



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 10:17 AM EST

PDB ID : 6PMJ
EMDB ID : EMD-20395
Title : Sigm28-transcription initiation complex with specific promoter at the state 2
Authors : Liu, B.; Shi, W.
Deposited on : 2019-07-02
Resolution : 3.91 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

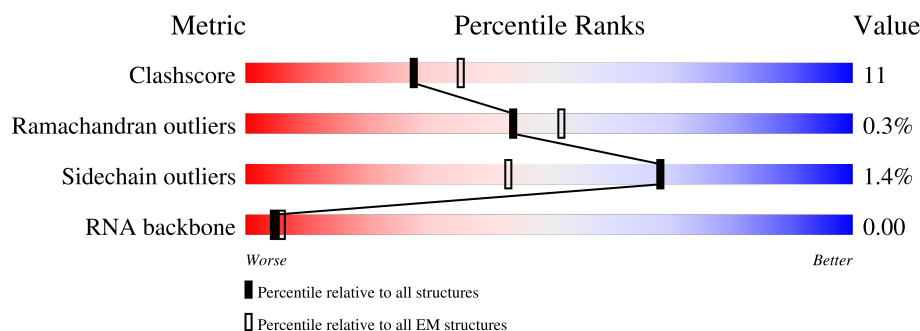
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.91 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
RNA backbone	4643	859

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	F	247	
6	1	54	

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Mol	Chain	Length	Quality of chain
7	2	54	<div><div></div><div>69%</div><div>30%</div><div>.</div></div>
8	3	3	<div><div></div><div>67%</div><div>33%</div><div></div></div>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 57995 atoms, of which 28620 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	230	Total	C	H	N	O	S	0	0
			3599	1112	1813	317	351	6		
1	B	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	1340	Total	C	H	N	O	S	0	0
			21152	6631	10582	1841	2055	43		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	D	1337	Total	C	H	N	O	S	0	0
			21010	6531	10614	1853	1962	50		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	79	Total	C	H	N	O	S	0	0
			1261	382	634	118	126	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	239	Total	C	H	N	O	S	0	0
			3871	1201	1936	356	374	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	240	LEU	-	expression tag	UNP P0AEM6

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Chain	Residue	Modelled	Actual	Comment	Reference
F	241	GLU	-	expression tag	UNP P0AEM6
F	242	HIS	-	expression tag	UNP P0AEM6
F	243	HIS	-	expression tag	UNP P0AEM6
F	244	HIS	-	expression tag	UNP P0AEM6
F	245	HIS	-	expression tag	UNP P0AEM6
F	246	HIS	-	expression tag	UNP P0AEM6
F	247	HIS	-	expression tag	UNP P0AEM6

- Molecule 6 is a DNA chain called SYNTHETIC NONTEMPLATE STRAND DNA (54-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	1	54	Total	C	H	N	O	P	0	0
			1712	526	611	194	327	54		

- Molecule 7 is a DNA chain called SYNTHETIC TEMPLATE STRAND DNA (54-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	2	54	Total	C	H	N	O	P	0	0
			1724	530	607	214	319	54		

- Molecule 8 is a RNA chain called Nascent RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	3	3	Total	C	H	N	O	P	0	0
			107	29	34	13	26	5		

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

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

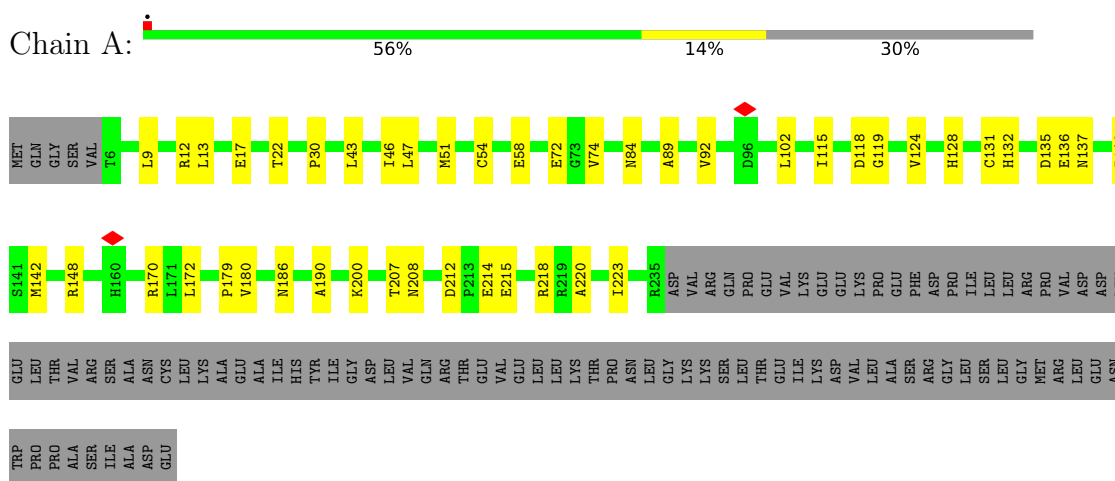
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

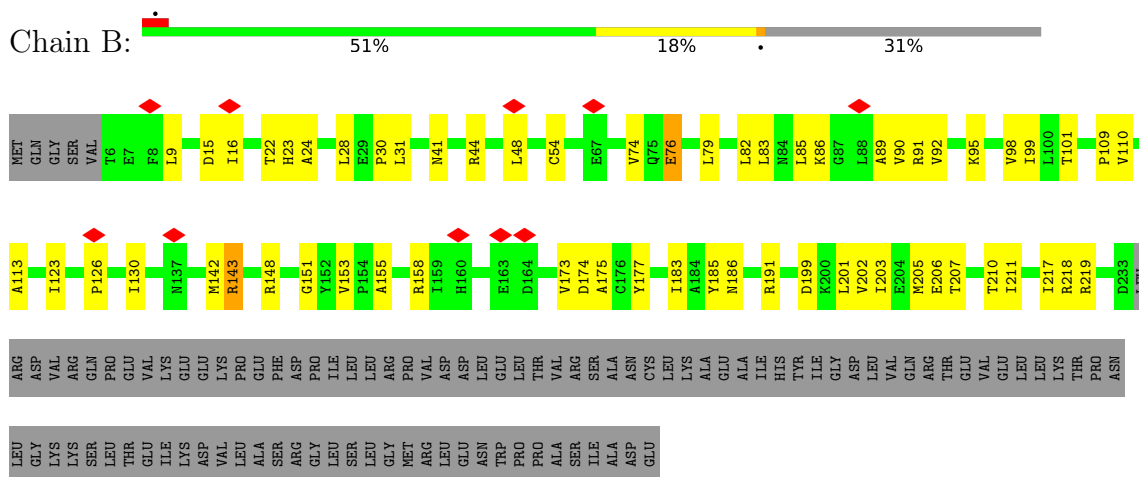
3 Residue-property plots

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



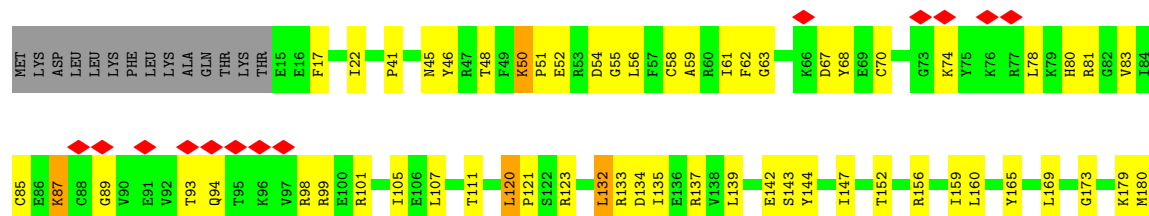
- Molecule 1: DNA-directed RNA polymerase subunit alpha

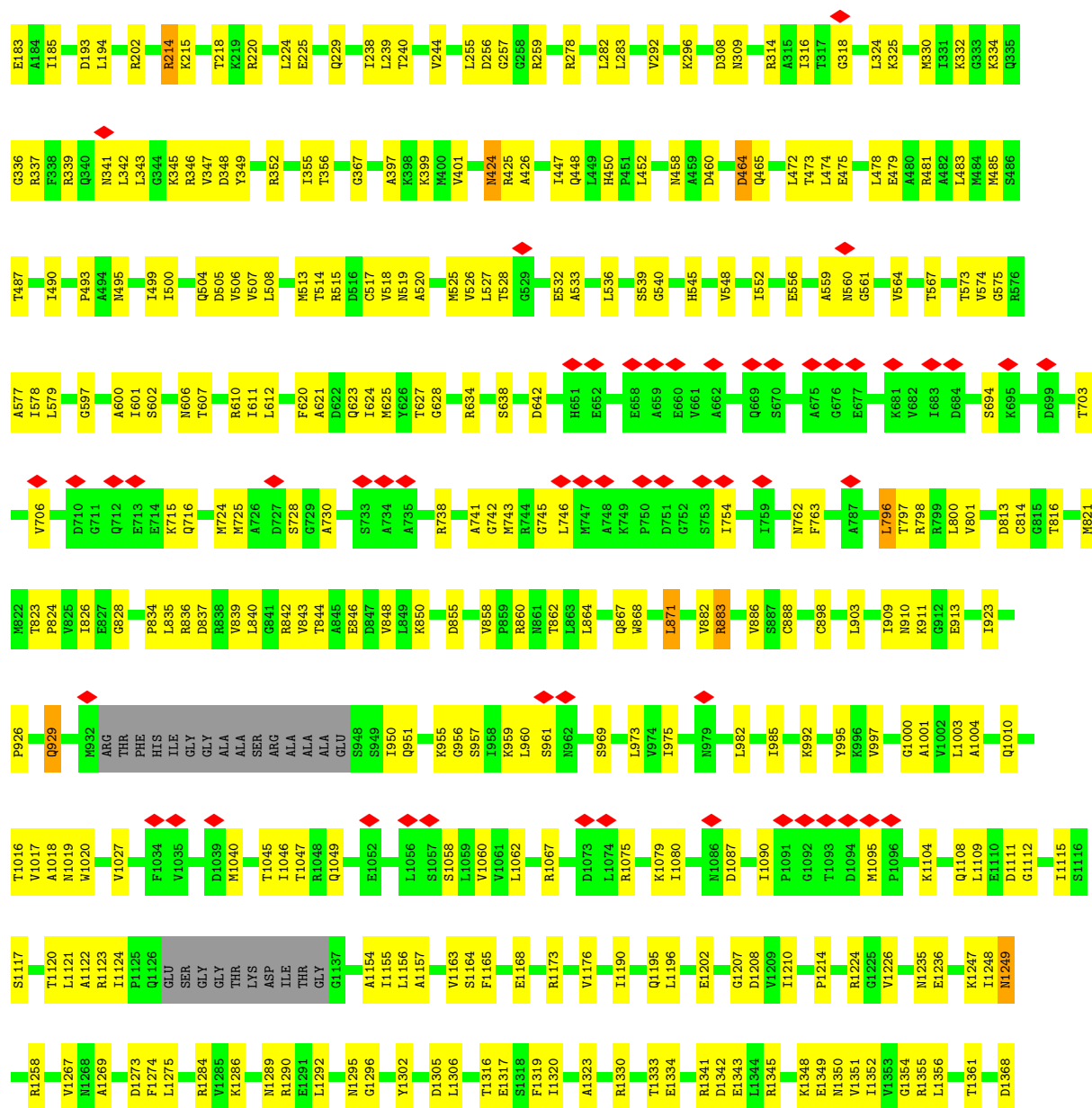


- Molecule 2: DNA-directed RNA polymerase subunit beta

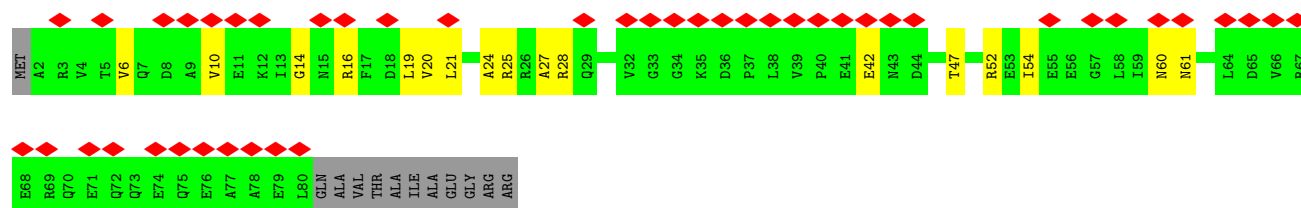


- Molecule 3: DNA-directed RNA polymerase subunit beta'

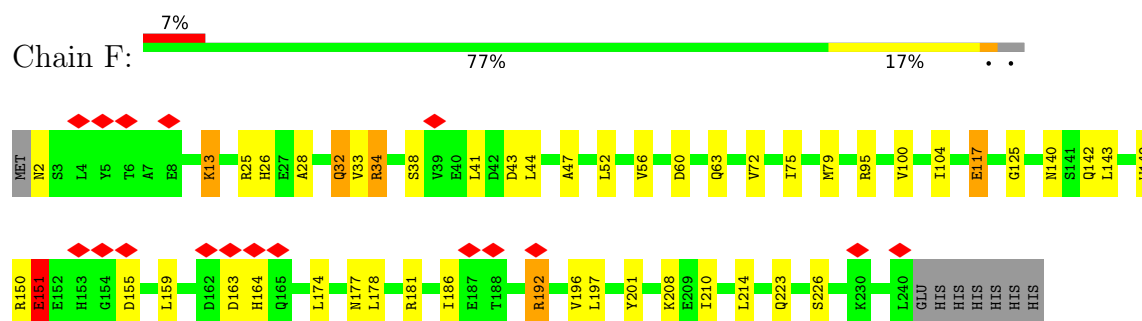




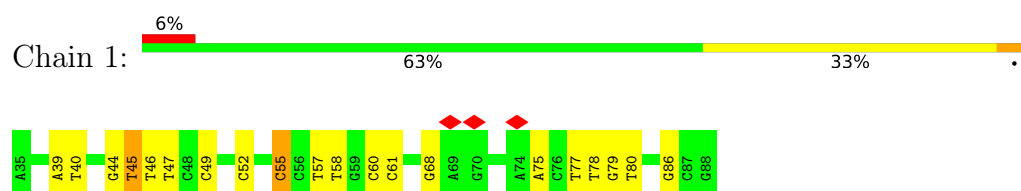
• Molecule 4: DNA-directed RNA polymerase subunit omega



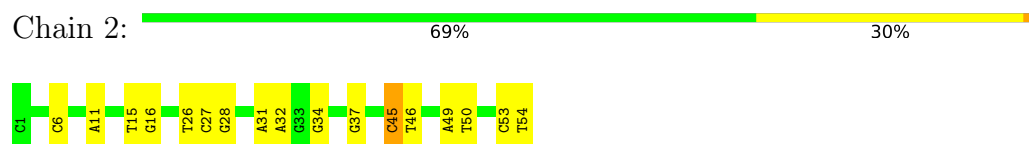
- Molecule 5: RNA polymerase sigma factor FliA



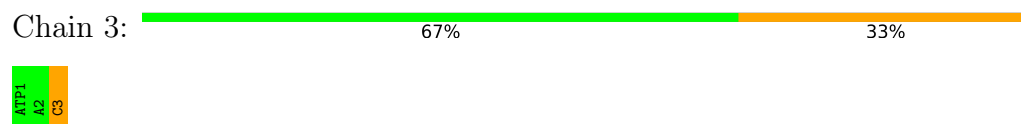
- Molecule 6: SYNTHETIC NONTEMPLATE STRAND DNA (54-MER)



- Molecule 7: SYNTHETIC TEMPLATE STRAND DNA (54-MER)



- Molecule 8: Nascent RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33687	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.449	Depositor
Minimum map value	-2.186	Depositor
Average map value	-0.020	Depositor
Map value standard deviation	0.289	Depositor
Recommended contour level	0.8	Depositor
Map size (\AA)	291.6, 291.6, 291.6	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.90000004, 0.90000004, 0.90000004	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.48	0/1808	0.68	0/2450
1	B	0.44	0/1789	0.71	1/2425 (0.0%)
2	C	0.53	0/10739	0.70	1/14489 (0.0%)
3	D	0.52	0/10553	0.74	4/14248 (0.0%)
4	E	0.30	0/629	0.60	0/847
5	F	0.51	0/1960	0.77	0/2649
6	1	1.02	1/1232 (0.1%)	1.17	6/1898 (0.3%)
7	2	1.09	0/1256	1.11	4/1938 (0.2%)
8	3	0.49	0/46	0.92	0/69
All	All	0.58	1/30012 (0.0%)	0.77	16/41013 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3
2	C	0	3
3	D	0	3
5	F	0	3
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	58	DT	C5-C7	-5.04	1.47	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	132	LEU	CA-CB-CG	6.93	131.25	115.30
7	2	45	DC	O4'-C4'-C3'	-6.66	101.84	104.50
1	B	219	ARG	NE-CZ-NH1	6.10	123.35	120.30
6	1	45	DT	O4'-C4'-C3'	-6.07	102.07	104.50
7	2	45	DC	O4'-C1'-N1	5.89	112.12	108.00
7	2	45	DC	C1'-O4'-C4'	-5.72	104.38	110.10
6	1	55	DC	C1'-O4'-C4'	-5.61	104.49	110.10
6	1	55	DC	O4'-C1'-N1	5.61	111.92	108.00
6	1	49	DC	O4'-C4'-C3'	-5.56	102.28	104.50
6	1	49	DC	C1'-O4'-C4'	-5.53	104.57	110.10
2	C	200	ARG	NE-CZ-NH1	5.52	123.06	120.30
7	2	16	DG	C1'-O4'-C4'	-5.49	104.61	110.10
3	D	871	LEU	CA-CB-CG	5.35	127.61	115.30
6	1	61	DC	OP1-P-O3'	5.20	116.63	105.20
3	D	1284	ARG	NE-CZ-NH2	-5.13	117.73	120.30
3	D	137	ARG	NE-CZ-NH2	-5.13	117.74	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	109	PRO	Peptide
1	B	191	ARG	Peptide
1	B	76	GLU	Peptide
2	C	1004	ASP	Peptide
2	C	1209	GLN	Peptide
2	C	57	PHE	Peptide
3	D	120	LEU	Peptide
3	D	67	ASP	Peptide
3	D	929	GLN	Peptide
5	F	149	TRP	Peptide
5	F	151	GLU	Peptide
5	F	32	GLN	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	1786	1813	1813	27	0
1	B	1767	1789	1789	35	0
2	C	10570	10582	10582	252	0
3	D	10396	10614	10616	259	0
4	E	627	634	634	21	0
5	F	1935	1936	1936	37	0
6	1	1101	611	611	16	0
7	2	1117	607	607	16	0
8	3	73	34	34	1	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
All	All	29375	28620	28622	613	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (613) 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)
3:D:425:ARG:NH1	3:D:426:ALA:O	2.07	0.87
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.48	0.86
3:D:475:GLU:OE1	4:E:28:ARG:NH2	2.10	0.85
3:D:473:THR:OG1	4:E:28:ARG:NH2	2.10	0.84
3:D:886:VAL:O	3:D:1258:ARG:NH1	2.10	0.83
2:C:1127:LYS:NZ	2:C:1131:MET:SD	2.53	0.81
2:C:145:ILE:HD11	2:C:456:VAL:HG13	1.63	0.81
2:C:408:SER:O	2:C:431:LYS:NZ	2.15	0.79
1:B:23:HIS:ND1	1:B:206:GLU:OE2	2.15	0.79
3:D:121:PRO:O	3:D:123:ARG:NH1	2.16	0.78
6:1:60:DC:N4	7:2:28:DG:O6	2.17	0.77
5:F:95:ARG:NH1	7:2:28:DG:OP2	2.16	0.77
2:C:1207:SER:OG	3:D:642:ASP:OD2	2.02	0.77
3:D:87:LYS:HB3	3:D:87:LYS:HZ3	1.48	0.77
3:D:68:TYR:OH	3:D:81:ARG:O	2.01	0.76
2:C:234:ASP:OD1	2:C:331:LYS:NZ	2.16	0.76
5:F:34:ARG:O	5:F:38:SER:OG	2.03	0.76
1:B:22:THR:OG1	1:B:207:THR:O	2.03	0.76
2:C:201:ARG:NH2	2:C:369:MET:O	2.18	0.76
1:B:41:ASN:ND2	2:C:1217:THR:O	2.19	0.76
3:D:225:GLU:OE1	3:D:229:GLN:NE2	2.18	0.76
1:B:91:ARG:NH1	1:B:92:VAL:O	2.20	0.75
3:D:552:ILE:O	3:D:567:THR:OG1	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:196:VAL:HG22	5:F:210:ILE:HG21	1.68	0.75
3:D:1173:ARG:O	3:D:1190:ILE:N	2.20	0.74
3:D:556:GLU:O	3:D:564:VAL:N	2.20	0.74
2:C:212:ALA:O	2:C:359:ARG:NH2	2.21	0.74
3:D:133:ARG:NH2	6:1:86:DG:OP1	2.20	0.74
3:D:214:ARG:NH1	3:D:218:THR:OG1	2.21	0.73
2:C:563:THR:OG1	2:C:569:ILE:O	2.04	0.73
2:C:760:ASN:OD1	2:C:761:GLN:NE2	2.22	0.73
2:C:1253:LEU:O	2:C:1256:GLN:NE2	2.21	0.73
3:D:17:PHE:O	3:D:1355:ARG:NH1	2.23	0.72
5:F:192:ARG:HG3	5:F:214:LEU:HD11	1.71	0.72
2:C:804:PHE:O	3:D:638:SER:OG	2.07	0.72
1:B:54:CYS:SG	1:B:91:ARG:NH2	2.63	0.71
5:F:72:VAL:HA	5:F:75:ILE:HD12	1.71	0.71
3:D:424:ASN:ND2	3:D:425:ARG:O	2.22	0.71
2:C:1120:ALA:HB1	2:C:1198:LEU:HD22	1.73	0.71
2:C:339:ASN:O	2:C:343:HIS:N	2.24	0.70
2:C:69:GLN:OE1	2:C:101:ARG:NH2	2.24	0.70
1:B:89:ALA:O	1:B:123:ILE:HG23	1.90	0.70
2:C:656:SER:OG	2:C:657:THR:N	2.22	0.70
1:A:207:THR:HG23	1:A:208:ASN:O	1.90	0.70
2:C:1222:GLU:OE2	3:D:634:ARG:NH1	2.23	0.70
1:B:153:VAL:O	1:B:175:ALA:N	2.24	0.70
2:C:1114:GLU:O	2:C:1118:GLY:N	2.25	0.69
2:C:292:ILE:HD13	2:C:322:LEU:HD13	1.73	0.69
3:D:495:ASN:ND2	3:D:1247:LYS:O	2.25	0.69
5:F:151:GLU:O	5:F:151:GLU:OE1	2.10	0.69
2:C:13:LYS:O	2:C:1183:ALA:N	2.24	0.69
2:C:839:VAL:O	2:C:886:LYS:NZ	2.16	0.69
2:C:1329:GLU:O	2:C:1332:SER:OG	2.03	0.69
3:D:1062:LEU:O	3:D:1067:ARG:NH2	2.26	0.69
2:C:692:THR:OG1	2:C:694:ARG:O	2.11	0.69
3:D:694:SER:OG	3:D:738:ARG:NH2	2.26	0.68
2:C:257:ALA:N	2:C:260:LYS:O	2.26	0.68
5:F:178:LEU:HD23	5:F:181:ARG:HD2	1.74	0.68
3:D:959:LYS:NZ	3:D:961:SER:OG	2.25	0.68
3:D:356:THR:N	3:D:447:ILE:O	2.27	0.68
2:C:559:CYS:SG	2:C:662:SER:N	2.66	0.68
2:C:1008:GLN:OE1	2:C:1008:GLN:N	2.26	0.67
1:B:44:ARG:NH2	1:B:183:ILE:O	2.27	0.67
3:D:202:ARG:NH2	3:D:225:GLU:OE2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:738:ARG:O	3:D:742:GLY:N	2.28	0.67
1:B:41:ASN:ND2	2:C:1217:THR:OG1	2.28	0.67
1:A:131:CYS:SG	1:A:132:HIS:N	2.68	0.67
2:C:295:LYS:O	2:C:317:LEU:N	2.27	0.67
3:D:111:THR:O	3:D:239:LEU:N	2.26	0.67
2:C:673:HIS:ND1	3:D:763:PHE:O	2.28	0.66
1:A:58:GLU:OE1	1:A:170:ARG:NH2	2.29	0.66
2:C:1220:GLN:O	3:D:634:ARG:NH2	2.30	0.65
2:C:659:GLN:N	2:C:659:GLN:OE1	2.29	0.65
2:C:297:VAL:HB	2:C:317:LEU:HD21	1.77	0.65
5:F:41:LEU:HD12	5:F:44:LEU:HD12	1.77	0.65
5:F:60:ASP:OD2	5:F:63:GLN:NE2	2.29	0.65
2:C:794:LEU:HD11	2:C:796:LEU:HD22	1.78	0.65
2:C:138:ILE:O	2:C:141:THR:OG1	2.10	0.65
2:C:989:LEU:O	2:C:997:TRP:NE1	2.30	0.65
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.30	0.64
2:C:820:GLU:OE1	2:C:820:GLU:N	2.30	0.64
2:C:564:PRO:HD3	2:C:572:ILE:HD11	1.79	0.64
2:C:1088:ASP:OD1	2:C:1091:GLY:N	2.31	0.63
2:C:718:ALA:N	2:C:781:ASP:O	2.29	0.63
3:D:50:LYS:NZ	3:D:52:GLU:OE1	2.24	0.63
1:A:207:THR:OG1	1:A:208:ASN:N	2.31	0.62
2:C:706:ARG:NH2	2:C:793:GLU:OE2	2.32	0.62
2:C:1080:ASN:ND2	2:C:1085:MET:SD	2.72	0.62
2:C:314:ASN:OD1	2:C:348:SER:OG	2.17	0.62
3:D:183:GLU:OE1	3:D:183:GLU:N	2.32	0.62
2:C:515:MET:O	2:C:760:ASN:ND2	2.32	0.62
2:C:542:ARG:NH1	6:1:78:DT:O5'	2.33	0.62
2:C:719:LYS:O	2:C:779:ARG:NE	2.32	0.62
3:D:950:ILE:HB	3:D:1018:ALA:HB3	1.82	0.62
1:A:102:LEU:HD13	1:A:115:ILE:HA	1.81	0.62
5:F:52:LEU:O	5:F:56:VAL:HG23	2.00	0.61
2:C:504:GLU:O	2:C:508:SER:N	2.33	0.61
2:C:592:ARG:N	2:C:653:MET:O	2.31	0.61
2:C:10:ARG:NH2	2:C:790:ASP:O	2.34	0.61
2:C:678:ARG:NE	2:C:1106:ARG:O	2.34	0.61
3:D:147:ILE:O	3:D:156:ARG:NH1	2.33	0.61
2:C:65:ASN:OD1	2:C:66:SER:N	2.33	0.61
5:F:32:GLN:O	5:F:34:ARG:N	2.33	0.61
2:C:399:ALA:O	2:C:403:MET:N	2.29	0.61
2:C:1131:MET:O	2:C:1135:GLN:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:117:GLU:N	5:F:117:GLU:OE1	2.32	0.61
2:C:839:VAL:HG23	2:C:1049:ILE:HG22	1.81	0.61
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.83	0.61
2:C:557:ARG:NH2	2:C:607:SER:O	2.34	0.61
3:D:1058:SER:OG	3:D:1109:LEU:O	2.18	0.61
2:C:1288:GLN:OE1	3:D:1356:LEU:HD21	2.01	0.60
3:D:607:THR:O	3:D:611:ILE:HD12	2.01	0.60
1:A:17:GLU:N	1:A:17:GLU:OE1	2.35	0.60
2:C:1283:ALA:HB1	3:D:479:GLU:OE1	2.01	0.60
3:D:1195:GLN:NE2	3:D:1196:LEU:O	2.34	0.60
4:E:10:VAL:O	4:E:14:GLY:N	2.34	0.60
3:D:814:CYS:SG	3:D:816:THR:OG1	2.47	0.60
4:E:25:ARG:NH1	4:E:61:ASN:OD1	2.35	0.60
2:C:576:SER:OG	2:C:659:GLN:O	2.17	0.60
3:D:61:ILE:O	3:D:98:ARG:NH1	2.34	0.60
2:C:794:LEU:CD1	2:C:796:LEU:HD22	2.31	0.60
3:D:45:ASN:OD1	3:D:46:TYR:N	2.34	0.60
3:D:1075:ARG:NH1	3:D:1168:GLU:OE2	2.34	0.60
3:D:1115:ILE:HG13	3:D:1121:LEU:HD23	1.84	0.60
5:F:208:LYS:NZ	7:2:45:DC:O5'	2.35	0.60
2:C:675:ASP:OD1	2:C:676:ALA:N	2.36	0.59
3:D:139:LEU:HD21	3:D:185:ILE:HD12	1.84	0.59
3:D:493:PRO:O	3:D:903:LEU:HD22	2.01	0.59
2:C:74:ARG:N	2:C:97:ARG:O	2.35	0.59
2:C:237:LEU:HD13	2:C:292:ILE:HD11	1.83	0.59
3:D:813:ASP:OD1	3:D:883:ARG:NH2	2.36	0.59
1:A:214:GLU:OE2	1:A:218:ARG:NE	2.36	0.59
2:C:592:ARG:O	2:C:653:MET:N	2.34	0.59
2:C:803:ALA:HB2	2:C:1227:VAL:HG22	1.85	0.59
2:C:241:LEU:HD21	2:C:246:LEU:HD12	1.83	0.59
2:C:867:GLU:OE2	2:C:944:ARG:NH1	2.36	0.59
2:C:175:ARG:NE	6:1:77:DT:O4	2.36	0.58
2:C:208:ILE:HG23	2:C:209:ILE:HD12	1.85	0.58
2:C:425:ILE:O	2:C:428:VAL:HG12	2.03	0.58
3:D:478:LEU:HB2	4:E:20:VAL:HG13	1.86	0.58
2:C:542:ARG:NH2	6:1:78:DT:H72	2.17	0.58
2:C:582:ASN:N	2:C:586:PHE:O	2.37	0.58
2:C:798:GLN:NE2	2:C:827:ARG:O	2.36	0.58
3:D:844:THR:HG21	3:D:858:VAL:HG11	1.84	0.58
3:D:913:GLU:N	3:D:913:GLU:OE1	2.37	0.58
2:C:1163:THR:OG1	2:C:1164:PHE:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ALA:HB2	1:A:200:LYS:HB3	1.85	0.58
5:F:223:GLN:O	5:F:226:SER:OG	2.17	0.58
2:C:748:ILE:HD12	2:C:748:ILE:O	2.04	0.57
3:D:1154:ALA:N	3:D:1214:PRO:O	2.37	0.57
1:A:135:ASP:OD2	1:A:137:ASN:N	2.37	0.57
3:D:725:MET:O	3:D:728:SER:OG	2.17	0.57
1:A:54:CYS:SG	1:A:148:ARG:NE	2.74	0.57
2:C:604:HIS:HB3	2:C:606:LEU:HD21	1.86	0.57
2:C:93:SER:OG	2:C:126:GLU:OE1	2.20	0.57
2:C:577:VAL:HG23	2:C:661:VAL:O	2.04	0.57
3:D:194:LEU:HB3	3:D:224:LEU:HD12	1.87	0.57
3:D:352:ARG:NH2	3:D:465:GLN:OE1	2.35	0.57
3:D:1371:ARG:O	3:D:1375:ALA:N	2.37	0.57
1:B:95:LYS:NZ	1:B:98:VAL:HG23	2.20	0.57
3:D:844:THR:OG1	3:D:858:VAL:HG21	2.05	0.57
6:1:52:DC:H42	7:2:37:DG:H22	1.52	0.56
2:C:18:ARG:NH1	2:C:621:SER:O	2.37	0.56
2:C:339:ASN:O	2:C:342:ASP:N	2.39	0.56
2:C:494:ASN:OD1	2:C:495:ALA:N	2.38	0.56
2:C:511:LEU:O	2:C:513:GLN:NE2	2.39	0.56
2:C:677:ASN:OD1	2:C:678:ARG:N	2.38	0.56
2:C:818:VAL:HG12	2:C:1096:ILE:HD12	1.88	0.56
3:D:886:VAL:HG11	3:D:1226:VAL:HG11	1.87	0.56
3:D:528:THR:OG1	3:D:532:GLU:OE2	2.23	0.56
5:F:47:ALA:HB3	5:F:79:MET:HE1	1.86	0.56
3:D:800:LEU:CD1	3:D:923:ILE:HD11	2.36	0.56
3:D:107:LEU:HD13	3:D:240:THR:C	2.26	0.56
5:F:186:ILE:HD12	5:F:197:LEU:HD12	1.88	0.56
2:C:1151:LEU:HD11	2:C:1197:GLU:HG3	1.88	0.56
2:C:901:LEU:HD21	5:F:201:TYR:CE2	2.42	0.55
3:D:575:GLY:HA2	3:D:578:ILE:HD12	1.88	0.55
2:C:753:LEU:O	2:C:755:LYS:NZ	2.31	0.55
3:D:526:VAL:C	3:D:527:LEU:HD22	2.27	0.55
3:D:513:MET:HG3	3:D:514:THR:HG23	1.89	0.55
2:C:405:PHE:O	2:C:409:LEU:N	2.40	0.55
2:C:628:HIS:ND1	2:C:629:PHE:O	2.40	0.55
1:B:48:LEU:HD21	3:D:539:SER:HB3	1.89	0.55
3:D:308:ASP:OD1	3:D:308:ASP:N	2.38	0.55
3:D:969:SER:N	3:D:1117:SER:O	2.40	0.55
3:D:478:LEU:HD23	4:E:47:THR:HG23	1.88	0.55
3:D:474:LEU:HD21	4:E:27:ALA:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:803:ALA:CB	2:C:1227:VAL:HG22	2.38	0.54
3:D:519:ASN:OD1	3:D:520:ALA:N	2.40	0.54
2:C:48:GLY:O	2:C:52:ALA:N	2.40	0.54
2:C:145:ILE:HD11	2:C:456:VAL:HG22	1.88	0.54
2:C:1278:LEU:HD22	2:C:1287:LEU:HD11	1.89	0.54
3:D:255:LEU:N	3:D:259:ARG:O	2.39	0.54
3:D:1269:ALA:HB2	3:D:1274:PHE:HA	1.89	0.54
3:D:1305:ASP:OD1	3:D:1306:LEU:N	2.40	0.54
2:C:452:ARG:NH1	2:C:453:ILE:O	2.40	0.54
3:D:54:ASP:N	3:D:58:CYS:SG	2.81	0.54
3:D:339:ARG:NH1	7:2:11:DA:OP1	2.40	0.54
3:D:843:VAL:O	3:D:882:VAL:HG13	2.07	0.54
3:D:850:LYS:NZ	3:D:855:ASP:O	2.40	0.54
2:C:189:ASP:OD1	2:C:193:ASN:N	2.41	0.54
2:C:243:PRO:HA	2:C:277:LEU:HD23	1.89	0.54
6:1:52:DC:N4	7:2:37:DG:H22	2.05	0.54
2:C:14:ASP:OD1	2:C:15:PHE:N	2.40	0.54
3:D:1348:LYS:HA	3:D:1351:VAL:HG22	1.89	0.54
2:C:148:GLN:NE2	2:C:533:LEU:O	2.40	0.53
5:F:100:VAL:O	5:F:104:ILE:HG22	2.08	0.53
2:C:18:ARG:NH2	2:C:620:ASN:O	2.41	0.53
2:C:397:LEU:O	2:C:398:SER:OG	2.23	0.53
3:D:460:ASP:O	3:D:464:ASP:OD2	2.27	0.53
2:C:145:ILE:HD11	2:C:456:VAL:CG1	2.35	0.53
3:D:193:ASP:OD1	3:D:194:LEU:N	2.41	0.53
3:D:800:LEU:HD13	3:D:923:ILE:HD11	1.88	0.53
5:F:34:ARG:NH1	7:2:26:DT:O4'	2.41	0.53
2:C:839:VAL:HG23	2:C:1049:ILE:CG2	2.39	0.53
2:C:1252:SER:OG	2:C:1256:GLN:N	2.42	0.53
1:A:43:LEU:O	1:A:47:LEU:HD13	2.09	0.53
2:C:656:SER:O	2:C:659:GLN:NE2	2.41	0.53
2:C:1272:GLU:OE1	2:C:1272:GLU:N	2.40	0.53
5:F:28:ALA:O	5:F:32:GLN:NE2	2.41	0.53
3:D:1286:LYS:O	3:D:1290:ARG:N	2.38	0.53
2:C:441:GLU:OE1	2:C:441:GLU:N	2.42	0.53
1:A:212:ASP:OD2	1:A:215:GLU:N	2.37	0.52
1:B:82:LEU:HD13	1:B:85:LEU:HD12	1.91	0.52
2:C:205:PRO:O	2:C:208:ILE:HG22	2.09	0.52
3:D:256:ASP:OD1	3:D:257:GLY:N	2.43	0.52
4:E:42:GLU:OE1	4:E:52:ARG:NH1	2.41	0.52
1:B:98:VAL:HG22	1:B:99:ILE:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:46:GLN:OE1	2:C:46:GLN:N	2.42	0.52
3:D:349:TYR:HD2	3:D:472:LEU:HD11	1.74	0.52
3:D:515:ARG:NH1	3:D:724:MET:SD	2.82	0.52
2:C:1103:VAL:O	2:C:1107:MET:N	2.41	0.52
3:D:536:LEU:O	3:D:540:GLY:N	2.43	0.52
3:D:1164:SER:O	3:D:1176:VAL:N	2.42	0.52
2:C:936:ARG:HG2	2:C:1042:LEU:HD23	1.91	0.52
2:C:1235:LEU:O	2:C:1238:LEU:HD21	2.10	0.52
3:D:142:GLU:N	3:D:142:GLU:OE1	2.43	0.52
2:C:1298:VAL:O	2:C:1302:THR:HG23	2.10	0.52
3:D:835:LEU:O	3:D:839:VAL:HG23	2.10	0.52
3:D:844:THR:CG2	3:D:858:VAL:HG11	2.39	0.51
1:A:179:PRO:HG2	1:A:180:VAL:HG23	1.92	0.51
2:C:320:ASP:OD1	2:C:321:LEU:N	2.42	0.51
2:C:851:THR:HG22	2:C:853:ASP:H	1.75	0.51
3:D:87:LYS:HB3	3:D:87:LYS:NZ	2.21	0.51
1:A:136:GLU:OE1	1:A:137:ASN:ND2	2.43	0.51
2:C:74:ARG:O	2:C:97:ARG:N	2.41	0.51
2:C:396:ASP:OD1	2:C:397:LEU:N	2.42	0.51
3:D:93:THR:HG22	3:D:94:GLN:N	2.25	0.51
3:D:910:ASN:OD1	3:D:911:LYS:N	2.44	0.51
2:C:1088:ASP:OD1	2:C:1092:THR:N	2.43	0.51
2:C:1120:ALA:HB1	2:C:1198:LEU:CD2	2.41	0.51
2:C:1211:ARG:C	2:C:1212:LEU:HD22	2.31	0.51
2:C:1324:ASN:OD1	2:C:1328:LYS:NZ	2.42	0.51
3:D:278:ARG:O	3:D:282:LEU:HD23	2.10	0.51
2:C:104:ILE:HG22	2:C:115:LYS:HD3	1.91	0.51
2:C:355:PRO:O	2:C:356:THR:HG23	2.10	0.51
2:C:445:ILE:O	2:C:451:ARG:NH1	2.44	0.51
2:C:658:GLN:N	2:C:659:GLN:OE1	2.44	0.51
3:D:955:LYS:O	3:D:992:LYS:NZ	2.43	0.51
2:C:270:THR:OG1	2:C:273:HIS:ND1	2.41	0.51
3:D:888:CYS:O	3:D:1258:ARG:NH2	2.43	0.51
2:C:104:ILE:HD12	2:C:116:ASP:HB3	1.93	0.51
2:C:217:THR:HA	2:C:220:ILE:HD12	1.92	0.51
3:D:1368:ASP:OD1	3:D:1371:ARG:NH1	2.43	0.51
5:F:192:ARG:O	5:F:196:VAL:HG23	2.11	0.51
2:C:1299:ASN:O	2:C:1302:THR:OG1	2.27	0.51
3:D:479:GLU:O	3:D:483:LEU:N	2.44	0.51
3:D:105:ILE:HD11	3:D:244:VAL:HG22	1.93	0.51
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1004:ALA:N	3:D:1017:VAL:O	2.43	0.51
1:B:155:ALA:N	1:B:174:ASP:OD1	2.36	0.50
2:C:398:SER:O	2:C:400:VAL:N	2.44	0.50
2:C:1278:LEU:HD13	2:C:1287:LEU:HD21	1.93	0.50
3:D:500:ILE:N	3:D:500:ILE:HD12	2.26	0.50
3:D:611:ILE:HB	3:D:612:LEU:HD22	1.94	0.50
1:B:210:THR:O	1:B:211:ILE:HD13	2.12	0.50
3:D:318:GLY:N	3:D:324:LEU:HD21	2.26	0.50
3:D:797:THR:O	3:D:801:VAL:HG23	2.12	0.50
2:C:866:ASP:OD1	2:C:870:ILE:N	2.43	0.50
1:B:74:VAL:HG12	1:B:76:GLU:N	2.27	0.50
2:C:772:SER:OG	2:C:775:GLU:OE1	2.28	0.50
2:C:1205:PRO:CG	2:C:1210:ILE:HD13	2.41	0.50
1:B:92:VAL:O	1:B:148:ARG:NH2	2.44	0.50
3:D:478:LEU:CB	4:E:20:VAL:HG13	2.41	0.50
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.93	0.50
1:B:79:LEU:O	1:B:83:LEU:HD23	2.12	0.50
2:C:230:PHE:CD1	2:C:237:LEU:HD11	2.46	0.50
3:D:973:LEU:HB3	3:D:1003:LEU:HD12	1.94	0.50
4:E:10:VAL:HG21	4:E:16:ARG:HD3	1.94	0.50
2:C:604:HIS:CB	2:C:606:LEU:HD21	2.42	0.50
3:D:743:MET:SD	3:D:745:GLY:N	2.85	0.50
3:D:1350:ASN:O	3:D:1354:GLY:N	2.45	0.50
1:B:202:VAL:O	1:B:203:ILE:HD13	2.12	0.49
2:C:241:LEU:HD23	2:C:277:LEU:HD21	1.93	0.49
3:D:1027:VAL:HG21	3:D:1122:ALA:HB3	1.94	0.49
5:F:2:ASN:OD1	5:F:13:LYS:NZ	2.41	0.49
2:C:1278:LEU:HD22	2:C:1287:LEU:CD1	2.43	0.49
3:D:283:LEU:HD13	3:D:283:LEU:O	2.12	0.49
3:D:505:ASP:O	3:D:508:LEU:N	2.45	0.49
1:A:22:THR:OG1	1:A:207:THR:O	2.24	0.49
3:D:532:GLU:N	3:D:532:GLU:OE1	2.45	0.49
3:D:1155:ILE:O	3:D:1210:ILE:N	2.42	0.49
3:D:1350:ASN:O	3:D:1355:ARG:N	2.46	0.49
5:F:174:LEU:HD22	5:F:177:ASN:HB2	1.93	0.49
2:C:699:LEU:HD23	2:C:1181:PRO:HB3	1.94	0.49
3:D:48:THR:O	3:D:50:LYS:N	2.45	0.49
3:D:1111:ASP:OD1	3:D:1112:GLY:N	2.45	0.49
1:A:72:GLU:O	1:A:74:VAL:HG23	2.13	0.49
2:C:417:SER:OG	2:C:418:GLY:N	2.46	0.49
2:C:462:ASN:O	2:C:466:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:759:SER:OG	2:C:763:THR:N	2.46	0.49
3:D:481:ARG:NE	4:E:47:THR:HG21	2.28	0.49
6:1:44:DG:N2	7:2:46:DT:O2	2.45	0.49
3:D:816:THR:O	3:D:860:ARG:NH2	2.40	0.49
5:F:163:ASP:OD1	5:F:164:HIS:N	2.45	0.49
2:C:207:THR:HA	2:C:210:LEU:HD23	1.95	0.49
2:C:714:VAL:O	2:C:767:GLN:NE2	2.45	0.49
3:D:620:PHE:CE2	3:D:624:ILE:HD11	2.47	0.49
3:D:951:GLN:OE1	3:D:1016:THR:OG1	2.13	0.49
2:C:843:THR:OG1	2:C:846:GLY:O	2.15	0.49
2:C:1277:ALA:O	2:C:1280:ALA:HB3	2.12	0.49
3:D:500:ILE:HG22	3:D:500:ILE:O	2.13	0.49
3:D:828:GLY:O	3:D:995:TYR:OH	2.28	0.49
5:F:155:ASP:HB2	5:F:159:LEU:HD12	1.95	0.49
2:C:20:GLN:OE1	2:C:22:LEU:N	2.40	0.48
3:D:956:GLY:N	3:D:1010:GLN:OE1	2.43	0.48
2:C:296:VAL:HG12	2:C:297:VAL:O	2.14	0.48
2:C:483:ASP:OD1	2:C:484:LEU:N	2.46	0.48
2:C:975:ILE:O	2:C:979:LEU:HD13	2.14	0.48
3:D:238:ILE:HD13	3:D:240:THR:HG23	1.95	0.48
3:D:481:ARG:HE	4:E:47:THR:HG21	1.78	0.48
2:C:398:SER:O	2:C:401:GLY:N	2.44	0.48
5:F:186:ILE:CD1	5:F:197:LEU:HD12	2.43	0.48
1:B:24:ALA:HB3	1:B:205:MET:SD	2.53	0.48
5:F:41:LEU:CD1	5:F:44:LEU:HD12	2.44	0.48
3:D:325:LYS:NZ	3:D:330:MET:SD	2.87	0.48
3:D:525:MET:H	3:D:548:VAL:HG13	1.78	0.48
2:C:1041:ASP:C	2:C:1042:LEU:HD22	2.34	0.48
1:A:172:LEU:HD23	1:A:172:LEU:H	1.79	0.48
2:C:400:VAL:HG22	2:C:584:TYR:HD1	1.78	0.48
2:C:768:MET:O	2:C:785:ASP:N	2.43	0.48
3:D:858:VAL:HG12	3:D:862:THR:CG2	2.44	0.48
2:C:1067:ALA:HB2	2:C:1073:LYS:HA	1.94	0.48
3:D:80:HIS:O	3:D:83:VAL:HG12	2.14	0.48
2:C:28:LEU:HD23	2:C:28:LEU:H	1.78	0.47
2:C:292:ILE:CD1	2:C:322:LEU:HD13	2.43	0.47
2:C:576:SER:OG	2:C:577:VAL:N	2.46	0.47
3:D:70:CYS:SG	3:D:74:LYS:N	2.85	0.47
3:D:1047:THR:HG22	3:D:1062:LEU:HG	1.96	0.47
7:2:53:DC:H2'	7:2:54:DT:H72	1.95	0.47
1:B:90:VAL:HA	1:B:123:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:111:GLU:O	2:C:113:THR:N	2.47	0.47
2:C:202:ARG:NH1	7:2:6:DC:OP1	2.48	0.47
3:D:1235:ASN:OD1	3:D:1236:GLU:N	2.47	0.47
4:E:19:LEU:CD1	4:E:54:ILE:HG21	2.44	0.47
2:C:306:THR:OG1	2:C:307:GLY:N	2.46	0.47
2:C:367:TYR:O	2:C:371:ARG:N	2.42	0.47
3:D:909:ILE:HG22	3:D:910:ASN:O	2.14	0.47
3:D:343:LEU:HD21	3:D:1352:ILE:HD11	1.94	0.47
3:D:545:HIS:O	3:D:545:HIS:ND1	2.47	0.47
3:D:1330:ARG:O	3:D:1333:THR:OG1	2.31	0.47
6:1:79:DG:H2''	6:1:80:DT:H71	1.95	0.47
2:C:1120:ALA:HB2	2:C:1199:LEU:HD21	1.96	0.47
3:D:479:GLU:HG3	4:E:20:VAL:HG11	1.95	0.47
3:D:1079:LYS:NZ	3:D:1087:ASP:OD1	2.27	0.47
4:E:6:VAL:HG12	4:E:6:VAL:O	2.15	0.47
2:C:617:ALA:HB3	2:C:653:MET:HG3	1.96	0.47
2:C:739:ASP:OD1	2:C:740:GLU:N	2.47	0.47
3:D:796:LEU:HD13	3:D:797:THR:N	2.29	0.47
3:D:1342:ASP:OD1	3:D:1343:GLU:N	2.45	0.47
1:A:89:ALA:HB1	1:A:124:VAL:CG2	2.45	0.47
2:C:660:VAL:HG13	2:C:661:VAL:HG13	1.96	0.47
2:C:667:LEU:HD22	2:C:705:GLU:OE2	2.15	0.47
3:D:621:ALA:HA	3:D:624:ILE:HD12	1.96	0.47
3:D:1207:GLY:O	3:D:1224:ARG:NH2	2.48	0.47
5:F:25:ARG:O	5:F:28:ALA:N	2.48	0.47
3:D:883:ARG:NH1	3:D:898:CYS:SG	2.88	0.46
3:D:837:ASP:HA	3:D:840:LEU:HD12	1.97	0.46
3:D:960:LEU:HD11	3:D:982:LEU:HD12	1.97	0.46
2:C:383:SER:O	2:C:387:ASN:ND2	2.48	0.46
3:D:597:GLY:O	3:D:601:ILE:HD12	2.15	0.46
5:F:192:ARG:O	5:F:196:VAL:N	2.42	0.46
2:C:145:ILE:HG22	2:C:512:SER:HB2	1.96	0.46
2:C:370:MET:HG2	2:C:384:LEU:HD21	1.98	0.46
2:C:1205:PRO:HG3	2:C:1210:ILE:HD13	1.98	0.46
1:B:91:ARG:HD2	1:B:210:THR:HG23	1.98	0.46
2:C:129:LEU:HD23	2:C:129:LEU:H	1.81	0.46
3:D:309:ASN:OD1	3:D:316:ILE:HD12	2.16	0.46
3:D:332:LYS:O	3:D:336:GLY:N	2.48	0.46
1:A:220:ALA:HA	1:A:223:ILE:HD12	1.97	0.46
3:D:574:VAL:O	3:D:577:ALA:HB3	2.15	0.46
3:D:824:PRO:HB2	3:D:826:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1047:THR:HG21	3:D:1049:GLN:NE2	2.30	0.46
3:D:499:ILE:N	3:D:500:ILE:HD12	2.31	0.46
2:C:208:ILE:CG2	2:C:209:ILE:HD12	2.45	0.46
3:D:926:PRO:O	3:D:929:GLN:N	2.47	0.46
2:C:402:ARG:NH2	2:C:419:ILE:O	2.48	0.45
2:C:618:GLN:NE2	2:C:620:ASN:OD1	2.47	0.45
3:D:575:GLY:O	3:D:579:LEU:HD13	2.15	0.45
1:A:46:ILE:HD11	1:A:223:ILE:HG21	1.97	0.45
1:A:92:VAL:O	1:A:148:ARG:NH2	2.44	0.45
3:D:59:ALA:O	3:D:63:GLY:N	2.48	0.45
3:D:347:VAL:HG12	3:D:348:ASP:O	2.17	0.45
3:D:957:SER:N	3:D:985:ILE:O	2.49	0.45
5:F:142:GLN:C	5:F:143:LEU:HD22	2.37	0.45
2:C:1049:ILE:O	2:C:1049:ILE:HD12	2.17	0.45
3:D:132:LEU:O	3:D:135:ILE:N	2.47	0.45
3:D:1361:THR:CG2	4:E:21:LEU:HD21	2.47	0.45
6:1:55:DC:H42	7:2:34:DG:H1	1.63	0.45
2:C:296:VAL:HG13	2:C:315:MET:N	2.32	0.45
2:C:371:ARG:HD2	2:C:384:LEU:HD22	1.99	0.45
3:D:143:SER:N	3:D:180:MET:SD	2.90	0.45
3:D:493:PRO:HA	3:D:903:LEU:HB2	1.98	0.45
3:D:1273:ASP:OD1	3:D:1274:PHE:N	2.46	0.45
2:C:39:ILE:HD12	2:C:40:GLU:N	2.31	0.45
2:C:230:PHE:HB3	2:C:237:LEU:HD11	1.97	0.45
1:A:84:ASN:O	1:A:128:HIS:NE2	2.47	0.45
2:C:1292:THR:O	2:C:1297:ASP:N	2.44	0.45
3:D:51:PRO:HG2	3:D:59:ALA:HB2	1.99	0.45
3:D:1345:ARG:N	3:D:1349:GLU:OE1	2.42	0.45
1:A:9:LEU:HD21	1:A:30:PRO:HG2	1.98	0.45
2:C:145:ILE:HG22	2:C:512:SER:CB	2.47	0.45
2:C:1278:LEU:HD13	2:C:1287:LEU:CD2	2.47	0.45
3:D:597:GLY:O	3:D:600:ALA:N	2.50	0.45
3:D:858:VAL:HG12	3:D:862:THR:OG1	2.16	0.45
2:C:56:VAL:HG12	2:C:56:VAL:O	2.17	0.45
3:D:517:CYS:SG	3:D:518:VAL:N	2.89	0.45
3:D:620:PHE:CD2	3:D:624:ILE:HD11	2.52	0.45
2:C:897:PRO:HA	2:C:900:LYS:HB3	1.99	0.45
2:C:1225:VAL:HG13	3:D:638:SER:OG	2.17	0.45
3:D:22:ILE:HD11	3:D:1319:PHE:CE2	2.52	0.45
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.99	0.44
2:C:1268:GLN:O	3:D:347:VAL:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:253:PHE:HZ	2:C:287:VAL:HG12	1.82	0.44
3:D:447:ILE:HG22	3:D:448:GLN:O	2.16	0.44
3:D:997:VAL:HG12	3:D:1001:ALA:HB3	1.98	0.44
3:D:1320:ILE:HD12	3:D:1342:ASP:OD2	2.17	0.44
2:C:127:ILE:HD12	2:C:128:PRO:O	2.17	0.44
2:C:189:ASP:OD1	2:C:192:ASP:N	2.50	0.44
3:D:62:PHE:O	3:D:78:LEU:HD13	2.17	0.44
3:D:292:VAL:HG12	3:D:296:LYS:NZ	2.31	0.44
3:D:356:THR:HG22	3:D:447:ILE:O	2.17	0.44
3:D:485:MET:SD	3:D:487:THR:OG1	2.74	0.44
3:D:515:ARG:O	3:D:573:THR:HG21	2.17	0.44
2:C:929:ILE:HD12	2:C:930:ASP:HB2	2.00	0.44
3:D:342:LEU:HD21	3:D:1352:ILE:HG23	1.98	0.44
3:D:134:ASP:HB3	3:D:159:ILE:HD11	1.98	0.44
3:D:278:ARG:NH2	5:F:43:ASP:OD1	2.51	0.44
3:D:846:GLU:O	3:D:848:VAL:HG13	2.17	0.44
3:D:1075:ARG:HE	3:D:1165:PHE:HB2	1.83	0.44
5:F:95:ARG:NH2	7:2:27:DC:OP2	2.50	0.44
2:C:180:ARG:O	2:C:396:ASP:N	2.50	0.44
2:C:804:PHE:CB	2:C:1098:LEU:HD22	2.47	0.44
3:D:85:CYS:O	3:D:89:GLY:N	2.51	0.44
2:C:43:PRO:O	2:C:54:ARG:NH2	2.51	0.44
1:B:185:TYR:HB2	1:B:201:LEU:HD11	2.00	0.44
2:C:689:ALA:HA	2:C:1235:LEU:HD23	1.99	0.44
3:D:214:ARG:HE	3:D:1275:LEU:HD21	1.83	0.44
3:D:165:TYR:CE2	3:D:169:LEU:HD12	2.53	0.44
1:B:199:ASP:OD1	1:B:199:ASP:N	2.47	0.43
2:C:246:LEU:O	2:C:274:ILE:HD11	2.18	0.43
2:C:138:ILE:HG22	2:C:139:ASN:OD1	2.17	0.43
2:C:671:LEU:HD12	2:C:1187:PHE:CZ	2.53	0.43
2:C:723:VAL:O	2:C:734:ILE:HD12	2.17	0.43
2:C:958:LYS:O	2:C:961:SER:OG	2.33	0.43
3:D:337:ARG:O	3:D:342:LEU:N	2.50	0.43
3:D:367:GLY:O	3:D:447:ILE:HD12	2.18	0.43
5:F:26:HIS:HB3	6:1:68:DG:C2	2.54	0.43
2:C:572:ILE:HD12	2:C:572:ILE:O	2.18	0.43
3:D:975:ILE:O	3:D:1000:GLY:N	2.45	0.43
1:A:43:LEU:HA	1:A:46:ILE:HG22	2.00	0.43
2:C:39:ILE:HD12	2:C:40:GLU:HA	2.01	0.43
2:C:869:GLY:C	2:C:870:ILE:HD12	2.39	0.43
2:C:1088:ASP:OD2	2:C:1092:THR:OG1	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:220:ARG:O	3:D:224:LEU:HD23	2.18	0.43
1:B:205:MET:CE	1:B:217:ILE:HD11	2.48	0.43
2:C:253:PHE:CZ	2:C:287:VAL:HG12	2.53	0.43
3:D:1267:VAL:HG23	3:D:1302:TYR:CA	2.49	0.43
3:D:1292:LEU:O	3:D:1295:ASN:N	2.47	0.43
2:C:622:ASN:O	2:C:630:VAL:HG23	2.19	0.43
3:D:508:LEU:O	3:D:508:LEU:HD23	2.19	0.43
3:D:706:VAL:O	3:D:706:VAL:HG23	2.19	0.43
2:C:292:ILE:O	2:C:295:LYS:N	2.45	0.43
3:D:483:LEU:HD21	4:E:16:ARG:HB3	2.01	0.43
3:D:597:GLY:O	3:D:600:ALA:HB3	2.19	0.43
3:D:623:GLN:O	3:D:627:THR:HG22	2.17	0.43
3:D:1040:MET:HE2	3:D:1046:ILE:HG21	2.01	0.43
1:B:95:LYS:HZ1	1:B:98:VAL:HG23	1.83	0.42
2:C:794:LEU:HD13	2:C:795:ALA:N	2.34	0.42
3:D:1080:ILE:HD11	3:D:1121:LEU:HD11	2.00	0.42
1:B:110:VAL:O	1:B:130:ILE:HD12	2.19	0.42
2:C:180:ARG:HE	2:C:181:GLY:H	1.68	0.42
2:C:701:GLY:O	2:C:1184:THR:N	2.47	0.42
2:C:1278:LEU:HD11	2:C:1286:THR:HG21	2.01	0.42
2:C:658:GLN:O	2:C:660:VAL:N	2.52	0.42
2:C:818:VAL:HG12	2:C:1096:ILE:CD1	2.49	0.42
2:C:1340:GLU:OE1	3:D:1341:ARG:NH2	2.46	0.42
3:D:120:LEU:HD12	3:D:1330:ARG:NH1	2.34	0.42
3:D:602:SER:O	3:D:606:ASN:ND2	2.52	0.42
3:D:1090:ILE:HD12	3:D:1095:MET:SD	2.59	0.42
1:A:140:ILE:HD11	1:A:142:MET:CE	2.49	0.42
2:C:177:ILE:HG23	2:C:183:TRP:NE1	2.33	0.42
2:C:561:ILE:HD11	2:C:680:LEU:N	2.35	0.42
2:C:1197:GLU:O	2:C:1200:LYS:HG2	2.19	0.42
3:D:194:LEU:HD22	3:D:224:LEU:CD1	2.49	0.42
3:D:858:VAL:HG12	3:D:862:THR:HG23	2.00	0.42
3:D:1045:THR:O	3:D:1067:ARG:NE	2.49	0.42
2:C:398:SER:OG	2:C:398:SER:O	2.38	0.42
2:C:700:VAL:O	2:C:700:VAL:HG23	2.19	0.42
2:C:1117:LEU:HA	2:C:1120:ALA:HB3	2.02	0.42
3:D:397:ALA:O	3:D:401:VAL:HG23	2.20	0.42
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.85	0.42
3:D:478:LEU:CD2	4:E:47:THR:HG23	2.49	0.42
1:A:13:LEU:HD23	1:A:13:LEU:H	1.85	0.42
2:C:342:ASP:OD1	2:C:439:LYS:NZ	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1154:ALA:O	3:D:1156:LEU:HD12	2.19	0.42
3:D:1319:PHE:O	3:D:1323:ALA:N	2.53	0.42
1:B:101:THR:HG22	1:B:143:ARG:HG3	2.02	0.42
3:D:87:LYS:NZ	6:1:47:DT:O3'	2.53	0.42
3:D:1120:THR:HG21	3:D:1123:ARG:HH11	1.85	0.42
1:B:15:ASP:OD1	1:B:16:ILE:N	2.53	0.42
2:C:310:ILE:HG23	2:C:324:LYS:HD3	2.01	0.42
2:C:714:VAL:HG13	2:C:715:THR:HG23	2.01	0.42
3:D:41:PRO:O	3:D:56:LEU:HD23	2.20	0.42
3:D:120:LEU:HD12	3:D:1330:ARG:CZ	2.50	0.42
3:D:259:ARG:CZ	5:F:140:ASN:HB3	2.50	0.42
3:D:867:GLN:OE1	3:D:871:LEU:HD12	2.19	0.42
3:D:1049:GLN:HB2	3:D:1060:VAL:HG21	2.00	0.42
2:C:769:PRO:HA	2:C:784:ALA:HA	2.02	0.42
3:D:559:ALA:O	3:D:561:GLY:N	2.52	0.42
3:D:601:ILE:HD12	3:D:601:ILE:H	1.85	0.42
3:D:1316:THR:HG22	3:D:1317:GLU:N	2.35	0.42
3:D:504:GLN:HA	3:D:730:ALA:HB1	2.02	0.42
3:D:1019:ASN:OD1	3:D:1020:TRP:N	2.53	0.42
3:D:1157:ALA:N	3:D:1208:ASP:O	2.45	0.42
3:D:1163:VAL:HG12	3:D:1202:GLU:O	2.19	0.42
2:C:200:ARG:NH2	6:1:75:DA:N3	2.67	0.41
2:C:338:THR:HG23	2:C:345:PRO:HD3	2.02	0.41
2:C:801:ARG:HA	2:C:1229:TYR:CD1	2.54	0.41
2:C:805:MET:SD	2:C:805:MET:N	2.93	0.41
2:C:1334:GLY:O	2:C:1335:ILE:HD13	2.20	0.41
4:E:60:ASN:OD1	4:E:61:ASN:N	2.52	0.41
2:C:611:GLU:OE1	2:C:611:GLU:N	2.48	0.41
2:C:1298:VAL:O	2:C:1301:ARG:HG2	2.20	0.41
1:B:28:LEU:CD2	1:B:31:LEU:HD11	2.51	0.41
1:B:151:GLY:O	1:B:177:TYR:N	2.53	0.41
2:C:718:ALA:HB3	2:C:780:GLY:N	2.35	0.41
2:C:818:VAL:O	2:C:1080:ASN:N	2.52	0.41
2:C:819:SER:OG	2:C:820:GLU:N	2.54	0.41
5:F:142:GLN:O	5:F:143:LEU:HD22	2.20	0.41
6:1:57:DT:O4	7:2:31:DA:N6	2.54	0.41
3:D:314:ARG:HA	3:D:314:ARG:NE	2.35	0.41
3:D:346:ARG:NH1	7:2:15:DT:OP2	2.54	0.41
3:D:533:ALA:HB1	3:D:574:VAL:CG1	2.50	0.41
3:D:1090:ILE:HD12	3:D:1095:MET:HB3	2.01	0.41
3:D:518:VAL:N	3:D:716:GLN:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:746:LEU:HD13	3:D:754:ILE:HG23	2.02	0.41
2:C:1094:VAL:HG12	2:C:1095:ASP:N	2.35	0.41
3:D:507:VAL:HG13	3:D:508:LEU:N	2.36	0.41
4:E:10:VAL:HG11	4:E:16:ARG:NH1	2.35	0.41
5:F:151:GLU:O	5:F:151:GLU:CD	2.59	0.41
2:C:693:LEU:HD23	2:C:694:ARG:N	2.36	0.41
2:C:961:SER:HG	2:C:962:GLU:H	1.69	0.41
2:C:1151:LEU:HD11	2:C:1197:GLU:CG	2.51	0.41
3:D:61:ILE:HG22	3:D:98:ARG:NH1	2.35	0.41
3:D:741:ALA:O	3:D:762:ASN:ND2	2.53	0.41
3:D:1333:THR:OG1	3:D:1334:GLU:N	2.53	0.41
2:C:671:LEU:HD13	2:C:671:LEU:O	2.21	0.41
3:D:868:TRP:CE3	3:D:871:LEU:HD13	2.56	0.41
1:A:118:ASP:OD1	1:A:119:GLY:N	2.54	0.41
2:C:979:LEU:HD11	2:C:1014:LEU:HD12	2.03	0.41
3:D:55:GLY:N	3:D:58:CYS:SG	2.86	0.41
3:D:703:THR:HG23	3:D:703:THR:O	2.21	0.41
7:2:31:DA:H2''	7:2:32:DA:C8	2.55	0.41
1:B:113:ALA:N	1:B:126:PRO:O	2.54	0.41
2:C:563:THR:O	2:C:680:LEU:HD21	2.20	0.41
2:C:901:LEU:HD21	5:F:201:TYR:CZ	2.56	0.41
2:C:1232:MET:N	2:C:1232:MET:SD	2.94	0.41
3:D:152:THR:HG22	3:D:152:THR:O	2.20	0.41
3:D:169:LEU:O	3:D:173:GLY:N	2.54	0.41
3:D:842:ARG:C	3:D:864:LEU:HD12	2.42	0.41
7:2:49:DA:C2'	7:2:50:DT:H72	2.51	0.41
1:B:9:LEU:HD21	1:B:30:PRO:HG2	2.02	0.40
1:B:86:LYS:HD3	1:B:173:VAL:HG11	2.03	0.40
2:C:1205:PRO:HG2	2:C:1210:ILE:HD13	2.02	0.40
3:D:214:ARG:HE	3:D:1275:LEU:CD2	2.34	0.40
3:D:425:ARG:NH2	8:3:3:C:O2'	2.54	0.40
3:D:460:ASP:OD1	3:D:460:ASP:N	2.53	0.40
3:D:478:LEU:HD12	4:E:24:ALA:HB2	2.03	0.40
3:D:1108:GLN:N	3:D:1108:GLN:OE1	2.54	0.40
3:D:1248:ILE:HD12	3:D:1249:ASN:C	2.42	0.40
2:C:623:LEU:HD13	2:C:629:PHE:HA	2.03	0.40
2:C:871:VAL:HG21	2:C:883:LEU:HD13	2.03	0.40
3:D:98:ARG:CB	3:D:101:ARG:HD2	2.51	0.40
6:1:39:DA:H2'	6:1:40:DT:H71	2.02	0.40
1:B:153:VAL:HB	1:B:175:ALA:HB3	2.03	0.40
2:C:878:THR:N	2:C:881:ASP:OD2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1160:ASP:OD1	2:C:1161:LEU:N	2.47	0.40
3:D:144:TYR:N	3:D:160:LEU:O	2.55	0.40
3:D:1295:ASN:OD1	3:D:1296:GLY:N	2.55	0.40
2:C:158:ASP:OD1	2:C:158:ASP:N	2.52	0.40
2:C:247:ARG:HA	2:C:274:ILE:HD11	2.03	0.40
2:C:857:VAL:CG1	2:C:862:LEU:HD11	2.51	0.40
2:C:1278:LEU:HD11	2:C:1286:THR:CG2	2.51	0.40
3:D:147:ILE:HD11	3:D:179:LYS:HG3	2.02	0.40
3:D:160:LEU:HD13	3:D:165:TYR:HD1	1.87	0.40
3:D:349:TYR:CD2	3:D:472:LEU:HD11	2.54	0.40
3:D:490:ILE:O	3:D:500:ILE:HD11	2.20	0.40
3:D:821:MET:HG2	3:D:823:THR:HG23	2.03	0.40
6:1:45:DT:H3'	6:1:46:DT:H72	2.03	0.40
2:C:835:GLU:O	2:C:836:LEU:HD23	2.22	0.40
3:D:960:LEU:HD11	3:D:982:LEU:CD1	2.52	0.40
3:D:1104:LYS:CB	3:D:1124:ILE:HG23	2.51	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%)	210 (92%)	18 (8%)	0	100	100
1	B	226/329 (69%)	213 (94%)	13 (6%)	0	100	100
2	C	1338/1342 (100%)	1205 (90%)	129 (10%)	4 (0%)	41	75
3	D	1331/1407 (95%)	1168 (88%)	161 (12%)	2 (0%)	47	79
4	E	77/91 (85%)	72 (94%)	5 (6%)	0	100	100
5	F	237/247 (96%)	201 (85%)	30 (13%)	6 (2%)	5	36
All	All	3437/3745 (92%)	3069 (89%)	356 (10%)	12 (0%)	44	75

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	33	VAL
2	C	399	ALA
2	C	659	GLN
5	F	34	ARG
5	F	117	GLU
5	F	150	ARG
2	C	57	PHE
2	C	819	SER
3	D	99	ARG
3	D	883	ARG
5	F	151	GLU
5	F	125	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/286 (69%)	195 (98%)	3 (2%)	65	80
1	B	196/286 (68%)	191 (97%)	5 (3%)	46	68
2	C	1155/1157 (100%)	1145 (99%)	10 (1%)	78	88
3	D	1120/1168 (96%)	1100 (98%)	20 (2%)	59	77
4	E	67/75 (89%)	67 (100%)	0	100	100
5	F	208/216 (96%)	206 (99%)	2 (1%)	76	86
All	All	2944/3188 (92%)	2904 (99%)	40 (1%)	68	81

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	51	MET
1	A	186	ASN
1	B	142	MET
1	B	143	ARG

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Mol	Chain	Res	Type
1	B	158	ARG
1	B	186	ASN
1	B	218	ARG
2	C	200	ARG
2	C	283	LYS
2	C	332	ARG
2	C	465	ARG
2	C	752	ASN
2	C	796	LEU
2	C	1009	ASN
2	C	1022	LYS
2	C	1129	ASN
2	C	1246	ARG
3	D	50	LYS
3	D	87	LYS
3	D	214	ARG
3	D	215	LYS
3	D	334	LYS
3	D	341	ASN
3	D	345	LYS
3	D	399	LYS
3	D	424	ASN
3	D	458	ASN
3	D	464	ASP
3	D	560	ASN
3	D	610	ARG
3	D	625	MET
3	D	796	LEU
3	D	798	ARG
3	D	834	PRO
3	D	836	ARG
3	D	1249	ASN
3	D	1289	ASN
5	F	13	LYS
5	F	192	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	137	ASN
1	A	186	ASN

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Mol	Chain	Res	Type
1	B	41	ASN
1	B	127	GLN
1	B	186	ASN
2	C	36	GLN
2	C	387	ASN
2	C	437	ASN
2	C	752	ASN
2	C	761	GLN
2	C	808	ASN
2	C	1017	GLN
3	D	424	ASN
3	D	450	HIS
3	D	458	ASN
3	D	560	ASN
4	E	15	ASN
5	F	14	HIS
5	F	32	GLN
5	F	63	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	3	1/3 (33%)	1 (100%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	3	3	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

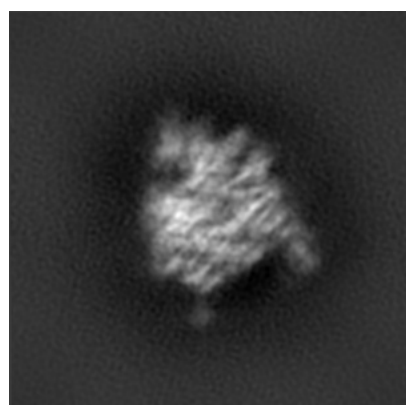
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20395. These allow visual inspection of the internal detail of the map and identification of artifacts.

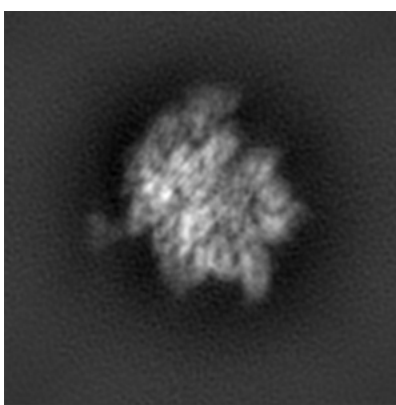
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

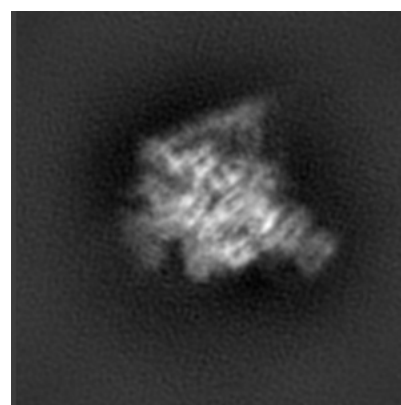
6.1.1 Primary map



X



Y

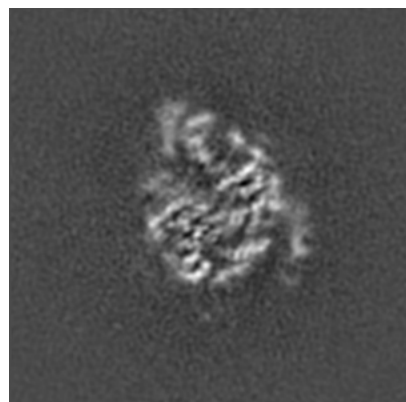


Z

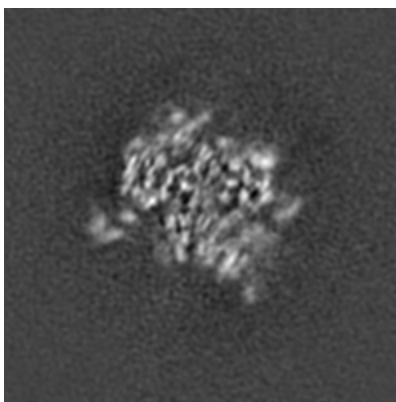
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

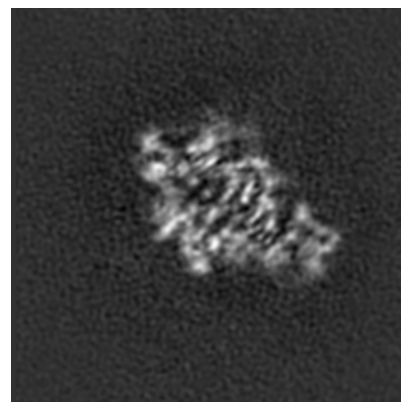
6.2.1 Primary map



X Index: 162



Y Index: 162

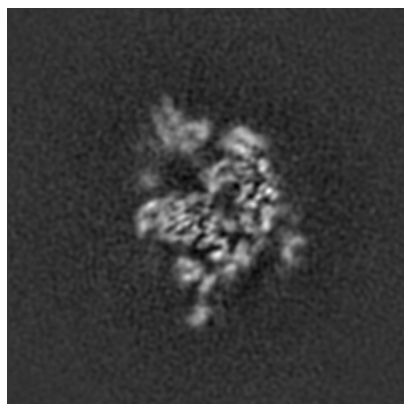


Z Index: 162

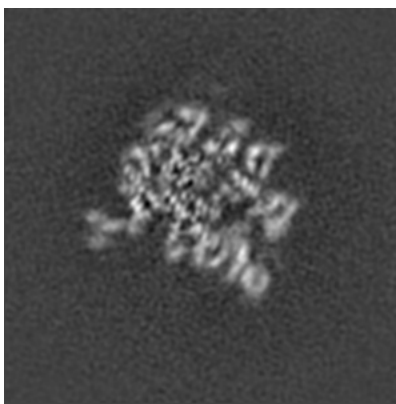
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

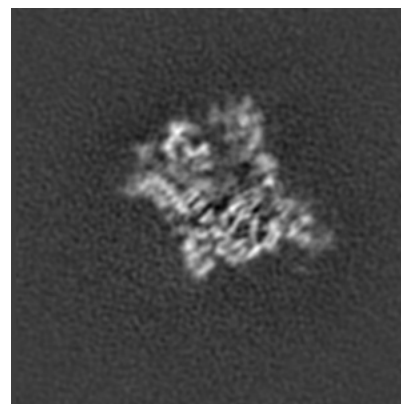
6.3.1 Primary map



X Index: 154



Y Index: 153

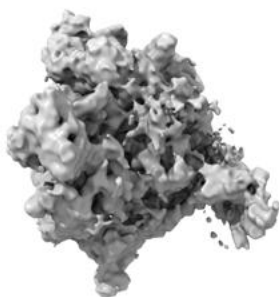


Z Index: 146

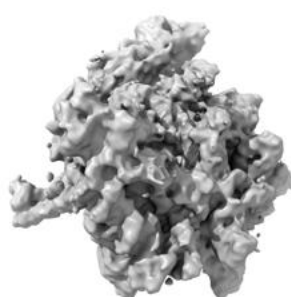
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

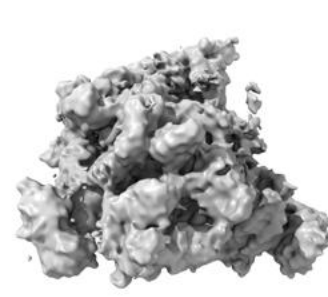
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

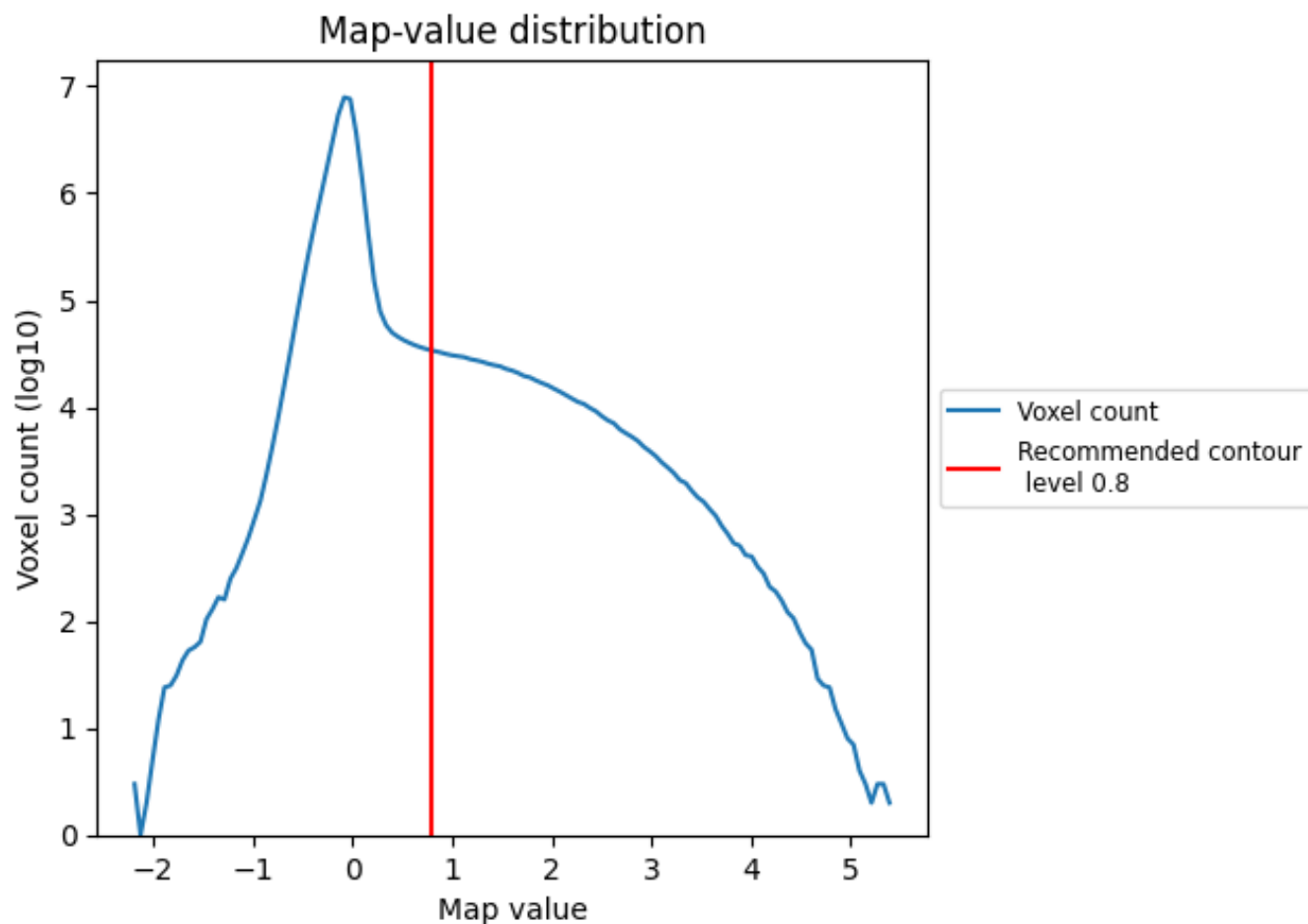
6.5 Mask visualisation

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

7 Map analysis [i](#)

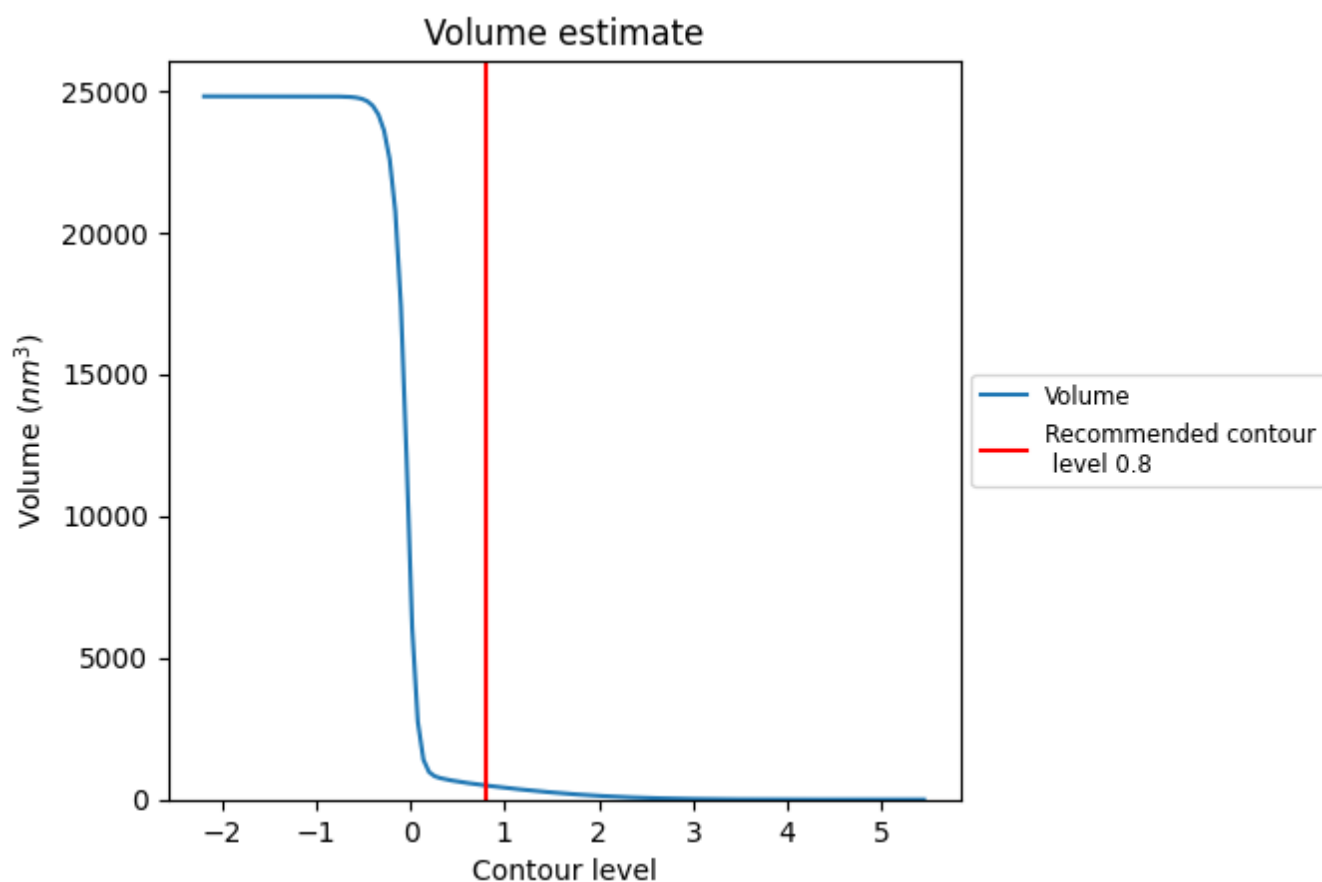
This section contains the results of statistical analysis of the map.

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.

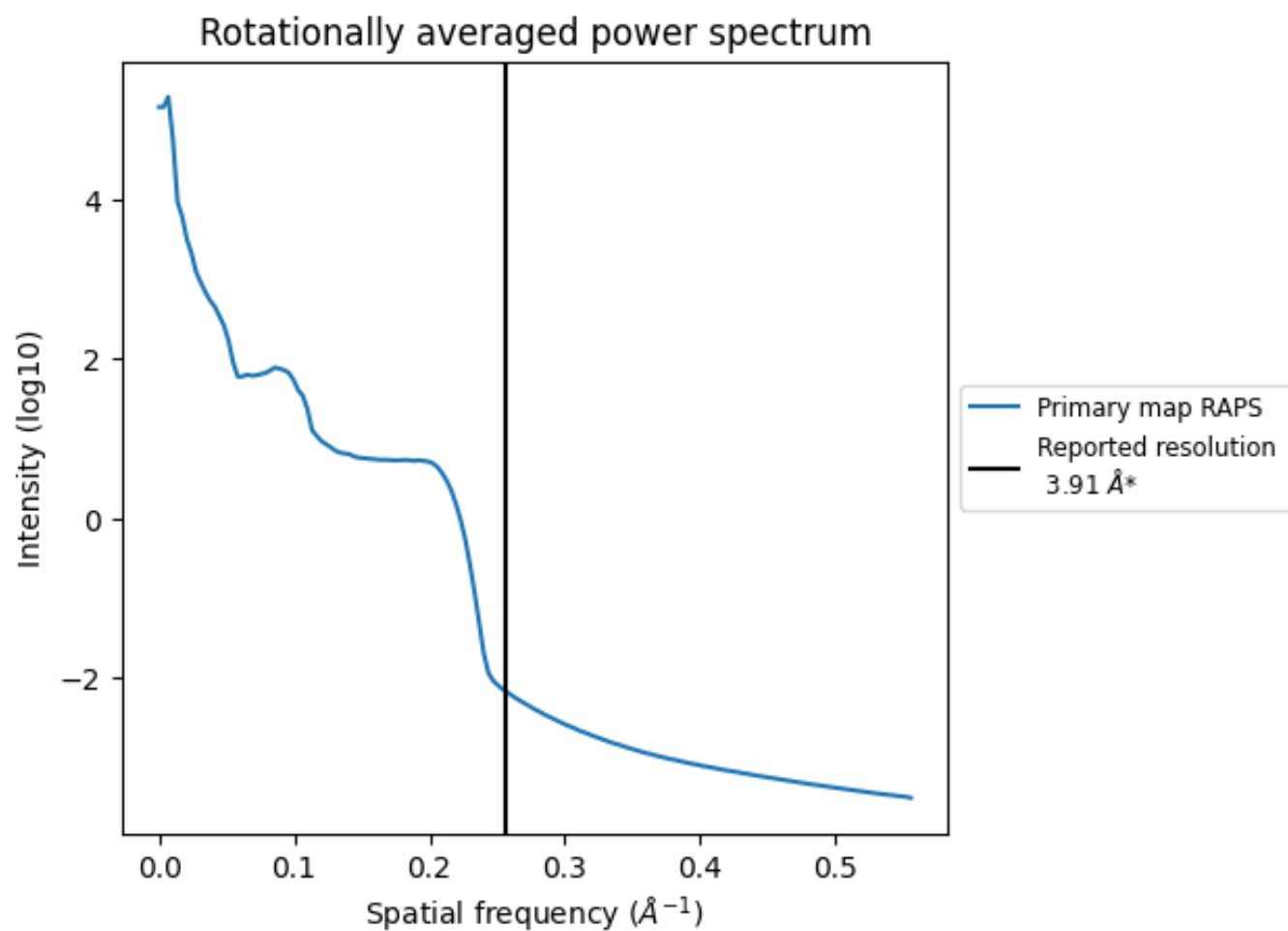
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 499 nm³; this corresponds to an approximate mass of 450 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 0.256 \AA^{-1}

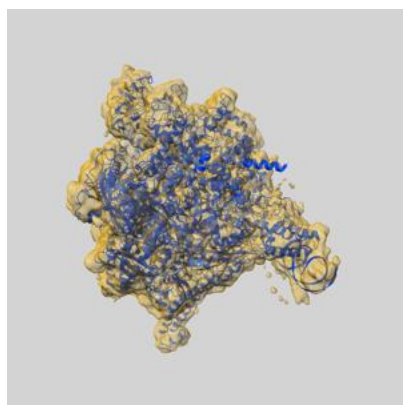
8 Fourier-Shell correlation ⓘ

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

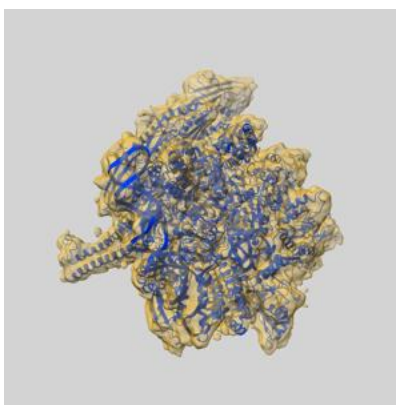
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20395 and PDB model 6PMJ. Per-residue inclusion information can be found in section 3 on page 6.

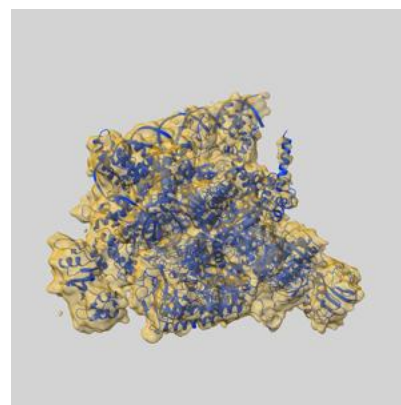
9.1 Map-model overlay [i](#)



X



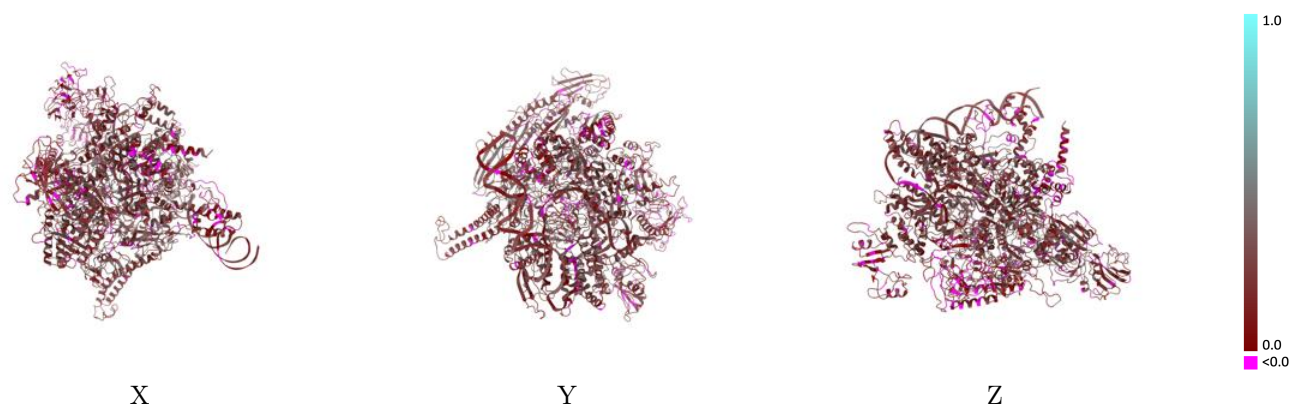
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 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](#)



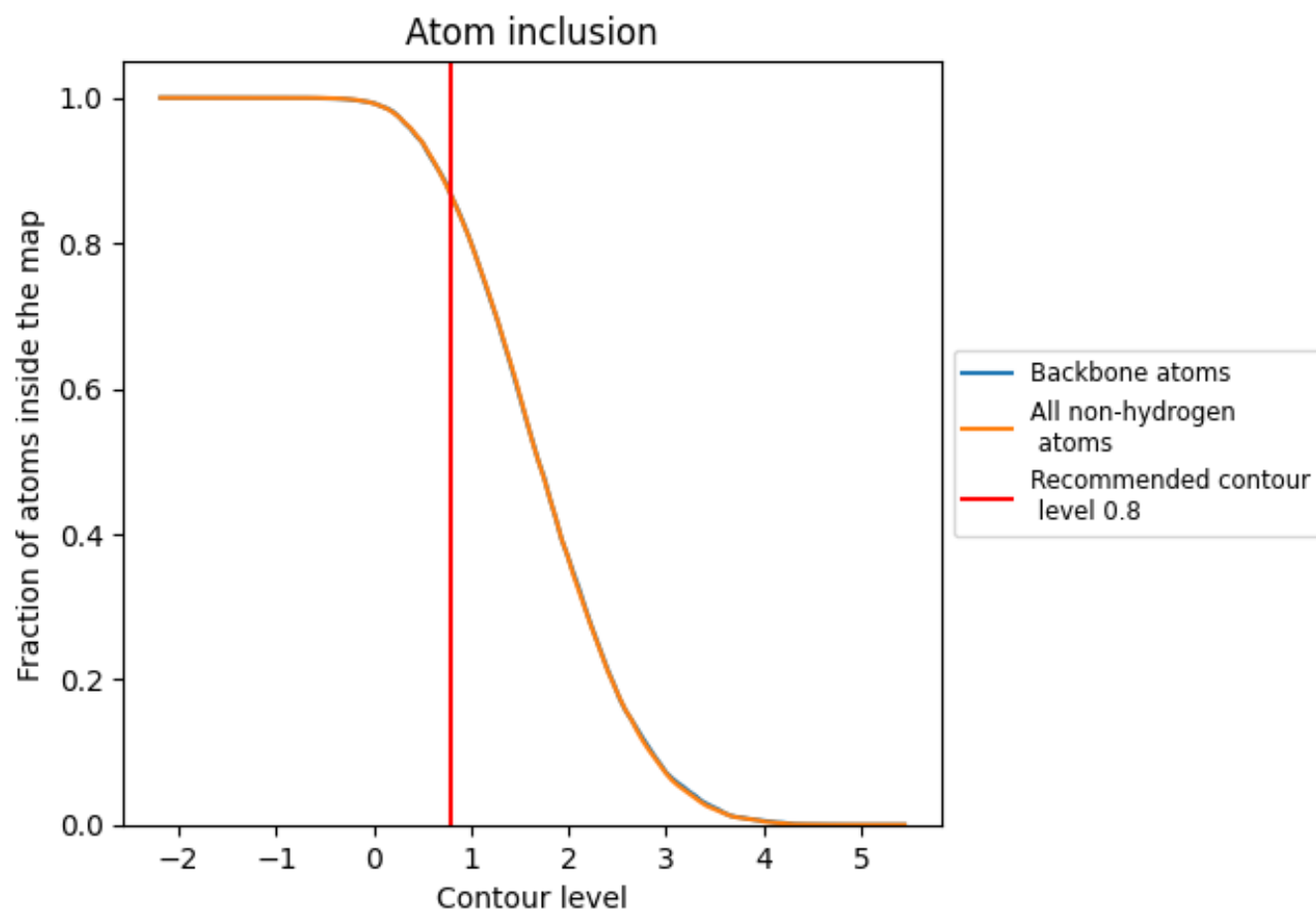
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 86% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8646</div>	<div><div></div>0.2070</div>
1	<div><div></div>0.8492</div>	<div><div></div>0.1720</div>
2	<div><div></div>0.8397</div>	<div><div></div>0.1760</div>
3	<div><div></div>0.8630</div>	<div><div></div>0.2650</div>
A	<div><div></div>0.9193</div>	<div><div></div>0.2470</div>
B	<div><div></div>0.8769</div>	<div><div></div>0.1840</div>
C	<div><div></div>0.9102</div>	<div><div></div>0.2350</div>
D	<div><div></div>0.8669</div>	<div><div></div>0.1970</div>
E	<div><div></div>0.3961</div>	<div><div></div>0.0520</div>
F	<div><div></div>0.8300</div>	<div><div></div>0.1790</div>

1.0

0.0

<0.0