



Full wwPDB EM Validation Report ⓘ

Nov 3, 2022 – 01:03 pm GMT

PDB ID : 7QWP
EMDB ID : EMD-14190
Title : CryoEM structure of bacterial transcription close complex (RPc)
Authors : Ye, F.Z.; Zhang, X.D.
Deposited on : 2022-01-25
Resolution : 3.40 Å(reported)
Based on initial model : 5NSR

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

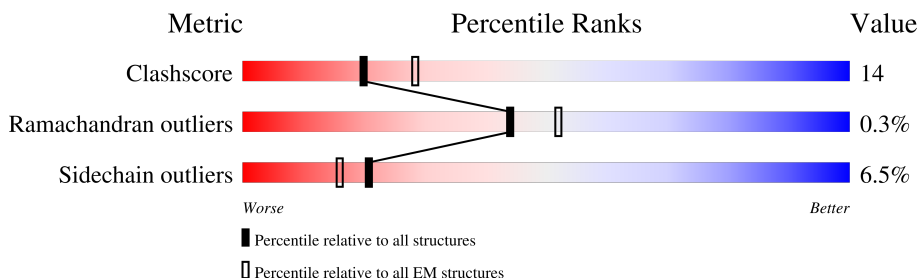
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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 $\leq 5\%$. 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	
4	E	91	
5	M	497	
6	N	63	
7	T	63	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 29006 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	309	Total	C	N	O	S	0	0
			2316	1450	404	455	7		
1	B	223	Total	C	N	O	S	0	0
			1673	1045	291	332	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1341	Total	C	N	O	S	0	0
			10135	6365	1764	1966	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1333	Total	C	N	O	S	0	0
			9638	6054	1731	1815	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	74	Total	C	N	O	S	0	0
			552	341	109	101	1		

- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	405	Total	C	N	O	S	0	0
			3216	2015	557	633	11		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	initiating methionine	UNP A0A0N9UTC1

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-18	GLY	-	expression tag	UNP A0A0N9UTC1
M	-17	SER	-	expression tag	UNP A0A0N9UTC1
M	-16	SER	-	expression tag	UNP A0A0N9UTC1
M	-15	HIS	-	expression tag	UNP A0A0N9UTC1
M	-14	HIS	-	expression tag	UNP A0A0N9UTC1
M	-13	HIS	-	expression tag	UNP A0A0N9UTC1
M	-12	HIS	-	expression tag	UNP A0A0N9UTC1
M	-11	HIS	-	expression tag	UNP A0A0N9UTC1
M	-10	HIS	-	expression tag	UNP A0A0N9UTC1
M	-9	SER	-	expression tag	UNP A0A0N9UTC1
M	-8	SER	-	expression tag	UNP A0A0N9UTC1
M	-7	GLY	-	expression tag	UNP A0A0N9UTC1
M	-6	LEU	-	expression tag	UNP A0A0N9UTC1
M	-5	VAL	-	expression tag	UNP A0A0N9UTC1
M	-4	PRO	-	expression tag	UNP A0A0N9UTC1
M	-3	ARG	-	expression tag	UNP A0A0N9UTC1
M	-2	GLY	-	expression tag	UNP A0A0N9UTC1
M	-1	SER	-	expression tag	UNP A0A0N9UTC1
M	0	HIS	-	expression tag	UNP A0A0N9UTC1
M	49	GLU	GLN	conflict	UNP A0A0N9UTC1

- Molecule 6 is a DNA chain called Non-Template promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	N	36	Total	C	N	O	P	0	0
			738	349	137	216	36		

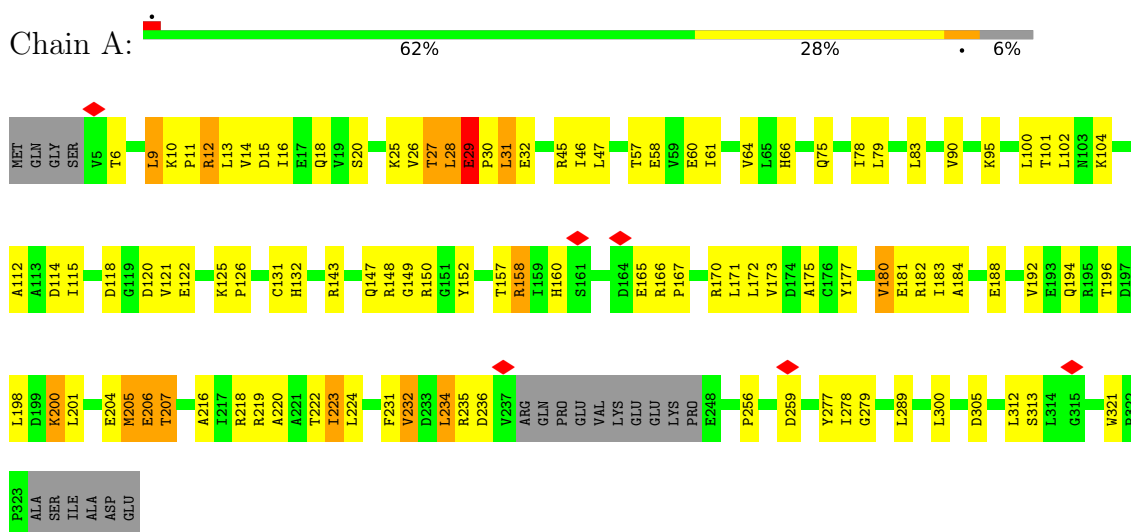
- Molecule 7 is a DNA chain called Template promoter DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	36	Total	C	N	O	P	0	0
			738	349	137	216	36		

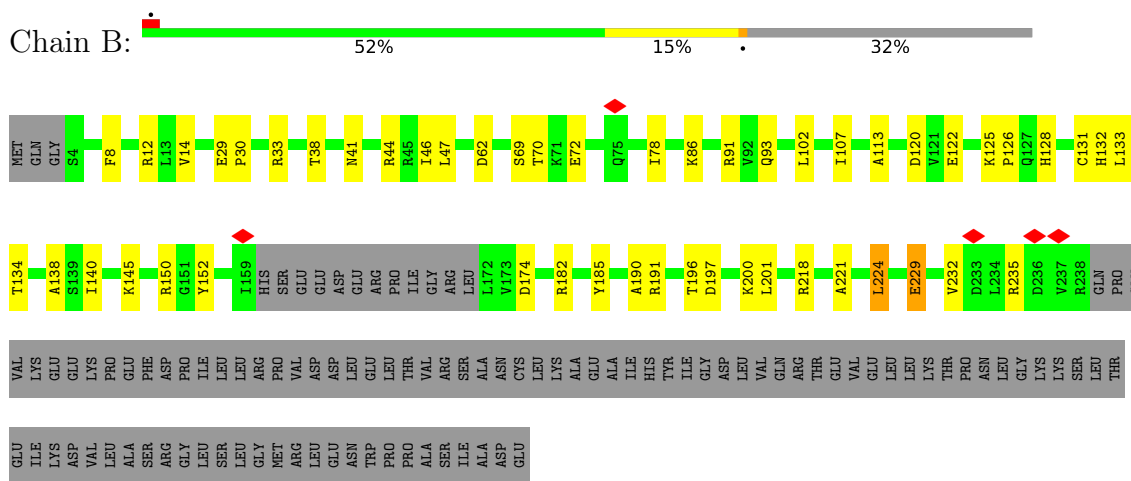
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

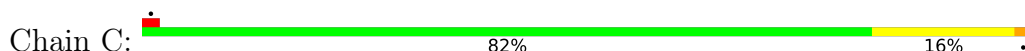
• Molecule 1: DNA-directed RNA polymerase subunit alpha

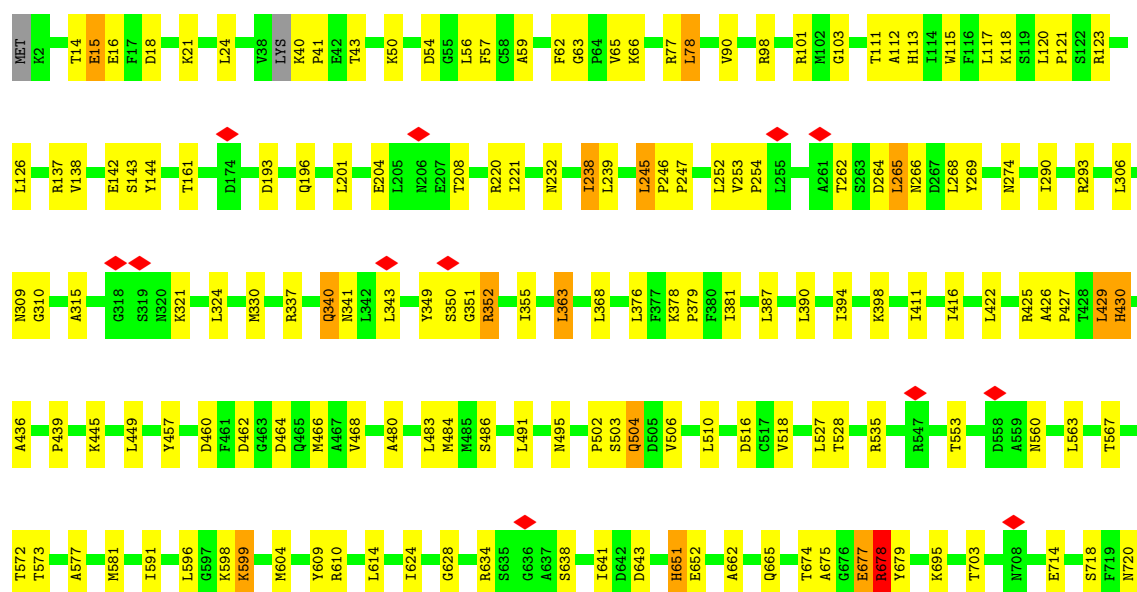


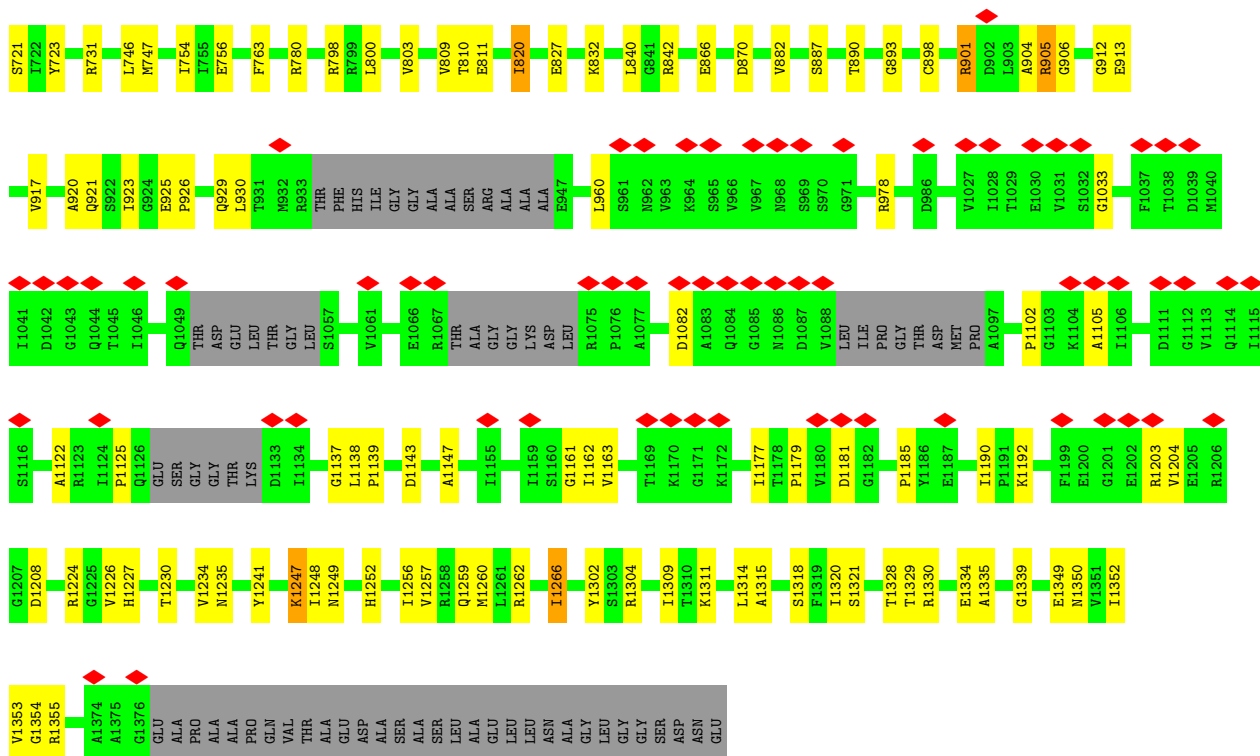
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta



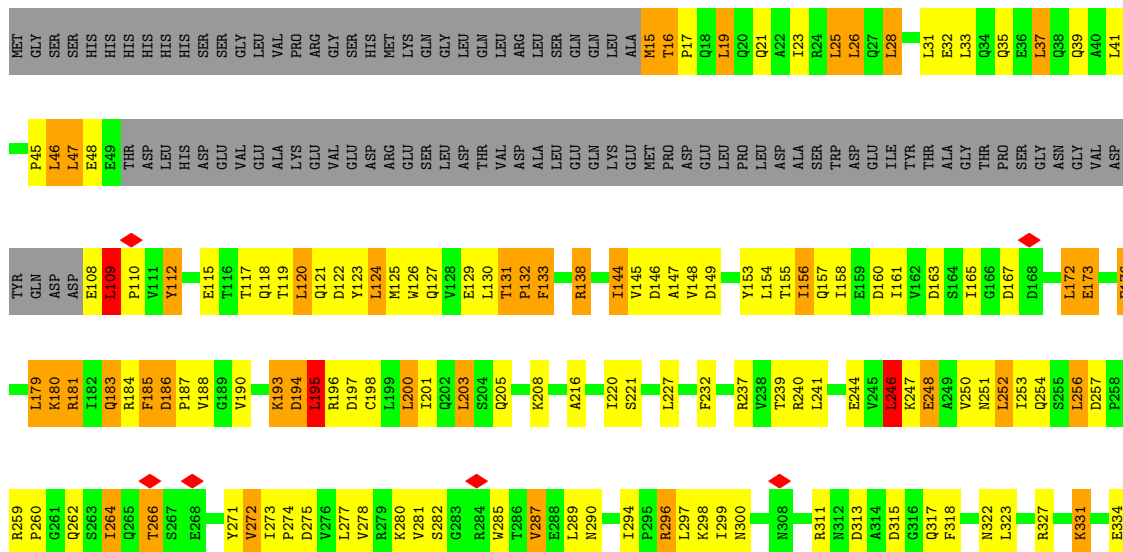




- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma-54 factor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31394	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1400	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.293	Depositor
Minimum map value	-0.159	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	281.6, 281.6, 281.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/2345	0.46	0/3195
1	B	0.23	0/1690	0.44	0/2297
2	C	0.23	0/10293	0.40	0/13952
3	D	0.24	0/9772	0.42	1/13273 (0.0%)
4	E	0.23	0/554	0.37	0/749
5	M	0.87	2/3263 (0.1%)	1.05	10/4420 (0.2%)
6	N	0.66	2/827 (0.2%)	0.85	3/1274 (0.2%)
7	T	1.15	12/827 (1.5%)	1.11	8/1274 (0.6%)
All	All	0.42	16/29571 (0.1%)	0.57	22/40434 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	-11	DC	C4'-O4'	-13.40	1.31	1.45
7	T	23	DT	C4'-O4'	13.16	1.58	1.45
7	T	17	DA	C4'-O4'	11.91	1.56	1.45
7	T	13	DG	O3'-P	-11.08	1.47	1.61
7	T	9	DT	O3'-P	-9.80	1.49	1.61
7	T	32	DT	C4'-O4'	8.81	1.53	1.45
7	T	20	DT	C4'-O4'	7.87	1.52	1.45
7	T	6	DT	C4'-O4'	6.95	1.52	1.45
7	T	10	DC	O3'-P	6.91	1.69	1.61
7	T	3	DG	C4'-O4'	6.85	1.51	1.45
7	T	7	DG	O3'-P	6.28	1.68	1.61
6	N	-11	DC	O3'-P	-6.05	1.53	1.61
7	T	31	DG	C4'-O4'	5.76	1.50	1.45
7	T	22	DG	C4'-O4'	5.34	1.50	1.45
5	M	133	PHE	CG-CD2	5.30	1.46	1.38
5	M	205	GLN	CG-CD	5.14	1.62	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	8	DA	O5'-P-OP2	-11.83	95.05	105.70
7	T	13	DG	C5'-C4'-O4'	11.06	130.32	109.30
7	T	7	DG	P-O3'-C3'	10.89	132.77	119.70
7	T	23	DT	C1'-O4'-C4'	-8.96	101.14	110.10
7	T	13	DG	O3'-P-O5'	8.45	120.05	104.00
7	T	8	DA	O5'-P-OP1	8.30	120.66	110.70
7	T	13	DG	P-O3'-C3'	8.04	129.35	119.70
6	N	-11	DC	O4'-C1'-C2'	-7.28	100.08	105.90
6	N	-11	DC	C5'-C4'-O4'	6.85	122.31	109.30
6	N	-11	DC	C3'-C2'-C1'	-6.65	94.52	102.50
7	T	17	DA	C1'-O4'-C4'	-5.89	104.21	110.10
5	M	277	LEU	CB-CG-CD2	5.68	120.65	111.00
5	M	275	ASP	CB-CG-OD1	5.61	123.35	118.30
5	M	399	LEU	CB-CG-CD2	5.51	120.38	111.00
5	M	163	ASP	CB-CG-OD2	5.32	123.08	118.30
5	M	264	ILE	CA-C-N	-5.29	105.57	117.20
5	M	144	ILE	CG1-CB-CG2	-5.25	99.86	111.40
3	D	870	ASP	CB-CG-OD2	5.18	122.97	118.30
5	M	25	LEU	CB-CG-CD1	5.17	119.80	111.00
5	M	246	LEU	CB-CG-CD2	-5.15	102.24	111.00
5	M	183	GLN	CB-CA-C	-5.10	100.20	110.40
5	M	160	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2316	0	2297	133	0
1	B	1673	0	1674	35	0
2	C	10135	0	9844	182	0
3	D	9638	0	9243	204	0
4	E	552	0	555	13	0
5	M	3216	0	3227	265	0
6	N	738	0	404	33	0
7	T	738	0	404	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29006	0	27648	774	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 14.

All (774) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:CG	1:A:30:PRO:HD3	1.57	1.34
5:M:23:ILE:CD1	7:T:12:DT:H71	1.65	1.26
4:E:3:ARG:HH12	4:E:55:GLU:CB	1.57	1.17
5:M:15:MET:HB2	6:N:-12:DA:N6	1.60	1.17
5:M:109:LEU:HB3	5:M:110:PRO:CD	1.75	1.17
1:A:12:ARG:O	1:A:29:GLU:HG2	1.45	1.16
1:A:104:LYS:HD2	1:A:114:ASP:OD2	1.39	1.16
3:D:111:THR:O	3:D:238:ILE:HG22	1.46	1.14
1:A:29:GLU:HG3	1:A:30:PRO:CD	1.78	1.13
5:M:186:ASP:HB3	5:M:187:PRO:CD	1.74	1.13
1:A:29:GLU:CB	1:A:30:PRO:CD	2.23	1.13
1:A:29:GLU:HB3	1:A:30:PRO:HD2	1.13	1.12
1:A:29:GLU:CG	1:A:30:PRO:CD	2.28	1.12
5:M:16:THR:HB	5:M:17:PRO:CD	1.81	1.11
5:M:23:ILE:HD13	7:T:12:DT:C7	1.81	1.10
1:A:14:VAL:HG12	1:A:29:GLU:OE1	1.49	1.10
1:A:29:GLU:HG3	1:A:30:PRO:HD3	1.13	1.10
5:M:154:LEU:HD21	5:M:193:LYS:HG3	1.28	1.09
5:M:287:VAL:HG22	5:M:348:VAL:HG21	1.34	1.09
3:D:112:ALA:HA	3:D:238:ILE:HG23	1.22	1.08
5:M:186:ASP:HB3	5:M:187:PRO:HD3	1.13	1.08
3:D:112:ALA:HA	3:D:238:ILE:CG2	1.84	1.08
5:M:203:LEU:HD21	5:M:256:LEU:HD21	1.14	1.08
5:M:144:ILE:HD13	5:M:179:LEU:HD23	1.31	1.08
5:M:287:VAL:HG21	5:M:344:SER:O	1.51	1.08
3:D:651:HIS:HD2	3:D:652:GLU:N	1.53	1.07
5:M:109:LEU:HB3	5:M:110:PRO:HD2	1.32	1.07
2:C:59:ILE:CD1	2:C:472:GLU:HG2	1.84	1.06
5:M:16:THR:HB	5:M:17:PRO:HD2	1.09	1.05
1:A:29:GLU:HB3	1:A:30:PRO:CD	1.78	1.05
5:M:124:LEU:HD23	5:M:145:VAL:HG12	1.38	1.03
3:D:253:VAL:HG13	5:M:112:TYR:HB3	1.39	1.01
5:M:203:LEU:CD2	5:M:256:LEU:HD21	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:CB	1:A:30:PRO:HD2	1.86	1.00
3:D:675:ALA:HA	3:D:678:ARG:HG2	1.43	1.00
5:M:16:THR:CB	5:M:17:PRO:HD2	1.91	1.00
2:C:169:LYS:HE2	2:C:169:LYS:HA	1.44	0.99
1:A:180:VAL:O	1:A:207:THR:HA	1.63	0.99
5:M:16:THR:HG23	6:N:-11:DC:H5	1.29	0.97
2:C:59:ILE:HD11	2:C:472:GLU:HG2	1.43	0.97
1:A:223:ILE:CD1	1:B:8:PHE:CZ	2.49	0.96
1:A:12:ARG:HH11	1:A:12:ARG:HB3	1.26	0.95
3:D:651:HIS:CD2	3:D:652:GLU:HG3	2.01	0.95
1:A:223:ILE:HD11	1:B:8:PHE:CE1	2.03	0.93
3:D:651:HIS:CD2	3:D:652:GLU:N	2.36	0.93
1:A:12:ARG:HB3	1:A:12:ARG:NH1	1.83	0.93
1:A:223:ILE:CD1	1:B:8:PHE:CE1	2.52	0.93
6:N:-11:DC:H42	7:T:11:DG:N2	1.66	0.93
5:M:203:LEU:HD21	5:M:256:LEU:CD2	1.98	0.92
6:N:-11:DC:N4	7:T:11:DG:H22	1.66	0.92
2:C:902:LEU:HD11	5:M:195:LEU:HB2	1.52	0.92
1:A:158:ARG:HH11	1:A:158:ARG:HG2	1.35	0.91
5:M:109:LEU:CB	5:M:110:PRO:HD2	2.00	0.91
5:M:272:VAL:HG13	5:M:274:PRO:HD3	1.53	0.90
1:A:223:ILE:HD11	1:B:8:PHE:CZ	2.07	0.90
2:C:454:ARG:HG3	2:C:454:ARG:HH21	1.37	0.90
5:M:109:LEU:CB	5:M:110:PRO:CD	2.47	0.89
5:M:33:LEU:CD1	5:M:336:ARG:HH12	1.85	0.89
2:C:916:SER:HB2	5:M:266:THR:OG1	1.72	0.88
5:M:16:THR:HG23	6:N:-11:DC:C5	2.08	0.88
1:A:13:LEU:HD23	1:A:28:LEU:HD13	1.55	0.88
7:T:33:DC:H2"	7:T:34:DT:C6	2.09	0.88
2:C:169:LYS:HA	2:C:169:LYS:CE	2.03	0.87
3:D:394:ILE:HG12	5:M:130:LEU:HD13	1.56	0.87
5:M:124:LEU:HD23	5:M:145:VAL:CG1	2.04	0.87
5:M:144:ILE:HG21	5:M:179:LEU:CD2	2.05	0.87
5:M:15:MET:HB2	6:N:-12:DA:H61	1.37	0.87
3:D:651:HIS:HD2	3:D:652:GLU:H	1.20	0.87
5:M:125:MET:CE	5:M:145:VAL:HG21	2.04	0.87
5:M:186:ASP:CB	5:M:187:PRO:HD3	2.03	0.87
2:C:902:LEU:HD11	5:M:195:LEU:CB	2.04	0.87
5:M:273:ILE:HG21	5:M:389:TYR:CD2	2.10	0.87
3:D:598:LYS:HB3	3:D:599:LYS:HE2	1.58	0.86
5:M:456:ARG:HE	7:T:25:DC:H41	1.20	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:-10:DG:H1	7:T:10:DC:H42	1.23	0.85
7:T:9:DT:H2"	7:T:10:DC:H5"	1.58	0.85
6:N:-11:DC:N4	7:T:11:DG:N2	2.24	0.85
5:M:15:MET:HB2	6:N:-12:DA:H62	1.42	0.85
5:M:23:ILE:CD1	7:T:12:DT:C7	2.49	0.84
5:M:273:ILE:CG2	5:M:389:TYR:CD2	2.60	0.84
3:D:905:ARG:HG3	3:D:905:ARG:HH11	1.43	0.84
1:A:183:ILE:HG12	1:A:205:MET:HB2	1.58	0.84
1:A:200:LYS:HZ2	1:A:200:LYS:HB3	1.42	0.84
5:M:124:LEU:CD2	5:M:145:VAL:HG12	2.08	0.84
5:M:23:ILE:HD13	7:T:12:DT:H71	0.86	0.83
4:E:3:ARG:NH1	4:E:55:GLU:CB	2.40	0.83
1:A:9:LEU:H	1:A:9:LEU:HD12	1.43	0.83
2:C:911:SER:HB3	5:M:259:ARG:NH2	1.93	0.83
5:M:132:PRO:O	5:M:132:PRO:HG2	1.76	0.82
3:D:254:PRO:HD2	5:M:112:TYR:CE2	2.15	0.82
3:D:112:ALA:CA	3:D:238:ILE:HG23	2.07	0.82
3:D:265:LEU:HD12	3:D:265:LEU:O	1.80	0.82
5:M:287:VAL:CG2	5:M:348:VAL:HG21	2.09	0.82
5:M:246:LEU:O	5:M:250:VAL:HG23	1.80	0.81
3:D:394:ILE:HG21	5:M:130:LEU:CD1	2.09	0.81
1:A:14:VAL:CG1	1:A:29:GLU:OE1	2.29	0.81
5:M:133:PHE:H	5:M:138:ARG:NH2	1.79	0.80
5:M:109:LEU:HB3	5:M:110:PRO:HD3	1.63	0.80
5:M:125:MET:HE2	5:M:145:VAL:HG21	1.63	0.80
1:A:104:LYS:CD	1:A:114:ASP:OD2	2.28	0.80
5:M:336:ARG:C	5:M:336:ARG:HD2	2.02	0.80
2:C:454:ARG:HG2	2:C:458:GLU:OE1	1.81	0.80
5:M:216:ALA:HB1	5:M:253:ILE:HD11	1.64	0.79
1:A:231:PHE:O	1:B:221:ALA:CB	2.30	0.79
5:M:158:ILE:HD11	5:M:193:LYS:HD3	1.64	0.78
5:M:273:ILE:CG2	5:M:389:TYR:CG	2.66	0.78
6:N:-11:DC:H42	7:T:11:DG:H22	1.23	0.78
1:A:25:LYS:HD2	1:A:204:GLU:HG2	1.66	0.78
5:M:16:THR:CG2	6:N:-11:DC:C5	2.66	0.78
2:C:911:SER:HB3	5:M:259:ARG:NH1	1.99	0.77
5:M:144:ILE:HD13	5:M:179:LEU:CD2	2.13	0.77
2:C:473:ARG:HG3	2:C:473:ARG:HH11	1.47	0.77
7:T:32:DT:H2"	7:T:33:DC:C5	2.20	0.77
2:C:879:GLY:HA2	2:C:923:GLY:HA2	1.67	0.77
5:M:131:THR:OG1	5:M:132:PRO:HD2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:186:ASP:CB	5:M:187:PRO:CD	2.60	0.77
5:M:112:TYR:HD1	5:M:112:TYR:H	1.33	0.76
5:M:273:ILE:HG21	5:M:389:TYR:CG	2.20	0.76
5:M:179:LEU:HD13	5:M:179:LEU:O	1.86	0.76
1:A:194:GLN:OE1	1:A:194:GLN:N	2.16	0.76
2:C:911:SER:HB3	5:M:259:ARG:CZ	2.16	0.76
5:M:33:LEU:CD1	5:M:336:ARG:NH1	2.48	0.75
2:C:50:GLU:O	2:C:54:ARG:HG2	1.86	0.75
5:M:144:ILE:CD1	5:M:179:LEU:HD23	2.14	0.75
5:M:456:ARG:HE	7:T:25:DC:N4	1.84	0.75
1:A:305:ASP:OD1	5:M:180:LYS:CD	2.35	0.75
5:M:144:ILE:HG21	5:M:179:LEU:HD23	1.68	0.75
1:A:223:ILE:HD13	1:B:8:PHE:CE1	2.21	0.75
6:N:-12:DA:N3	6:N:-12:DA:H3'	2.01	0.75
2:C:911:SER:HB3	5:M:259:ARG:HH22	1.49	0.75
1:A:10:LYS:HD2	1:B:229:GLU:OE1	1.87	0.74
1:A:223:ILE:HD13	1:B:8:PHE:CZ	2.22	0.74
2:C:473:ARG:HG3	2:C:473:ARG:NH1	2.00	0.74
5:M:15:MET:N	6:N:-11:DC:N4	2.35	0.74
5:M:172:LEU:HD22	5:M:172:LEU:O	1.86	0.74
1:A:9:LEU:CD1	1:A:32:GLU:OE2	2.35	0.73
1:A:9:LEU:HD11	1:A:32:GLU:OE2	1.88	0.73
5:M:16:THR:HG22	6:N:-11:DC:C6	2.24	0.73
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.71	0.73
5:M:15:MET:N	6:N:-11:DC:H41	1.87	0.73
3:D:651:HIS:CD2	3:D:652:GLU:H	2.04	0.72
2:C:903:ARG:HG3	2:C:910:ALA:HB2	1.71	0.72
2:C:59:ILE:HD12	2:C:472:GLU:OE1	1.89	0.72
1:A:9:LEU:HD12	1:A:9:LEU:N	2.01	0.71
1:A:47:LEU:CD2	1:A:220:ALA:HB2	2.19	0.71
1:A:149:GLY:HA3	1:A:177:TYR:CD2	2.24	0.71
1:A:234:LEU:N	1:A:234:LEU:HD23	2.05	0.71
1:A:158:ARG:HG2	1:A:158:ARG:NH1	1.99	0.71
3:D:1247:LYS:HB2	3:D:1247:LYS:NZ	2.05	0.71
5:M:154:LEU:HD21	5:M:193:LYS:CG	2.14	0.71
1:A:200:LYS:HB3	1:A:200:LYS:NZ	2.06	0.71
5:M:125:MET:HE1	5:M:145:VAL:HG21	1.72	0.71
2:C:916:SER:HA	5:M:266:THR:HG21	1.73	0.71
5:M:33:LEU:HD12	5:M:336:ARG:HH12	1.55	0.71
1:A:29:GLU:CD	1:A:30:PRO:HD3	2.11	0.70
3:D:651:HIS:NE2	3:D:652:GLU:HG3	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ASP:OD1	5:M:180:LYS:HD2	1.93	0.69
2:C:59:ILE:CD1	2:C:472:GLU:CG	2.68	0.69
5:M:16:THR:CG2	6:N:-11:DC:H5	2.04	0.69
1:A:218:ARG:HG3	1:B:232:VAL:HA	1.74	0.68
2:C:59:ILE:HD12	2:C:472:GLU:HG2	1.72	0.68
3:D:111:THR:O	3:D:238:ILE:CG2	2.32	0.68
3:D:674:THR:O	3:D:678:ARG:HB3	1.93	0.68
5:M:248:GLU:HA	5:M:251:ASN:HD22	1.58	0.68
3:D:913:GLU:HG2	4:E:17:PHE:CE2	2.28	0.68
3:D:398:LYS:HD2	5:M:126:TRP:CH2	2.29	0.68
2:C:678:ARG:NH1	2:C:681:MET:SD	2.67	0.68
5:M:41:LEU:CD1	5:M:48:GLU:HB2	2.24	0.68
1:A:167:PRO:HG2	1:A:170:ARG:HE	1.58	0.68
5:M:195:LEU:HD23	5:M:195:LEU:N	2.08	0.67
7:T:8:DA:H1'	7:T:9:DT:H5'	1.76	0.67
3:D:394:ILE:HG21	5:M:130:LEU:HD13	1.74	0.67
2:C:213:LEU:O	2:C:214:ASN:ND2	2.27	0.67
5:M:341:LEU:O	5:M:345:ARG:HG2	1.95	0.67
5:M:172:LEU:C	5:M:172:LEU:HD13	2.14	0.67
5:M:158:ILE:HG22	5:M:172:LEU:HD21	1.76	0.67
5:M:46:LEU:HD12	5:M:46:LEU:C	2.16	0.66
2:C:911:SER:HB3	5:M:259:ARG:HH12	1.58	0.66
3:D:123:ARG:HH22	3:D:1334:GLU:HG2	1.60	0.66
1:A:149:GLY:O	1:A:177:TYR:HB3	1.95	0.66
2:C:54:ARG:NH1	2:C:54:ARG:HG3	2.11	0.66
3:D:1230:THR:HG22	3:D:1257:VAL:HG11	1.76	0.66
1:A:57:THR:HG21	1:A:147:GLN:OE1	1.96	0.66
3:D:913:GLU:HG2	4:E:17:PHE:HE2	1.61	0.66
5:M:46:LEU:CD1	5:M:298:LYS:O	2.44	0.66
2:C:678:ARG:HH21	2:C:1106:ARG:HD3	1.60	0.65
5:M:120:LEU:HD22	5:M:120:LEU:C	2.16	0.65
5:M:232:PHE:HE1	5:M:250:VAL:HG11	1.62	0.65
3:D:254:PRO:HD2	5:M:112:TYR:CZ	2.32	0.65
2:C:889:PRO:HA	2:C:912:ASP:O	1.97	0.65
5:M:252:LEU:HD22	5:M:252:LEU:O	1.95	0.65
2:C:617:ALA:HB3	2:C:653:MET:HG2	1.78	0.65
1:B:62:ASP:HB2	1:B:140:ILE:HD11	1.79	0.65
1:A:45:ARG:NH1	1:B:38:THR:OG1	2.28	0.64
5:M:173:GLU:CD	5:M:173:GLU:H	1.99	0.64
5:M:23:ILE:HD11	7:T:12:DT:H6	1.62	0.64
5:M:287:VAL:HG11	5:M:344:SER:OG	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:16:THR:HG22	6:N:-11:DC:H6	1.61	0.64
5:M:153:TYR:OH	5:M:259:ARG:HG2	1.96	0.64
3:D:510:LEU:HB3	3:D:596:LEU:HD23	1.79	0.64
5:M:345:ARG:HG3	5:M:345:ARG:NH1	2.12	0.64
3:D:137:ARG:HG2	3:D:143:SER:HB2	1.79	0.64
1:A:9:LEU:HD11	1:A:32:GLU:CD	2.18	0.64
1:B:134:THR:HB	1:B:138:ALA:HB3	1.80	0.64
3:D:238:ILE:N	3:D:238:ILE:HD13	2.13	0.64
5:M:296:ARG:HG2	5:M:296:ARG:HH21	1.63	0.64
3:D:1226:VAL:HG11	3:D:1304:ARG:HD2	1.80	0.63
1:A:47:LEU:HD23	1:A:220:ALA:HB2	1.80	0.63
2:C:1177:ARG:HG3	2:C:1178:LYS:HD2	1.81	0.63
5:M:33:LEU:HD13	5:M:336:ARG:HH22	1.63	0.63
2:C:528:ARG:NH1	2:C:576:SER:O	2.31	0.63
3:D:905:ARG:HH11	3:D:905:ARG:CG	2.12	0.63
5:M:47:LEU:CD1	5:M:300:ASN:ND2	2.62	0.63
5:M:132:PRO:O	5:M:132:PRO:CG	2.45	0.63
5:M:197:ASP:HA	5:M:200:LEU:HD23	1.81	0.63
5:M:318:PHE:O	5:M:322:ASN:ND2	2.32	0.63
5:M:156:ILE:HG13	5:M:157:GLN:H	1.64	0.63
2:C:398:SER:O	2:C:401:GLY:N	2.26	0.62
2:C:454:ARG:HG3	2:C:454:ARG:NH2	2.12	0.62
2:C:1061:GLN:NE2	2:C:1240:ASP:OD1	2.31	0.62
2:C:102:LEU:HD12	2:C:489:PRO:HB3	1.80	0.62
5:M:15:MET:HA	5:M:19:LEU:HD13	1.81	0.62
5:M:120:LEU:HD22	5:M:120:LEU:O	1.98	0.62
2:C:843:THR:HB	5:M:271:TYR:CD2	2.35	0.62
5:M:273:ILE:HG22	5:M:389:TYR:CG	2.33	0.62
5:M:345:ARG:HG3	5:M:345:ARG:HH11	1.64	0.62
1:A:312:LEU:HD22	5:M:181:ARG:HH22	1.64	0.62
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.81	0.62
2:C:902:LEU:HD11	5:M:195:LEU:HB3	1.80	0.62
5:M:120:LEU:O	5:M:120:LEU:HD13	1.98	0.62
2:C:915:ASP:O	2:C:919:ARG:NH2	2.32	0.61
2:C:843:THR:HB	5:M:271:TYR:CE2	2.35	0.61
5:M:133:PHE:HB2	5:M:138:ARG:HH21	1.65	0.61
3:D:78:LEU:HB2	5:M:146:ASP:OD2	2.00	0.61
2:C:54:ARG:HG3	2:C:54:ARG:HH11	1.65	0.61
5:M:41:LEU:O	5:M:41:LEU:HD23	2.01	0.61
5:M:144:ILE:HG21	5:M:179:LEU:HD21	1.82	0.61
3:D:1181:ASP:HA	3:D:1185:PRO:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1335:ALA:O	3:D:1339:GLY:N	2.34	0.61
5:M:23:ILE:HD11	7:T:12:DT:C6	2.36	0.61
5:M:183:GLN:HB3	5:M:201:ILE:HD13	1.83	0.61
5:M:455:ARG:NH2	6:N:-26:DG:N7	2.41	0.61
3:D:1177:ILE:HG12	3:D:1179:PRO:HD2	1.82	0.60
5:M:158:ILE:CD1	5:M:193:LYS:HD3	2.31	0.60
3:D:394:ILE:HG21	5:M:130:LEU:HD12	1.84	0.60
5:M:462:ARG:NH2	6:N:-26:DG:OP2	2.32	0.60
1:A:157:THR:HG22	1:A:157:THR:O	2.00	0.60
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.83	0.60
5:M:244:GLU:O	5:M:247:LYS:HB3	2.01	0.60
5:M:456:ARG:NE	7:T:25:DC:H41	1.96	0.60
3:D:63:GLY:HA2	3:D:101:ARG:HD2	1.83	0.60
1:A:305:ASP:OD1	5:M:180:LYS:HD3	2.01	0.60
2:C:905:ILE:O	5:M:254:GLN:NE2	2.35	0.60
3:D:677:GLU:C	3:D:679:TYR:H	2.05	0.60
5:M:133:PHE:H	5:M:138:ARG:HH22	1.47	0.60
3:D:1208:ASP:HB2	3:D:1224:ARG:HE	1.67	0.60
1:A:235:ARG:O	1:B:14:VAL:HG23	2.01	0.59
2:C:166:SER:O	2:C:166:SER:OG	2.20	0.59
5:M:183:GLN:OE1	5:M:201:ILE:HD11	2.03	0.59
5:M:109:LEU:N	5:M:109:LEU:HD22	2.17	0.59
5:M:173:GLU:OE1	5:M:173:GLU:N	2.35	0.59
3:D:506:VAL:HG13	3:D:628:GLY:HA3	1.84	0.59
1:A:95:LYS:NZ	1:A:120:ASP:HB2	2.18	0.59
1:B:93:GLN:H	1:B:120:ASP:HB3	1.66	0.59
5:M:165:ILE:HG23	5:M:167:ASP:H	1.67	0.59
5:M:273:ILE:HG22	5:M:273:ILE:O	2.01	0.59
3:D:398:LYS:HD2	5:M:126:TRP:HH2	1.66	0.59
1:A:231:PHE:O	1:B:221:ALA:HB2	2.01	0.59
1:B:12:ARG:H	1:B:30:PRO:HG2	1.67	0.59
3:D:651:HIS:CD2	3:D:652:GLU:CG	2.82	0.59
2:C:150:HIS:CD2	2:C:454:ARG:HH22	2.21	0.59
2:C:563:THR:O	2:C:684:ASN:ND2	2.31	0.59
2:C:54:ARG:HH11	2:C:54:ARG:CG	2.14	0.59
3:D:112:ALA:HA	3:D:238:ILE:HG22	1.81	0.59
3:D:254:PRO:HG2	5:M:112:TYR:CE2	2.38	0.59
6:N:-12:DA:H2'	6:N:-11:DC:H4'	1.85	0.59
2:C:540:ARG:HG2	2:C:542:ARG:H	1.67	0.59
5:M:158:ILE:HG12	5:M:193:LYS:HD2	1.85	0.58
5:M:455:ARG:HD3	5:M:455:ARG:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:-7:DC:H2"	6:N:-6:DA:C8	2.38	0.58
2:C:421:SER:OG	2:C:423:ASP:OD1	2.20	0.58
2:C:589:THR:OG1	2:C:659:GLN:NE2	2.36	0.58
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.85	0.58
3:D:842:ARG:HH11	3:D:882:VAL:HG11	1.69	0.58
2:C:150:HIS:CD2	2:C:454:ARG:NH2	2.72	0.58
2:C:911:SER:CB	5:M:259:ARG:HH22	2.16	0.58
3:D:840:LEU:HD11	3:D:866:GLU:HG2	1.86	0.58
3:D:599:LYS:HD3	3:D:599:LYS:N	2.18	0.58
1:A:188:GLU:HG3	1:A:200:LYS:NZ	2.19	0.58
2:C:17:LYS:NZ	2:C:1194:GLU:OE2	2.35	0.58
1:A:25:LYS:CD	1:A:204:GLU:HG2	2.34	0.57
5:M:196:ARG:O	5:M:200:LEU:HD22	2.04	0.57
3:D:355:ILE:HD11	3:D:449:LEU:HB2	1.86	0.57
5:M:112:TYR:CD1	5:M:112:TYR:N	2.72	0.57
1:A:29:GLU:OE2	1:A:29:GLU:HA	2.05	0.57
1:A:231:PHE:O	1:B:221:ALA:HB3	2.04	0.57
2:C:1296:ASP:HB3	2:C:1321:GLU:H	1.70	0.57
3:D:351:GLY:HA3	3:D:468:VAL:H	1.67	0.57
1:A:47:LEU:CD2	1:A:220:ALA:CB	2.82	0.57
2:C:155:VAL:HG22	2:C:176:ILE:HB	1.85	0.57
2:C:474:ALA:O	2:C:477:GLU:HG3	2.04	0.57
2:C:515:MET:SD	2:C:517:GLN:NE2	2.77	0.57
3:D:1247:LYS:HB2	3:D:1247:LYS:HZ2	1.69	0.57
5:M:374:VAL:O	5:M:376:MET:HG2	2.05	0.57
3:D:483:LEU:CD2	4:E:16:ARG:HD2	2.34	0.57
3:D:651:HIS:HD2	3:D:652:GLU:HG3	1.63	0.57
1:A:149:GLY:HA3	1:A:177:TYR:CE2	2.39	0.57
5:M:196:ARG:O	5:M:196:ARG:HG2	2.03	0.57
2:C:797:GLY:HA3	2:C:1232:MET:O	2.05	0.57
3:D:913:GLU:CG	4:E:17:PHE:HE2	2.18	0.57
1:A:13:LEU:HD23	1:A:28:LEU:CD1	2.32	0.56
3:D:811:GLU:HG2	3:D:890:THR:HG21	1.87	0.56
3:D:253:VAL:CG1	5:M:112:TYR:HB3	2.26	0.56
3:D:1311:LYS:HD2	3:D:1314:LEU:HD12	1.87	0.56
1:A:12:ARG:HH11	1:A:12:ARG:CB	2.09	0.56
2:C:524:ILE:HD12	2:C:708:VAL:HG13	1.88	0.56
2:C:1276:TRP:HH2	3:D:798:ARG:HD2	1.70	0.56
3:D:112:ALA:CA	3:D:238:ILE:CG2	2.71	0.56
5:M:33:LEU:HD11	5:M:336:ARG:NH1	2.20	0.56
5:M:117:THR:HG23	5:M:119:THR:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:GLN:NE2	1:A:20:SER:O	2.38	0.56
1:A:61:ILE:HB	1:A:64:VAL:HG12	1.85	0.56
2:C:462:ASN:N	2:C:462:ASN:HD22	2.03	0.56
2:C:59:ILE:CD1	2:C:472:GLU:OE1	2.53	0.56
5:M:129:GLU:OE1	5:M:129:GLU:HA	2.06	0.56
5:M:296:ARG:HH21	5:M:296:ARG:CG	2.18	0.56
5:M:351:GLN:OE1	5:M:363:LYS:N	2.34	0.56
7:T:20:DT:H2"	7:T:21:DC:C6	2.40	0.56
2:C:724:VAL:HG22	2:C:734:ILE:HG12	1.88	0.56
2:C:1065:LYS:NZ	3:D:462:ASP:O	2.38	0.56
3:D:63:GLY:HA3	3:D:98:ARG:HG3	1.87	0.56
3:D:930:LEU:HD21	3:D:1137:GLY:HA2	1.88	0.56
5:M:216:ALA:O	5:M:220:ILE:HG13	2.06	0.56
5:M:220:ILE:HD11	5:M:253:ILE:HG13	1.88	0.56
1:B:46:ILE:HG13	1:B:224:LEU:HG	1.87	0.56
2:C:823:VAL:HA	2:C:1060:ILE:HD11	1.87	0.56
3:D:1122:ALA:HB1	3:D:1125:PRO:HD3	1.87	0.56
3:D:510:LEU:HD11	3:D:624:ILE:HG23	1.87	0.56
5:M:112:TYR:HD1	5:M:112:TYR:N	2.02	0.56
5:M:118:GLN:O	5:M:122:ASP:HB2	2.06	0.56
7:T:33:DC:H2"	7:T:34:DT:H6	1.63	0.56
3:D:917:VAL:O	3:D:921:GLN:HB2	2.06	0.55
5:M:196:ARG:NH1	5:M:221:SER:O	2.40	0.55
1:A:131:CYS:SG	1:A:132:HIS:N	2.78	0.55
2:C:463:GLN:HG2	2:C:505:PHE:HB2	1.88	0.55
3:D:137:ARG:HG3	3:D:142:GLU:HG3	1.88	0.55
3:D:262:THR:HB	3:D:266:ASN:HD22	1.70	0.55
1:A:219:ARG:HA	1:A:222:THR:HG22	1.88	0.55
1:A:58:GLU:OE2	1:A:170:ARG:NH2	2.35	0.55
1:A:312:LEU:HD22	5:M:181:ARG:NH2	2.21	0.55
1:B:152:TYR:OH	3:D:535:ARG:NH2	2.39	0.55
3:D:720:ASN:HB3	3:D:723:TYR:HB3	1.89	0.55
2:C:454:ARG:HH21	2:C:454:ARG:CG	2.13	0.55
1:A:100:LEU:CD2	1:A:121:VAL:HG21	2.36	0.55
3:D:121:PRO:HG2	3:D:123:ARG:HH21	1.72	0.55
5:M:455:ARG:HD3	5:M:455:ARG:C	2.27	0.55
1:B:41:ASN:OD1	1:B:44:ARG:NH1	2.39	0.55
2:C:402:ARG:HH12	2:C:420:LEU:HB3	1.72	0.55
3:D:483:LEU:HD21	4:E:16:ARG:HD2	1.89	0.55
3:D:504:GLN:HE22	3:D:731:ARG:HH11	1.53	0.55
3:D:553:THR:HG22	3:D:567:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:SER:HB2	1:B:78:ILE:HG21	1.89	0.54
2:C:143:ARG:NH2	2:C:512:SER:O	2.40	0.54
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.89	0.54
5:M:187:PRO:HB3	5:M:260:PRO:HB2	1.90	0.54
2:C:678:ARG:HH12	2:C:1073:LYS:HE2	1.73	0.54
1:A:192:VAL:HB	1:A:194:GLN:HE22	1.72	0.54
2:C:150:HIS:NE2	2:C:454:ARG:NH2	2.55	0.54
3:D:65:VAL:HG22	3:D:66:LYS:H	1.71	0.54
3:D:254:PRO:CD	5:M:112:TYR:CE2	2.89	0.54
5:M:16:THR:CG2	6:N:-11:DC:C6	2.88	0.54
5:M:41:LEU:HD13	5:M:48:GLU:HB2	1.87	0.54
1:B:131:CYS:SG	1:B:132:HIS:N	2.80	0.54
2:C:1060:ILE:HD13	2:C:1060:ILE:H	1.73	0.54
2:C:1151:LEU:HD21	2:C:1201:LEU:HD22	1.90	0.54
2:C:1275:VAL:HG11	3:D:343:LEU:HD22	1.89	0.54
1:A:152:TYR:CD1	1:A:175:ALA:O	2.61	0.54
1:A:188:GLU:HG3	1:A:200:LYS:HZ1	1.73	0.54
3:D:1033:GLY:HA3	3:D:1082:ASP:HA	1.88	0.54
7:T:33:DC:H2'	7:T:34:DT:H72	1.89	0.54
1:A:64:VAL:HG21	1:A:78:ILE:HG21	1.90	0.54
3:D:126:LEU:O	3:D:220:ARG:NH1	2.40	0.54
2:C:1311:GLY:O	4:E:31:GLN:NE2	2.41	0.54
5:M:216:ALA:HB1	5:M:253:ILE:CD1	2.38	0.54
3:D:425:ARG:NH2	3:D:464:ASP:OD2	2.41	0.53
3:D:355:ILE:HB	3:D:466:MET:HB2	1.90	0.53
5:M:158:ILE:CG1	5:M:193:LYS:HD3	2.39	0.53
5:M:262:GLN:C	5:M:264:ILE:H	2.11	0.53
5:M:248:GLU:HA	5:M:248:GLU:OE1	2.09	0.53
2:C:1268:GLN:HB2	3:D:350:SER:HB2	1.91	0.53
1:B:185:TYR:HB2	1:B:201:LEU:HD11	1.90	0.53
3:D:610:ARG:NH1	3:D:866:GLU:OE2	2.41	0.53
5:M:345:ARG:HH11	5:M:345:ARG:CG	2.21	0.53
1:A:158:ARG:NH2	1:A:173:VAL:O	2.42	0.53
2:C:473:ARG:HH11	2:C:473:ARG:CG	2.14	0.53
2:C:1238:LEU:HD13	2:C:1240:ASP:HB2	1.91	0.53
2:C:1272:GLU:OE1	3:D:798:ARG:NH2	2.41	0.53
2:C:731:ARG:HH22	2:C:959:ASP:HB3	1.74	0.53
3:D:1318:SER:OG	3:D:1321:SER:OG	2.26	0.53
5:M:28:LEU:HB2	5:M:32:GLU:HG3	1.90	0.53
3:D:803:VAL:O	3:D:1259:GLN:NE2	2.42	0.53
3:D:1102:PRO:O	3:D:1105:ALA:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:677:GLU:OE2	3:D:677:GLU:HA	2.09	0.53
5:M:154:LEU:CD2	5:M:193:LYS:HG3	2.19	0.53
3:D:887:SER:HB3	3:D:1227:HIS:CE1	2.45	0.52
2:C:12:ARG:NH2	2:C:793:GLU:OE1	2.43	0.52
1:A:31:LEU:N	1:A:31:LEU:CD2	2.73	0.52
3:D:677:GLU:C	3:D:679:TYR:N	2.62	0.52
1:A:29:GLU:OE2	1:A:30:PRO:HD3	2.10	0.52
2:C:902:LEU:CD1	5:M:195:LEU:HB2	2.32	0.52
5:M:190:VAL:O	5:M:190:VAL:HG13	2.09	0.52
1:A:118:ASP:HB3	1:A:121:VAL:HG12	1.92	0.52
1:A:165:GLU:OE1	1:A:165:GLU:HA	2.10	0.52
1:B:125:LYS:HE2	1:B:128:HIS:HB2	1.92	0.52
2:C:706:ARG:NH2	2:C:791:LEU:O	2.42	0.52
5:M:273:ILE:HG21	5:M:389:TYR:CE2	2.45	0.52
5:M:348:VAL:O	5:M:352:GLN:HG3	2.09	0.52
2:C:532:ALA:HB1	2:C:538:LEU:HD23	1.90	0.52
2:C:560:PRO:O	3:D:780:ARG:NH2	2.42	0.52
2:C:916:SER:CA	5:M:266:THR:HG21	2.39	0.52
2:C:1219:GLU:OE1	3:D:634:ARG:NH1	2.42	0.52
3:D:57:PHE:HD2	3:D:98:ARG:HH12	1.56	0.52
5:M:23:ILE:HD11	7:T:12:DT:C7	2.39	0.52
3:D:599:LYS:N	3:D:599:LYS:CD	2.73	0.52
2:C:675:ASP:HB3	2:C:678:ARG:HB2	1.91	0.52
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.92	0.52
2:C:1254:VAL:HG12	2:C:1255:THR:HG23	1.92	0.51
3:D:62:PHE:HB3	3:D:247:PRO:HG3	1.92	0.51
1:B:113:ALA:HB2	1:B:126:PRO:HB2	1.91	0.51
1:A:16:ILE:HG13	1:A:26:VAL:HG22	1.92	0.51
1:A:101:THR:HG22	1:A:143:ARG:HG2	1.91	0.51
1:A:152:TYR:HD1	1:A:175:ALA:O	1.92	0.51
1:A:234:LEU:N	1:A:234:LEU:CD2	2.73	0.51
2:C:906:PHE:HA	5:M:254:GLN:HE21	1.74	0.51
2:C:1246:ARG:HH22	2:C:1258:PRO:HB3	1.76	0.51
2:C:657:THR:HB	2:C:1187:PHE:HB2	1.93	0.51
2:C:661:VAL:HG11	2:C:1186:VAL:HG11	1.93	0.51
3:D:422:LEU:HA	3:D:436:ALA:HA	1.93	0.51
5:M:147:ALA:O	5:M:155:THR:OG1	2.26	0.51
2:C:887:VAL:HB	2:C:913:VAL:HB	1.93	0.51
5:M:181:ARG:O	5:M:181:ARG:HG3	2.08	0.51
6:N:-10:DG:H2''	6:N:-9:DA:H5'	1.92	0.51
3:D:62:PHE:HE1	3:D:103:GLY:HA3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:643:ASP:OD2	3:D:721:SER:OG	2.27	0.51
3:D:426:ALA:HB3	3:D:427:PRO:HD3	1.92	0.51
3:D:309:ASN:HD21	3:D:315:ALA:HB3	1.76	0.51
5:M:158:ILE:HG12	5:M:193:LYS:CD	2.41	0.51
5:M:195:LEU:N	5:M:195:LEU:CD2	2.72	0.51
1:A:102:LEU:HD13	1:A:115:ILE:HG12	1.92	0.50
1:A:256:PRO:HA	1:A:277:TYR:HB3	1.93	0.50
2:C:972:PHE:HE1	2:C:993:PRO:HB3	1.75	0.50
2:C:1268:GLN:HG2	3:D:352:ARG:HH11	1.76	0.50
5:M:176:GLU:OE1	5:M:180:LYS:NZ	2.44	0.50
1:A:279:GLY:HA3	1:A:321:TRP:HZ2	1.77	0.50
2:C:902:LEU:CD1	5:M:195:LEU:CB	2.83	0.50
3:D:254:PRO:HD2	5:M:112:TYR:CD2	2.45	0.50
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.94	0.50
1:B:190:ALA:HB2	1:B:200:LYS:HD2	1.94	0.50
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.93	0.50
5:M:366:VAL:HG12	5:M:367:LEU:H	1.77	0.50
3:D:394:ILE:CG2	5:M:130:LEU:HD13	2.42	0.50
4:E:3:ARG:O	4:E:4:VAL:C	2.49	0.50
2:C:873:ILE:HD13	2:C:873:ILE:H	1.76	0.50
1:A:83:LEU:HD13	2:C:694:ARG:HD2	1.93	0.50
6:N:-34:DA:H2''	6:N:-33:DG:C8	2.46	0.50
2:C:454:ARG:NH2	2:C:454:ARG:CG	2.73	0.50
3:D:901:ARG:NH1	3:D:906:GLY:O	2.45	0.50
1:A:192:VAL:HG23	1:A:192:VAL:O	2.12	0.49
2:C:812:PHE:N	2:C:815:SER:OG	2.45	0.49
2:C:916:SER:HB2	5:M:266:THR:CB	2.42	0.49
5:M:35:GLN:O	5:M:39:GLN:HB3	2.12	0.49
3:D:43:THR:HG22	3:D:56:LEU:HB2	1.94	0.49
5:M:366:VAL:HG12	5:M:367:LEU:N	2.27	0.49
1:A:47:LEU:HD21	1:A:220:ALA:HB2	1.93	0.49
1:A:180:VAL:O	1:A:206:GLU:O	2.30	0.49
3:D:651:HIS:CD2	3:D:651:HIS:C	2.85	0.49
5:M:184:ARG:NH1	5:M:201:ILE:HG12	2.28	0.49
5:M:203:LEU:CD2	5:M:256:LEU:HD11	2.42	0.49
1:A:9:LEU:HD13	1:A:9:LEU:O	2.13	0.49
2:C:848:GLU:HG2	2:C:889:PRO:HD2	1.95	0.49
3:D:341:ASN:HD21	3:D:1352:ILE:HG23	1.77	0.49
3:D:1247:LYS:NZ	3:D:1247:LYS:CB	2.73	0.49
3:D:1230:THR:O	3:D:1234:VAL:HG12	2.13	0.49
1:A:224:LEU:O	1:A:224:LEU:HG	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:VAL:HG22	1:B:235:ARG:H	1.77	0.49
3:D:746:LEU:HD23	3:D:754:ILE:HG21	1.94	0.49
5:M:26:LEU:HB3	5:M:336:ARG:HG2	1.95	0.49
5:M:37:LEU:HD11	5:M:297:LEU:HD22	1.94	0.49
5:M:232:PHE:CE1	5:M:250:VAL:HG11	2.46	0.49
2:C:69:GLN:O	2:C:101:ARG:N	2.46	0.49
2:C:1129:ASN:OD1	2:C:1177:ARG:NH2	2.41	0.49
3:D:265:LEU:CD2	3:D:330:MET:HE1	2.43	0.49
1:A:121:VAL:O	1:A:121:VAL:HG13	2.13	0.49
2:C:10:ARG:HE	2:C:791:LEU:HD12	1.78	0.49
5:M:158:ILE:CG1	5:M:193:LYS:CD	2.91	0.49
1:A:205:MET:HG2	1:A:205:MET:O	2.13	0.48
2:C:175:ARG:HH12	2:C:177:ILE:HD11	1.78	0.48
7:T:7:DG:H1'	7:T:8:DA:H5''	1.93	0.48
2:C:152:SER:H	2:C:451:ARG:HA	1.78	0.48
2:C:196:VAL:HG23	2:C:206:ALA:HA	1.96	0.48
2:C:1246:ARG:NH2	2:C:1265:PHE:O	2.46	0.48
3:D:59:ALA:HB1	3:D:90:VAL:HG22	1.95	0.48
3:D:368:LEU:HD12	3:D:439:PRO:HB3	1.95	0.48
3:D:1350:ASN:O	3:D:1354:GLY:N	2.42	0.48
2:C:807:TRP:N	2:C:811:ASN:HD21	2.11	0.48
3:D:40:LYS:N	3:D:54:ASP:O	2.45	0.48
3:D:1234:VAL:O	3:D:1235:ASN:C	2.50	0.48
1:A:47:LEU:HD21	1:A:220:ALA:CB	2.43	0.48
3:D:678:ARG:NH2	3:D:756:GLU:OE1	2.47	0.48
5:M:273:ILE:HG22	5:M:389:TYR:CB	2.44	0.48
2:C:444:ASP:O	2:C:450:ASN:ND2	2.46	0.48
3:D:429:LEU:HD13	3:D:925:GLU:HG2	1.95	0.48
7:T:10:DC:H2''	7:T:11:DG:N7	2.29	0.48
2:C:582:ASN:ND2	2:C:588:GLU:OE2	2.46	0.48
2:C:675:ASP:OD1	2:C:676:ALA:N	2.46	0.48
5:M:278:VAL:HG22	5:M:287:VAL:HG13	1.95	0.48
5:M:290:ASN:O	5:M:294:ILE:HG12	2.14	0.48
7:T:0:DC:H2''	7:T:1:DA:C8	2.48	0.48
2:C:472:GLU:OE1	2:C:476:LYS:HE3	2.14	0.48
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.94	0.48
2:C:1246:ARG:HH21	2:C:1266:GLY:HA2	1.79	0.48
2:C:23:ASP:OD1	2:C:24:VAL:N	2.45	0.48
2:C:444:ASP:HB3	2:C:447:HIS:HB2	1.95	0.48
3:D:290:ILE:HG12	3:D:293:ARG:HH21	1.78	0.48
1:A:29:GLU:HG3	1:A:30:PRO:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HD11	1:B:8:PHE:HE1	1.73	0.47
2:C:555:TYR:OH	2:C:654:ASP:OD2	2.32	0.47
3:D:516:ASP:OD1	3:D:516:ASP:N	2.46	0.47
1:A:31:LEU:CD2	1:A:31:LEU:H	2.26	0.47
3:D:1266:ILE:HG22	3:D:1302:TYR:HB3	1.96	0.47
5:M:41:LEU:HD12	5:M:297:LEU:HD11	1.96	0.47
5:M:296:ARG:HG2	5:M:296:ARG:O	2.13	0.47
7:T:33:DC:C2'	7:T:34:DT:C6	2.92	0.47
2:C:1282:GLY:HA3	4:E:17:PHE:HE1	1.78	0.47
2:C:185:ASP:HB2	2:C:197:ARG:HB3	1.96	0.47
3:D:252:LEU:HA	3:D:262:THR:HG22	1.97	0.47
7:T:32:DT:H2''	7:T:33:DC:C6	2.49	0.47
2:C:27:LEU:HD21	2:C:663:VAL:HG11	1.96	0.47
2:C:509:SER:HB3	2:C:512:SER:HB3	1.97	0.47
3:D:923:ILE:HD13	3:D:1248:ILE:HG21	1.97	0.47
1:A:312:LEU:CD2	5:M:181:ARG:HH22	2.25	0.47
2:C:801:ARG:HD3	2:C:1094:VAL:HA	1.96	0.47
2:C:802:VAL:HG12	2:C:1096:ILE:HB	1.97	0.47
2:C:1070:HIS:NE2	2:C:1114:GLU:OE1	2.38	0.47
3:D:502:PRO:HB2	3:D:506:VAL:HB	1.96	0.47
3:D:978:ARG:NH1	3:D:1203:ARG:O	2.45	0.47
5:M:296:ARG:CG	5:M:296:ARG:NH2	2.76	0.47
3:D:349:TYR:HD1	3:D:376:LEU:HD22	1.80	0.47
3:D:1247:LYS:HB2	3:D:1247:LYS:HZ3	1.77	0.47
5:M:187:PRO:CB	5:M:260:PRO:HB2	2.44	0.47
2:C:169:LYS:HE2	2:C:169:LYS:CA	2.30	0.47
2:C:692:THR:OG1	2:C:693:LEU:N	2.48	0.47
5:M:127:GLN:NE2	5:M:186:ASP:HB2	2.29	0.46
5:M:252:LEU:HD22	5:M:252:LEU:C	2.34	0.46
2:C:10:ARG:HH11	2:C:791:LEU:HB2	1.80	0.46
3:D:609:TYR:HE1	3:D:614:LEU:HD13	1.80	0.46
5:M:33:LEU:HD13	5:M:336:ARG:NH2	2.28	0.46
7:T:33:DC:H2''	7:T:34:DT:C5	2.50	0.46
3:D:809:VAL:HB	3:D:912:GLY:H	1.81	0.46
1:A:46:ILE:CD1	1:A:224:LEU:HB2	2.45	0.46
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.96	0.46
2:C:1290:MET:HA	2:C:1294:LYS:HD2	1.97	0.46
5:M:133:PHE:N	5:M:138:ARG:NH2	2.57	0.46
5:M:456:ARG:HG3	7:T:24:DG:N7	2.30	0.46
6:N:-12:DA:OP2	6:N:-12:DA:H2	1.98	0.46
5:M:145:VAL:HA	5:M:148:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1272:GLU:HG2	3:D:343:LEU:HB2	1.98	0.46
5:M:37:LEU:HD22	5:M:37:LEU:HA	1.79	0.46
5:M:426:LYS:HB2	5:M:426:LYS:HE3	1.68	0.46
1:A:28:LEU:HD13	1:A:28:LEU:HA	1.56	0.46
2:C:394:ARG:O	2:C:394:ARG:HG2	2.14	0.46
2:C:906:PHE:HA	5:M:254:GLN:NE2	2.30	0.46
1:A:200:LYS:O	1:A:200:LYS:HG2	2.16	0.46
3:D:40:LYS:HZ3	3:D:41:PRO:HD2	1.80	0.46
5:M:239:THR:HG23	5:M:241:LEU:HG	1.98	0.46
2:C:458:GLU:O	2:C:462:ASN:ND2	2.48	0.46
2:C:562:GLU:OE1	2:C:662:SER:OG	2.27	0.46
3:D:24:LEU:HG	3:D:232:ASN:HD22	1.80	0.46
3:D:1162:ILE:HG22	3:D:1163:VAL:H	1.81	0.46
3:D:1249:ASN:HB3	3:D:1252:HIS:CD2	2.51	0.46
1:B:86:LYS:HE2	1:B:174:ASP:HB2	1.98	0.46
1:A:9:LEU:H	1:A:9:LEU:CD1	2.15	0.45
1:A:66:HIS:HB3	2:C:874:GLY:HA2	1.98	0.45
5:M:47:LEU:CD1	5:M:300:ASN:HD22	2.28	0.45
2:C:59:ILE:HD12	2:C:472:GLU:CG	2.40	0.45
3:D:254:PRO:CG	5:M:112:TYR:CE2	2.99	0.45
5:M:273:ILE:HG21	5:M:389:TYR:CD1	2.50	0.45
1:A:15:ASP:O	1:A:27:THR:HG22	2.16	0.45
1:A:15:ASP:O	1:A:27:THR:CG2	2.64	0.45
3:D:1190:ILE:HG22	3:D:1192:LYS:H	1.81	0.45
5:M:336:ARG:NH1	5:M:336:ARG:HG3	2.30	0.45
6:N:-12:DA:N3	6:N:-12:DA:C3'	2.77	0.45
2:C:207:THR:HG22	2:C:210:LEU:HD12	1.99	0.45
3:D:337:ARG:HH11	3:D:340:GLN:HE22	1.65	0.45
5:M:41:LEU:HD11	5:M:48:GLU:HB2	1.98	0.45
2:C:179:TYR:OH	2:C:462:ASN:OD1	2.23	0.45
2:C:1257:GLN:NE2	3:D:340:GLN:OE1	2.48	0.45
2:C:1268:GLN:HG2	3:D:352:ARG:HD2	1.98	0.45
5:M:176:GLU:OE1	5:M:180:LYS:CE	2.64	0.45
5:M:377:HIS:O	5:M:381:ILE:HG13	2.16	0.45
1:A:312:LEU:CD2	5:M:181:ARG:NH2	2.79	0.45
2:C:1108:ASN:O	2:C:1111:GLN:HG2	2.17	0.45
3:D:309:ASN:OD1	3:D:310:GLY:N	2.49	0.45
3:D:363:LEU:O	3:D:486:SER:OG	2.28	0.45
1:A:6:THR:OG1	1:B:150:ARG:NH2	2.49	0.45
1:A:13:LEU:CD2	1:A:28:LEU:HD13	2.39	0.45
2:C:350:THR:O	2:C:354:ASP:OD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:PRO:HB2	2:C:354:ASP:OD2	2.17	0.45
2:C:402:ARG:NH2	2:C:418:GLY:O	2.42	0.45
3:D:120:LEU:HB2	3:D:121:PRO:HD3	1.98	0.45
3:D:265:LEU:CD2	3:D:330:MET:CE	2.95	0.45
3:D:480:ALA:HA	3:D:484:MET:HB2	1.98	0.45
5:M:172:LEU:O	5:M:172:LEU:HD13	2.17	0.45
7:T:6:DT:H2''	7:T:7:DG:C8	2.51	0.45
5:M:176:GLU:O	5:M:180:LYS:HB2	2.16	0.45
2:C:519:ASN:ND2	2:C:689:ALA:O	2.50	0.45
2:C:520:PRO:HA	2:C:523:GLU:HG3	1.98	0.45
2:C:856:ASN:HA	5:M:257:ASP:OD2	2.17	0.45
1:B:91:ARG:NH2	1:B:122:GLU:OE1	2.47	0.44
2:C:1065:LYS:HG2	2:C:1235:LEU:HD12	2.00	0.44
3:D:905:ARG:HG3	3:D:905:ARG:NH1	2.20	0.44
2:C:1080:ASN:HB3	2:C:1085:MET:HE2	1.98	0.44
3:D:1320:ILE:HG22	3:D:1352:ILE:HD12	1.99	0.44
6:N:-12:DA:OP2	6:N:-12:DA:C2	2.70	0.44
7:T:12:DT:H2'	7:T:12:DT:O2	2.16	0.44
2:C:398:SER:O	2:C:400:VAL:N	2.50	0.44
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.98	0.44
5:M:441:LYS:O	5:M:445:MET:HG2	2.18	0.44
5:M:455:ARG:C	5:M:455:ARG:CD	2.86	0.44
1:A:45:ARG:NH2	2:C:1084:ASP:OD1	2.50	0.44
3:D:662:ALA:O	3:D:665:GLN:HG3	2.18	0.44
5:M:123:TYR:O	5:M:123:TYR:CD1	2.70	0.44
1:A:31:LEU:H	1:A:31:LEU:HD23	1.82	0.44
1:A:289:LEU:HD12	1:A:300:LEU:HD13	2.00	0.44
1:A:305:ASP:CG	5:M:180:LYS:HD2	2.37	0.44
5:M:25:LEU:HD13	5:M:25:LEU:O	2.18	0.44
5:M:193:LYS:HB2	5:M:193:LYS:HE2	1.58	0.44
5:M:281:VAL:O	5:M:282:SER:OG	2.33	0.44
3:D:394:ILE:HG12	5:M:130:LEU:CD1	2.39	0.44
3:D:820:ILE:HG22	3:D:1227:HIS:CE1	2.53	0.44
6:N:-33:DG:H2''	6:N:-32:DA:N7	2.32	0.44
2:C:852:ALA:HB2	2:C:869:GLY:HA2	1.99	0.44
2:C:1225:VAL:HG22	3:D:638:SER:HB2	1.99	0.44
3:D:201:LEU:HB3	3:D:221:ILE:HG12	2.00	0.44
3:D:398:LYS:HD2	5:M:126:TRP:CZ3	2.52	0.44
5:M:280:LYS:CB	5:M:285:TRP:HE3	2.31	0.44
3:D:340:GLN:HE21	3:D:340:GLN:HB3	1.67	0.44
3:D:390:LEU:HD22	3:D:411:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:46:LEU:HG	5:M:46:LEU:O	2.18	0.44
2:C:13:LYS:NZ	2:C:1149:TYR:O	2.50	0.43
3:D:887:SER:CB	3:D:1227:HIS:CE1	3.00	0.43
5:M:126:TRP:CZ2	5:M:130:LEU:HD11	2.53	0.43
3:D:677:GLU:O	3:D:679:TYR:N	2.51	0.43
3:D:1330:ARG:NH1	3:D:1334:GLU:OE2	2.51	0.43
2:C:594:VAL:HG21	2:C:653:MET:HG3	2.01	0.43
3:D:703:THR:HA	3:D:718:SER:H	1.83	0.43
1:A:196:THR:O	1:A:198:LEU:HG	2.18	0.43
2:C:548:ARG:NH2	2:C:567:PRO:O	2.51	0.43
3:D:193:ASP:HB3	3:D:196:GLN:HB3	2.00	0.43
3:D:204:GLU:O	3:D:208:THR:OG1	2.32	0.43
3:D:572:THR:OG1	3:D:573:THR:N	2.52	0.43
2:C:932:GLN:N	2:C:1051:LYS:O	2.51	0.43
1:A:158:ARG:NH1	1:A:172:LEU:HD23	2.34	0.43
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	2.00	0.43
3:D:15:GLU:OE1	3:D:16:GLU:N	2.51	0.43
2:C:205:PRO:CB	2:C:354:ASP:OD2	2.66	0.43
2:C:1192:GLU:HG2	2:C:1196:LYS:HE2	2.00	0.43
5:M:46:LEU:HD21	5:M:297:LEU:CD2	2.49	0.43
1:A:216:ALA:O	1:A:220:ALA:N	2.51	0.43
2:C:463:GLN:OE1	2:C:463:GLN:HA	2.18	0.43
3:D:430:HIS:HB3	3:D:925:GLU:HG3	2.01	0.43
3:D:905:ARG:CG	3:D:905:ARG:NH1	2.73	0.43
1:A:75:GLN:HB3	1:A:132:HIS:HB2	2.00	0.43
1:A:167:PRO:CG	1:A:170:ARG:HE	2.30	0.43
1:A:9:LEU:HD12	1:A:32:GLU:OE2	2.19	0.42
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.34	0.42
3:D:65:VAL:HG12	3:D:90:VAL:HG11	2.00	0.42
3:D:121:PRO:HB2	3:D:123:ARG:HE	1.84	0.42
3:D:1138:LEU:HB3	3:D:1139:PRO:HD3	2.01	0.42
6:N:-9:DA:C2	6:N:-8:DT:C2	3.07	0.42
1:A:180:VAL:HG23	1:A:181:GLU:H	1.84	0.42
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	2.01	0.42
3:D:1328:THR:O	3:D:1329:THR:C	2.57	0.42
5:M:15:MET:O	6:N:-12:DA:N6	2.48	0.42
5:M:280:LYS:HA	5:M:285:TRP:HB3	2.01	0.42
1:B:70:THR:OG1	1:B:72:GLU:OE2	2.30	0.42
2:C:229:ILE:HG21	2:C:240:GLU:HB2	2.02	0.42
5:M:46:LEU:HD11	5:M:298:LYS:O	2.18	0.42
5:M:125:MET:HE1	5:M:145:VAL:CG2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:29:DC:H2"	7:T:30:DC:C6	2.54	0.42
1:A:150:ARG:HG2	1:A:150:ARG:HH21	1.84	0.42
2:C:931:VAL:HG12	2:C:1052:VAL:HG13	2.01	0.42
3:D:138:VAL:HA	3:D:143:SER:HB3	2.01	0.42
5:M:158:ILE:HG22	5:M:172:LEU:CD2	2.45	0.42
5:M:455:ARG:HD2	5:M:456:ARG:NH2	2.34	0.42
2:C:902:LEU:CD1	5:M:195:LEU:HB3	2.48	0.42
3:D:1234:VAL:HG13	3:D:1235:ASN:H	1.84	0.42
5:M:15:MET:CB	6:N:-12:DA:H62	2.23	0.42
5:M:287:VAL:CG2	5:M:348:VAL:CG2	2.89	0.42
1:A:32:GLU:OE1	1:A:32:GLU:HA	2.20	0.42
1:B:191:ARG:HB3	1:B:196:THR:HG22	2.01	0.42
3:D:66:LYS:H	3:D:66:LYS:HD2	1.85	0.42
2:C:54:ARG:HD3	2:C:70:TYR:OH	2.20	0.42
3:D:245:LEU:HD22	3:D:246:PRO:O	2.20	0.42
1:A:60:GLU:HG3	1:A:143:ARG:HB2	2.02	0.42
2:C:673:HIS:ND1	3:D:763:PHE:O	2.41	0.42
2:C:1246:ARG:NH2	2:C:1266:GLY:HA2	2.34	0.42
3:D:269:TYR:CD1	3:D:306:LEU:HD11	2.55	0.42
3:D:677:GLU:N	3:D:677:GLU:CD	2.73	0.42
3:D:1262:ARG:HH12	3:D:1315:ALA:HB3	1.85	0.42
5:M:343:VAL:O	5:M:343:VAL:HG12	2.19	0.42
5:M:347:ILE:HG23	5:M:365:MET:HE1	2.01	0.42
1:A:158:ARG:C	1:A:160:HIS:N	2.73	0.41
1:A:232:VAL:O	1:B:218:ARG:HG3	2.20	0.41
3:D:449:LEU:HD21	3:D:457:TYR:HD2	1.85	0.41
5:M:313:ASP:O	5:M:317:GLN:HG3	2.20	0.41
2:C:785:ASP:OD2	2:C:791:LEU:N	2.45	0.41
7:T:6:DT:H2"	7:T:7:DG:N7	2.36	0.41
2:C:836:LEU:HD23	2:C:1054:LEU:HD13	2.03	0.41
3:D:378:LYS:HB3	3:D:379:PRO:HD3	2.01	0.41
5:M:123:TYR:HE2	5:M:186:ASP:CG	2.24	0.41
1:A:313:SER:HB2	5:M:181:ARG:HD3	2.02	0.41
3:D:77:ARG:HD2	5:M:147:ALA:HA	2.01	0.41
3:D:416:ILE:HG12	3:D:439:PRO:HG2	2.02	0.41
3:D:1143:ASP:O	3:D:1147:ALA:N	2.54	0.41
2:C:911:SER:CB	5:M:259:ARG:NH2	2.73	0.41
3:D:113:HIS:CD2	3:D:115:TRP:HB2	2.55	0.41
3:D:495:ASN:OD1	3:D:1247:LYS:HG3	2.20	0.41
2:C:805:MET:O	2:C:811:ASN:ND2	2.53	0.41
4:E:10:VAL:O	4:E:14:GLY:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:MET:HB3	2:C:130:MET:HE2	1.92	0.41
3:D:460:ASP:N	3:D:460:ASP:OD1	2.53	0.41
3:D:803:VAL:HG11	3:D:1309:ILE:HD11	2.02	0.41
5:M:120:LEU:C	5:M:120:LEU:CD2	2.85	0.41
5:M:123:TYR:CE2	5:M:186:ASP:CG	2.94	0.41
5:M:331:LYS:HB3	5:M:331:LYS:HE3	1.58	0.41
6:N:-33:DG:H2"	6:N:-32:DA:C8	2.55	0.41
1:A:232:VAL:O	1:A:232:VAL:HG13	2.21	0.41
2:C:360:LEU:HA	2:C:363:LEU:HG	2.03	0.41
3:D:599:LYS:CD	3:D:599:LYS:H	2.33	0.41
3:D:929:GLN:HE22	3:D:1241:TYR:HA	1.86	0.41
3:D:1257:VAL:O	3:D:1260:MET:HG2	2.21	0.41
4:E:66:VAL:HG22	4:E:69:ARG:HH12	1.86	0.41
5:M:47:LEU:HD12	5:M:300:ASN:HD22	1.85	0.41
2:C:519:ASN:O	2:C:521:LEU:N	2.54	0.41
2:C:874:GLY:H	2:C:928:VAL:HG13	1.85	0.41
5:M:31:LEU:HD13	5:M:31:LEU:HA	1.89	0.41
5:M:194:ASP:N	5:M:194:ASP:OD1	2.54	0.41
5:M:220:ILE:HD11	5:M:253:ILE:CG1	2.50	0.41
1:A:29:GLU:CG	1:A:30:PRO:HD2	2.21	0.41
3:D:827:GLU:HB2	3:D:832:LYS:HE2	2.03	0.41
3:D:1266:ILE:HD13	3:D:1266:ILE:H	1.85	0.41
5:M:161:ILE:O	5:M:161:ILE:HG22	2.21	0.41
5:M:208:LYS:HE3	5:M:208:LYS:HB2	1.88	0.41
2:C:228:VAL:HG22	2:C:229:ILE:HG22	2.03	0.40
3:D:1161:GLY:HA3	3:D:1204:VAL:HG23	2.03	0.40
3:D:1349:GLU:O	3:D:1353:VAL:HG23	2.21	0.40
5:M:148:VAL:HG12	5:M:149:ASP:N	2.35	0.40
1:A:235:ARG:O	1:A:236:ASP:HB2	2.22	0.40
3:D:381:ILE:HD13	3:D:381:ILE:HA	1.97	0.40
1:A:182:ARG:HB3	1:A:206:GLU:HG2	2.03	0.40
6:N:-1:DT:H2"	6:N:0:DG:C8	2.56	0.40
1:A:90:VAL:HG23	1:A:122:GLU:O	2.22	0.40
1:B:29:GLU:HB3	1:B:30:PRO:HD3	2.04	0.40
3:D:560:ASN:OD1	3:D:560:ASN:N	2.55	0.40
3:D:923:ILE:HG13	3:D:1256:ILE:HD11	2.03	0.40
5:M:118:GLN:HE21	5:M:118:GLN:HB2	1.67	0.40
2:C:201:ARG:HG2	2:C:202:ARG:H	1.86	0.40
2:C:1210:ILE:HD12	2:C:1210:ILE:HA	1.97	0.40
3:D:503:SER:OG	3:D:504:GLN:N	2.53	0.40
3:D:577:ALA:O	3:D:581:MET:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:591:ILE:HG23	3:D:604:MET:HE2	2.03	0.40
5:M:297:LEU:HD12	5:M:297:LEU:HA	1.98	0.40
5:M:323:LEU:O	5:M:327:ARG:HG3	2.21	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	305/329 (93%)	274 (90%)	29 (10%)	2 (1%)	22	55
1	B	219/329 (67%)	206 (94%)	13 (6%)	0	100	100
2	C	1339/1342 (100%)	1266 (94%)	72 (5%)	1 (0%)	51	82
3	D	1319/1407 (94%)	1229 (93%)	89 (7%)	1 (0%)	51	82
4	E	72/91 (79%)	69 (96%)	2 (3%)	1 (1%)	11	37
5	M	401/497 (81%)	361 (90%)	33 (8%)	7 (2%)	9	34
All	All	3655/3995 (92%)	3405 (93%)	238 (6%)	12 (0%)	44	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
5	M	195	LEU
5	M	185	PHE
2	C	399	ALA
5	M	45	PRO
5	M	186	ASP
4	E	4	VAL
5	M	109	LEU
3	D	678	ARG

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Mol	Chain	Res	Type
5	M	16	THR
5	M	156	ILE
1	A	11	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/286 (87%)	225 (91%)	23 (9%)	9	31
1	B	180/286 (63%)	170 (94%)	10 (6%)	21	51
2	C	1049/1157 (91%)	1005 (96%)	44 (4%)	30	59
3	D	914/1168 (78%)	868 (95%)	46 (5%)	24	54
4	E	54/75 (72%)	49 (91%)	5 (9%)	9	31
5	M	358/440 (81%)	303 (85%)	55 (15%)	2	11
All	All	2803/3412 (82%)	2620 (94%)	183 (6%)	21	46

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	ARG
1	A	27	THR
1	A	28	LEU
1	A	29	GLU
1	A	31	LEU
1	A	79	LEU
1	A	125	LYS
1	A	148	ARG
1	A	158	ARG
1	A	166	ARG
1	A	171	LEU
1	A	180	VAL
1	A	200	LYS
1	A	201	LEU

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Mol	Chain	Res	Type
1	A	205	MET
1	A	206	GLU
1	A	207	THR
1	A	223	ILE
1	A	232	VAL
1	A	234	LEU
1	A	259	ASP
1	A	278	ILE
1	B	33	ARG
1	B	47	LEU
1	B	102	LEU
1	B	107	ILE
1	B	133	LEU
1	B	145	LYS
1	B	182	ARG
1	B	197	ASP
1	B	224	LEU
1	B	229	GLU
2	C	30	ILE
2	C	37	LYS
2	C	54	ARG
2	C	169	LYS
2	C	170	VAL
2	C	200	ARG
2	C	209	ILE
2	C	214	ASN
2	C	228	VAL
2	C	360	LEU
2	C	394	ARG
2	C	397	LEU
2	C	411	ARG
2	C	451	ARG
2	C	453	ILE
2	C	454	ARG
2	C	463	GLN
2	C	465	ARG
2	C	473	ARG
2	C	484	LEU
2	C	487	LEU
2	C	540	ARG
2	C	589	THR
2	C	697	LYS

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Mol	Chain	Res	Type
2	C	700	VAL
2	C	741	MET
2	C	811	ASN
2	C	817	LEU
2	C	873	ILE
2	C	895	LEU
2	C	960	LEU
2	C	1014	LEU
2	C	1026	GLU
2	C	1027	LYS
2	C	1060	ILE
2	C	1069	ARG
2	C	1073	LYS
2	C	1084	ASP
2	C	1103	VAL
2	C	1140	LYS
2	C	1161	LEU
2	C	1238	LEU
2	C	1275	VAL
2	C	1319	MET
3	D	14	THR
3	D	15	GLU
3	D	18	ASP
3	D	21	LYS
3	D	50	LYS
3	D	78	LEU
3	D	117	LEU
3	D	118	LYS
3	D	144	TYR
3	D	161	THR
3	D	238	ILE
3	D	239	LEU
3	D	245	LEU
3	D	264	ASP
3	D	265	LEU
3	D	274	ASN
3	D	321	LYS
3	D	324	LEU
3	D	340	GLN
3	D	352	ARG
3	D	363	LEU
3	D	387	LEU

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Mol	Chain	Res	Type
3	D	429	LEU
3	D	430	HIS
3	D	445	LYS
3	D	504	GLN
3	D	518	VAL
3	D	527	LEU
3	D	528	THR
3	D	563	LEU
3	D	599	LYS
3	D	641	ILE
3	D	651	HIS
3	D	677	GLU
3	D	678	ARG
3	D	695	LYS
3	D	714	GLU
3	D	747	MET
3	D	820	ILE
3	D	898	CYS
3	D	901	ARG
3	D	905	ARG
3	D	960	LEU
3	D	1247	LYS
3	D	1266	ILE
3	D	1355	ARG
4	E	3	ARG
4	E	11	GLU
4	E	35	LYS
4	E	39	VAL
4	E	47	THR
5	M	15	MET
5	M	19	LEU
5	M	21	GLN
5	M	26	LEU
5	M	28	LEU
5	M	37	LEU
5	M	46	LEU
5	M	47	LEU
5	M	108	GLU
5	M	109	LEU
5	M	112	TYR
5	M	115	GLU
5	M	120	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	M	121	GLN
5	M	124	LEU
5	M	131	THR
5	M	132	PRO
5	M	138	ARG
5	M	172	LEU
5	M	173	GLU
5	M	176	GLU
5	M	179	LEU
5	M	180	LYS
5	M	181	ARG
5	M	185	PHE
5	M	188	VAL
5	M	193	LYS
5	M	194	ASP
5	M	195	LEU
5	M	198	CYS
5	M	200	LEU
5	M	203	LEU
5	M	227	LEU
5	M	237	ARG
5	M	240	ARG
5	M	246	LEU
5	M	248	GLU
5	M	252	LEU
5	M	256	LEU
5	M	266	THR
5	M	272	VAL
5	M	287	VAL
5	M	289	LEU
5	M	296	ARG
5	M	299	ILE
5	M	311	ARG
5	M	315	ASP
5	M	331	LYS
5	M	334	GLU
5	M	336	ARG
5	M	345	ARG
5	M	409	THR
5	M	423	LEU
5	M	425	LYS
5	M	455	ARG

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

Mol	Chain	Res	Type
1	A	41	ASN
2	C	659	GLN
2	C	1013	GLN
2	C	1257	GLN
3	D	340	GLN
3	D	504	GLN
3	D	594	GLN
3	D	651	HIS
3	D	680	ASN
3	D	1227	HIS
4	E	31	GLN
5	M	21	GLN
5	M	118	GLN
5	M	223	HIS
5	M	251	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

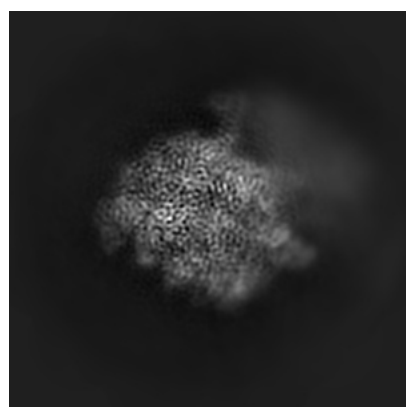
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14190. These allow visual inspection of the internal detail of the map and identification of artifacts.

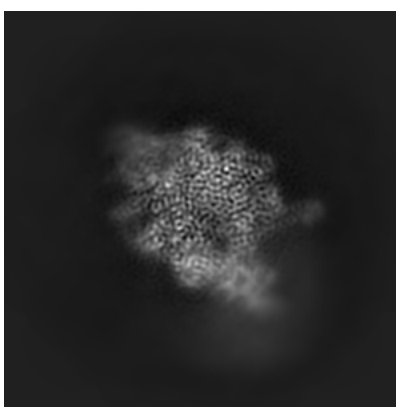
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

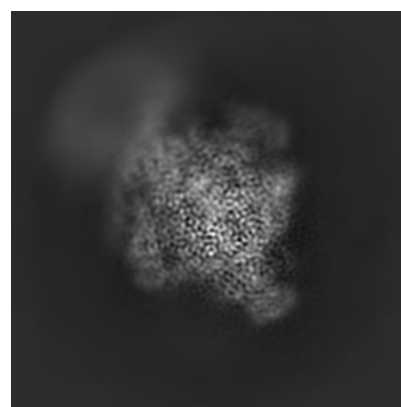
6.1.1 Primary map



X



Y

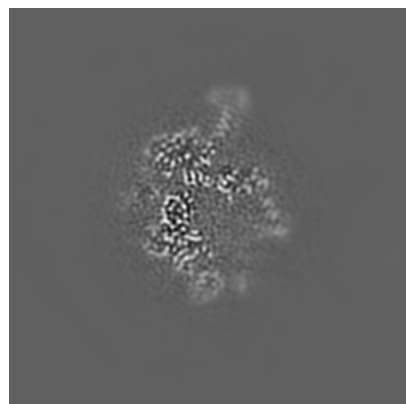


Z

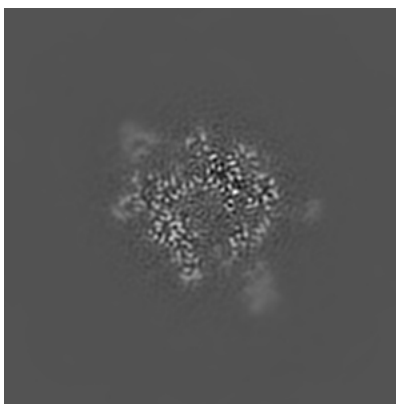
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

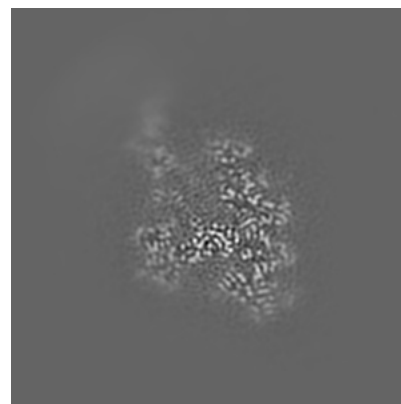
6.2.1 Primary map



X Index: 128



Y Index: 128

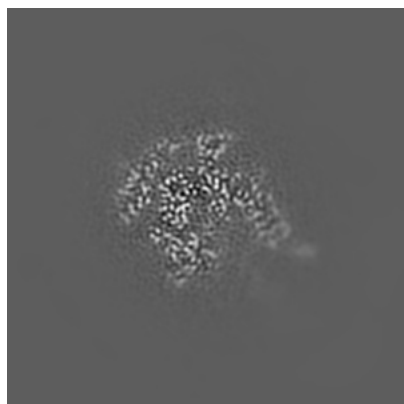


Z Index: 128

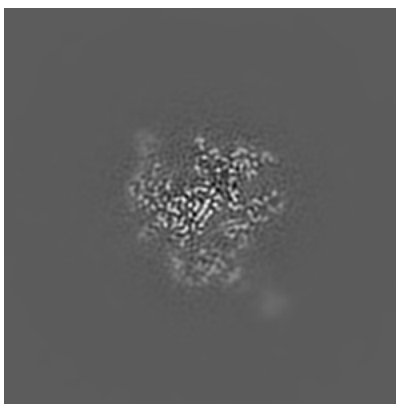
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

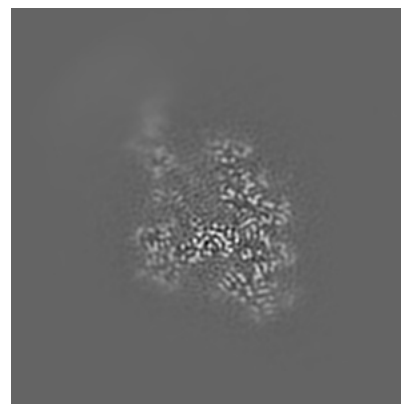
6.3.1 Primary map



X Index: 139



Y Index: 112

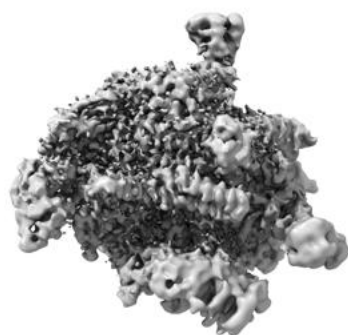


Z Index: 128

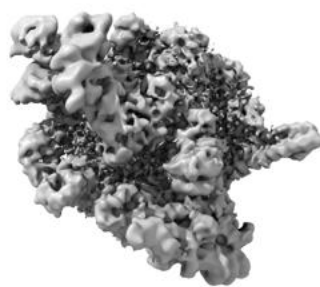
The images above show the largest variance slices of the map in three orthogonal directions.

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

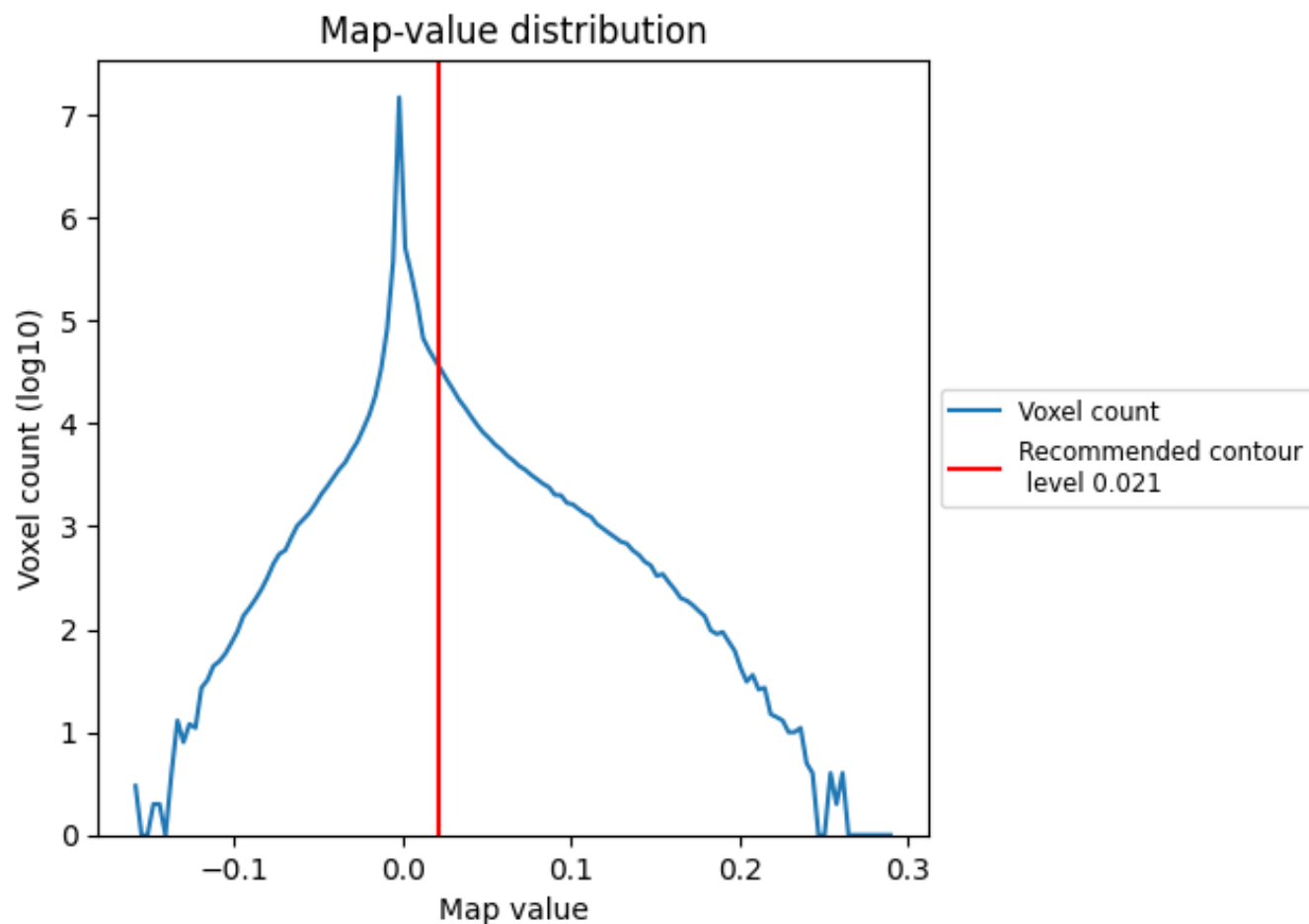
6.5 Mask visualisation

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

7 Map analysis [i](#)

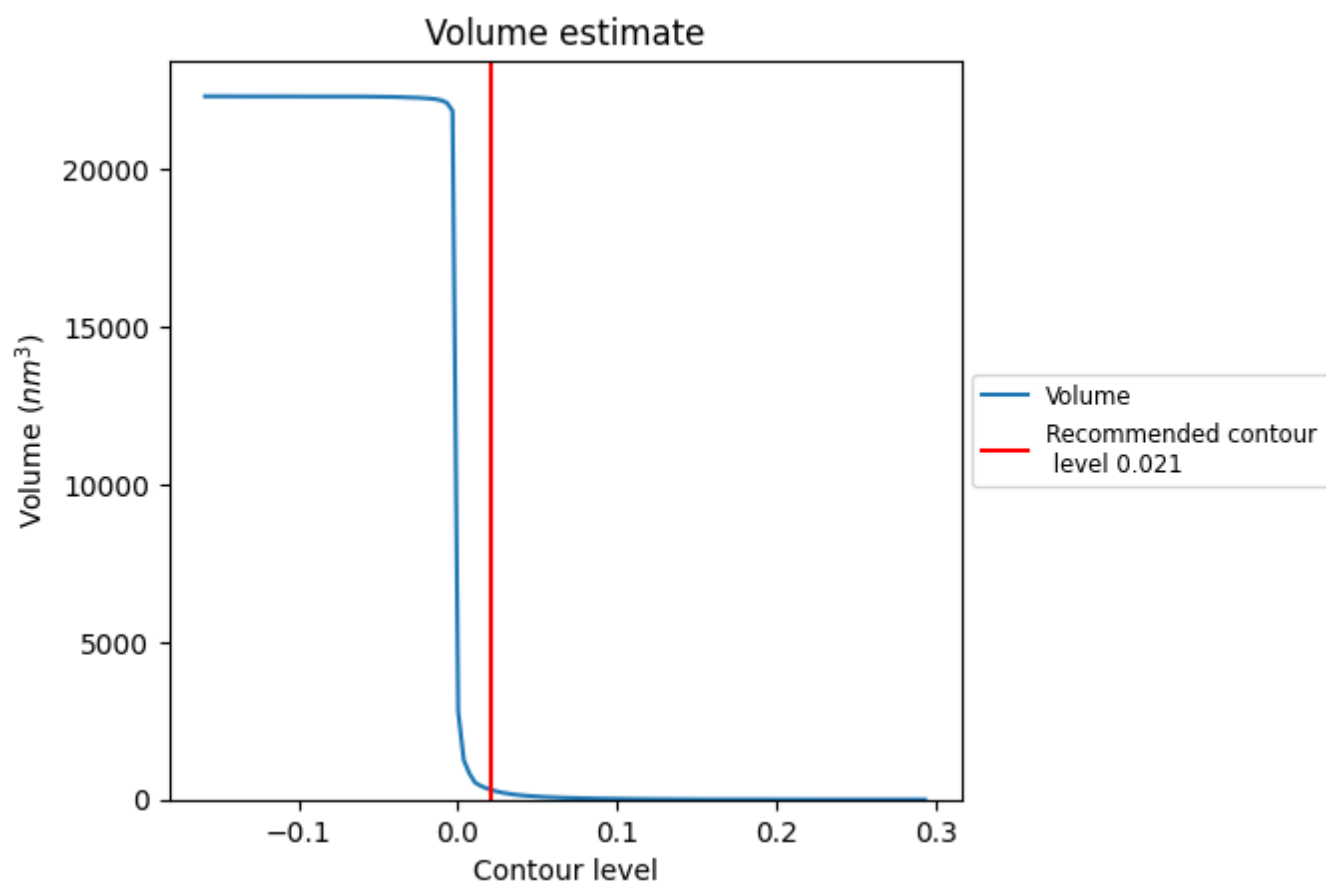
This section contains the results of statistical analysis of the map.

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.

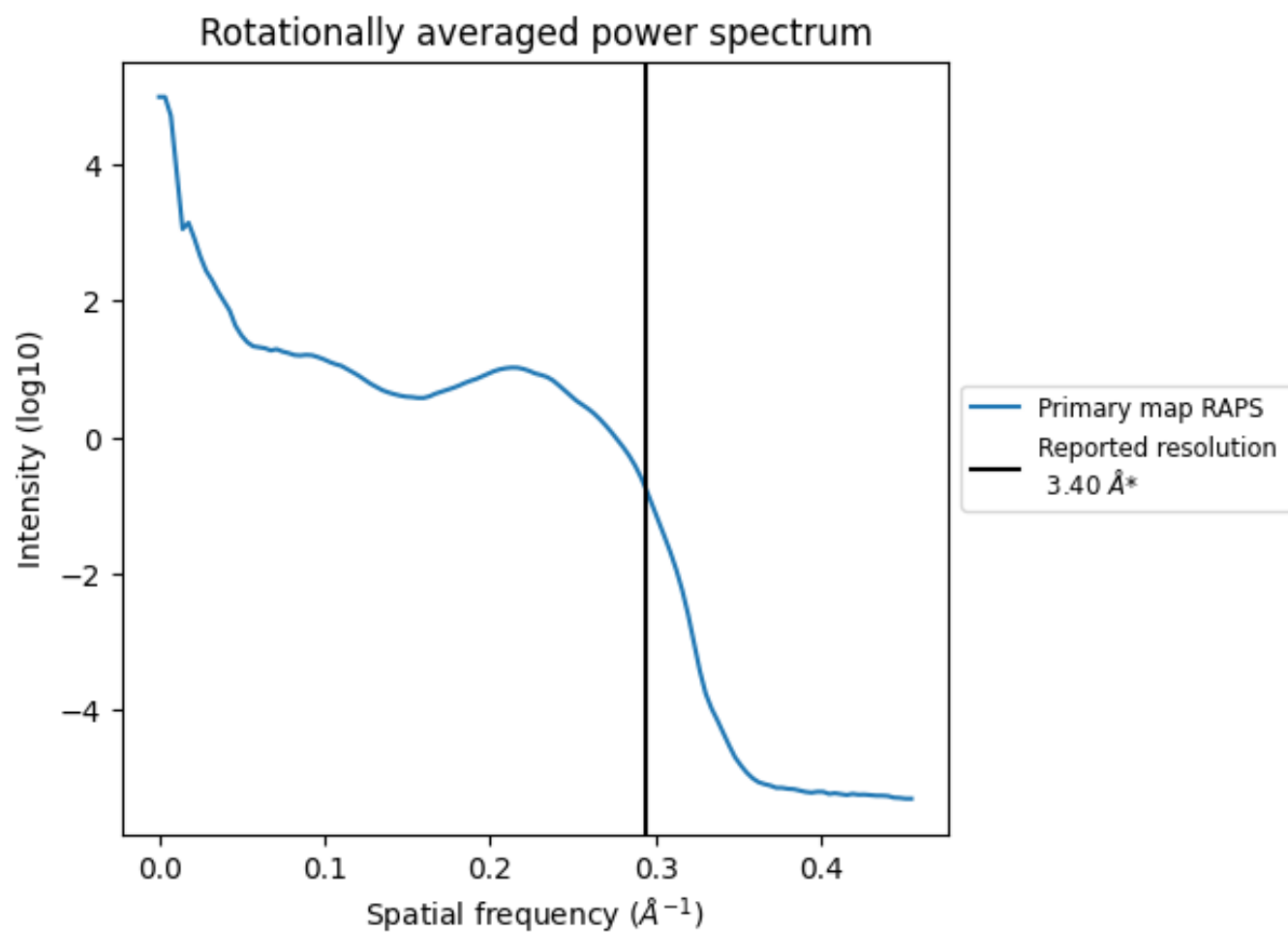
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm³; this corresponds to an approximate mass of 277 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 0.294 Å⁻¹

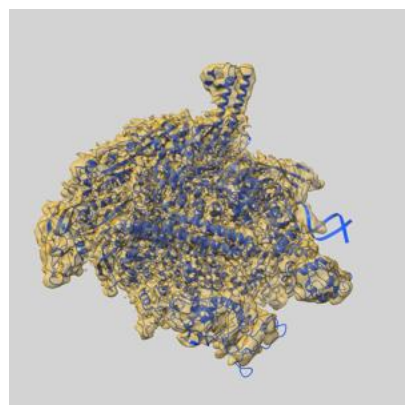
8 Fourier-Shell correlation ⓘ

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

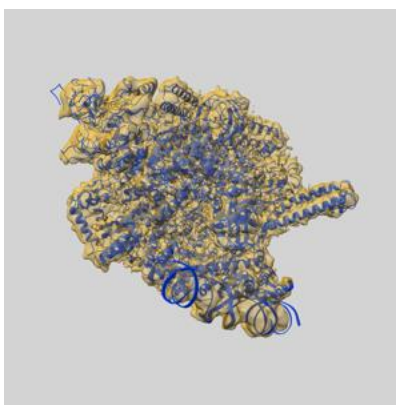
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14190 and PDB model 7QWP. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

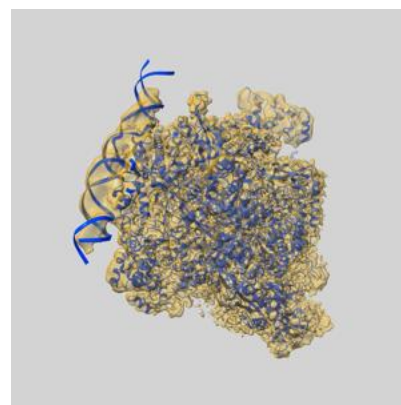
9.1 Map-model overlay [i](#)



X



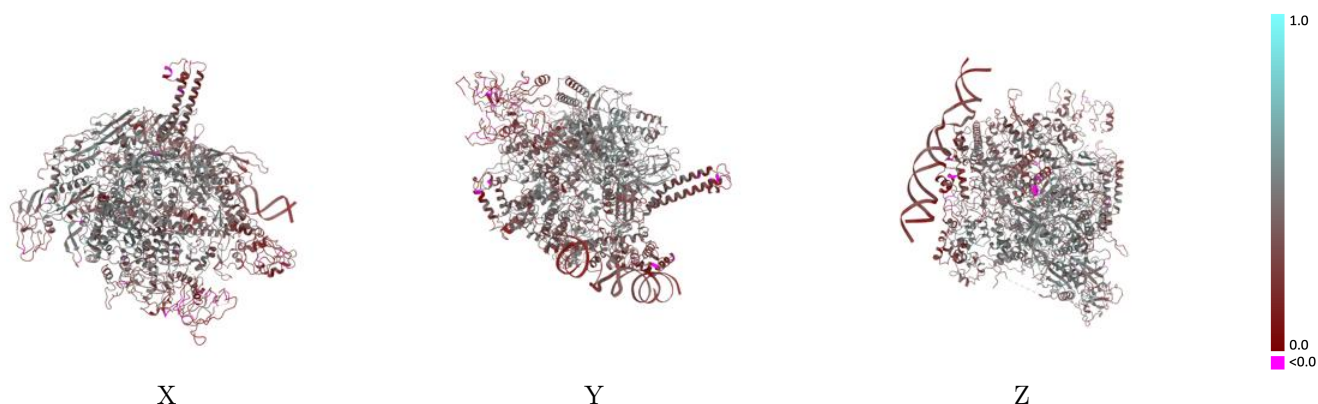
Y



Z

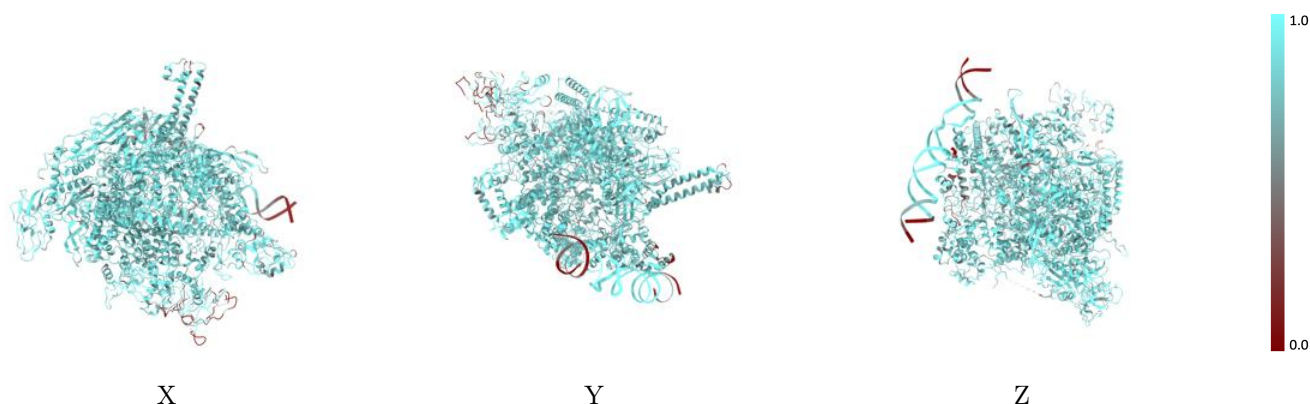
The images above show the 3D surface view of the map at the recommended contour level 0.021 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



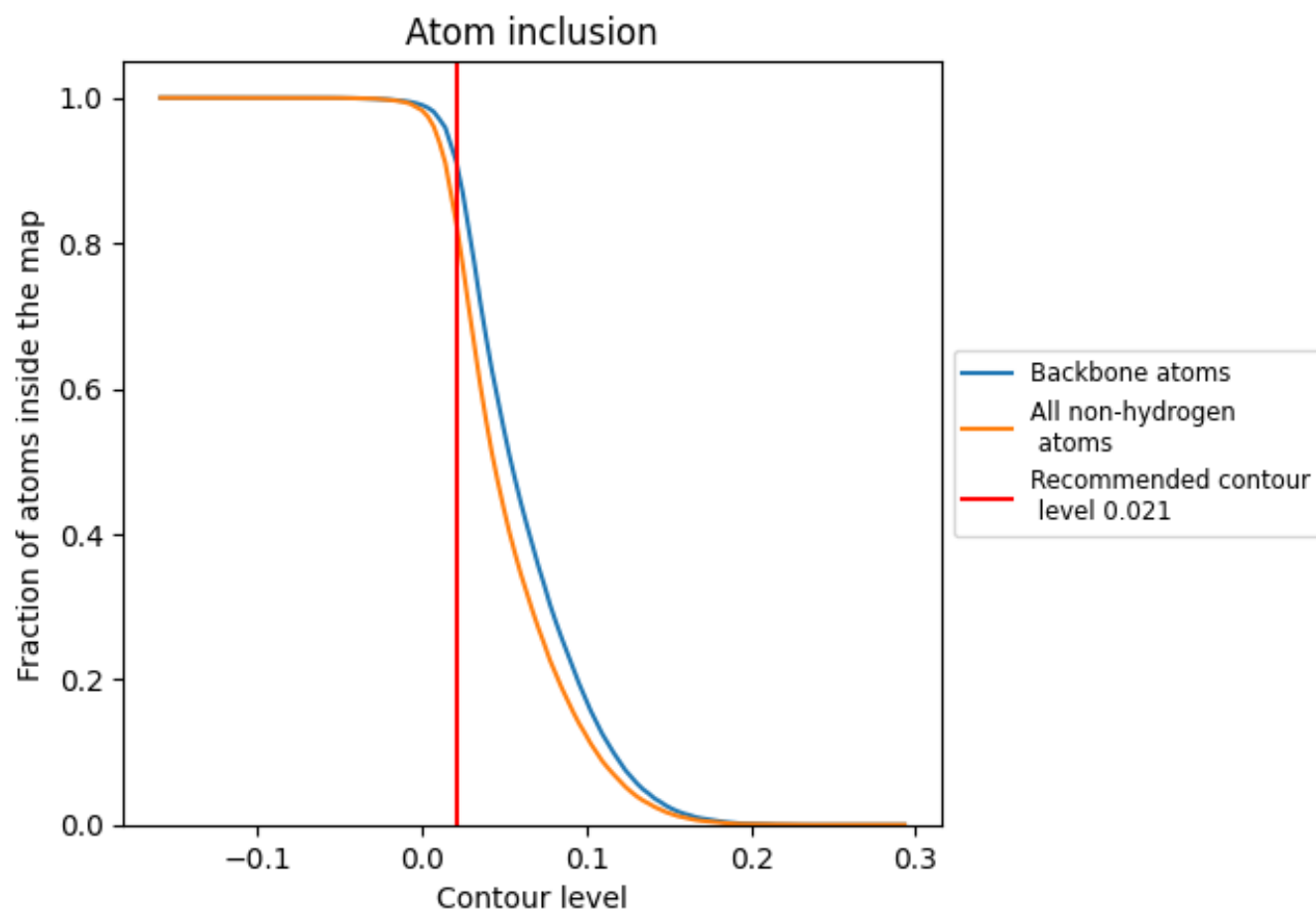
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.021).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 83% 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 (0.021) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8281	<div></div> 0.3780
A	<div></div> 0.8593	<div></div> 0.4250
B	<div></div> 0.8411	<div></div> 0.3820
C	<div></div> 0.8474	<div></div> 0.3970
D	<div></div> 0.8300	<div></div> 0.3780
E	<div></div> 0.8694	<div></div> 0.4290
M	<div></div> 0.7905	<div></div> 0.3390
N	<div></div> 0.7182	<div></div> 0.2390
T	<div></div> 0.6585	<div></div> 0.2340

1.0

0.0

<0.0