
1:B:10:LYS:HE2	1:B:12:ARG:HH22	1.76	0.50
5:F:576:VAL:HG11	5:F:587:ILE:HG21	1.92	0.50
6:1:47:DA:C2	7:2:45:DG:C6	3.00	0.50
3:D:818:GLU:HG3	3:D:845:ALA:HB1	1.93	0.50
1:A:619:LEU:HD13	1:A:624:LEU:HB3	1.94	0.50
3:D:517:CYS:SG	3:D:519:ASN:CG	2.95	0.50
1:A:92:VAL:O	1:A:148:ARG:NH2	2.44	0.50
3:D:260:PHE:O	5:F:505:ILE:HD12	2.11	0.50
3:D:1330:ARG:O	3:D:1333:THR:OG1	2.29	0.50
3:D:150:GLY:H	3:D:176:PHE:HA	1.77	0.50
5:F:330:LEU:HD12	5:F:333:VAL:HG11	1.90	0.50
2:C:16:GLY:HA3	2:C:1156:ARG:HH21	1.77	0.50
2:C:300:ASP:HB3	2:C:309:LEU:HD21	1.94	0.50
3:D:121:PRO:HB3	3:D:126:LEU:CD2	2.38	0.50
3:D:965:SER:HB3	3:D:975:ILE:HG23	1.94	0.50
1:A:34:GLY:O	1:A:38:THR:OG1	2.30	0.49
2:C:934:PHE:HB2	2:C:1049:ILE:HB	1.94	0.49
6:1:30:DG:H1'	6:1:31:DC:C6	2.46	0.49
8:G:24:LEU:O	8:G:28:ALA:N	2.42	0.49
1:A:603:ALA:HA	8:I:234:THR:HG21	1.93	0.49
2:C:98:VAL:HG21	2:C:124:MET:HE2	1.94	0.49
2:C:314:ASN:ND2	2:C:348:SER:O	2.40	0.49
2:C:911:SER:OG	2:C:912:ASP:N	2.44	0.49
2:C:947:GLU:O	2:C:951:MET:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.44	0.49
2:C:292:ILE:HD11	2:C:322:LEU:HD22	1.94	0.49
2:C:739:ASP:OD1	2:C:739:ASP:N	2.43	0.49
2:C:802:VAL:HG22	2:C:1096:ILE:HB	1.94	0.49
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.77	0.49
3:D:512:TYR:HE2	3:D:544:LEU:HD23	1.73	0.49
3:D:955:LYS:O	3:D:992:LYS:NZ	2.43	0.49
2:C:363:LEU:HG	2:C:381:ALA:HB1	1.94	0.49
3:D:610:ARG:HE	3:D:866:GLU:HG2	1.77	0.49
3:D:790:THR:OG1	7:2:12:DA:N6	2.45	0.49
5:F:137:TYR:HA	5:F:353:LEU:HD21	1.94	0.49
1:A:626:LYS:HZ1	6:1:28:DC:H5"	1.76	0.49
3:D:821:MET:HE3	3:D:881:LYS:HG3	1.93	0.49
3:D:725:MET:O	3:D:728:SER:OG	2.28	0.49
3:D:978:ARG:HE	3:D:1197:ASN:HD21	1.61	0.49
3:D:1047:THR:HB	3:D:1062:LEU:HD11	1.94	0.49
8:G:18:LEU:HD11	8:G:57:ARG:HB3	1.84	0.49
3:D:199:GLU:HA	3:D:202:ARG:HB2	1.95	0.49
3:D:255:LEU:N	3:D:259:ARG:O	2.45	0.49
1:B:192:VAL:CG2	1:B:198:LEU:HD12	2.43	0.49
2:C:296:VAL:HB	2:C:336:LEU:HD22	1.93	0.49
2:C:427:ASP:HA	2:C:430:LYS:HB2	1.95	0.49
8:G:13:TRP:O	8:G:17:HIS:N	2.46	0.49
1:B:82:LEU:HA	1:B:85:LEU:HD12	1.94	0.49
5:F:330:LEU:HD12	5:F:333:VAL:CG1	2.40	0.49
1:A:207:THR:OG1	1:A:208:ASN:O	2.29	0.49
2:C:939:VAL:HG11	2:C:1047:LEU:HD22	1.95	0.49
3:D:308:ASP:HB3	3:D:311:ARG:HB2	1.95	0.49
5:F:249:ILE:HA	5:F:252:LEU:HB3	1.94	0.48
2:C:188:PHE:HZ	2:C:433:ILE:HG12	1.78	0.48
2:C:262:TYR:O	2:C:267:ARG:NH1	2.45	0.48
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.95	0.48
3:D:984:LEU:HB3	3:D:993:GLU:HB2	1.95	0.48
1:B:33:ARG:HH12	2:C:1081:PRO:HG3	1.78	0.48
3:D:1263:LYS:NZ	3:D:1279:GLN:OE1	2.46	0.48
4:E:5:THR:HG22	4:E:7:GLN:H	1.76	0.48
2:C:1002:LEU:HD11	2:C:1011:LEU:HD11	1.95	0.48
2:C:1015:ALA:HA	2:C:1018:TYR:HB2	1.95	0.48
4:E:60:ASN:H	4:E:63:ILE:HB	1.77	0.48
5:F:544:THR:O	5:F:548:LEU:N	2.44	0.48
6:1:30:DG:O6	8:G:40:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:505:ILE:HG22	5:F:509:THR:HG21	1.96	0.48
8:G:46:THR:HG22	8:G:120:LEU:HD11	1.96	0.48
8:I:275:ARG:HD2	8:I:276:PRO:HD2	1.95	0.48
2:C:1257:GLN:HG2	3:D:346:ARG:HB2	1.96	0.48
3:D:361:LEU:HD13	3:D:366:CYS:HA	1.95	0.48
3:D:848:VAL:HG21	3:D:880:VAL:HG23	1.96	0.48
1:A:45:ARG:HG2	2:C:1083:GLU:HB3	1.95	0.48
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.95	0.48
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.34	0.48
3:D:405:GLU:HB2	3:D:408:VAL:HG23	1.95	0.48
3:D:570:LYS:HE2	3:D:589:TYR:HB3	1.96	0.48
3:D:1155:ILE:HG22	3:D:1211:SER:HB3	1.96	0.48
4:E:10:VAL:HG21	4:E:16:ARG:HH11	1.77	0.48
7:2:17:DA:H2"	7:2:18:DG:C4	2.49	0.48
2:C:421:SER:OG	2:C:424:ASP:OD2	2.27	0.48
3:D:520:ALA:HB3	3:D:546:ALA:CB	2.39	0.48
3:D:1003:LEU:HD22	3:D:1017:VAL:HG12	1.96	0.48
3:D:1158:GLU:OE2	3:D:1222:ARG:NH2	2.40	0.48
8:I:145:TYR:HE2	8:I:198:TYR:H	1.60	0.48
2:C:127:ILE:HG22	2:C:502:VAL:HG11	1.95	0.48
3:D:291:ILE:HG23	5:F:406:GLN:HE22	1.79	0.48
3:D:1060:VAL:HG22	3:D:1106:ILE:HG23	1.95	0.48
8:I:143:GLN:NE2	8:I:159:MET:SD	2.80	0.48
1:A:234:LEU:HD21	1:B:13:LEU:H	1.78	0.47
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.96	0.47
3:D:237:MET:HE3	3:D:237:MET:HB3	1.78	0.47
3:D:517:CYS:SG	3:D:545:HIS:ND1	2.68	0.47
3:D:728:SER:OG	3:D:729:GLY:N	2.47	0.47
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.96	0.47
8:G:8:ARG:HB2	8:I:243:VAL:HB	1.96	0.47
2:C:689:ALA:HA	2:C:1235:LEU:HA	1.96	0.47
3:D:884:SER:OG	3:D:885:VAL:N	2.47	0.47
3:D:1021:ASP:HB3	3:D:1024:THR:HG22	1.96	0.47
5:F:309:ASN:ND2	5:F:314:THR:OG1	2.46	0.47
3:D:222:LYS:O	3:D:226:ALA:N	2.47	0.47
3:D:721:SER:O	3:D:721:SER:OG	2.28	0.47
3:D:1288:ALA:HA	3:D:1292:LEU:HD13	1.95	0.47
5:F:314:THR:HA	5:F:317:ASN:HB2	1.95	0.47
2:C:895:LEU:HD13	2:C:899:GLU:HB3	1.97	0.47
3:D:1069:ALA:HA	3:D:1072:LYS:HB2	1.95	0.47
5:F:505:ILE:HD12	5:F:505:ILE:N	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:473:THR:OG1	3:D:475:GLU:OE1	2.32	0.47
6:1:31:DC:C2	6:1:32:DA:N7	2.82	0.47
2:C:201:ARG:HH21	2:C:370:MET:HE3	1.79	0.47
2:C:594:VAL:HG21	2:C:629:PHE:HZ	1.80	0.47
2:C:1244:HIS:NE2	2:C:1266:GLY:O	2.37	0.47
3:D:475:GLU:HA	3:D:478:LEU:HD12	1.95	0.47
3:D:903:LEU:HD21	3:D:1249:ASN:HD22	1.79	0.47
4:E:68:GLU:O	4:E:72:GLN:N	2.47	0.47
3:D:490:ILE:HG22	3:D:498:PRO:HB3	1.95	0.47
3:D:825:VAL:HG12	3:D:833:GLU:HB3	1.96	0.47
3:D:836:ARG:HA	3:D:839:VAL:HB	1.97	0.47
3:D:1026:PRO:HB2	3:D:1028:ILE:HG23	1.96	0.47
1:A:19:VAL:HB	1:A:23:HIS:HB3	1.97	0.47
3:D:141:PHE:HE1	3:D:181:GLY:HA2	1.80	0.47
3:D:799:ARG:HE	3:D:799:ARG:HB2	1.57	0.47
6:1:85:DA:H2'	6:1:86:DT:C6	2.49	0.47
8:G:57:ARG:NH2	8:G:117:PRO:HB3	2.29	0.47
1:B:44:ARG:HD2	1:B:185:TYR:HE1	1.80	0.47
2:C:46:GLN:HG3	2:C:51:ALA:HB2	1.96	0.47
3:D:518:VAL:HG22	3:D:709:ARG:NE	2.30	0.47
4:E:2:ALA:N	4:E:5:THR:O	2.48	0.47
8:I:223:GLU:O	8:I:256:ARG:NH2	2.39	0.47
1:A:594:ARG:HH22	1:A:625:GLY:HA3	1.80	0.46
1:B:211:ILE:HD11	1:B:219:ARG:HD3	1.98	0.46
2:C:55:SER:OG	2:C:465:ARG:NH1	2.48	0.46
3:D:247:PRO:HA	3:D:250:ARG:HG3	1.97	0.46
5:F:296:LYS:HB3	5:F:297:MET:H	1.63	0.46
1:B:118:ASP:H	1:B:121:VAL:HB	1.80	0.46
2:C:896:THR:HG23	2:C:899:GLU:H	1.80	0.46
3:D:161:THR:O	3:D:165:TYR:N	2.47	0.46
3:D:512:TYR:CD2	3:D:544:LEU:HD23	2.49	0.46
5:F:370:ALA:HA	5:F:373:ARG:HB3	1.96	0.46
8:G:9:ASP:HB2	8:I:241:LEU:HD11	1.97	0.46
8:I:186:PRO:HG3	8:I:194:GLN:HE21	1.80	0.46
2:C:63:SER:OG	2:C:65:ASN:OD1	2.32	0.46
3:D:275:ARG:NH1	3:D:301:GLU:OE1	2.46	0.46
1:A:45:ARG:NH2	1:B:34:GLY:O	2.48	0.46
1:B:194:GLN:C	1:B:195:ARG:HG3	2.39	0.46
6:1:30:DG:N2	7:2:61:DC:N3	2.61	0.46
2:C:800:MET:HB3	2:C:827:ARG:HH22	1.80	0.46
2:C:1311:GLY:O	4:E:31:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:481:ARG:HH12	4:E:3:ARG:HA	1.81	0.46
8:G:56:ALA:HB3	8:G:115:ARG:HG2	1.94	0.46
3:D:179:LYS:HB2	3:D:184:ALA:HB2	1.97	0.46
2:C:93:SER:OG	2:C:94:ALA:O	2.33	0.46
3:D:826:ILE:HG22	3:D:831:VAL:HA	1.98	0.46
5:F:426:LYS:HG3	5:F:428:SER:H	1.81	0.46
2:C:342:ASP:O	2:C:437:ASN:ND2	2.49	0.46
2:C:969:ALA:HA	2:C:972:PHE:HD2	1.81	0.46
1:A:102:LEU:HB2	1:A:115:ILE:HG22	1.97	0.45
2:C:810:TYR:HB3	2:C:817:LEU:HD13	1.99	0.45
3:D:1368:ASP:OD1	3:D:1371:ARG:NH1	2.49	0.45
5:F:108:VAL:O	5:F:385:ARG:NH2	2.49	0.45
5:F:589:GLN:O	5:F:593:LYS:NZ	2.45	0.45
3:D:259:ARG:HG3	5:F:502:LYS:HG2	1.98	0.45
5:F:166:VAL:HG13	5:F:168:PRO:HD3	1.97	0.45
5:F:341:LEU:HG	5:F:345:GLN:HE22	1.81	0.45
6:1:31:DC:H41	8:G:36:TRP:HB3	1.76	0.45
6:1:75:DG:H2"	6:1:76:DC:H5"	1.98	0.45
7:2:52:DC:H2"	7:2:53:DA:C8	2.52	0.45
1:A:594:ARG:HH12	1:A:625:GLY:H	1.65	0.45
2:C:199:ASP:N	2:C:199:ASP:OD1	2.47	0.45
1:B:47:LEU:HD22	1:B:180:VAL:HG21	1.98	0.45
1:B:192:VAL:HG12	1:B:195:ARG:N	2.30	0.45
2:C:24:VAL:HG22	2:C:578:TYR:HE1	1.82	0.45
3:D:553:THR:HG23	3:D:567:THR:HB	1.98	0.45
3:D:985:ILE:HA	3:D:991:THR:HA	1.99	0.45
3:D:1352:ILE:HG13	3:D:1353:VAL:HG13	1.97	0.45
6:1:80:DC:N4	6:1:81:DA:N6	2.65	0.45
8:I:148:SER:OG	8:I:150:GLU:OE1	2.33	0.45
1:B:212:ASP:O	1:B:216:ALA:N	2.49	0.45
2:C:732:ILE:HD11	2:C:783:LEU:HB3	1.99	0.45
3:D:625:MET:HE2	3:D:625:MET:HB3	1.83	0.45
8:I:181:LEU:HD22	8:I:261:ILE:HG12	1.98	0.45
3:D:1047:THR:OG1	3:D:1048:ARG:N	2.50	0.45
6:1:82:DC:H42	7:2:9:DG:H1	1.65	0.45
1:B:82:LEU:HD11	1:B:173:VAL:HG13	1.98	0.45
3:D:50:LYS:HE2	3:D:71:LEU:HD13	1.98	0.45
3:D:527:LEU:HB2	3:D:550:VAL:HG22	1.99	0.45
1:A:27:THR:HG22	1:A:202:VAL:HG22	1.99	0.45
2:C:300:ASP:OD1	2:C:313:ALA:N	2.50	0.45
2:C:900:LYS:HG3	2:C:903:ARG:HH21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:555:TYR:HB2	3:D:585:LYS:HB3	1.98	0.45
3:D:1062:LEU:O	3:D:1067:ARG:NH2	2.40	0.45
2:C:964:LEU:O	2:C:968:GLU:N	2.45	0.45
2:C:398:SER:O	2:C:401:GLY:N	2.40	0.44
3:D:97:VAL:HB	3:D:101:ARG:HG3	1.99	0.44
5:F:333:VAL:O	5:F:333:VAL:HG22	2.17	0.44
1:A:627:LYS:N	8:G:32:GLY:O	2.50	0.44
2:C:633:LEU:HD12	2:C:644:LEU:HD13	1.98	0.44
3:D:846:GLU:HG2	3:D:881:LYS:HB2	1.98	0.44
5:F:253:SER:O	5:F:257:LYS:N	2.50	0.44
5:F:551:LEU:HD22	5:F:555:GLU:HG2	1.99	0.44
8:G:56:ALA:CB	8:G:115:ARG:CG	2.82	0.44
1:A:152:TYR:CZ	2:C:824:GLN:HA	2.51	0.44
2:C:237:LEU:HD21	2:C:292:ILE:HG23	1.98	0.44
3:D:798:ARG:HH22	3:D:1325:PHE:HB2	1.83	0.44
3:D:1322:ALA:HA	3:D:1325:PHE:HE1	1.82	0.44
2:C:731:ARG:HA	2:C:753:LEU:HG	2.00	0.44
3:D:53:ARG:HG3	3:D:60:ARG:HD2	1.99	0.44
6:1:84:DG:H2''	6:1:85:DA:C5'	2.31	0.44
1:A:582:LEU:HD22	1:A:639:ARG:HD2	1.99	0.44
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.99	0.44
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.98	0.44
2:C:169:LYS:HD3	2:C:190:PRO:HA	2.00	0.44
2:C:935:THR:HG21	2:C:941:LYS:HG2	2.00	0.44
2:C:1315:MET:HE3	2:C:1315:MET:HB2	1.75	0.44
1:B:191:ARG:HA	1:B:196:THR:HG23	2.00	0.44
3:D:73:GLY:HA2	3:D:76:LYS:HE3	2.00	0.44
3:D:259:ARG:HD2	5:F:502:LYS:HE2	1.99	0.44
3:D:759:ILE:HG22	3:D:761:ALA:H	1.83	0.44
2:C:201:ARG:NH2	2:C:370:MET:HE3	2.32	0.44
2:C:297:VAL:HG11	2:C:311:CYS:HB3	2.00	0.44
2:C:378:ARG:NE	2:C:382:GLU:OE2	2.39	0.44
2:C:624:ASP:HB3	2:C:627:GLY:HA3	2.00	0.44
3:D:975:ILE:HG21	3:D:980:THR:HG21	1.99	0.44
4:E:10:VAL:HG21	4:E:16:ARG:HD3	1.99	0.44
2:C:1051:LYS:HB3	2:C:1051:LYS:HE3	1.87	0.44
2:C:548:ARG:NH1	2:C:570:GLY:H	2.16	0.43
2:C:714:VAL:HG13	2:C:715:THR:HG23	2.00	0.43
2:C:880:GLY:H	2:C:920:VAL:HB	1.82	0.43
3:D:1279:GLN:H	3:D:1279:GLN:HG2	1.57	0.43
2:C:960:LEU:HB3	2:C:1025:PHE:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:984:LEU:N	3:D:993:GLU:O	2.50	0.43
5:F:271:ASN:HA	5:F:274:ARG:HB3	2.00	0.43
8:G:25:ASP:O	8:G:29:ALA:N	2.51	0.43
2:C:251:ALA:HB2	2:C:269:ILE:HG13	2.00	0.43
3:D:121:PRO:HB3	3:D:126:LEU:HD13	2.00	0.43
3:D:430:HIS:HA	3:D:921:GLN:HB3	2.00	0.43
2:C:685:MET:HE3	2:C:685:MET:HB2	1.74	0.43
2:C:811:ASN:OD1	2:C:811:ASN:N	2.50	0.43
3:D:42:GLU:OE2	5:F:451:ARG:NE	2.50	0.43
8:G:6:ILE:H	8:I:246:THR:H	1.66	0.43
2:C:1209:GLN:NE2	2:C:1224:PRO:O	2.51	0.43
3:D:969:SER:O	3:D:969:SER:OG	2.34	0.43
3:D:1115:ILE:HD11	3:D:1119:ASP:HB3	1.99	0.43
2:C:523:GLU:OE1	2:C:527:LYS:NZ	2.51	0.43
2:C:615:VAL:HG23	2:C:651:ASP:H	1.83	0.43
2:C:914:LYS:NZ	2:C:915:ASP:O	2.50	0.43
2:C:1287:LEU:HD12	2:C:1287:LEU:HA	1.85	0.43
2:C:715:THR:HG21	2:C:789:THR:HG21	2.01	0.43
2:C:796:LEU:HD11	2:C:1233:LEU:HD21	1.96	0.43
6:1:33:DC:H42	7:2:57:DA:N6	2.16	0.43
1:A:10:LYS:HB2	1:A:10:LYS:HE2	1.88	0.43
2:C:194:LEU:HD21	2:C:429:MET:HG2	2.00	0.43
2:C:667:LEU:HD22	2:C:705:GLU:HG3	2.00	0.43
3:D:254:PRO:HA	3:D:260:PHE:HA	2.00	0.43
3:D:530:PRO:HB2	3:D:581:MET:HE3	2.00	0.43
8:G:12:ILE:HG12	8:I:149:LEU:HD13	2.01	0.43
3:D:1155:ILE:HG12	3:D:1210:ILE:CG1	2.49	0.43
4:E:52:ARG:NH2	4:E:55:GLU:OE1	2.52	0.43
6:1:86:DT:H2'	6:1:87:DG:H8	1.84	0.43
1:B:97:GLU:OE1	1:B:147:GLN:NE2	2.51	0.43
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.86	0.43
3:D:726:ALA:HB1	3:D:733:SER:HA	2.01	0.43
3:D:759:ILE:HD12	3:D:771:GLN:HG2	2.01	0.43
2:C:263:VAL:HA	2:C:267:ARG:HH11	1.84	0.42
2:C:335:THR:OG1	2:C:336:LEU:N	2.52	0.42
2:C:800:MET:HB3	2:C:800:MET:HE2	1.73	0.42
3:D:366:CYS:O	3:D:440:VAL:N	2.52	0.42
5:F:166:VAL:HB	5:F:259:PHE:HD1	1.83	0.42
5:F:248:GLU:O	5:F:252:LEU:N	2.43	0.42
6:1:30:DG:C4	6:1:31:DC:C5	3.07	0.42
7:2:48:DT:H4'	8:G:93:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:LEU:HD12	1:A:596:ALA:HB2	2.01	0.42
2:C:896:THR:OG1	2:C:898:GLU:OE1	2.27	0.42
2:C:941:LYS:HD3	2:C:946:LEU:HD21	2.01	0.42
2:C:1084:ASP:OD1	2:C:1084:ASP:N	2.37	0.42
2:C:1289:GLU:HG2	2:C:1294:LYS:HD2	2.00	0.42
3:D:370:LYS:HB3	3:D:409:TRP:HZ3	1.83	0.42
3:D:441:LEU:HD23	3:D:441:LEU:HA	1.86	0.42
3:D:587:LEU:HD23	3:D:591:ILE:HG21	2.00	0.42
6:1:38:DT:H3	7:2:53:DA:H61	1.67	0.42
8:I:261:ILE:HB	8:I:284:LEU:HB3	1.99	0.42
1:B:81:ILE:HG23	1:B:130:ILE:HG22	2.01	0.42
2:C:682:GLY:O	2:C:686:GLN:N	2.49	0.42
2:C:808:ASN:HA	3:D:629:PHE:HB3	2.01	0.42
6:1:54:DT:H3'	6:1:55:DC:C6	2.54	0.42
7:2:21:DT:H2''	7:2:22:DA:C8	2.55	0.42
2:C:720:ARG:HE	2:C:720:ARG:HB2	1.71	0.42
2:C:762:ASN:HD22	2:C:762:ASN:HA	1.64	0.42
2:C:1073:LYS:HD2	3:D:462:ASP:HB2	2.01	0.42
5:F:338:HIS:HA	5:F:341:LEU:HB3	2.01	0.42
5:F:426:LYS:HG2	6:1:68:DA:H3'	2.01	0.42
8:G:18:LEU:CD1	8:G:57:ARG:HB3	2.47	0.42
1:A:98:VAL:HG23	1:A:146:VAL:HB	2.02	0.42
1:A:650:TRP:CD2	1:A:651:PRO:HD3	2.54	0.42
1:B:102:LEU:HD11	1:B:115:ILE:HG22	2.02	0.42
2:C:91:THR:OG1	2:C:139:ASN:N	2.52	0.42
2:C:176:ILE:HD11	2:C:428:VAL:HG21	2.02	0.42
3:D:501:VAL:HA	3:D:502:PRO:HD3	1.91	0.42
3:D:863:LEU:HD11	3:D:901:ARG:HG3	2.01	0.42
5:F:111:LEU:HD12	5:F:115:GLY:HA3	2.01	0.42
5:F:402:LEU:HD12	5:F:405:ILE:HD12	2.02	0.42
1:A:593:VAL:HG13	8:G:13:TRP:CG	2.55	0.42
2:C:314:ASN:OD1	2:C:352:ARG:NE	2.41	0.42
2:C:634:VAL:N	2:C:645:PHE:O	2.48	0.42
3:D:836:ARG:O	3:D:840:LEU:N	2.52	0.42
5:F:530:LEU:HB2	5:F:533:ASP:HB2	2.01	0.42
8:G:59:LEU:HD22	8:G:96:PHE:HE1	1.83	0.42
1:A:157:THR:HA	1:A:160:HIS:HB2	2.01	0.42
2:C:606:LEU:HD23	2:C:606:LEU:HA	1.92	0.42
3:D:114:ILE:HD12	3:D:114:ILE:HA	1.88	0.42
3:D:299:LEU:O	3:D:303:VAL:N	2.43	0.42
3:D:715:LYS:HA	3:D:715:LYS:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1154:ALA:HB3	3:D:1214:PRO:O	2.20	0.42
2:C:925:SER:OG	2:C:926:GLY:N	2.53	0.42
3:D:332:LYS:HZ3	3:D:1329:THR:HG1	1.62	0.42
3:D:821:MET:HA	3:D:881:LYS:HA	2.01	0.42
5:F:451:ARG:NH2	6:1:61:DC:OP1	2.36	0.42
8:I:191:ASP:OD1	8:I:191:ASP:N	2.52	0.42
1:A:155:ALA:HB3	1:A:172:LEU:HD11	2.00	0.42
1:B:192:VAL:HG21	1:B:198:LEU:HD12	2.02	0.42
2:C:680:LEU:O	2:C:684:ASN:ND2	2.52	0.42
3:D:329:ASP:HA	3:D:332:LYS:HB3	2.02	0.42
4:E:25:ARG:NH2	4:E:61:ASN:OD1	2.47	0.42
2:C:590:PRO:HG3	2:C:605:TYR:HD1	1.85	0.41
3:D:484:MET:HE3	3:D:484:MET:HB2	1.90	0.41
3:D:789:LYS:HE2	3:D:931:THR:HG21	2.01	0.41
3:D:1369:ARG:HG2	3:D:1373:ARG:HH21	1.84	0.41
5:F:122:ARG:HH22	5:F:374:ARG:HH11	1.68	0.41
5:F:441:ARG:NH1	6:1:63:DA:OP2	2.51	0.41
7:2:10:DT:H2'	7:2:11:DG:C8	2.55	0.41
1:A:594:ARG:NH2	8:G:31:ALA:O	2.53	0.41
1:B:44:ARG:HD2	1:B:185:TYR:CE1	2.55	0.41
2:C:12:ARG:HA	2:C:1181:PRO:HG2	2.01	0.41
2:C:1324:ASN:OD1	2:C:1324:ASN:N	2.50	0.41
7:2:43:DT:C7	7:2:44:DT:O4	2.68	0.41
7:2:56:DC:H2''	7:2:57:DA:C8	2.55	0.41
1:A:15:ASP:OD1	1:A:15:ASP:N	2.52	0.41
2:C:81:ASP:N	2:C:81:ASP:OD1	2.50	0.41
2:C:678:ARG:HD3	2:C:1106:ARG:HD2	2.02	0.41
2:C:1085:MET:HE3	2:C:1086:PRO:HD2	2.03	0.41
3:D:118:LYS:HD2	3:D:118:LYS:HA	1.62	0.41
3:D:520:ALA:CB	3:D:545:HIS:O	2.68	0.41
3:D:968:ASN:OD1	3:D:971:GLY:N	2.54	0.41
3:D:1040:MET:HE1	3:D:1078:LEU:HG	2.02	0.41
8:G:18:LEU:HD13	8:G:58:ARG:N	2.34	0.41
8:I:281:CYS:SG	8:I:282:GLU:N	2.93	0.41
2:C:188:PHE:HE1	2:C:194:LEU:HB2	1.84	0.41
2:C:1315:MET:HG2	2:C:1317:PRO:HD3	2.03	0.41
3:D:804:ALA:HB1	3:D:916:GLY:HA3	2.03	0.41
3:D:960:LEU:N	3:D:1007:ASP:OD1	2.53	0.41
7:2:36:DG:H2'	7:2:37:DA:O4'	2.20	0.41
2:C:28:LEU:HD22	2:C:527:LYS:HD2	2.02	0.41
2:C:540:ARG:HH11	2:C:567:PRO:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:520:ALA:HB2	3:D:545:HIS:O	2.20	0.41
6:1:87:DG:H2''	6:1:88:DC:H5''	2.02	0.41
2:C:1058:ARG:HH21	2:C:1240:ASP:HB3	1.84	0.41
3:D:112:ALA:HA	3:D:238:ILE:HG23	2.01	0.41
3:D:249:LEU:HD13	3:D:249:LEU:HA	1.87	0.41
3:D:518:VAL:HG22	3:D:518:VAL:O	2.20	0.41
5:F:391:ALA:O	5:F:395:THR:N	2.53	0.41
1:B:62:ASP:N	1:B:62:ASP:OD1	2.51	0.41
2:C:838:CYS:HB3	2:C:1050:VAL:HG13	2.02	0.41
5:F:505:ILE:CG2	5:F:509:THR:HG21	2.51	0.41
8:I:149:LEU:HA	8:I:152:ILE:HB	2.02	0.41
2:C:198:ILE:O	2:C:201:ARG:CG	2.64	0.41
2:C:799:ASN:OD1	2:C:799:ASN:N	2.53	0.41
3:D:144:TYR:CG	3:D:180:MET:HB2	2.56	0.41
8:G:25:ASP:HA	8:G:28:ALA:HB3	2.03	0.41
8:I:182:ASN:N	8:I:260:ASP:O	2.49	0.41
1:A:627:LYS:HA	1:A:627:LYS:HD3	1.84	0.41
1:A:630:THR:O	1:A:634:ASP:N	2.54	0.41
2:C:212:ALA:O	2:C:359:ARG:NE	2.49	0.41
2:C:403:MET:HE3	2:C:403:MET:HB3	1.96	0.41
2:C:633:LEU:HB2	2:C:644:LEU:HB3	2.02	0.41
2:C:905:ILE:O	5:F:599:ARG:NH1	2.54	0.41
2:C:1028:LYS:HB3	2:C:1028:LYS:HE2	1.89	0.41
3:D:211:GLU:O	3:D:215:LYS:N	2.47	0.41
3:D:514:THR:HG21	3:D:596:LEU:HD23	2.03	0.41
3:D:822:MET:HB2	3:D:880:VAL:HG13	2.02	0.41
3:D:1058:SER:HB3	3:D:1107:VAL:HB	2.03	0.41
4:E:73:GLN:O	4:E:77:ALA:N	2.53	0.41
5:F:552:THR:O	5:F:556:ALA:N	2.47	0.41
7:2:24:DT:H6	7:2:24:DT:H2'	1.73	0.41
2:C:421:SER:OG	2:C:423:ASP:OD1	2.38	0.40
3:D:809:VAL:H	3:D:809:VAL:HG22	1.64	0.40
3:D:1075:ARG:NH2	3:D:1166:GLY:O	2.54	0.40
3:D:1152:GLU:O	3:D:1214:PRO:HG2	2.21	0.40
3:D:1367:GLN:HA	3:D:1370:MET:HB3	2.03	0.40
5:F:121:LYS:HA	5:F:124:GLU:HG3	2.02	0.40
5:F:242:HIS:HB3	5:F:245:ALA:HB3	2.03	0.40
5:F:474:MET:HE2	5:F:476:ARG:O	2.21	0.40
1:A:582:LEU:HD12	1:A:607:ILE:HB	2.02	0.40
2:C:623:LEU:HD12	2:C:623:LEU:HA	1.85	0.40
3:D:1145:PHE:HE2	3:D:1237:VAL:HG21	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1285:VAL:O	3:D:1289:ASN:ND2	2.55	0.40
6:1:55:DC:C2'	6:1:56:DA:O5'	2.38	0.40
6:1:85:DA:C8	6:1:86:DT:C4	3.09	0.40
2:C:1251:TYR:OH	3:D:348:ASP:OD2	2.33	0.40
6:1:56:DA:H2''	6:1:57:DC:C5	2.57	0.40
2:C:1333:LEU:HD21	3:D:327:LEU:HB3	2.03	0.40
3:D:1256:ILE:O	3:D:1260:MET:N	2.54	0.40
3:D:1335:ALA:HA	3:D:1340:LYS:HD2	2.04	0.40
1:B:192:VAL:HG12	1:B:195:ARG:H	1.86	0.40
2:C:240:GLU:HB3	2:C:283:LYS:HE3	2.04	0.40
2:C:1232:MET:C	2:C:1233:LEU:HD12	2.47	0.40
5:F:505:ILE:O	5:F:506:SER:CB	2.70	0.40
6:1:30:DG:H2''	6:1:31:DC:OP2	2.20	0.40
6:1:85:DA:C2'	6:1:86:DT:O4'	2.62	0.40
8:I:249:PRO:HA	8:I:252:ASN:H	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	291/329 (88%)	260 (89%)	31 (11%)	0	100	100
1	B	226/329 (69%)	213 (94%)	13 (6%)	0	100	100
2	C	1335/1342 (100%)	1216 (91%)	118 (9%)	1 (0%)	48	81
3	D	1320/1407 (94%)	1198 (91%)	122 (9%)	0	100	100
4	E	77/91 (85%)	76 (99%)	1 (1%)	0	100	100
5	F	470/613 (77%)	419 (89%)	45 (10%)	6 (1%)	9	41
8	G	108/289 (37%)	99 (92%)	9 (8%)	0	100	100
8	I	160/289 (55%)	148 (92%)	11 (7%)	1 (1%)	21	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3987/4689 (85%)	3629 (91%)	350 (9%)	8 (0%)	44	75

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	296	LYS
5	F	506	SER
5	F	507	MET
2	C	399	ALA
5	F	310	GLU
5	F	490	PRO
5	F	581	ASP
8	I	249	PRO

5.3.2 Protein sidechains ⓘ

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	269/286 (94%)	265 (98%)	4 (2%)	57	70
1	B	196/286 (68%)	194 (99%)	2 (1%)	68	76
2	C	1152/1157 (100%)	1142 (99%)	10 (1%)	70	76
3	D	1104/1168 (94%)	1094 (99%)	10 (1%)	70	76
4	E	67/75 (89%)	67 (100%)	0	100	100
5	F	422/540 (78%)	413 (98%)	9 (2%)	47	65
8	G	94/247 (38%)	92 (98%)	2 (2%)	47	65
8	I	146/247 (59%)	145 (99%)	1 (1%)	76	79
All	All	3450/4006 (86%)	3412 (99%)	38 (1%)	63	74

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	VAL
1	A	98	VAL

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Mol	Chain	Res	Type
1	A	153	VAL
1	A	183	ILE
1	B	187	VAL
1	B	194	GLN
2	C	199	ASP
2	C	207	THR
2	C	854	ILE
2	C	888	THR
2	C	1014	LEU
2	C	1050	VAL
2	C	1054	LEU
2	C	1112	ILE
2	C	1233	LEU
2	C	1293	VAL
3	D	118	LYS
3	D	208	THR
3	D	501	VAL
3	D	706	VAL
3	D	809	VAL
3	D	849	LEU
3	D	1155	ILE
3	D	1265	THR
3	D	1316	THR
3	D	1329	THR
5	F	261	LEU
5	F	296	LYS
5	F	332	ASP
5	F	402	LEU
5	F	487	MET
5	F	488	LEU
5	F	579	GLN
5	F	580	PHE
5	F	587	ILE
8	G	50	ILE
8	G	58	ARG
8	I	211	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	B	84	ASN

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Mol	Chain	Res	Type
1	B	93	GLN
1	B	127	GLN
1	B	147	GLN
1	B	186	ASN
1	B	208	ASN
2	C	31	GLN
2	C	120	GLN
2	C	133	ASN
2	C	273	HIS
2	C	276	GLN
2	C	387	ASN
2	C	406	ASN
2	C	462	ASN
2	C	494	ASN
2	C	551	HIS
2	C	568	ASN
2	C	573	ASN
2	C	620	ASN
2	C	622	ASN
2	C	659	GLN
2	C	688	GLN
2	C	737	ASN
2	C	762	ASN
2	C	1017	GLN
2	C	1175	ASN
2	C	1220	GLN
2	C	1256	GLN
2	C	1268	GLN
3	D	158	GLN
3	D	274	ASN
3	D	276	ASN
3	D	277	ASN
3	D	335	GLN
3	D	488	ASN
3	D	504	GLN
3	D	519	ASN
3	D	651	HIS
3	D	680	ASN
3	D	910	ASN
3	D	1049	GLN
3	D	1086	ASN
3	D	1108	GLN

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Mol	Chain	Res	Type
3	D	1235	ASN
4	E	31	GLN
5	F	246	GLN
5	F	309	ASN
5	F	323	ASN
5	F	338	HIS
5	F	342	GLN
5	F	362	ASN
5	F	406	GLN
5	F	409	ASN
5	F	568	ASN
8	I	157	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

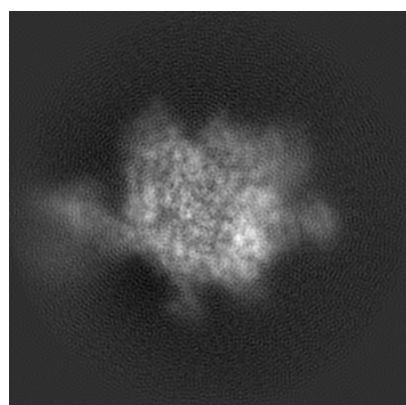
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32166. These allow visual inspection of the internal detail of the map and identification of artifacts.

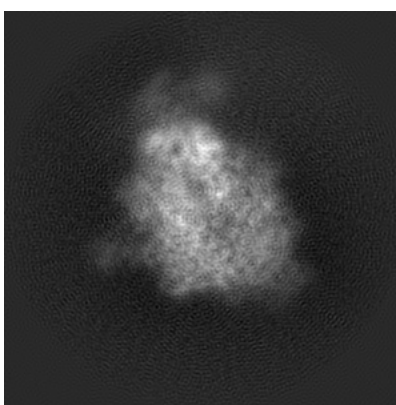
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

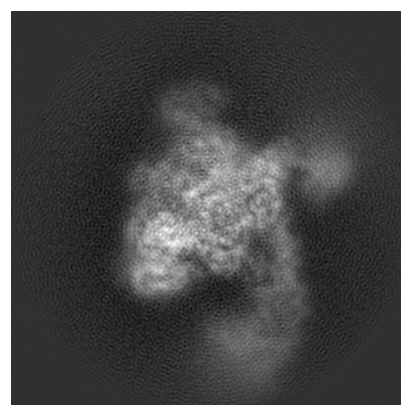
6.1.1 Primary map



X



Y

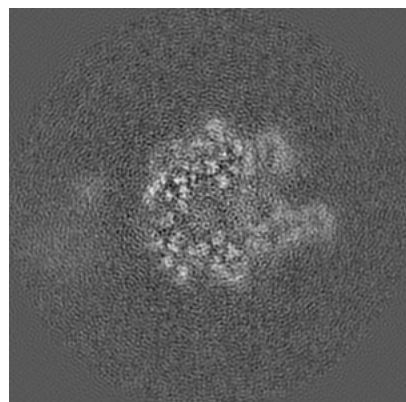


Z

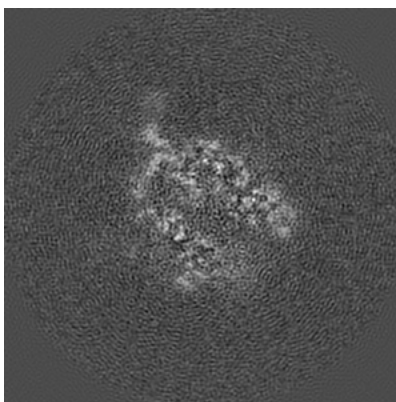
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

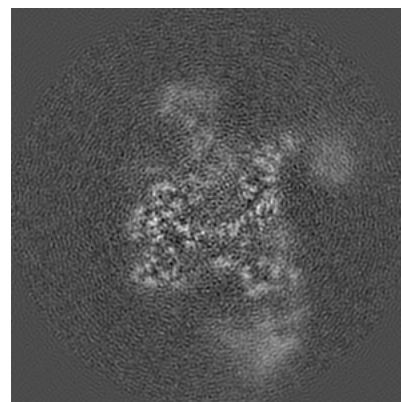
6.2.1 Primary map



X Index: 120



Y Index: 120

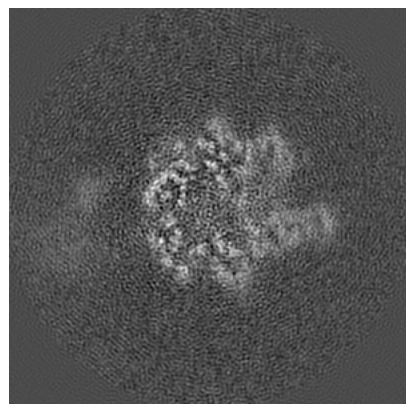


Z Index: 120

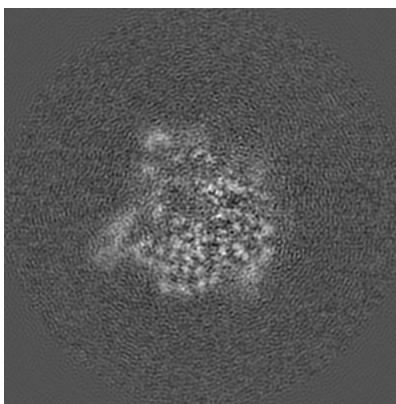
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

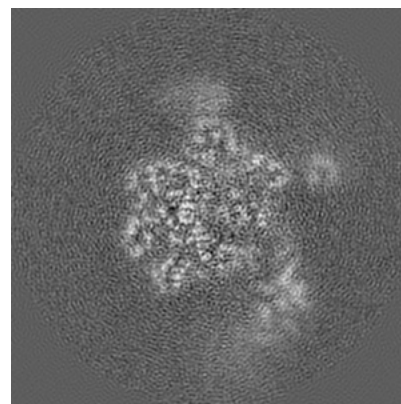
6.3.1 Primary map



X Index: 121



Y Index: 108

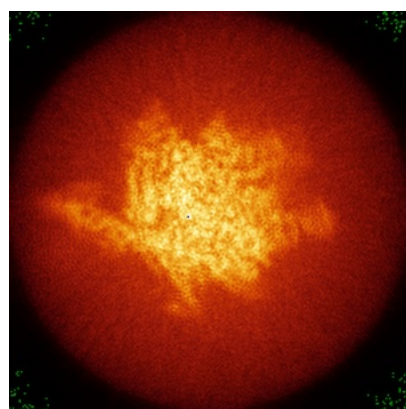


Z Index: 106

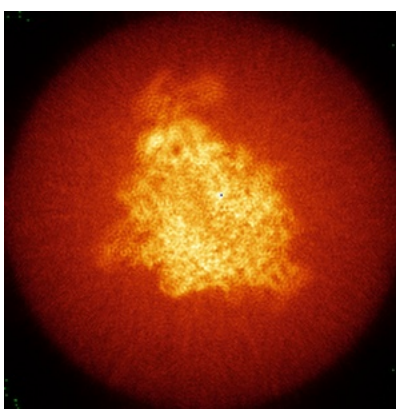
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

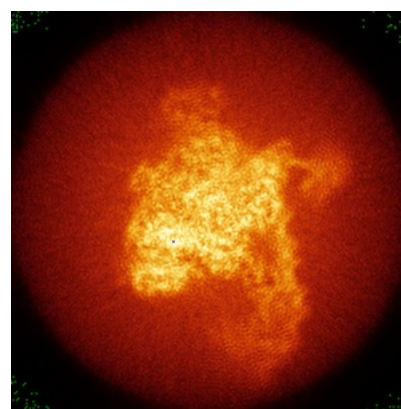
6.4.1 Primary map



X



Y

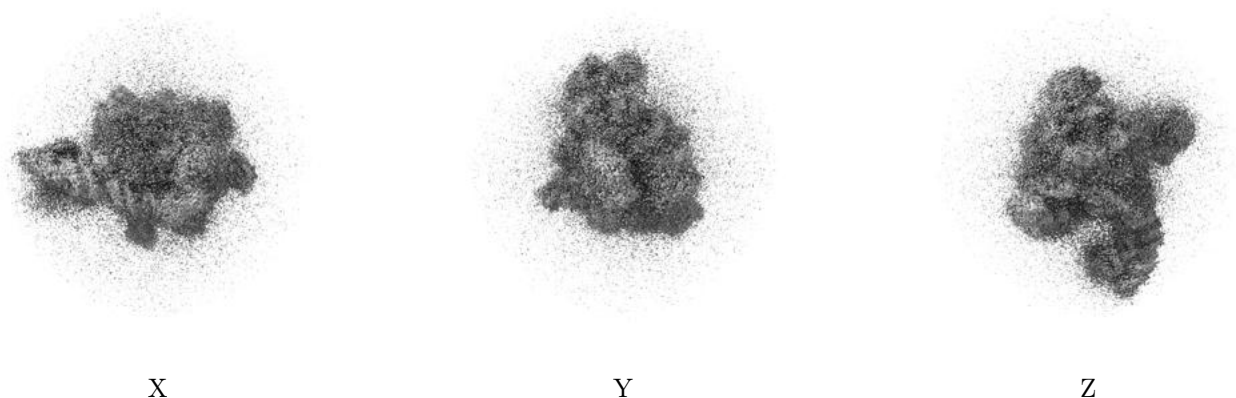


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

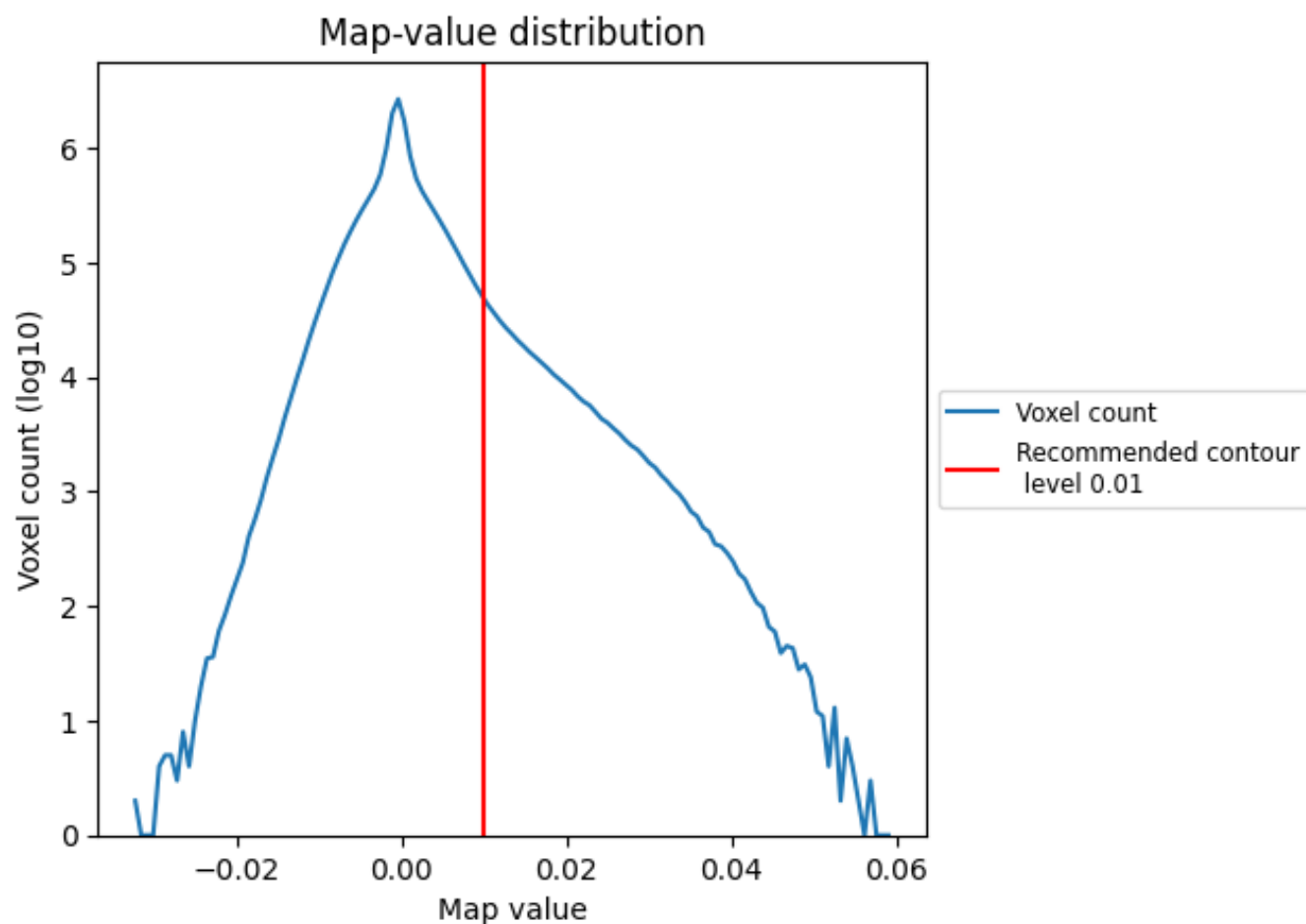
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

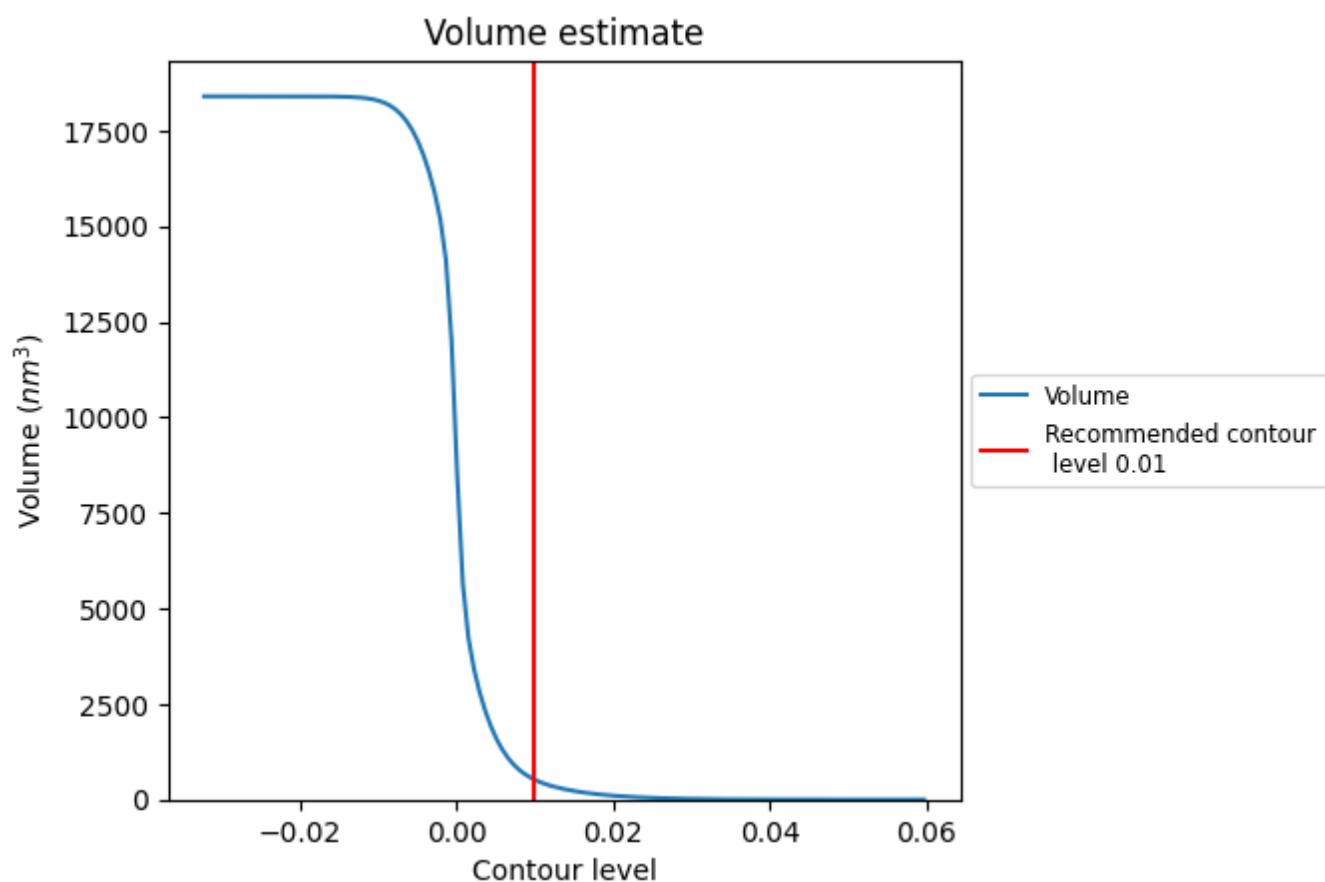
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

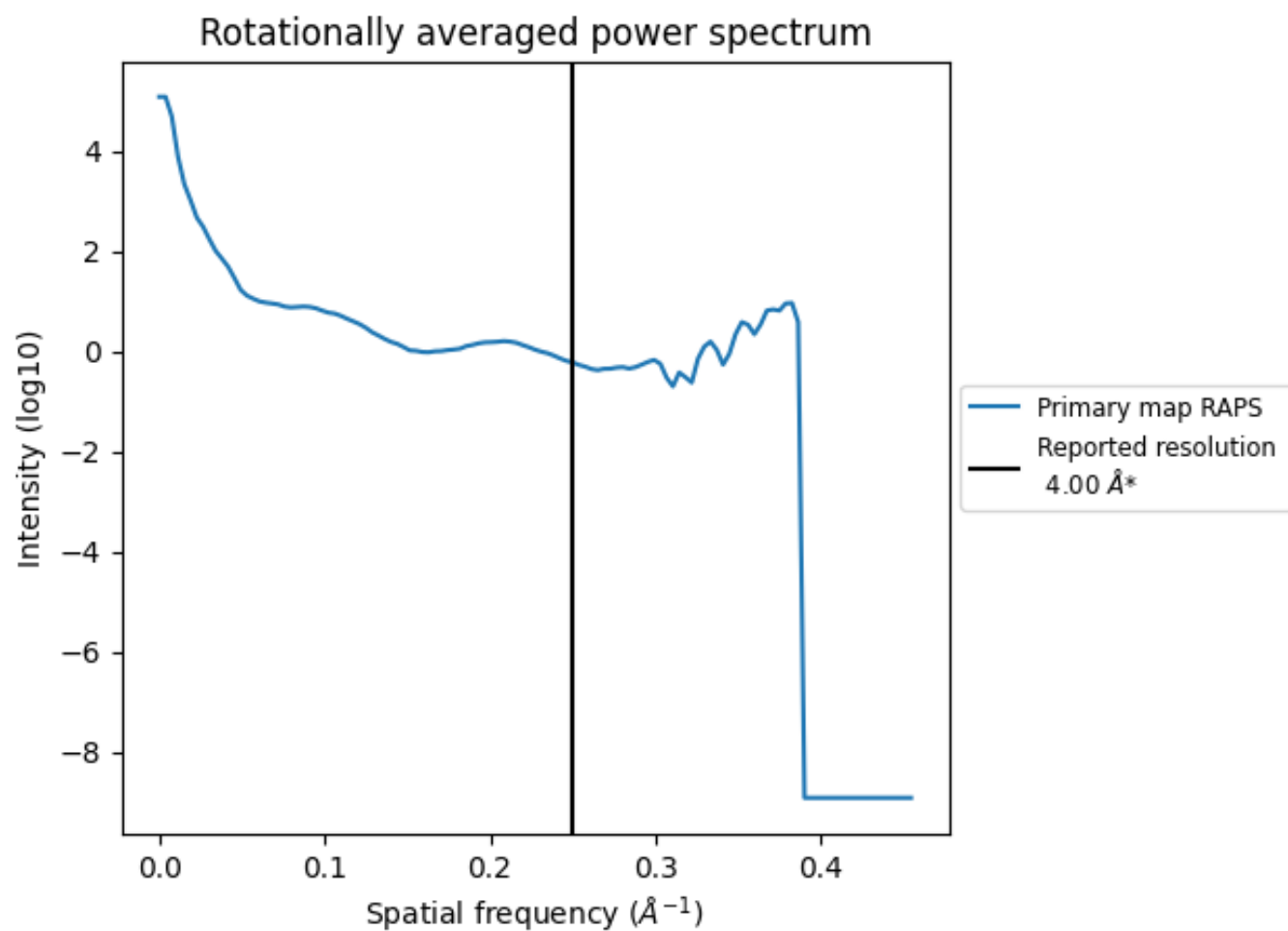
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 519 nm³; this corresponds to an approximate mass of 468 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

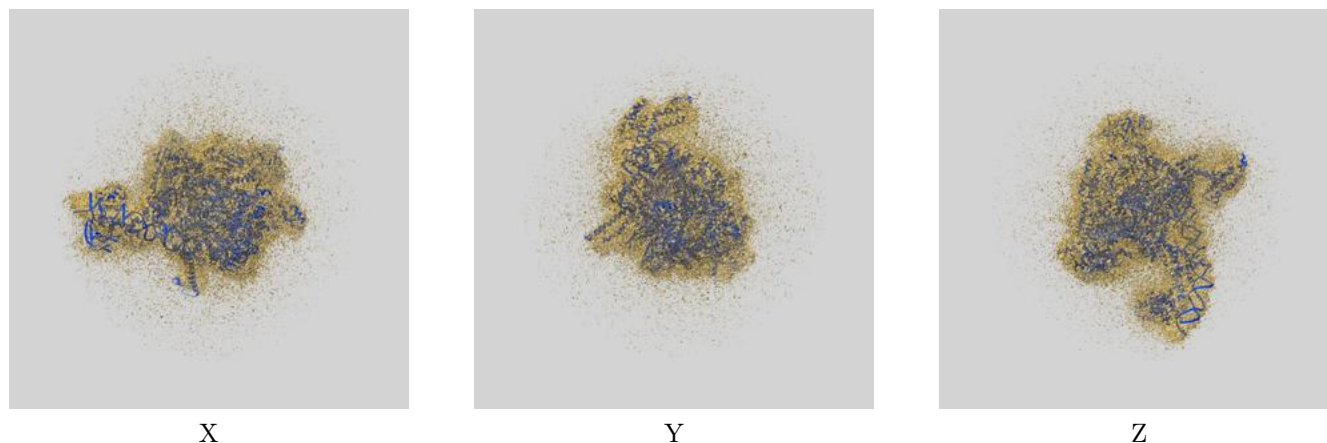
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

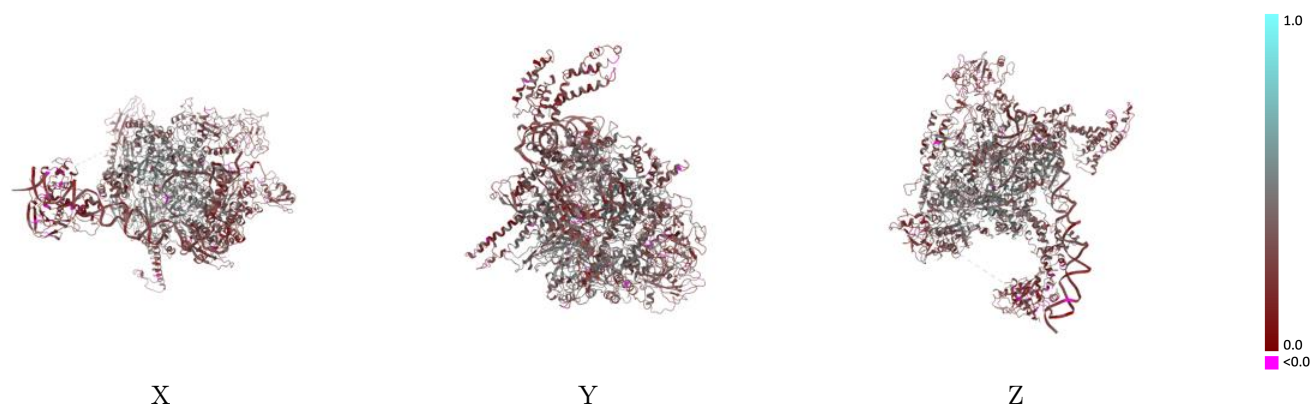
This section contains information regarding the fit between EMDB map EMD-32166 and PDB model 7VWZ. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.01 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](#)

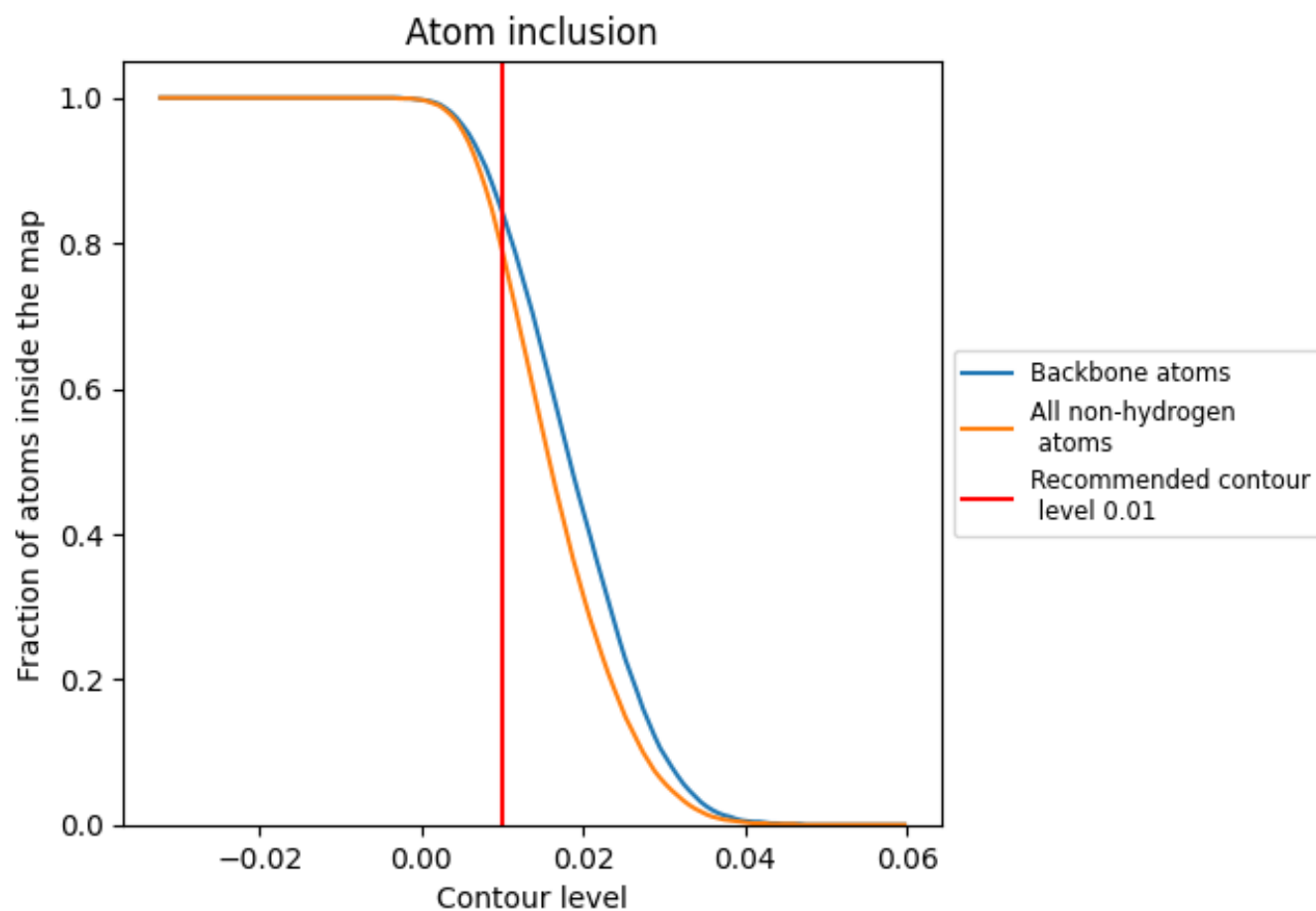


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 79% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7890	0.3450
1	0.8850	0.2550
2	0.7750	0.2470
A	0.7880	0.3610
B	0.7660	0.3120
C	0.8550	0.3880
D	0.8100	0.3710
E	0.7770	0.3790
F	0.7630	0.3000
G	0.7380	0.2240
I	0.1740	0.2120

1.0
0.0
<0.0