



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 01:52 AM UTC

PDB ID : 6CA0 / pdb_00006ca0
EMDB ID : EMD-7439
Title : Cryo-EM structure of E. coli RNAP sigma70 open complex
Authors : Narayanan, A.; Vago, F.; Li, K.; Qayyum, M.Z.; Yernool, D.; Jiang, W.;
Murakami, K.S.
Deposited on : 2018-01-29
Resolution : 5.75 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:

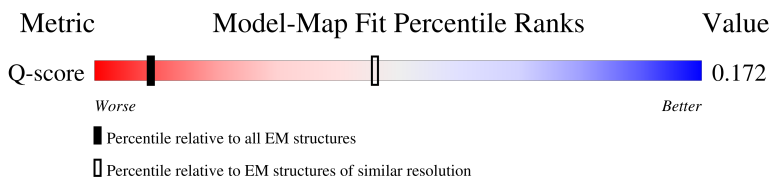
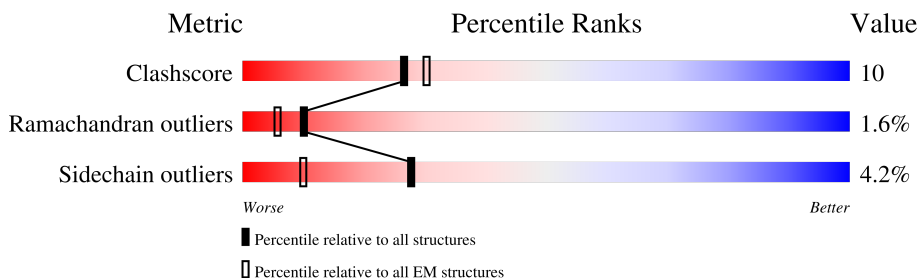
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 5.75 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.



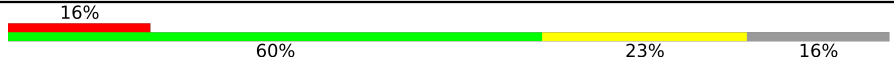
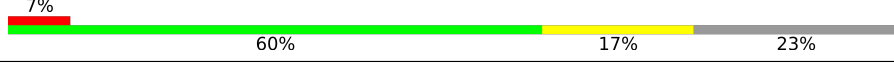

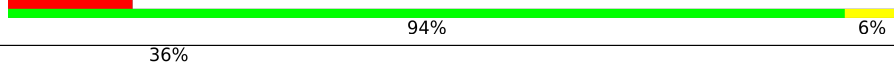

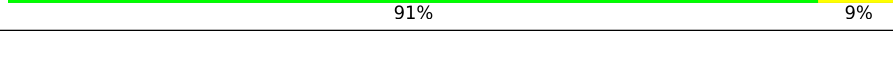
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	476 (5.25 - 6.25)

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	 46% 22% 30%
1	B	329	 41% 27% 31%
2	C	1342	 70% 28%
3	D	1407	 10% 67% 27%

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Mol	Chain	Length	Quality of chain
4	E	91	
5	F	613	
6	G	45	
7	H	35	
8	I	11	
9	J	11	

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 31098 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
			Total	C	N	O	S		
1	A	230	Total	C	N	O	S	0	0
			1787	1112	317	352	6		
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
			Total	C	N	O	S		
2	C	1340	Total	C	N	O	S	0	0
			10570	6631	1841	2055	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1352	Total	C	N	O	S	0	0
			10428	6547	1855	1976	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	76	Total	C	N	O	S	0	0
			605	368	115	121	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	472	Total	C	N	O	S	0	0
			3845	2408	685	729	23		

- Molecule 6 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	G	45	923	441	165	272	45	0	0

- Molecule 7 is a DNA chain called DNA (35-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	H	35	719	343	131	210	35	0	0

- Molecule 8 is a DNA chain called DNA (5'-D(P*TP*CP*TP*GP*AP*CP*GP*CP*GP*GP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	I	11	225	106	41	67	11	0	0

- Molecule 9 is a DNA chain called DNA (5'-D(P*GP*CP*CP*GP*CP*GP*TP*CP*AP*GP*A)-3').

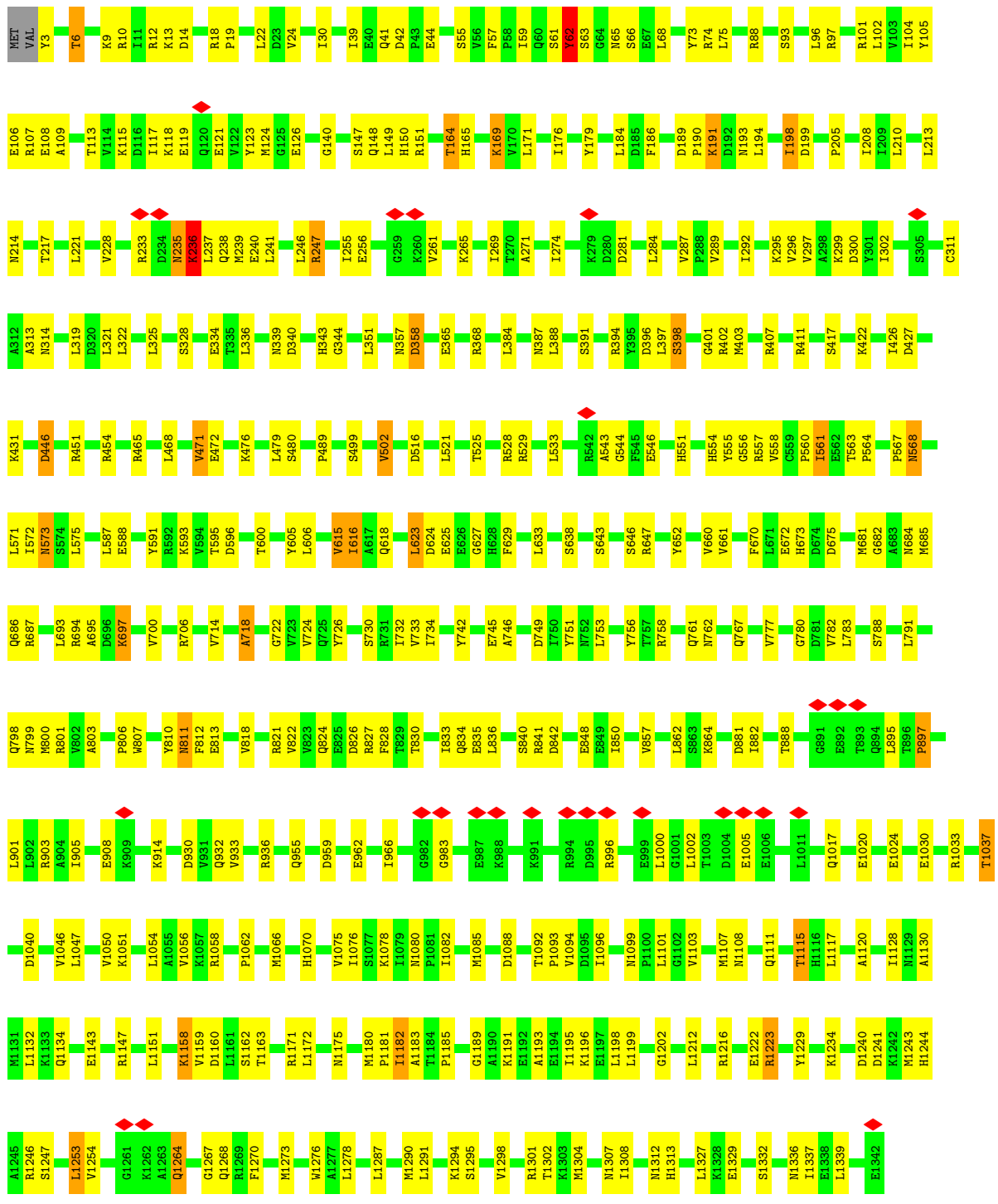
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	J	11	226	106	44	65	11	0	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

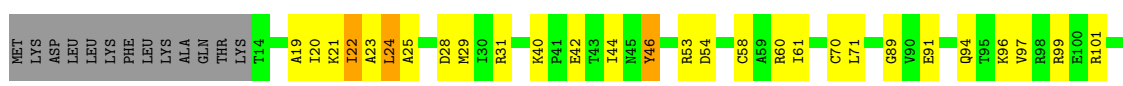
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	D	1	1	1	0

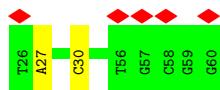
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

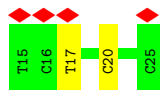
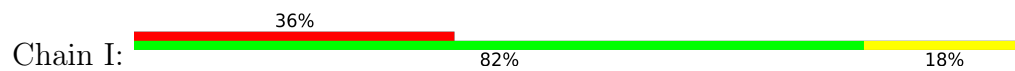


• Molecule 3: DNA-directed RNA polymerase subunit beta'

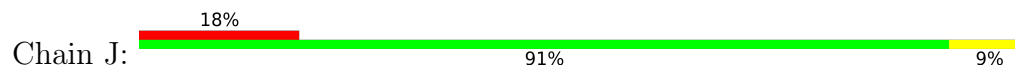




- Molecule 8: DNA (5'-D(P*TP*CP*TP*GP*AP*CP*GP*CP*GP*GP*C)-3')



- Molecule 9: DNA (5'-D(P*GP*CP*CP*GP*CP*GP*TP*CP*AP*GP*A)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	96067	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.022	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	315.84, 315.84, 315.84	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.316, 1.316, 1.316	Depositor

5 Model quality i

5.1 Standard geometry i

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	0.35	0/1809	1.04	2/2451 (0.1%)
1	B	0.37	0/1789	1.08	6/2425 (0.2%)
2	C	0.35	0/10739	1.03	28/14489 (0.2%)
3	D	0.36	0/10586	1.05	17/14303 (0.1%)
4	E	0.20	0/607	0.55	0/817
5	F	0.38	0/3896	1.07	11/5236 (0.2%)
6	G	0.27	0/1034	0.54	0/1594
7	H	0.25	0/806	0.49	0/1242
8	I	0.20	0/251	0.44	0/385
9	J	0.26	0/253	0.44	0/388
All	All	0.35	0/31770	1.00	64/43330 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
3	D	0	3
All	All	0	6

There are no bond length outliers.

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	567	PRO	CA-C-N	10.67	142.30	121.18
2	C	567	PRO	C-N-CA	10.67	142.30	121.18
2	C	722	GLY	N-CA-C	9.45	122.67	110.20
2	C	236	LYS	N-CA-C	8.35	121.46	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	57	PHE	C-N-CD	-8.18	102.60	120.60
3	D	1343	GLU	CA-C-N	8.06	136.93	121.54
3	D	1343	GLU	C-N-CA	8.06	136.93	121.54
2	C	397	LEU	CA-C-N	7.71	136.26	121.54
2	C	397	LEU	C-N-CA	7.71	136.26	121.54
2	C	568	ASN	CA-C-O	-7.60	109.17	119.05
1	B	135	ASP	CA-C-N	7.43	135.73	121.54
1	B	135	ASP	C-N-CA	7.43	135.73	121.54
3	D	805	GLN	N-CA-C	7.37	120.25	111.33
5	F	323	ASN	CA-C-N	6.69	130.84	120.60
5	F	323	ASN	C-N-CA	6.69	130.84	120.60
3	D	1184	ASP	N-CA-C	6.39	123.93	109.81
2	C	1160	ASP	CA-C-N	6.26	132.97	121.70
2	C	1160	ASP	C-N-CA	6.26	132.97	121.70
2	C	233	ARG	CA-C-N	6.24	133.46	121.54
2	C	233	ARG	C-N-CA	6.24	133.46	121.54
2	C	811	ASN	CA-C-N	5.95	132.91	121.54
2	C	811	ASN	C-N-CA	5.95	132.91	121.54
1	B	229	GLU	N-CA-C	5.95	121.13	111.37
2	C	164	THR	CA-C-N	5.90	132.81	121.54
2	C	164	THR	C-N-CA	5.90	132.81	121.54
3	D	1053	LEU	N-CA-C	5.86	120.98	111.37
2	C	1264	GLN	N-CA-C	-5.81	96.17	107.62
2	C	1159	VAL	N-CA-C	5.70	117.33	109.46
2	C	396	ASP	CA-C-N	-5.56	111.23	120.68
2	C	396	ASP	C-N-CA	-5.56	111.23	120.68
3	D	1255	VAL	CA-CB-CG2	5.51	119.77	110.40
2	C	624	ASP	CA-C-N	5.51	132.07	121.54
2	C	624	ASP	C-N-CA	5.51	132.07	121.54
5	F	565	ILE	CA-C-N	5.42	130.54	122.74
5	F	565	ILE	C-N-CA	5.42	130.54	122.74
3	D	318	GLY	CA-C-N	5.38	131.81	121.54
3	D	318	GLY	C-N-CA	5.38	131.81	121.54
5	F	153	ALA	CA-C-N	5.34	131.73	121.54
5	F	153	ALA	C-N-CA	5.34	131.73	121.54
5	F	234	THR	N-CA-C	5.32	122.14	110.80
1	B	75	GLN	CA-CB-CG	5.32	124.74	114.10
3	D	1341	ARG	N-CA-C	-5.32	98.71	108.02
5	F	493	LYS	CA-C-O	-5.30	114.80	120.42
5	F	584	ARG	CA-CB-CG	5.30	124.70	114.10
2	C	140	GLY	N-CA-C	-5.26	105.74	114.48
3	D	861	ASN	N-CA-C	5.25	121.98	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	297	MET	N-CA-C	5.24	121.39	109.81
3	D	900	GLY	N-CA-C	5.23	125.58	113.18
2	C	1151	LEU	CA-CB-CG	5.19	134.45	116.30
3	D	1140	ARG	CA-CB-CG	5.18	124.47	114.10
1	B	20	SER	CA-C-N	5.18	131.43	121.54
1	B	20	SER	C-N-CA	5.18	131.43	121.54
3	D	768	ASN	CA-C-N	5.13	131.20	121.97
3	D	768	ASN	C-N-CA	5.13	131.20	121.97
1	A	161	SER	CA-C-N	5.12	127.91	120.79
1	A	161	SER	C-N-CA	5.12	127.91	120.79
2	C	983	GLY	N-CA-C	-5.10	101.09	113.18
3	D	1168	GLU	CA-C-N	5.05	129.99	122.82
3	D	1168	GLU	C-N-CA	5.05	129.99	122.82
2	C	718	ALA	CA-C-N	-5.04	113.55	122.26
2	C	718	ALA	C-N-CA	-5.04	113.55	122.26
3	D	357	VAL	N-CA-C	5.04	119.81	109.34
5	F	100	MET	N-CA-CB	5.02	117.29	110.01
2	C	1327	LEU	CA-CB-CG	5.01	133.83	116.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	198	ILE	Peptide
2	C	236	LYS	Peptide
2	C	595	THR	Peptide
3	D	1184	ASP	Peptide
3	D	715	LYS	Peptide
3	D	901	ARG	Peptide

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	1787	0	1810	47	0
1	B	1767	0	1789	62	0
2	C	10570	0	10582	239	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	10428	0	10573	236	0
4	E	605	0	612	14	0
5	F	3845	0	3913	57	0
6	G	923	0	510	10	0
7	H	719	0	396	2	0
8	I	225	0	124	2	0
9	J	226	0	123	1	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
All	All	31098	0	30432	608	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 10.

All (608) 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)
5:F:360:ASP:O	5:F:364:ARG:HB2	1.80	0.80
2:C:1033:ARG:O	2:C:1037:THR:HB	1.86	0.73
3:D:362:ARG:H	3:D:365:GLN:HE21	1.38	0.72
2:C:557:ARG:HD3	2:C:587:LEU:HB3	1.71	0.71
3:D:1075:ARG:HH21	3:D:1173:ARG:HD3	1.56	0.70
2:C:1103:VAL:HG21	3:D:639:VAL:HG11	1.74	0.69
3:D:648:GLU:HG3	3:D:649:LYS:HG2	1.75	0.69
3:D:1273:ASP:HB2	3:D:1276:GLU:HB2	1.77	0.67
2:C:798:GLN:HB3	2:C:827:ARG:HH21	1.59	0.67
2:C:1313:HIS:HB3	3:D:474:LEU:H	1.60	0.67
5:F:530:LEU:HD13	5:F:532:LEU:HB2	1.76	0.67
1:A:234:LEU:HD22	1:B:214:GLU:HG3	1.77	0.66
2:C:97:ARG:HB3	2:C:121:GLU:HB3	1.79	0.65
1:B:211:ILE:HG12	1:B:219:ARG:HH22	1.62	0.64
2:C:297:VAL:HG11	2:C:311:CYS:HB2	1.79	0.64
1:B:44:ARG:HG3	1:B:183:ILE:HD13	1.80	0.64
2:C:660:VAL:HG23	2:C:661:VAL:HG13	1.78	0.64
1:A:84:ASN:ND2	1:A:130:ILE:O	2.30	0.64
2:C:14:ASP:HA	2:C:1183:ALA:HB3	1.80	0.64
3:D:526:VAL:HG12	3:D:549:LYS:HB3	1.81	0.63
1:A:45:ARG:NH1	1:B:34:GLY:O	2.31	0.63
3:D:1046:ILE:HB	3:D:1059:LEU:HD22	1.81	0.63
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.63	0.63
3:D:1161:GLY:HA3	3:D:1179:PRO:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1253:LEU:HG	5:F:525:ASP:HB2	1.81	0.63
2:C:1295:SER:O	2:C:1301:ARG:NH2	2.32	0.62
3:D:275:ARG:HG2	3:D:278:ARG:HH2	1.64	0.62
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.62	0.62
2:C:117:ILE:HD12	2:C:489:PRO:HD3	1.81	0.62
2:C:239:MET:HE2	2:C:241:LEU:HD13	1.81	0.62
3:D:160:LEU:HD22	3:D:164:GLN:HB3	1.81	0.62
2:C:842:ASP:HB2	2:C:1047:LEU:HG	1.81	0.62
2:C:1254:VAL:O	3:D:99:ARG:NH2	2.32	0.62
1:B:180:VAL:HG23	3:D:535:ARG:HH2	1.64	0.62
3:D:910:ASN:ND2	4:E:14:GLY:O	2.33	0.62
2:C:403:MET:SD	2:C:407:ARG:NH2	2.73	0.62
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.81	0.61
2:C:670:PHE:HB3	2:C:673:HIS:HD2	1.65	0.61
2:C:9:LYS:O	2:C:1171:ARG:NH1	2.33	0.61
2:C:623:LEU:HB2	2:C:627:GLY:HA2	1.81	0.61
3:D:850:LYS:HD2	3:D:855:ASP:HB3	1.81	0.61
3:D:1239:ASP:OD1	3:D:1242:ARG:NH1	2.33	0.61
3:D:1362:GLY:O	3:D:1366:HIS:ND1	2.26	0.61
2:C:1246:ARG:HA	2:C:1264:GLN:HE21	1.66	0.61
3:D:1198:VAL:HB	3:D:1210:ILE:HD12	1.83	0.61
3:D:857:LEU:HD12	3:D:858:VAL:HG13	1.82	0.61
2:C:558:VAL:HG11	2:C:573:ASN:HB3	1.82	0.60
3:D:515:ARG:NH1	3:D:724:MET:SD	2.73	0.60
2:C:1120:ALA:HB2	2:C:1199:LEU:HD23	1.83	0.60
3:D:568:SER:OG	3:D:569:LEU:N	2.34	0.60
2:C:97:ARG:HE	2:C:123:TYR:HD1	1.47	0.60
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.82	0.60
2:C:1294:LYS:HE3	3:D:349:TYR:HD2	1.66	0.60
3:D:1069:ALA:HA	3:D:1072:LYS:HE2	1.84	0.60
2:C:1143:GLU:OE2	2:C:1147:ARG:NH1	2.31	0.59
1:A:96:ASP:OD1	1:A:148:ARG:NH1	2.34	0.59
2:C:101:ARG:HH11	2:C:118:LYS:HZ1	1.50	0.59
2:C:237:LEU:HB3	2:C:292:ILE:HD12	1.83	0.59
1:A:59:VAL:HG22	1:A:144:ILE:HG23	1.85	0.59
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.84	0.59
3:D:126:LEU:HD13	3:D:220:ARG:HG3	1.85	0.59
5:F:320:ILE:HA	5:F:327:SER:HB3	1.85	0.59
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.85	0.58
3:D:694:SER:HB2	3:D:738:ARG:HE	1.68	0.58
1:B:22:THR:OG1	1:B:207:THR:O	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:88:ARG:HH22	2:C:1040:ASP:HA	1.68	0.58
2:C:1307:ASN:OD1	2:C:1312:ASN:ND2	2.37	0.58
2:C:1103:VAL:HG11	3:D:639:VAL:HG21	1.85	0.58
3:D:1025:MET:HB3	3:D:1124:ILE:HB	1.86	0.58
3:D:297:ARG:HD2	5:F:97:PRO:HB3	1.86	0.58
2:C:557:ARG:HB3	2:C:587:LEU:HD13	1.85	0.58
3:D:137:ARG:HG3	3:D:142:GLU:HB2	1.84	0.58
3:D:425:ARG:NH1	3:D:457:TYR:O	2.36	0.58
1:A:86:LYS:NZ	2:C:826:ASP:OD2	2.37	0.58
1:B:133:LEU:HD21	1:B:140:ILE:HB	1.86	0.58
2:C:718:ALA:O	2:C:780:GLY:N	2.36	0.58
2:C:905:ILE:O	5:F:599:ARG:NH1	2.37	0.58
5:F:98:VAL:HG11	6:G:44:DG:H1	1.69	0.58
2:C:151:ARG:HA	2:C:451:ARG:HD3	1.86	0.58
2:C:693:LEU:HD23	2:C:694:ARG:HG3	1.86	0.57
5:F:106:GLY:HA2	5:F:385:ARG:HH21	1.69	0.57
2:C:189:ASP:OD1	2:C:193:ASN:N	2.30	0.57
3:D:259:ARG:HH21	5:F:505:ILE:HG13	1.68	0.57
3:D:482:ALA:O	3:D:488:ASN:ND2	2.37	0.57
2:C:41:GLN:NE2	2:C:73:TYR:O	2.38	0.57
2:C:897:PRO:HB3	5:F:563:PHE:HB3	1.86	0.57
5:F:437:GLN:HB2	7:H:27:DA:H62	1.70	0.56
2:C:104:ILE:HB	2:C:115:LYS:HB3	1.87	0.56
2:C:271:ALA:HA	2:C:274:ILE:HD12	1.87	0.56
1:A:218:ARG:NH1	1:B:231:PHE:O	2.38	0.56
2:C:186:PHE:HB3	2:C:194:LEU:HD11	1.88	0.56
2:C:176:ILE:HB	2:C:184:LEU:HB3	1.88	0.56
2:C:516:ASP:OD1	2:C:761:GLN:NE2	2.39	0.56
3:D:1344:LEU:O	3:D:1346:GLY:N	2.29	0.56
1:B:86:LYS:NZ	3:D:526:VAL:O	2.38	0.56
2:C:1111:GLN:O	2:C:1115:THR:OG1	2.23	0.56
2:C:149:LEU:HD11	2:C:451:ARG:HG3	1.88	0.56
3:D:530:PRO:HG3	3:D:552:ILE:HG22	1.88	0.56
3:D:836:ARG:HD2	3:D:873:GLU:HB2	1.88	0.56
1:A:189:ALA:HA	1:A:199:ASP:HA	1.87	0.55
3:D:156:ARG:HH21	3:D:191:SER:HG	1.54	0.55
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.88	0.55
3:D:120:LEU:HD11	8:I:20:DC:H4'	1.87	0.55
1:A:14:VAL:HG11	1:A:29:GLU:HG2	1.87	0.55
2:C:73:TYR:HB2	2:C:96:LEU:HD11	1.88	0.55
2:C:836:LEU:HD13	2:C:1054:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1262:ARG:HE	3:D:1312:ALA:HB1	1.71	0.55
2:C:1246:ARG:HH11	2:C:1267:GLY:H	1.55	0.55
3:D:335:GLN:HG2	9:J:13:DA:H5''	1.88	0.55
3:D:1148:ARG:HH21	8:I:17:DT:H4'	1.72	0.55
3:D:515:ARG:NH2	3:D:717:VAL:O	2.29	0.55
1:B:102:LEU:HB2	1:B:142:MET:HG2	1.87	0.55
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.40	0.55
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.89	0.55
3:D:251:PRO:HB2	3:D:253:VAL:HG13	1.88	0.55
5:F:355:ILE:HA	5:F:358:VAL:HB	1.88	0.55
2:C:803:ALA:HB2	2:C:1094:VAL:HG21	1.89	0.55
3:D:44:ILE:HG13	3:D:46:TYR:H	1.72	0.55
3:D:600:ALA:HA	3:D:603:LYS:HG2	1.88	0.55
4:E:25:ARG:NH2	4:E:68:GLU:OE1	2.40	0.55
3:D:814:CYS:HG	3:D:890:THR:HG1	1.55	0.55
3:D:843:VAL:HG13	3:D:883:ARG:HB2	1.89	0.55
2:C:1268:GLN:HE22	3:D:352:ARG:HD3	1.72	0.55
2:C:1304:MET:HA	2:C:1307:ASN:HD22	1.72	0.55
5:F:441:ARG:NH2	6:G:33:DG:OP2	2.40	0.55
2:C:12:ARG:NH1	2:C:1182:ILE:O	2.40	0.54
2:C:65:ASN:HB3	2:C:105:TYR:HB2	1.88	0.54
2:C:446:ASP:N	2:C:446:ASP:OD1	2.39	0.54
2:C:1033:ARG:O	2:C:1037:THR:CB	2.54	0.54
2:C:1336:ASN:HB2	3:D:25:ALA:HA	1.89	0.54
3:D:91:GLU:OE2	3:D:101:ARG:NH2	2.41	0.54
2:C:1336:ASN:ND2	3:D:29:MET:SD	2.80	0.54
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.89	0.54
3:D:840:LEU:HG	3:D:901:ARG:HH22	1.71	0.54
2:C:807:TRP:HZ2	2:C:1216:ARG:HD3	1.73	0.54
3:D:1033:GLY:HA3	3:D:1082:ASP:HA	1.90	0.54
1:A:75:GLN:HE21	1:A:132:HIS:HB2	1.73	0.54
2:C:240:GLU:HA	2:C:284:LEU:HA	1.89	0.54
2:C:930:ASP:OD2	2:C:932:GLN:NE2	2.37	0.54
3:D:1143:ASP:HA	3:D:1148:ARG:HH11	1.73	0.54
2:C:932:GLN:HB2	2:C:1051:LYS:HB2	1.90	0.54
2:C:1172:LEU:HA	2:C:1175:ASN:HD22	1.71	0.54
5:F:560:ARG:NH1	5:F:566:ASP:OD2	2.41	0.54
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.90	0.53
2:C:9:LYS:HA	2:C:1171:ARG:HH22	1.73	0.53
2:C:560:PRO:HB2	3:D:776:THR:HG21	1.89	0.53
3:D:531:LYS:HG2	3:D:581:MET:HE1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:243:ALA:N	5:F:246:GLN:OE1	2.42	0.53
1:B:210:THR:OG1	1:B:211:ILE:N	2.41	0.53
2:C:593:LYS:O	2:C:600:THR:N	2.40	0.53
2:C:745:GLU:OE2	2:C:1017:GLN:NE2	2.41	0.53
3:D:975:ILE:HD13	3:D:980:THR:HG21	1.90	0.53
5:F:145:LEU:HD22	5:F:225:ARG:HE	1.72	0.53
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.89	0.53
4:E:26:ARG:HG3	4:E:30:MET:HE2	1.90	0.53
1:A:58:GLU:HG2	1:A:145:LYS:HB3	1.90	0.53
3:D:473:THR:HG23	3:D:476:ALA:H	1.74	0.53
2:C:13:LYS:O	2:C:1183:ALA:N	2.39	0.53
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.74	0.53
3:D:475:GLU:HG3	4:E:24:ALA:HB1	1.89	0.53
2:C:247:ARG:O	2:C:339:ASN:ND2	2.41	0.53
2:C:675:ASP:HB2	2:C:1107:MET:HB2	1.90	0.53
2:C:164:THR:HB	2:C:171:LEU:HD12	1.91	0.53
2:C:1198:LEU:O	2:C:1202:GLY:N	2.39	0.53
5:F:136:GLU:OE1	5:F:364:ARG:NH2	2.36	0.53
1:A:16:ILE:HG23	1:A:26:VAL:HG12	1.91	0.53
3:D:825:VAL:HG22	3:D:838:ARG:HD2	1.91	0.52
3:D:1080:ILE:HB	3:D:1097:ALA:HB3	1.90	0.52
1:B:9:LEU:HD21	1:B:30:PRO:HG2	1.91	0.52
1:B:158:ARG:HB2	1:B:172:LEU:HD21	1.90	0.52
2:C:237:LEU:HG	2:C:289:VAL:HG23	1.91	0.52
3:D:367:GLY:H	3:D:448:GLN:HB2	1.75	0.52
2:C:1130:ALA:O	2:C:1134:GLN:NE2	2.42	0.52
3:D:126:LEU:HD11	3:D:223:LEU:HD23	1.92	0.52
2:C:358:ASP:OD1	2:C:358:ASP:N	2.38	0.52
5:F:471:LEU:HG	5:F:478:PRO:HD3	1.91	0.52
3:D:1079:LYS:HA	3:D:1098:GLN:HA	1.91	0.52
3:D:1221:LEU:HG	3:D:1306:LEU:HB2	1.91	0.52
1:B:74:VAL:HG22	1:B:133:LEU:HG	1.91	0.52
3:D:107:LEU:HD11	3:D:242:LEU:HB2	1.92	0.52
1:A:104:LYS:HE3	1:A:110:VAL:HG22	1.90	0.52
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.92	0.52
2:C:848:GLU:HG2	2:C:888:THR:HG22	1.92	0.52
5:F:327:SER:HA	5:F:330:LEU:HG	1.92	0.52
1:A:158:ARG:HH12	1:A:172:LEU:HG	1.75	0.51
1:B:92:VAL:HG22	1:B:121:VAL:HG22	1.93	0.51
2:C:673:HIS:ND1	3:D:763:PHE:O	2.36	0.51
3:D:1356:LEU:O	3:D:1366:HIS:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:9:ALA:HB1	4:E:19:LEU:HD11	1.92	0.51
5:F:392:LYS:HA	5:F:395:THR:HG23	1.93	0.51
2:C:726:TYR:HB3	2:C:733:VAL:HB	1.92	0.51
3:D:337:ARG:HH12	3:D:1320:ILE:HG23	1.75	0.51
2:C:888:THR:O	2:C:914:LYS:N	2.39	0.51
2:C:1270:PHE:HZ	2:C:1278:LEU:HD12	1.75	0.51
4:E:25:ARG:HD3	4:E:64:LEU:HD13	1.91	0.51
2:C:213:LEU:HD22	2:C:422:LYS:HD3	1.93	0.51
3:D:390:LEU:HD23	3:D:407:VAL:HG13	1.92	0.51
2:C:169:LYS:HE2	2:C:190:PRO:HB3	1.91	0.51
3:D:140:TYR:OH	3:D:312:ARG:NH1	2.41	0.51
3:D:722:ILE:HA	3:D:725:MET:HE3	1.92	0.51
1:B:35:PHE:HA	1:B:38:THR:HG22	1.93	0.51
2:C:150:HIS:CD2	2:C:454:ARG:HE	2.29	0.51
2:C:339:ASN:O	2:C:343:HIS:N	2.42	0.51
2:C:734:ILE:HB	2:C:749:ASP:HB2	1.93	0.51
3:D:190:LYS:HZ1	3:D:235:GLU:HG2	1.76	0.51
3:D:1108:GLN:OE1	3:D:1123:ARG:NH1	2.44	0.51
2:C:499:SER:HA	2:C:502:VAL:HG12	1.91	0.51
2:C:801:ARG:NH2	2:C:1092:THR:O	2.40	0.51
3:D:425:ARG:HG2	3:D:427:PRO:HD2	1.93	0.51
3:D:840:LEU:HD11	3:D:866:GLU:HG3	1.93	0.51
3:D:1173:ARG:N	3:D:1190:ILE:O	2.44	0.51
3:D:1262:ARG:HG3	3:D:1263:LYS:HG2	1.92	0.51
2:C:1030:GLU:OE1	2:C:1033:ARG:NH2	2.40	0.50
3:D:418:GLU:HG3	4:E:45:LYS:H	1.77	0.50
3:D:1143:ASP:HA	3:D:1148:ARG:HD2	1.94	0.50
3:D:362:ARG:H	3:D:365:GLN:NE2	2.06	0.50
3:D:592:VAL:HA	3:D:596:LEU:HD21	1.92	0.50
1:B:100:LEU:O	1:B:144:ILE:N	2.40	0.50
2:C:682:GLY:O	2:C:686:GLN:HB2	2.11	0.50
2:C:1243:MET:O	2:C:1244:HIS:ND1	2.44	0.50
1:A:7:GLU:OE2	1:A:195:ARG:NH1	2.44	0.50
1:A:79:LEU:HA	1:A:82:LEU:HD12	1.93	0.50
2:C:525:THR:HG23	2:C:529:ARG:HH21	1.77	0.50
3:D:863:LEU:HD21	3:D:901:ARG:HB3	1.94	0.50
5:F:116:GLU:HA	5:F:379:MET:HE1	1.93	0.50
2:C:238:GLN:HA	2:C:287:VAL:HG22	1.92	0.50
2:C:864:LYS:NZ	2:C:881:ASP:OD2	2.45	0.50
3:D:414:GLU:O	4:E:45:LYS:NZ	2.44	0.50
3:D:416:ILE:HG23	3:D:439:PRO:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:638:SER:OG	3:D:639:VAL:N	2.42	0.50
1:B:113:ALA:N	1:B:126:PRO:O	2.45	0.50
1:B:73:GLY:O	1:B:134:THR:N	2.41	0.49
2:C:1108:ASN:OD1	2:C:1108:ASN:N	2.35	0.49
2:C:1247:SER:HB3	3:D:376:LEU:HA	1.94	0.49
3:D:201:LEU:HB3	3:D:217:LEU:HD11	1.94	0.49
3:D:786:THR:O	3:D:790:THR:OG1	2.25	0.49
4:E:46:THR:HA	4:E:49:ILE:HB	1.94	0.49
2:C:106:GLU:HB3	2:C:109:ALA:HB2	1.94	0.49
3:D:608:CYS:O	3:D:612:LEU:HB2	2.12	0.49
3:D:959:LYS:HD2	3:D:985:ILE:HG13	1.92	0.49
2:C:588:GLU:HB2	2:C:605:TYR:HB3	1.95	0.49
2:C:1088:ASP:OD1	2:C:1092:THR:N	2.45	0.49
2:C:1196:LYS:HD3	2:C:1199:LEU:HD12	1.94	0.49
3:D:156:ARG:NH2	3:D:188:LEU:O	2.42	0.49
5:F:310:GLU:HG2	5:F:344:LEU:HD21	1.93	0.49
1:B:28:LEU:HB3	1:B:201:LEU:HB3	1.95	0.49
2:C:93:SER:HB2	2:C:126:GLU:HB3	1.94	0.49
2:C:1336:ASN:N	3:D:23:ALA:O	2.40	0.49
3:D:232:ASN:ND2	3:D:1337:VAL:O	2.46	0.49
3:D:1161:GLY:HA2	3:D:1180:VAL:HG23	1.93	0.49
2:C:1291:LEU:HD11	3:D:1354:GLY:HA2	1.95	0.49
2:C:1337:ILE:HB	3:D:22:ILE:HG13	1.95	0.49
3:D:144:TYR:OH	3:D:293:ARG:NH2	2.45	0.49
5:F:497:VAL:O	5:F:501:ALA:N	2.46	0.49
2:C:555:TYR:OH	2:C:618:GLN:OE1	2.26	0.49
1:A:91:ARG:HD2	1:A:210:THR:HA	1.95	0.49
1:A:224:LEU:HG	1:B:228:LEU:HD11	1.94	0.49
2:C:1276:TRP:HH2	3:D:798:ARG:HG3	1.78	0.49
3:D:1031:VAL:HG23	3:D:1080:ILE:HG21	1.94	0.49
3:D:1175:LEU:HD22	3:D:1190:ILE:HD11	1.95	0.49
1:B:78:ILE:HA	1:B:81:ILE:HD12	1.95	0.49
3:D:156:ARG:NH2	3:D:191:SER:OG	2.39	0.49
3:D:1310:THR:O	3:D:1313:SER:OG	2.28	0.49
1:A:34:GLY:O	1:B:45:ARG:NH1	2.46	0.49
2:C:593:LYS:HB3	2:C:600:THR:HB	1.95	0.48
2:C:1085:MET:HB3	2:C:1094:VAL:HG12	1.95	0.48
2:C:1273:MET:HB3	3:D:428:THR:HB	1.95	0.48
3:D:1178:THR:HG23	3:D:1184:ASP:HB3	1.95	0.48
2:C:732:ILE:HG13	2:C:753:LEU:HD11	1.95	0.48
3:D:501:VAL:HG22	3:D:502:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:THR:HG23	1:B:39:LEU:HD23	1.95	0.48
2:C:3:TYR:HE1	2:C:1158:LYS:HE3	1.78	0.48
2:C:476:LYS:HA	2:C:479:LEU:HD12	1.95	0.48
2:C:962:GLU:O	2:C:966:ILE:HG13	2.13	0.48
2:C:1240:ASP:OD1	2:C:1241:ASP:N	2.47	0.48
3:D:556:GLU:HB3	3:D:564:VAL:HB	1.95	0.48
3:D:1263:LYS:HA	3:D:1279:GLN:HA	1.94	0.48
1:B:6:THR:OG1	1:B:7:GLU:N	2.46	0.48
1:B:91:ARG:HD2	1:B:210:THR:HB	1.95	0.48
3:D:826:ILE:H	3:D:826:ILE:HG12	1.37	0.48
3:D:984:LEU:HB3	3:D:993:GLU:H	1.78	0.48
3:D:268:LEU:HD11	3:D:324:LEU:HD13	1.96	0.48
3:D:865:HIS:CE1	3:D:867:GLN:HB2	2.49	0.48
1:B:9:LEU:HD11	1:B:192:VAL:HG21	1.95	0.48
2:C:365:GLU:OE2	2:C:368:ARG:NH2	2.46	0.48
3:D:94:GLN:HG3	3:D:97:VAL:HG23	1.96	0.48
3:D:510:LEU:HD22	3:D:601:ILE:HD12	1.96	0.48
1:B:162:GLU:HG3	1:B:166:ARG:HH12	1.79	0.48
2:C:903:ARG:HA	2:C:908:GLU:HB2	1.94	0.48
3:D:521:LYS:NZ	3:D:540:GLY:O	2.43	0.48
3:D:361:LEU:HB3	3:D:365:GLN:HG3	1.95	0.47
5:F:256:PHE:HZ	5:F:261:LEU:HD23	1.77	0.47
3:D:475:GLU:OE2	4:E:28:ARG:NH2	2.45	0.47
5:F:272:SER:O	5:F:276:MET:HB2	2.14	0.47
1:B:60:GLU:HB2	1:B:170:ARG:HH11	1.80	0.47
2:C:933:VAL:HG13	2:C:1050:VAL:HG22	1.95	0.47
3:D:484:MET:HB3	3:D:484:MET:HE2	1.73	0.47
3:D:1028:ILE:HG23	3:D:1118:GLY:HA2	1.95	0.47
1:B:81:ILE:HG12	1:B:131:CYS:HB3	1.96	0.47
2:C:955:GLN:NE2	2:C:959:ASP:OD2	2.44	0.47
3:D:587:LEU:HD23	3:D:591:ILE:HG21	1.96	0.47
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.96	0.47
1:B:33:ARG:HD2	1:B:197:ASP:HB2	1.96	0.47
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.97	0.47
1:B:20:SER:O	1:B:22:THR:N	2.47	0.47
1:B:154:PRO:HD2	1:B:157:THR:HB	1.97	0.47
2:C:402:ARG:NH2	2:C:417:SER:O	2.46	0.47
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.96	0.47
5:F:547:VAL:HG21	5:F:607:LEU:HD11	1.96	0.47
1:B:100:LEU:N	1:B:144:ILE:O	2.46	0.47
2:C:62:TYR:HB2	2:C:480:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.95	0.47
4:E:3:ARG:NH1	4:E:55:GLU:OE1	2.48	0.47
5:F:432:THR:OG1	6:G:40:DA:N7	2.43	0.47
2:C:561:ILE:HD13	3:D:772:TYR:HE2	1.80	0.47
4:E:5:THR:HB	4:E:7:GLN:H	1.79	0.47
1:B:145:LYS:HB2	1:B:170:ARG:HH22	1.79	0.47
2:C:189:ASP:OD2	2:C:191:LYS:NZ	2.48	0.47
3:D:1060:VAL:HG13	3:D:1104:LYS:HA	1.97	0.47
1:B:219:ARG:O	1:B:223:ILE:HG13	2.15	0.46
2:C:387:ASN:HA	2:C:391:SER:HB2	1.97	0.46
2:C:615:VAL:HB	2:C:638:SER:HB2	1.97	0.46
2:C:800:MET:HE1	2:C:828:PHE:HZ	1.80	0.46
3:D:720:ASN:O	3:D:724:MET:HG3	2.15	0.46
5:F:428:SER:O	5:F:432:THR:OG1	2.33	0.46
3:D:865:HIS:HE1	3:D:867:GLN:HB2	1.81	0.46
3:D:909:ILE:HD11	3:D:913:GLU:HG2	1.97	0.46
3:D:1150:PRO:HG3	3:D:1214:PRO:HB2	1.97	0.46
5:F:545:HIS:CE1	5:F:560:ARG:HH22	2.34	0.46
3:D:770:LEU:O	3:D:774:ILE:HG13	2.16	0.46
3:D:859:PRO:HG2	3:D:862:THR:HG21	1.98	0.46
5:F:362:ASN:OD1	5:F:363:ARG:N	2.49	0.46
5:F:426:LYS:NZ	6:G:40:DA:OP1	2.48	0.46
2:C:228:VAL:HG11	2:C:239:MET:HE3	1.97	0.46
3:D:368:LEU:HD21	3:D:373:ALA:HB2	1.97	0.46
1:A:60:GLU:HB2	1:A:170:ARG:HD3	1.98	0.46
1:A:124:VAL:HG21	1:A:209:GLY:HA3	1.97	0.46
2:C:633:LEU:HA	2:C:646:SER:HA	1.98	0.46
2:C:1070:HIS:HB3	2:C:1108:ASN:HD22	1.80	0.46
2:C:1302:THR:HA	5:F:531:PRO:HB3	1.98	0.46
2:C:1066:MET:HG2	2:C:1234:LYS:HA	1.98	0.46
3:D:156:ARG:NH2	3:D:191:SER:HG	2.14	0.46
3:D:1163:VAL:HG23	3:D:1177:ILE:HG22	1.97	0.46
1:A:12:ARG:NH1	1:A:13:LEU:O	2.49	0.46
1:A:93:GLN:N	1:A:120:ASP:O	2.45	0.46
1:B:181:GLU:N	1:B:206:GLU:O	2.44	0.46
2:C:74:ARG:NH1	2:C:121:GLU:OE2	2.49	0.46
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.98	0.46
3:D:641:ILE:O	3:D:764:ARG:NH1	2.46	0.46
3:D:883:ARG:NH2	3:D:895:CYS:SG	2.89	0.46
2:C:1078:LYS:NZ	2:C:1080:ASN:OD1	2.41	0.46
3:D:322:ARG:HH11	5:F:510:PRO:HD2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1313:SER:O	3:D:1316:THR:OG1	2.33	0.46
1:B:60:GLU:HB2	1:B:170:ARG:HD2	1.98	0.46
3:D:70:CYS:SG	3:D:71:LEU:N	2.89	0.46
3:D:485:MET:HB3	3:D:488:ASN:ND2	2.31	0.46
3:D:1025:MET:N	3:D:1124:ILE:O	2.36	0.46
3:D:1263:LYS:HD3	3:D:1279:GLN:HG3	1.97	0.46
1:A:182:ARG:HB3	1:A:206:GLU:HB3	1.98	0.45
1:B:196:THR:O	1:B:198:LEU:N	2.49	0.45
2:C:672:GLU:HG3	2:C:673:HIS:CD2	2.51	0.45
3:D:53:ARG:HH12	3:D:89:GLY:H	1.62	0.45
2:C:543:ALA:HA	2:C:544:GLY:HA3	1.75	0.45
3:D:1059:LEU:O	3:D:1106:ILE:HA	2.16	0.45
5:F:510:PRO:HA	5:F:518:HIS:HA	1.97	0.45
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.98	0.45
2:C:299:LYS:NZ	2:C:334:GLU:HB2	2.31	0.45
3:D:53:ARG:HA	3:D:54:ASP:HA	1.77	0.45
3:D:473:THR:OG1	3:D:475:GLU:OE1	2.28	0.45
5:F:234:THR:OG1	5:F:248:GLU:OE1	2.25	0.45
2:C:6:THR:HB	2:C:706:ARG:HH12	1.81	0.45
2:C:476:LYS:HA	2:C:479:LEU:HB2	1.97	0.45
2:C:813:GLU:HB2	3:D:461:PHE:HD2	1.82	0.45
3:D:424:ASN:N	3:D:467:ALA:O	2.38	0.45
1:B:80:GLU:O	3:D:551:ARG:NH2	2.47	0.45
2:C:800:MET:HE2	2:C:800:MET:HB3	1.81	0.45
3:D:511:TYR:HA	3:D:514:THR:HG22	1.98	0.45
3:D:849:LEU:HD12	3:D:855:ASP:H	1.82	0.45
5:F:520:GLY:HA2	5:F:523:ILE:HD12	1.98	0.45
1:A:13:LEU:HB3	1:B:231:PHE:HE1	1.82	0.45
1:A:15:ASP:HB3	1:A:27:THR:HB	1.99	0.45
1:A:92:VAL:HG12	1:A:121:VAL:HG22	1.99	0.45
3:D:279:LEU:HD12	3:D:295:GLU:HG3	1.99	0.45
3:D:1036:ARG:HD2	3:D:1079:LYS:HD3	1.98	0.45
5:F:292:VAL:HG11	5:F:299:LYS:HE2	1.98	0.45
3:D:701:LEU:HD12	3:D:723:TYR:CD2	2.52	0.45
3:D:1205:GLU:N	3:D:1208:ASP:OD2	2.41	0.45
2:C:179:TYR:HB2	2:C:398:SER:HB3	1.98	0.44
2:C:295:LYS:HG3	2:C:296:VAL:H	1.82	0.44
3:D:579:LEU:HD12	3:D:582:ILE:HD12	1.99	0.44
3:D:1057:SER:OG	3:D:1107:VAL:O	2.23	0.44
3:D:1356:LEU:HB3	3:D:1366:HIS:HE1	1.82	0.44
5:F:484:ALA:HB1	5:F:491:GLU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:762:ASN:O	2:C:833:ILE:N	2.47	0.44
4:E:39:VAL:HG21	4:E:52:ARG:HE	1.81	0.44
1:A:61:ILE:HG12	1:A:142:MET:HE2	1.99	0.44
1:B:68:TYR:HA	1:B:79:LEU:HD23	1.99	0.44
1:B:205:MET:HE3	1:B:213:PRO:HB3	1.99	0.44
3:D:845:ALA:HA	3:D:883:ARG:HG3	1.99	0.44
3:D:1106:ILE:N	3:D:1123:ARG:O	2.44	0.44
5:F:145:LEU:HD13	5:F:225:ARG:HD3	1.99	0.44
5:F:392:LYS:HE3	6:G:43:DT:H4'	1.98	0.44
2:C:300:ASP:OD1	2:C:313:ALA:N	2.50	0.44
2:C:391:SER:HB3	2:C:394:ARG:HB2	1.98	0.44
2:C:821:ARG:HB2	2:C:1082:ILE:HG12	1.98	0.44
2:C:936:ARG:NH2	2:C:1046:VAL:O	2.50	0.44
2:C:1304:MET:O	2:C:1308:ILE:HG12	2.16	0.44
3:D:147:ILE:HA	3:D:188:LEU:HD21	1.99	0.44
3:D:749:LYS:HB3	3:D:755:ILE:HD11	1.99	0.44
3:D:1221:LEU:HD23	3:D:1229:VAL:HG11	1.99	0.44
2:C:528:ARG:NH2	2:C:575:LEU:O	2.51	0.44
3:D:624:ILE:HA	3:D:627:THR:HG22	2.00	0.44
2:C:205:PRO:O	2:C:208:ILE:HG22	2.18	0.44
2:C:830:THR:O	2:C:1058:ARG:N	2.46	0.44
2:C:821:ARG:HA	2:C:824:GLN:HB2	1.99	0.44
3:D:186:GLN:HB2	3:D:238:ILE:HG13	1.99	0.44
3:D:475:GLU:HA	3:D:478:LEU:HD12	2.00	0.44
1:B:191:ARG:HH11	1:B:193:GLU:HA	1.83	0.44
2:C:681:MET:HB3	2:C:685:MET:HE2	2.00	0.44
2:C:1020:GLU:O	2:C:1024:GLU:CB	2.66	0.44
2:C:1062:PRO:HA	2:C:1076:ILE:HG23	2.00	0.44
3:D:598:LYS:HA	3:D:601:ILE:HG22	1.98	0.44
1:A:154:PRO:O	1:A:157:THR:OG1	2.35	0.43
2:C:75:LEU:HD13	2:C:75:LEU:HA	1.85	0.43
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.99	0.43
3:D:28:ASP:HA	3:D:31:ARG:HD2	2.00	0.43
3:D:380:PHE:HB3	3:D:415:VAL:HG11	2.00	0.43
3:D:525:MET:HG3	3:D:527:LEU:HD11	1.99	0.43
2:C:1020:GLU:O	2:C:1024:GLU:HB3	2.17	0.43
3:D:1314:LEU:HA	3:D:1326:GLN:HE22	1.83	0.43
1:B:182:ARG:NH1	3:D:581:MET:SD	2.91	0.43
2:C:1270:PHE:CZ	2:C:1278:LEU:HD12	2.54	0.43
3:D:812:ASP:HB2	3:D:911:LYS:HZ3	1.83	0.43
3:D:275:ARG:HH11	3:D:302:ALA:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:VAL:HG13	1:A:71:LYS:HE2	2.00	0.43
2:C:148:GLN:NE2	2:C:533:LEU:O	2.51	0.43
2:C:357:ASN:OD1	2:C:357:ASN:N	2.44	0.43
3:D:746:LEU:HB3	3:D:754:ILE:HD11	2.00	0.43
3:D:836:ARG:HG3	3:D:869:CYS:HB3	1.99	0.43
3:D:957:SER:HB3	3:D:985:ILE:HB	1.99	0.43
1:A:12:ARG:H	1:A:30:PRO:HG2	1.84	0.43
2:C:758:ARG:NH2	2:C:835:GLU:OE1	2.46	0.43
2:C:1196:LYS:HD3	2:C:1196:LYS:HA	1.89	0.43
2:C:1339:LEU:HA	3:D:20:ILE:HG23	2.00	0.43
3:D:288:PRO:HG2	3:D:291:ILE:HD12	1.99	0.43
3:D:710:ASP:OD1	3:D:711:GLY:N	2.51	0.43
5:F:585:GLU:O	5:F:588:ARG:HG2	2.18	0.43
1:A:191:ARG:HA	1:A:191:ARG:HD3	1.78	0.43
2:C:107:ARG:HA	2:C:108:GLU:HA	1.61	0.43
3:D:24:LEU:HB2	3:D:236:TRP:HE3	1.84	0.43
2:C:10:ARG:HE	2:C:706:ARG:HH21	1.67	0.43
3:D:24:LEU:HD23	3:D:232:ASN:HB3	2.01	0.43
4:E:12:LYS:HD2	4:E:57:GLY:HA2	2.01	0.43
5:F:137:TYR:HA	5:F:138:PRO:HD3	1.90	0.43
2:C:208:ILE:HD11	2:C:365:GLU:HB3	2.01	0.43
2:C:516:ASP:HA	2:C:761:GLN:HE22	1.84	0.43
2:C:564:PRO:HD2	2:C:572:ILE:HG21	2.01	0.43
2:C:1329:GLU:O	2:C:1332:SER:OG	2.32	0.43
3:D:1258:ARG:HA	3:D:1261:LEU:HG	2.00	0.43
1:B:188:GLU:O	1:B:200:LYS:N	2.46	0.43
2:C:13:LYS:HB2	2:C:1180:MET:HE2	2.00	0.43
2:C:105:TYR:HA	2:C:113:THR:HA	2.00	0.43
2:C:568:ASN:HA	2:C:571:LEU:HD12	2.01	0.43
2:C:568:ASN:HB2	2:C:572:ILE:HD11	2.01	0.43
2:C:810:TYR:CD2	3:D:359:PRO:HG2	2.54	0.43
2:C:1294:LYS:HB3	2:C:1294:LYS:HE2	1.85	0.43
3:D:314:ARG:HA	3:D:314:ARG:HD2	1.85	0.43
3:D:406:ALA:HA	3:D:409:TRP:HD1	1.84	0.43
5:F:305:LEU:HD22	5:F:315:TRP:HB3	2.00	0.43
1:A:45:ARG:NH2	2:C:1216:ARG:O	2.52	0.42
2:C:322:LEU:HA	2:C:325:LEU:HG	2.00	0.42
3:D:96:LYS:HE3	3:D:96:LYS:HB3	1.82	0.42
3:D:356:THR:N	3:D:447:ILE:O	2.48	0.42
3:D:375:GLU:OE2	3:D:378:LYS:NZ	2.49	0.42
3:D:450:HIS:CE1	3:D:452:LEU:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:861:ASN:HD22	3:D:883:ARG:NH1	2.17	0.42
3:D:1173:ARG:HH22	3:D:1175:LEU:HD13	1.84	0.42
2:C:718:ALA:HB2	2:C:783:LEU:HD21	2.01	0.42
2:C:857:VAL:HG23	2:C:862:LEU:HD11	2.01	0.42
3:D:40:LYS:HB3	3:D:42:GLU:OE1	2.19	0.42
3:D:135:ILE:O	3:D:139:LEU:HG	2.20	0.42
3:D:615:LYS:HE2	3:D:615:LYS:HB2	1.84	0.42
1:B:26:VAL:HB	1:B:203:ILE:HB	2.01	0.42
2:C:319:LEU:HA	2:C:322:LEU:HD12	2.01	0.42
1:A:19:VAL:HG13	1:A:23:HIS:HB3	2.02	0.42
1:A:45:ARG:HA	1:A:45:ARG:HD3	1.88	0.42
2:C:256:GLU:HA	2:C:261:VAL:HA	2.01	0.42
2:C:897:PRO:HB3	5:F:564:GLY:H	1.84	0.42
2:C:903:ARG:NH1	2:C:908:GLU:OE1	2.51	0.42
3:D:1282:TYR:HA	3:D:1285:VAL:HG22	2.00	0.42
5:F:469:GLN:O	5:F:472:GLN:HG3	2.19	0.42
2:C:61:SER:O	2:C:63:SER:N	2.51	0.42
2:C:758:ARG:HG2	2:C:762:ASN:HA	2.02	0.42
3:D:555:TYR:HB2	3:D:585:LYS:HB3	2.01	0.42
3:D:559:ALA:HB3	3:D:562:GLU:HB2	2.01	0.42
3:D:915:ILE:O	3:D:918:ILE:HG12	2.18	0.42
5:F:463:LEU:HD21	5:F:494:ILE:HG12	2.01	0.42
1:A:97:GLU:HB3	1:A:147:GLN:HG2	2.02	0.42
1:B:48:LEU:HG	3:D:535:ARG:HH21	1.85	0.42
1:B:134:THR:O	1:B:138:ALA:HB2	2.20	0.42
2:C:822:VAL:HG13	2:C:827:ARG:HD3	2.01	0.42
2:C:1180:MET:HA	2:C:1181:PRO:HD3	1.88	0.42
3:D:860:ARG:HG2	3:D:861:ASN:H	1.85	0.42
3:D:861:ASN:OD1	3:D:861:ASN:N	2.53	0.42
6:G:4:DC:H2''	6:G:5:DG:C8	2.55	0.42
1:B:151:GLY:O	1:B:177:TYR:HB2	2.20	0.42
1:B:155:ALA:H	1:B:174:ASP:HA	1.85	0.42
1:B:197:ASP:OD1	1:B:197:ASP:N	2.52	0.42
2:C:556:GLY:HA2	2:C:660:VAL:HA	2.00	0.42
3:D:334:LYS:HA	3:D:335:GLN:HA	1.85	0.42
3:D:1229:VAL:O	3:D:1233:ILE:HG12	2.20	0.42
5:F:453:PRO:HG3	6:G:31:DC:H3'	2.00	0.42
1:B:203:ILE:HD13	1:B:203:ILE:HA	1.94	0.42
2:C:59:ILE:HB	2:C:68:LEU:HB3	2.00	0.42
2:C:119:GLU:HB2	2:C:489:PRO:HD2	2.02	0.42
2:C:834:GLN:N	2:C:1054:LEU:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1272:SER:OG	3:D:1273:ASP:N	2.53	0.42
2:C:124:MET:HE2	2:C:124:MET:HB3	1.78	0.42
2:C:431:LYS:HA	2:C:431:LYS:HD3	1.90	0.42
2:C:818:VAL:HG13	2:C:1096:ILE:HG12	2.01	0.42
3:D:412:LEU:HD21	3:D:441:LEU:HG	2.00	0.42
3:D:436:ALA:HB3	3:D:485:MET:HA	2.02	0.42
2:C:695:ALA:HB2	2:C:788:SER:HA	2.02	0.41
2:C:801:ARG:HB2	2:C:1229:TYR:HE1	1.85	0.41
3:D:118:LYS:O	3:D:311:ARG:NH1	2.53	0.41
3:D:1173:ARG:O	3:D:1190:ILE:N	2.44	0.41
2:C:714:VAL:O	2:C:767:GLN:NE2	2.53	0.41
2:C:806:PRO:HA	2:C:811:ASN:ND2	2.33	0.41
2:C:1223:ARG:HG3	3:D:636:GLY:O	2.21	0.41
1:A:232:VAL:O	1:B:218:ARG:NE	2.53	0.41
2:C:55:SER:OG	2:C:465:ARG:NH1	2.53	0.41
3:D:555:TYR:HD1	3:D:563:LEU:HB3	1.85	0.41
3:D:796:LEU:O	3:D:800:LEU:HD12	2.20	0.41
5:F:126:GLY:HA3	5:F:372:ALA:HB2	2.02	0.41
5:F:261:LEU:HD11	5:F:266:PHE:HD1	1.85	0.41
6:G:27:DC:H2"	6:G:28:DA:C8	2.55	0.41
3:D:118:LYS:NZ	3:D:311:ARG:HB3	2.35	0.41
3:D:1265:THR:O	3:D:1303:SER:N	2.41	0.41
2:C:749:ASP:HB3	2:C:751:TYR:HE2	1.85	0.41
3:D:21:LYS:HD3	3:D:1341:ARG:HB2	2.01	0.41
3:D:485:MET:HG3	3:D:487:THR:H	1.86	0.41
3:D:968:ASN:ND2	3:D:1117:SER:O	2.53	0.41
5:F:489:MET:HE1	5:F:494:ILE:HG13	2.02	0.41
5:F:511:ILE:HD12	5:F:511:ILE:HA	1.90	0.41
5:F:533:ASP:O	5:F:536:THR:OG1	2.28	0.41
2:C:299:LYS:HE3	2:C:299:LYS:HB3	1.81	0.41
2:C:629:PHE:O	2:C:647:ARG:NH1	2.53	0.41
3:D:60:ARG:HG3	3:D:61:ILE:HG13	2.03	0.41
3:D:221:ILE:HD12	3:D:221:ILE:HA	1.89	0.41
3:D:1348:LYS:HA	3:D:1351:VAL:HB	2.02	0.41
5:F:423:ARG:HG3	6:G:37:DA:C6	2.55	0.41
1:A:100:LEU:N	1:A:144:ILE:O	2.48	0.41
2:C:235:ASN:ND2	2:C:236:LYS:H	2.19	0.41
2:C:422:LYS:O	2:C:426:ILE:HG13	2.20	0.41
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.96	0.41
3:D:316:ILE:HG22	3:D:323:PRO:HA	2.03	0.41
3:D:1138:LEU:HD12	3:D:1138:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:HB2	1:A:122:GLU:HB3	2.02	0.41
1:B:82:LEU:HD23	1:B:82:LEU:HA	1.95	0.41
1:B:208:ASN:O	1:B:210:THR:N	2.49	0.41
2:C:74:ARG:NH2	2:C:121:GLU:OE1	2.54	0.41
3:D:709:ARG:HG3	3:D:710:ASP:H	1.85	0.41
7:H:30:DC:H6	7:H:30:DC:H2'	1.73	0.41
1:A:45:ARG:HG2	1:B:38:THR:HG21	2.03	0.41
1:A:90:VAL:HG21	1:A:146:VAL:HG11	2.02	0.41
2:C:3:TYR:OH	2:C:1158:LYS:O	2.27	0.41
2:C:221:LEU:HD22	2:C:336:LEU:HD11	2.03	0.41
2:C:311:CYS:HB3	2:C:321:LEU:HD21	2.01	0.41
2:C:724:VAL:HG13	2:C:734:ILE:HD13	2.03	0.41
2:C:800:MET:H	2:C:800:MET:HG2	1.76	0.41
2:C:801:ARG:NH1	2:C:1093:PRO:O	2.53	0.41
2:C:1000:LEU:HD23	2:C:1000:LEU:HA	1.92	0.41
3:D:147:ILE:HG22	3:D:188:LEU:HG	2.03	0.41
3:D:557:LYS:HE2	3:D:557:LYS:HB2	1.80	0.41
3:D:643:ASP:O	3:D:720:ASN:ND2	2.48	0.41
3:D:848:VAL:HG11	3:D:880:VAL:HG13	2.01	0.41
3:D:865:HIS:CE1	3:D:868:TRP:HD1	2.39	0.41
2:C:210:LEU:HD23	2:C:210:LEU:HA	1.92	0.41
2:C:799:ASN:OD1	2:C:799:ASN:N	2.47	0.41
6:G:44:DG:H2''	6:G:45:DT:C6	2.56	0.41
1:A:152:TYR:HD1	1:A:176:CYS:HA	1.86	0.40
2:C:340:ASP:HA	2:C:344:GLY:HA2	2.04	0.40
2:C:681:MET:O	2:C:685:MET:HG3	2.21	0.40
2:C:1162:SER:OG	2:C:1163:THR:N	2.54	0.40
1:A:190:ALA:HB2	1:A:200:LYS:HB2	2.03	0.40
2:C:325:LEU:O	2:C:328:SER:OG	2.33	0.40
2:C:1290:MET:SD	3:D:347:VAL:HG11	2.61	0.40
3:D:736:GLN:O	3:D:740:LEU:HD12	2.20	0.40
3:D:1319:PHE:O	3:D:1323:ALA:HB2	2.22	0.40
2:C:18:ARG:HA	2:C:19:PRO:HD3	1.84	0.40
2:C:66:SER:HB3	2:C:102:LEU:HD11	2.03	0.40
2:C:551:HIS:H	2:C:554:HIS:HD2	1.68	0.40
2:C:684:ASN:OD1	2:C:687:ARG:NH1	2.54	0.40
2:C:742:TYR:O	2:C:746:ALA:HB2	2.22	0.40
2:C:1099:ASN:HD21	2:C:1101:LEU:HB2	1.86	0.40
3:D:972:LYS:HB2	3:D:974:VAL:HG23	2.02	0.40
5:F:380:VAL:HG13	5:F:412:LEU:HD23	2.02	0.40
1:B:72:GLU:HB3	1:B:137:ASN:ND2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:ASP:O	2:C:44:GLU:N	2.53	0.40
5:F:474:MET:HE3	5:F:474:MET:HB3	1.98	0.40
1:A:45:ARG:O	1:A:49:SER:OG	2.33	0.40
1:A:66:HIS:ND1	1:A:68:TYR:HB2	2.37	0.40
1:A:234:LEU:HB2	1:B:218:ARG:HH21	1.85	0.40
2:C:398:SER:HG	2:C:401:GLY:H	1.65	0.40
2:C:932:GLN:O	2:C:1051:LYS:N	2.53	0.40
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.92	0.40
3:D:923:ILE:HD11	3:D:1252:HIS:HB3	2.04	0.40
3:D:1260:MET:HE3	3:D:1309:ILE:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/329 (69%)	201 (88%)	25 (11%)	2 (1%)	14	50
1	B	226/329 (69%)	202 (89%)	21 (9%)	3 (1%)	9	41
2	C	1338/1342 (100%)	1200 (90%)	115 (9%)	23 (2%)	7	36
3	D	1348/1407 (96%)	1189 (88%)	134 (10%)	25 (2%)	6	31
4	E	74/91 (81%)	67 (90%)	7 (10%)	0	100	100
5	F	466/613 (76%)	427 (92%)	32 (7%)	7 (2%)	8	39
All	All	3680/4111 (90%)	3286 (89%)	334 (9%)	60 (2%)	10	37

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	SER
2	C	62	TYR

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Mol	Chain	Res	Type
2	C	246	LEU
2	C	398	SER
2	C	625	GLU
2	C	756	TYR
3	D	590	SER
3	D	861	ASN
3	D	1200	GLU
3	D	1345	ARG
5	F	154	GLU
5	F	515	GLU
1	A	15	ASP
1	B	197	ASP
2	C	214	ASN
2	C	281	ASP
2	C	314	ASN
2	C	643	SER
2	C	730	SER
2	C	812	PHE
3	D	148	GLU
3	D	404	GLU
3	D	860	ARG
3	D	1024	THR
5	F	568	ASN
1	B	193	GLU
2	C	165	HIS
2	C	247	ARG
2	C	546	GLU
2	C	573	ASN
2	C	596	ASP
2	C	1005	GLU
2	C	1158	LYS
2	C	1223	ARG
3	D	500	ILE
3	D	851	PRO
3	D	1114	GLN
5	F	234	THR
5	F	447	ALA
2	C	199	ASP
2	C	235	ASN
3	D	744	ARG
3	D	769	VAL
3	D	962	ASN

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Mol	Chain	Res	Type
3	D	1022	PRO
3	D	1087	ASP
1	A	30	PRO
3	D	19	ALA
3	D	928	THR
3	D	1097	ALA
2	C	897	PRO
3	D	46	TYR
3	D	828	GLY
3	D	1052	GLU
3	D	1106	ILE
5	F	478	PRO
3	D	850	LYS
5	F	91	ILE
2	C	697	LYS
3	D	745	GLY

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	198/286 (69%)	189 (96%)	9 (4%)	24	46
1	B	196/286 (68%)	187 (95%)	9 (5%)	24	45
2	C	1155/1157 (100%)	1107 (96%)	48 (4%)	26	48
3	D	1111/1168 (95%)	1056 (95%)	55 (5%)	22	42
4	E	65/75 (87%)	65 (100%)	0	100	100
5	F	420/540 (78%)	409 (97%)	11 (3%)	40	61
All	All	3145/3512 (90%)	3013 (96%)	132 (4%)	28	48

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	VAL
1	A	56	VAL

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Mol	Chain	Res	Type
1	A	65	LEU
1	A	100	LEU
1	A	107	ILE
1	A	146	VAL
1	A	153	VAL
1	A	174	ASP
1	A	222	THR
1	B	13	LEU
1	B	14	VAL
1	B	31	LEU
1	B	39	LEU
1	B	82	LEU
1	B	129	VAL
1	B	171	LEU
1	B	173	VAL
1	B	183	ILE
2	C	6	THR
2	C	22	LEU
2	C	24	VAL
2	C	30	ILE
2	C	39	ILE
2	C	62	TYR
2	C	147	SER
2	C	169	LYS
2	C	191	LYS
2	C	198	ILE
2	C	255	ILE
2	C	265	LYS
2	C	269	ILE
2	C	302	ILE
2	C	358	ASP
2	C	384	LEU
2	C	388	LEU
2	C	446	ASP
2	C	471	VAL
2	C	472	GLU
2	C	502	VAL
2	C	521	LEU
2	C	561	ILE
2	C	563	THR
2	C	615	VAL
2	C	616	ILE

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Mol	Chain	Res	Type
2	C	623	LEU
2	C	697	LYS
2	C	700	VAL
2	C	777	VAL
2	C	782	VAL
2	C	791	LEU
2	C	882	ILE
2	C	895	LEU
2	C	901	LEU
2	C	1002	LEU
2	C	1037	THR
2	C	1056	VAL
2	C	1075	VAL
2	C	1115	THR
2	C	1128	ILE
2	C	1132	LEU
2	C	1182	ILE
2	C	1212	LEU
2	C	1222	GLU
2	C	1253	LEU
2	C	1287	LEU
2	C	1298	VAL
3	D	22	ILE
3	D	24	LEU
3	D	58	CYS
3	D	132	LEU
3	D	138	VAL
3	D	146	VAL
3	D	190	LYS
3	D	208	THR
3	D	214	ARG
3	D	219	LYS
3	D	252	LEU
3	D	306	LEU
3	D	324	LEU
3	D	330	MET
3	D	354	VAL
3	D	374	LEU
3	D	398	LYS
3	D	501	VAL
3	D	506	VAL
3	D	534	GLU

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Mol	Chain	Res	Type
3	D	536	LEU
3	D	573	THR
3	D	574	VAL
3	D	619	ILE
3	D	653	ILE
3	D	674	THR
3	D	701	LEU
3	D	717	VAL
3	D	753	SER
3	D	755	ILE
3	D	769	VAL
3	D	776	THR
3	D	807	LEU
3	D	814	CYS
3	D	826	ILE
3	D	830	ASP
3	D	857	LEU
3	D	858	VAL
3	D	928	THR
3	D	948	SER
3	D	973	LEU
3	D	974	VAL
3	D	980	THR
3	D	986	ASP
3	D	1024	THR
3	D	1029	THR
3	D	1031	VAL
3	D	1037	PHE
3	D	1057	SER
3	D	1088	VAL
3	D	1196	LEU
3	D	1318	SER
3	D	1321	SER
3	D	1331	VAL
3	D	1340	LYS
5	F	110	LEU
5	F	132	CYS
5	F	305	LEU
5	F	387	VAL
5	F	414	LYS
5	F	417	ASP
5	F	449	THR

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Mol	Chain	Res	Type
5	F	454	VAL
5	F	461	ASN
5	F	516	ASP
5	F	530	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	75	GLN
1	A	117	HIS
1	A	227	GLN
1	B	137	ASN
2	C	235	ASN
2	C	437	ASN
2	C	463	GLN
2	C	490	GLN
2	C	554	HIS
2	C	573	ASN
2	C	752	ASN
2	C	760	ASN
2	C	808	ASN
2	C	811	ASN
2	C	922	ASN
2	C	1090	ASN
2	C	1134	GLN
2	C	1175	ASN
2	C	1220	GLN
2	C	1237	HIS
2	C	1264	GLN
2	C	1268	GLN
2	C	1324	ASN
2	C	1336	ASN
3	D	186	GLN
3	D	206	ASN
3	D	300	GLN
3	D	320	ASN
3	D	365	GLN
3	D	419	HIS
3	D	424	ASN
3	D	450	HIS
3	D	488	ASN

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Mol	Chain	Res	Type
3	D	489	ASN
3	D	504	GLN
3	D	665	GLN
3	D	929	GLN
3	D	1019	ASN
3	D	1238	GLN
3	D	1289	ASN
3	D	1350	ASN
4	E	62	GLN
5	F	301	ASN
5	F	342	GLN
5	F	400	GLN
5	F	464	ASN
5	F	545	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.

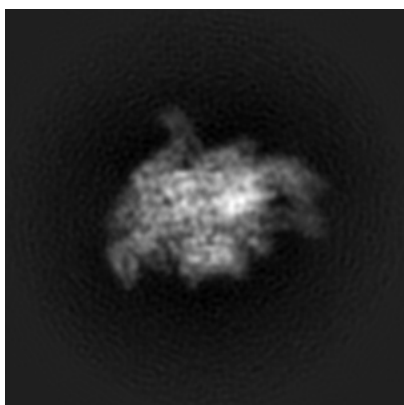
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7439. These allow visual inspection of the internal detail of the map and identification of artifacts.

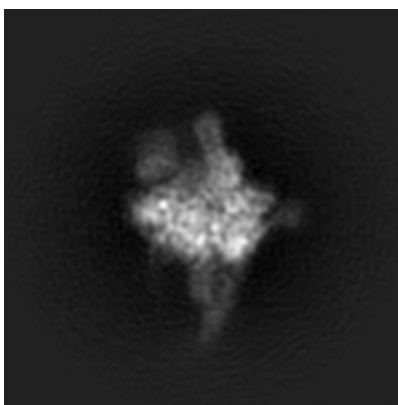
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

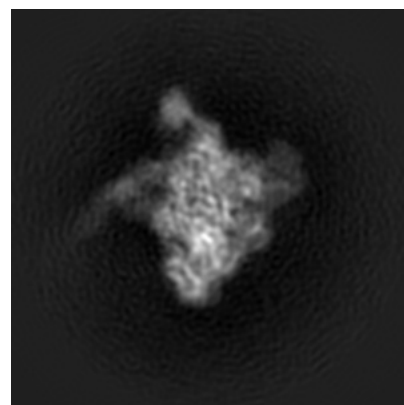
6.1.1 Primary map



X



Y

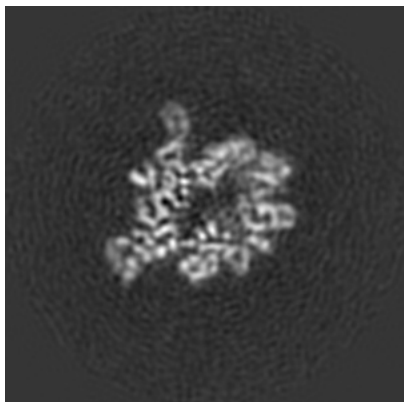


Z

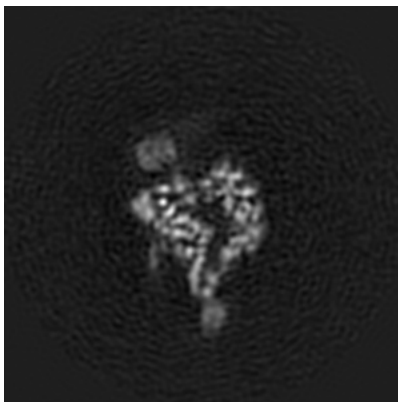
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

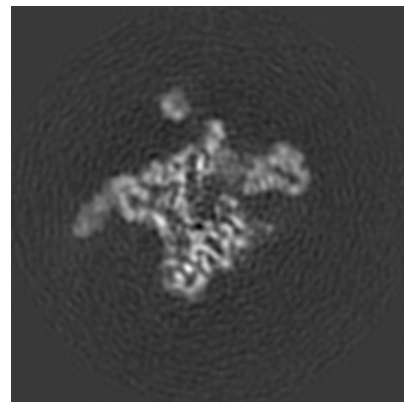
6.2.1 Primary map



X Index: 120



Y Index: 120

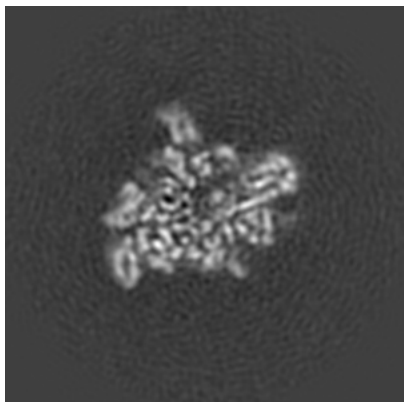


Z Index: 120

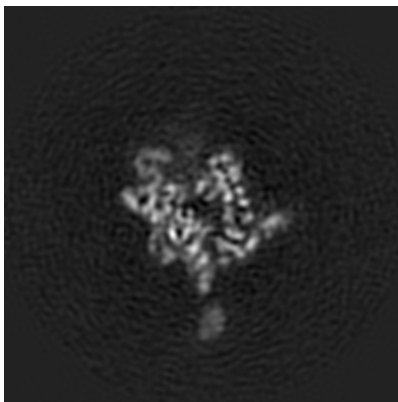
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

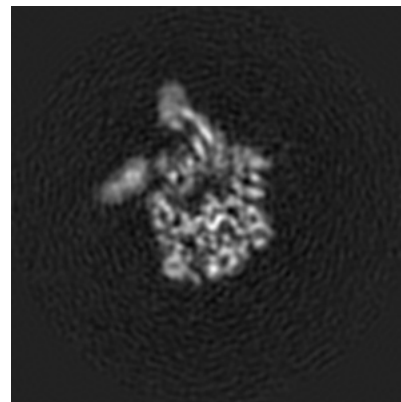
6.3.1 Primary map



X Index: 113



Y Index: 113

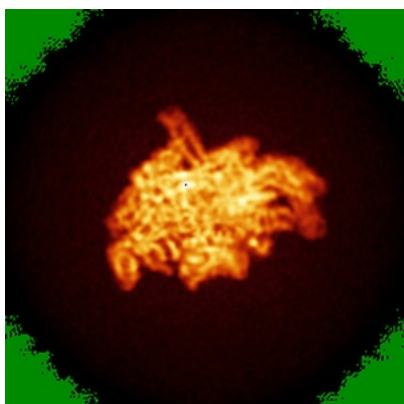


Z Index: 134

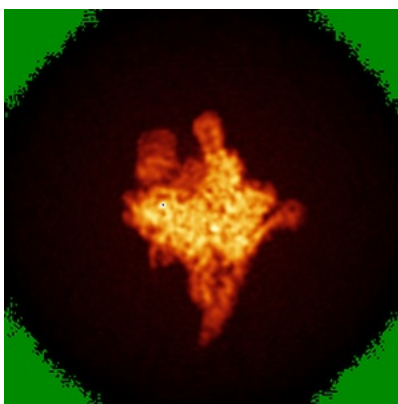
The images above show the largest variance slices of the map in three orthogonal directions.

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

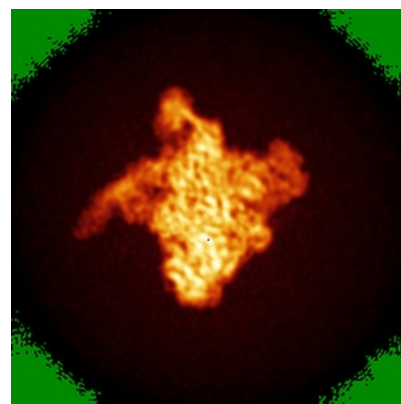
6.4.1 Primary map



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

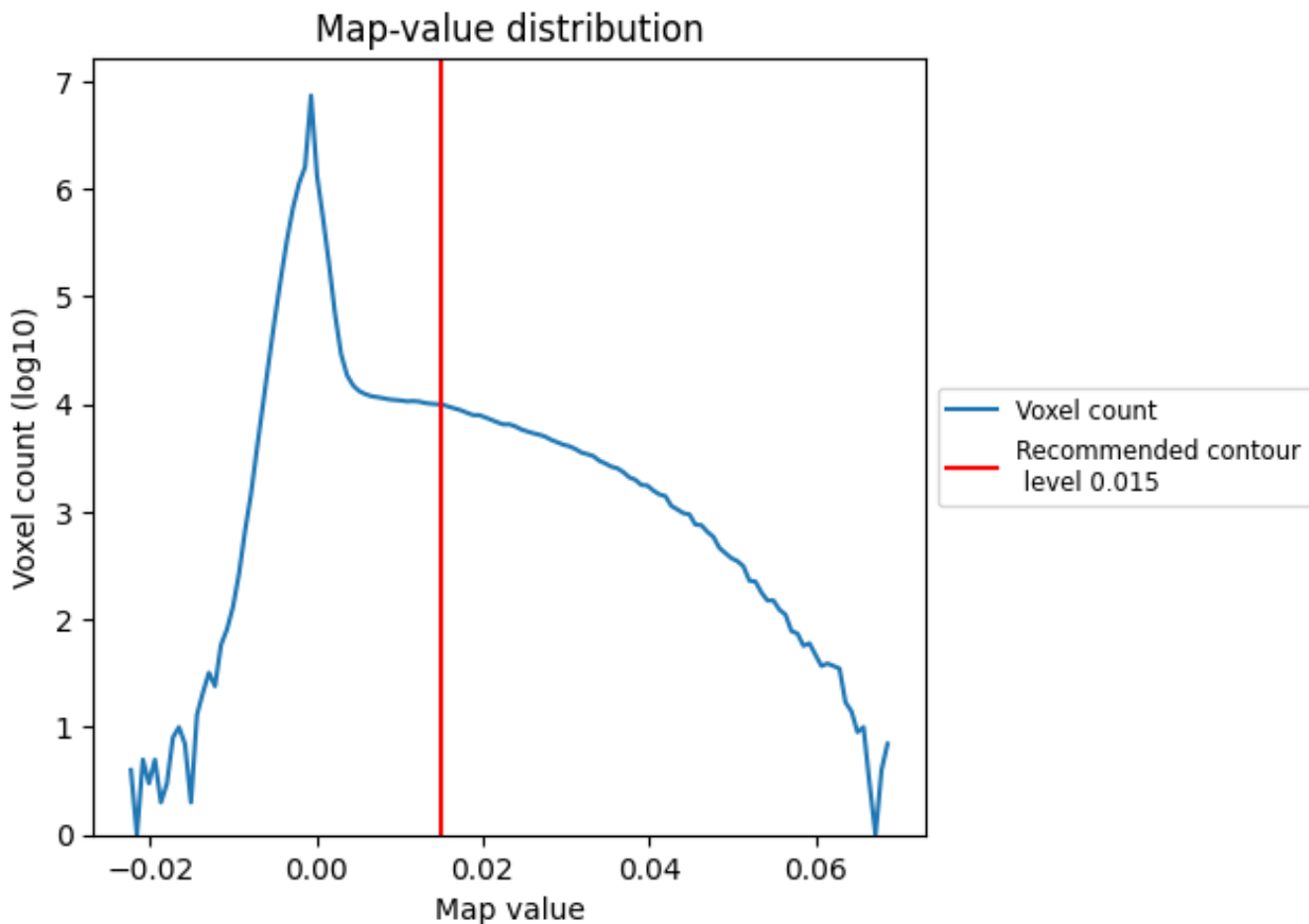
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

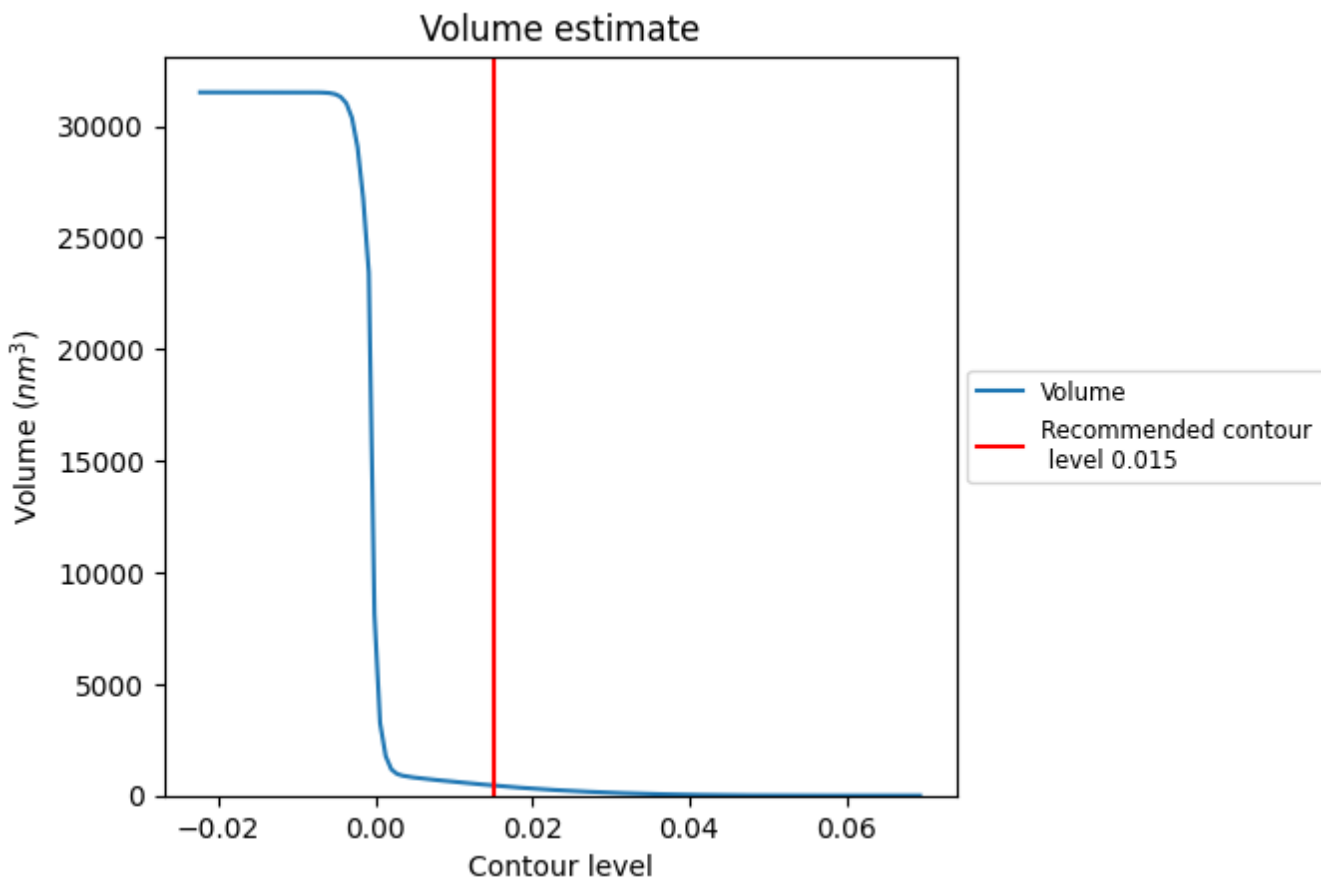
This section contains the results of statistical analysis of the map.

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.

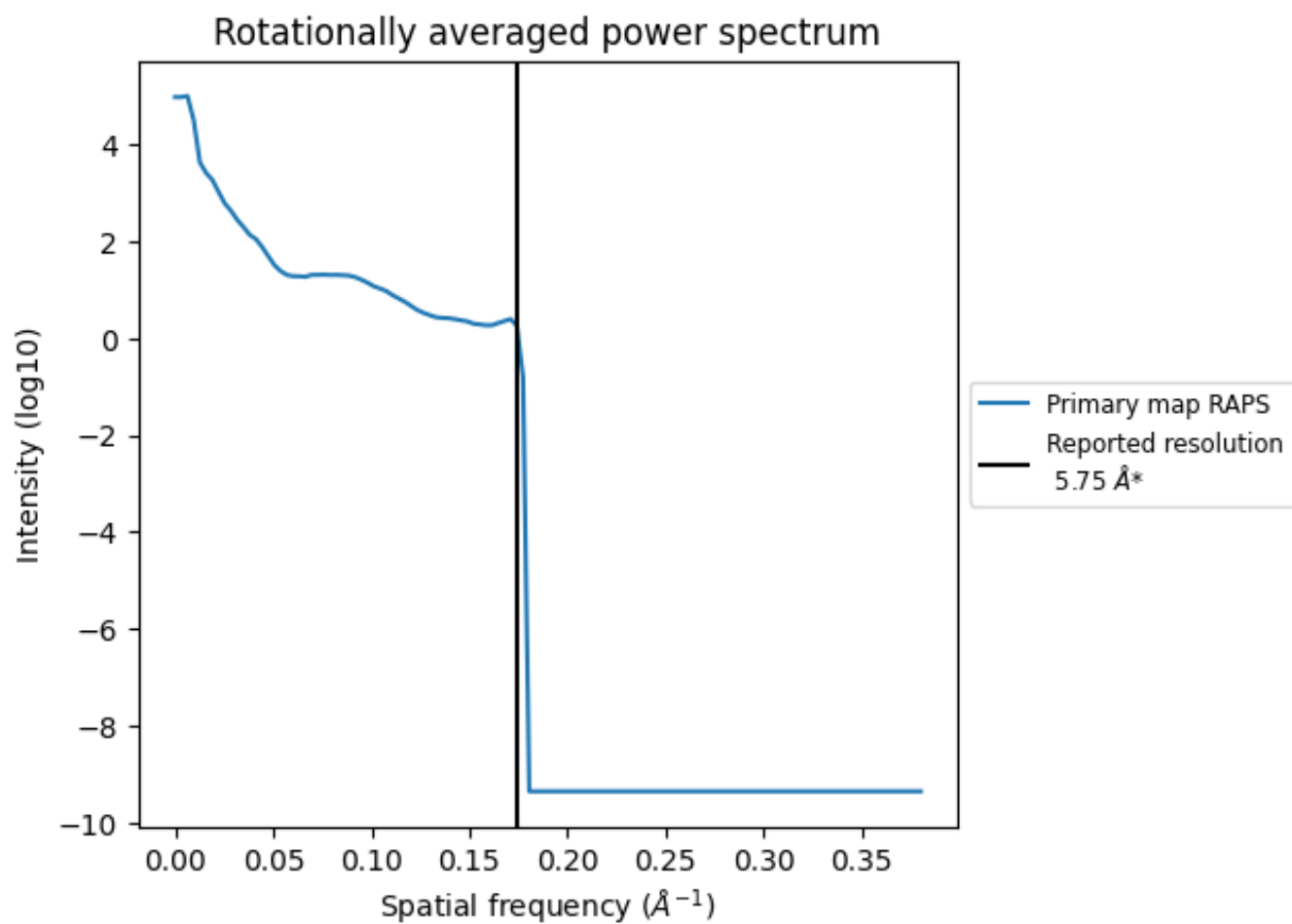
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 454 nm³; this corresponds to an approximate mass of 410 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.174 Å⁻¹

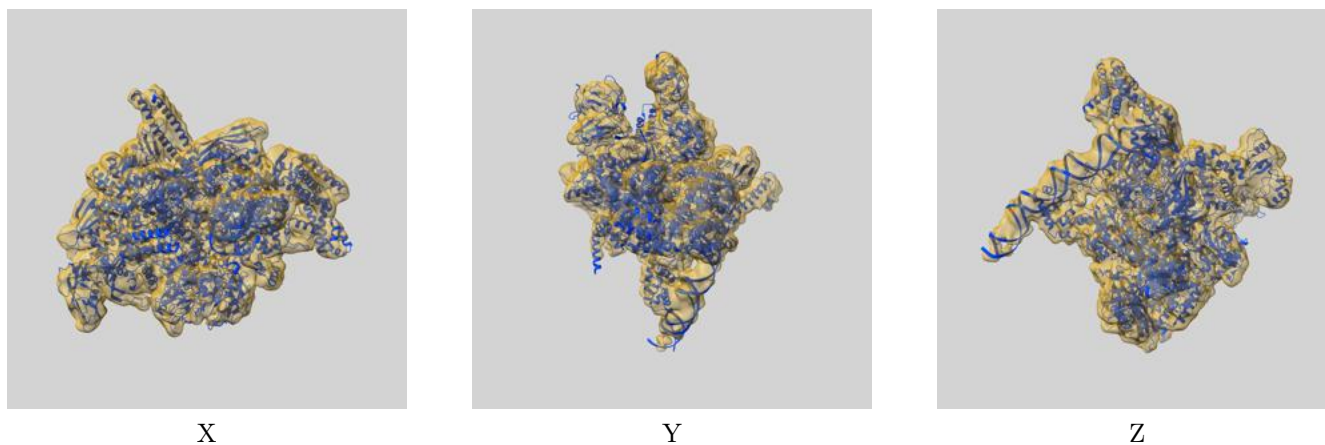
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

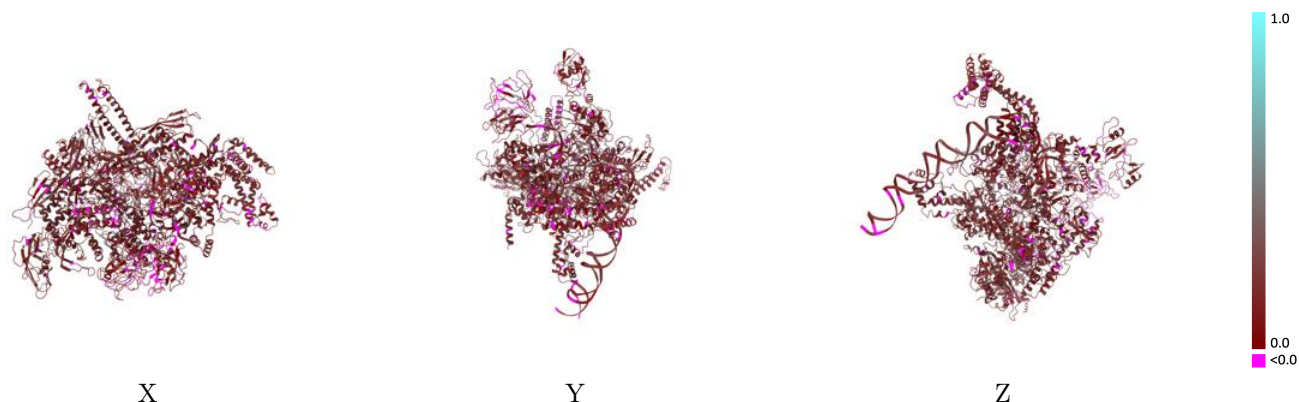
This section contains information regarding the fit between EMDB map EMD-7439 and PDB model 6CA0. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



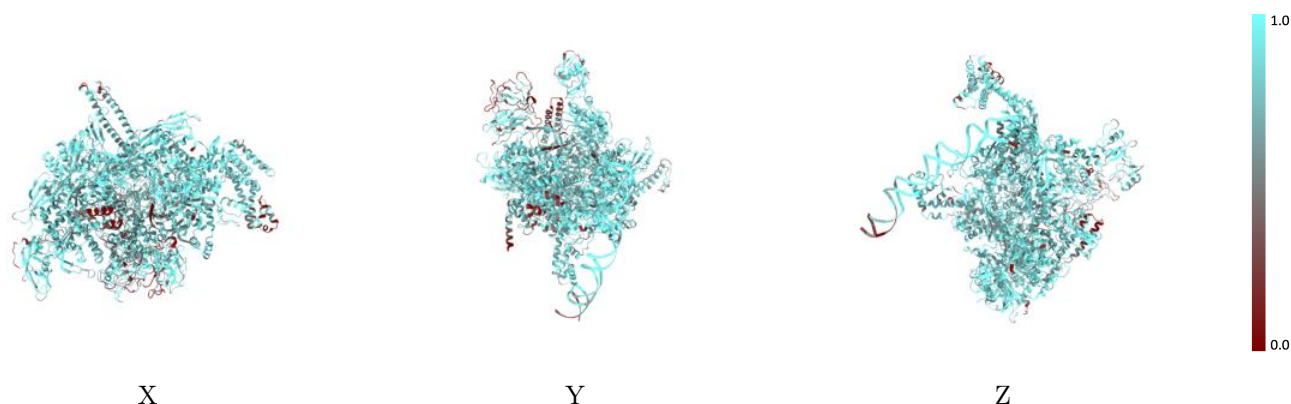
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



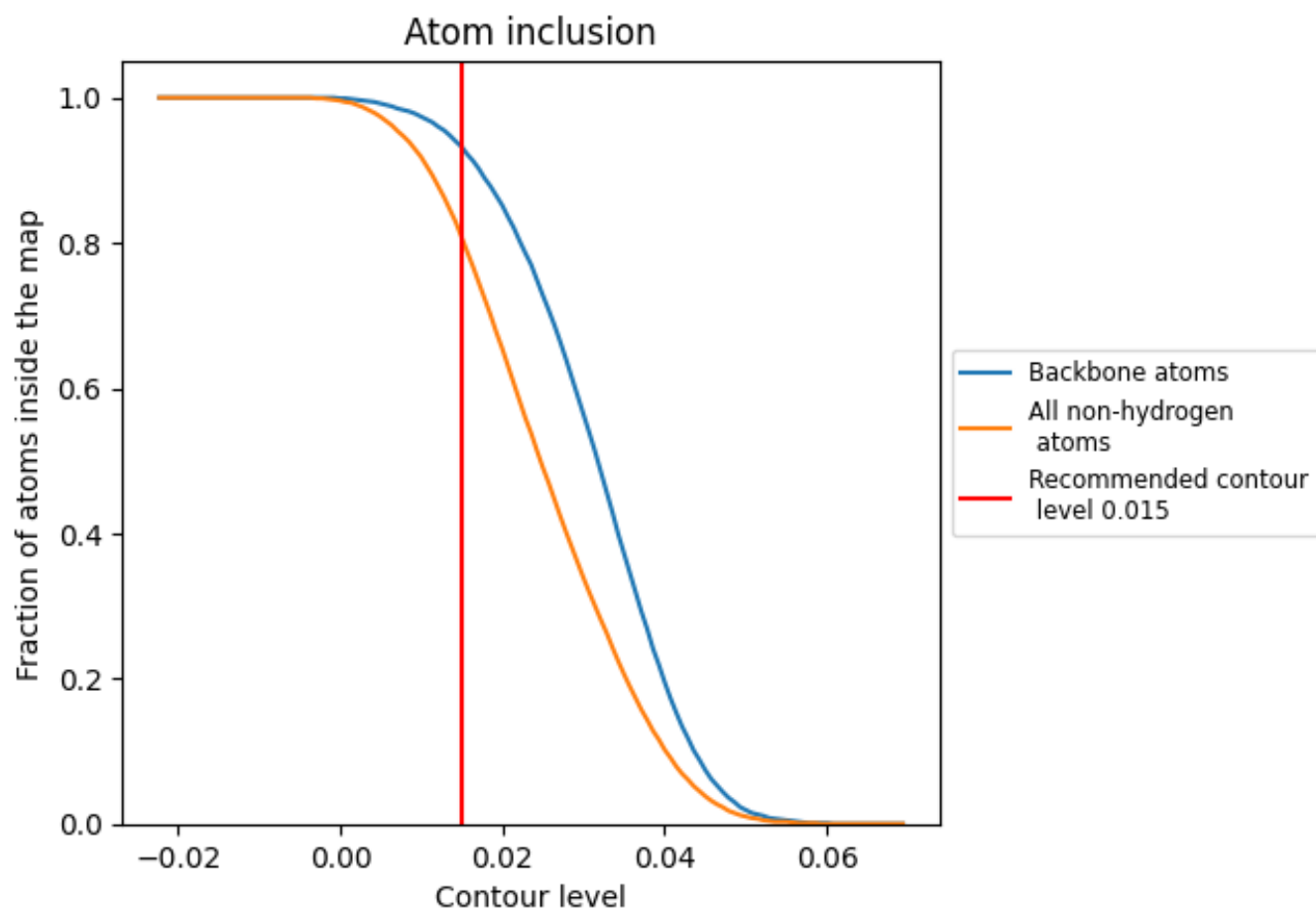
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).























9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8070	 0.1720
A	 0.8800	 0.1940
B	 0.8600	 0.1720
C	 0.8480	 0.1860
D	 0.7650	 0.1630
E	 0.5960	 0.1730
F	 0.8090	 0.1520
G	 0.8310	 0.1860
H	 0.7870	 0.1550
I	 0.5240	 0.1310
J	 0.6280	 0.1440

