



Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 06:44 AM EST

PDB ID : 6PB5
EMDB ID : EMD-20287
Title : The E. coli class-II CAP-dependent transcription activation complex at the state 1 architecture
Authors : Liu, B.; Shi, W.
Deposited on : 2019-06-13
Resolution : 4.52 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
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

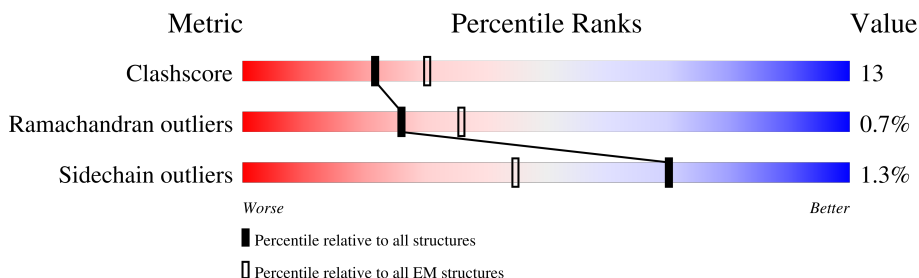
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.52 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
2	C	1342	
3	D	1407	
4	E	91	
5	F	628	
6	G	210	
6	H	210	

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Mol	Chain	Length	Quality of chain
7	1	78	<div><div>24%</div><div>78%</div><div>15%</div><div>6%</div></div>
8	2	78	<div><div>28%</div><div>85%</div><div>15%</div></div>

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 69718 atoms, of which 34341 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	1334	Total	C	H	N	O	S	0	0
			21054	6603	10532	1831	2045	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
			21012	6531	10616	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 RpoD.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	482	Total	C	H	N	O	S	0	0
			7892	2449	3975	700	745	23		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	expression tag	UNP P00579

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-13	ARG	-	expression tag	UNP P00579
F	-12	GLY	-	expression tag	UNP P00579
F	-11	SER	-	expression tag	UNP P00579
F	-10	HIS	-	expression tag	UNP P00579
F	-9	HIS	-	expression tag	UNP P00579
F	-8	HIS	-	expression tag	UNP P00579
F	-7	HIS	-	expression tag	UNP P00579
F	-6	HIS	-	expression tag	UNP P00579
F	-5	HIS	-	expression tag	UNP P00579
F	-4	THR	-	expression tag	UNP P00579
F	-3	ASP	-	expression tag	UNP P00579
F	-2	GLN	-	expression tag	UNP P00579
F	-1	PHE	-	expression tag	UNP P00579
F	0	THR	-	expression tag	UNP P00579

- Molecule 6 is a protein called cAMP-activated global transcriptional regulator CRP.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	G	197	Total	C	H	N	O	S	0	0
			3154	986	1598	273	288	9		
6	H	197	Total	C	H	N	O	S	0	0
			3155	986	1599	273	288	9		

- Molecule 7 is a DNA chain called SYNTHETIC NONTEMPLATE STRAND DNA (78-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
7	1	78	Total	C	H	N	O	P	0	0
			2480	765	889	264	484	78		

- Molecule 8 is a DNA chain called SYNTHETIC TEMPLATE STRAND DNA (78-MER).

Mol	Chain	Residues	Atoms						AltConf	Trace
8	2	78	Total	C	H	N	O	P	0	0
			2486	767	874	313	454	78		

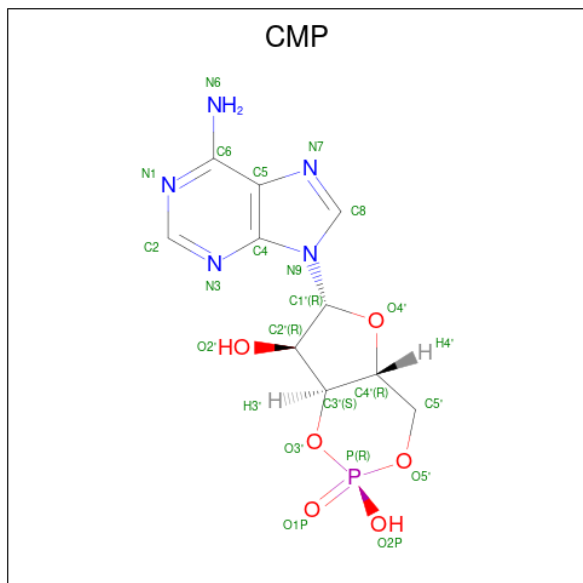
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

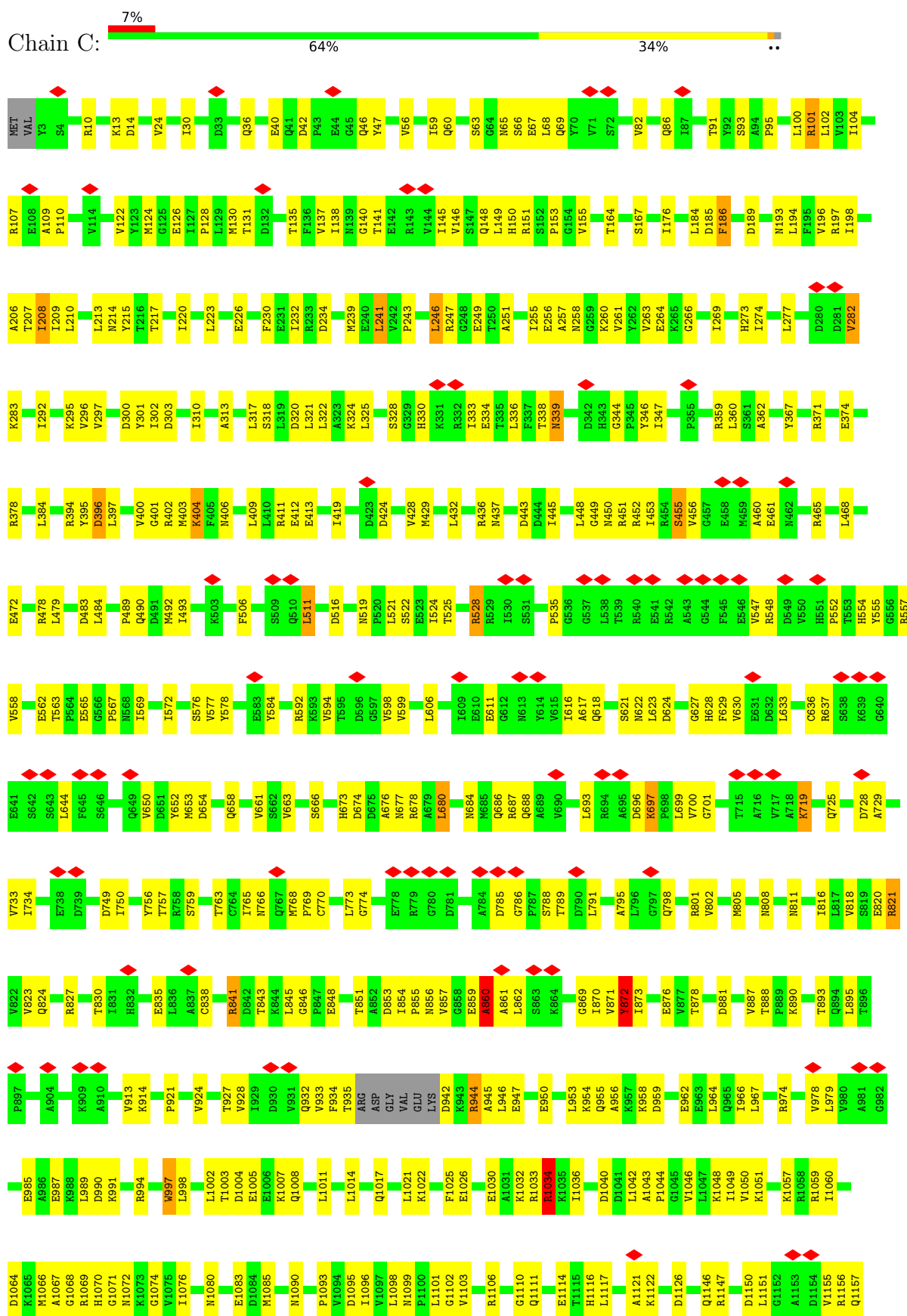
- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

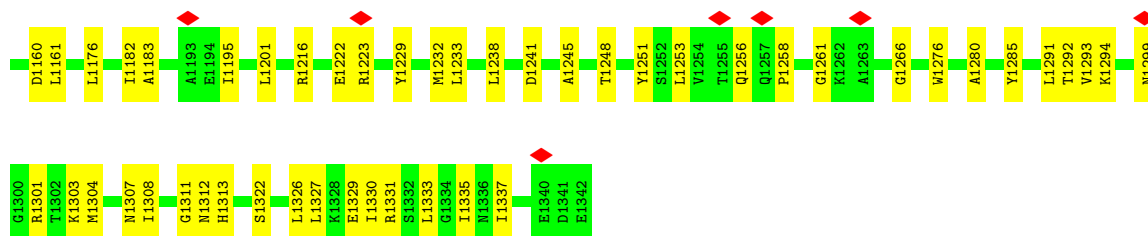
Mol	Chain	Residues	Atoms		AltConf
10	D	1	Total	Mg	0
			1	1	

- Molecule 11 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C₁₀H₁₂N₅O₆P) (labeled as "Ligand of Interest" by depositor).



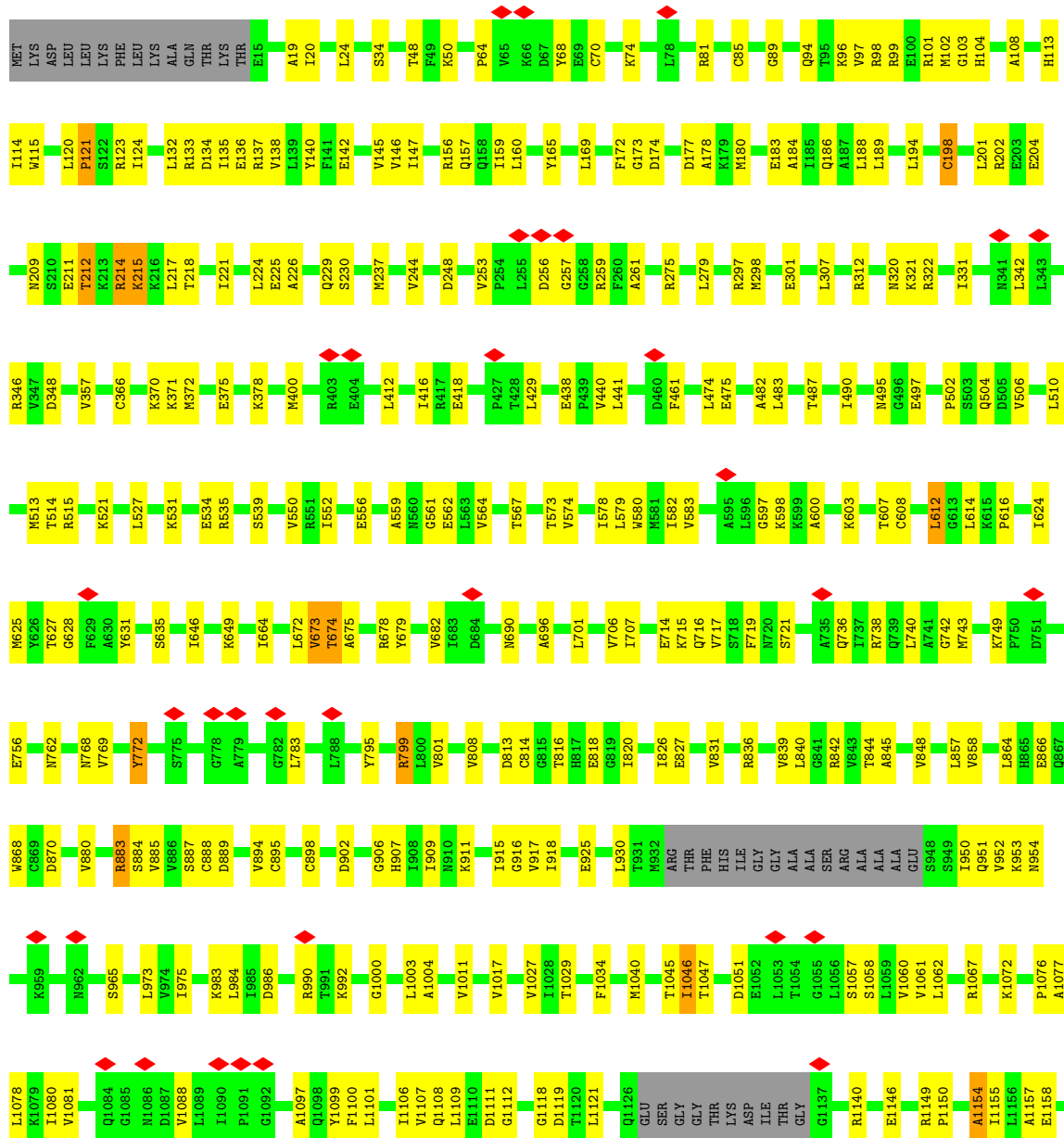
Mol	Chain	Residues	Atoms							AltConf
11	G	1	Total 33	C 10	H 11	N 5	O 6	P 1	0	
11	H	1	Total 33	C 10	H 11	N 5	O 6	P 1	0	



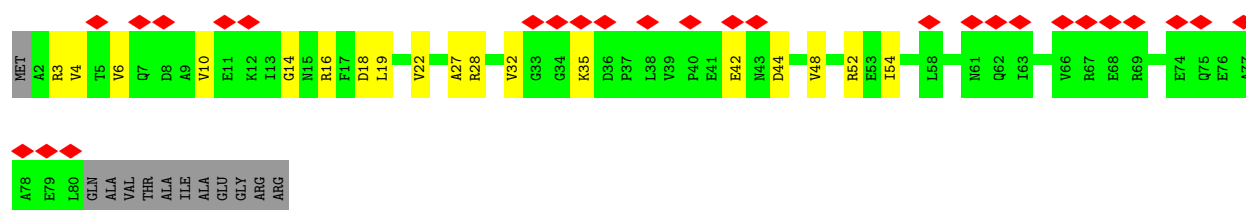


• Molecule 3: DNA-directed RNA polymerase subunit beta'

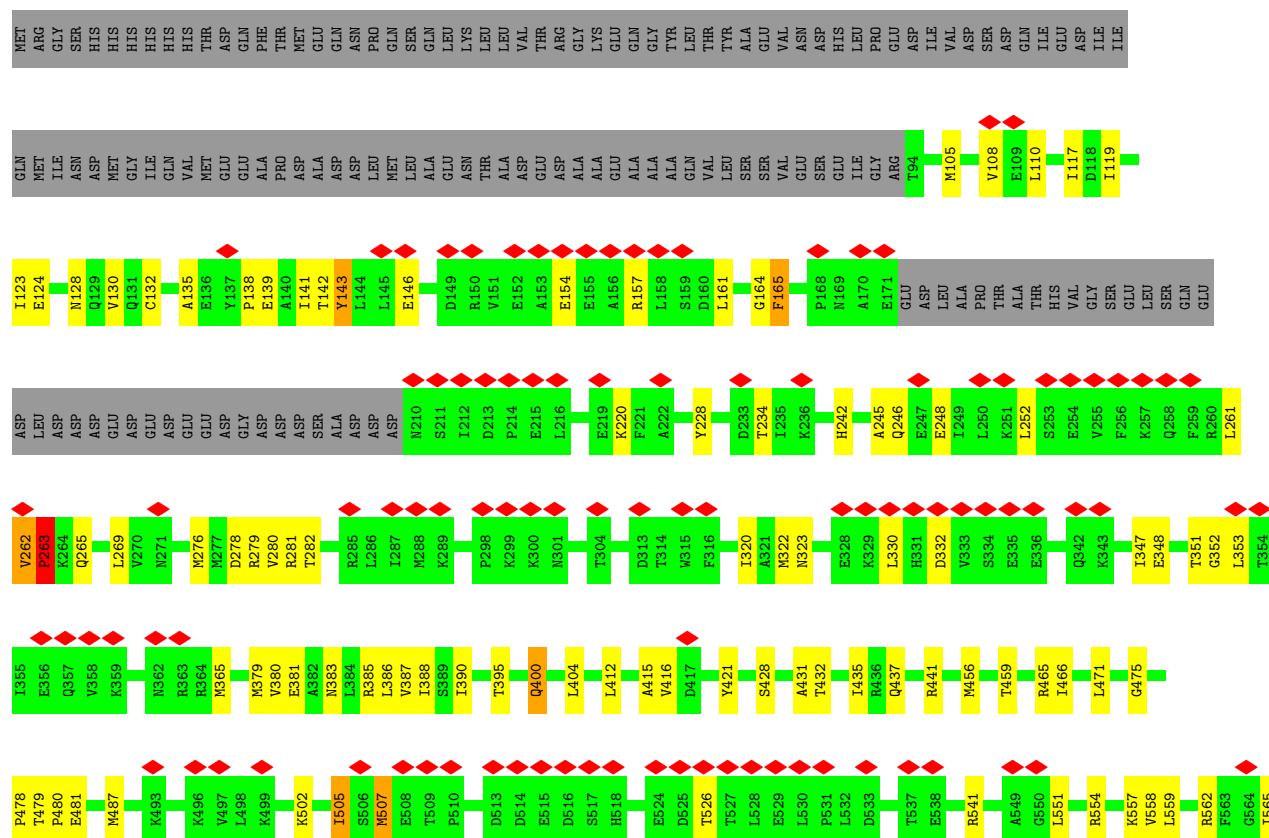
Chain D: 69% 25% 5%

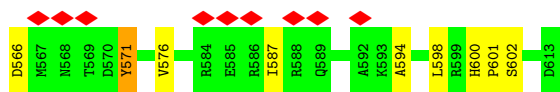


- Molecule 4: DNA-directed RNA polymerase subunit omega

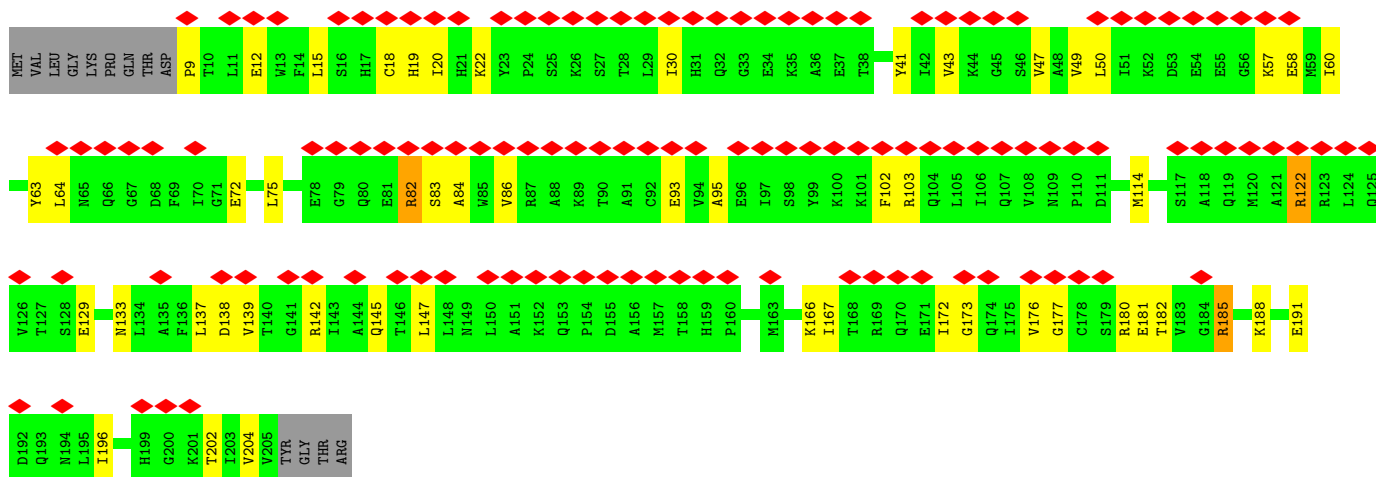


- Molecule 5: RNA polymerase sigma factor RpoD

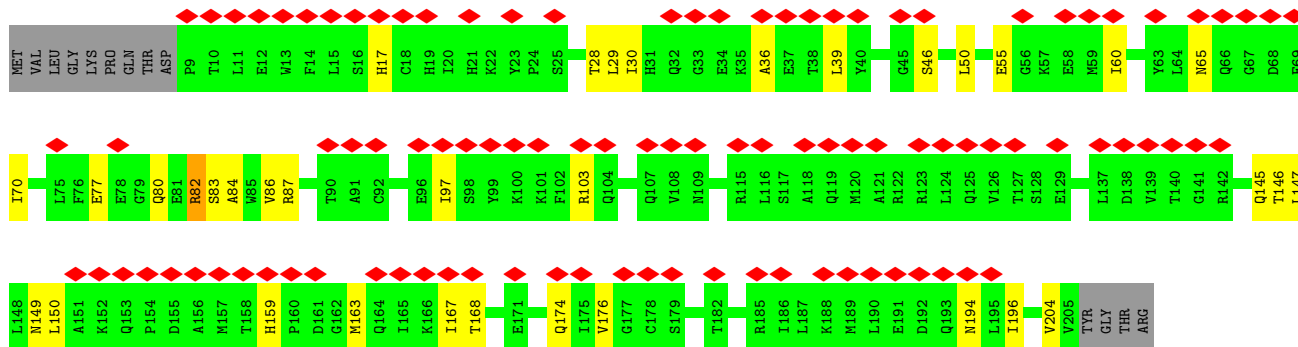
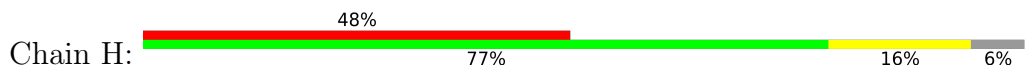




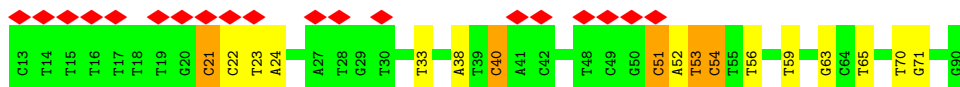
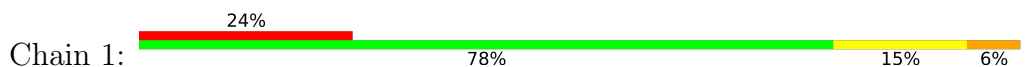
- Molecule 6: cAMP-activated global transcriptional regulator CRP



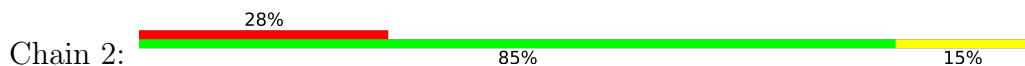
- Molecule 6: cAMP-activated global transcriptional regulator CRP

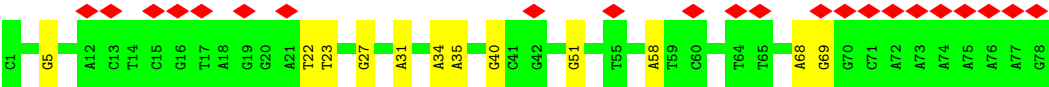


- Molecule 7: SYNTHETIC NONTEMPLATE STRAND DNA (78-MER)



- Molecule 8: SYNTHETIC TEMPLATE STRAND DNA (78-MER)





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30296	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 ($e^-/\text{\AA}^2$)	36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	5.780	Depositor
Minimum map value	-1.761	Depositor
Average map value	-0.020	Depositor
Map value standard deviation	0.262	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	345.59998, 345.59998, 345.59998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8999999, 0.8999999, 0.8999999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CMP, 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	0.55	0/1808	0.87	3/2450 (0.1%)
1	B	0.55	0/1789	0.79	2/2425 (0.1%)
2	C	0.54	1/10690 (0.0%)	0.79	11/14423 (0.1%)
3	D	0.50	4/10553 (0.0%)	0.76	4/14248 (0.0%)
4	E	0.37	0/629	0.62	0/847
5	F	0.46	1/3971 (0.0%)	0.73	2/5340 (0.0%)
6	G	0.47	0/1580	0.77	2/2127 (0.1%)
6	H	0.49	0/1580	0.77	1/2127 (0.0%)
7	1	1.11	3/1777 (0.2%)	1.27	8/2741 (0.3%)
8	2	1.02	2/1815 (0.1%)	1.08	1/2800 (0.0%)
All	All	0.59	11/36192 (0.0%)	0.83	34/49528 (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
1	A	0	10
1	B	0	1
2	C	0	20
3	D	0	11
5	F	0	9
6	H	0	3
All	All	0	54

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	772	TYR	CD2-CE2	-7.59	1.27	1.39
8	2	35	DA	C3'-O3'	6.44	1.52	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1	51	DC	C1'-N1	5.88	1.56	1.49
7	1	21	DC	C1'-N1	5.57	1.56	1.49
8	2	31	DA	N9-C4	-5.52	1.34	1.37
3	D	198	CYS	CB-SG	-5.50	1.72	1.81
2	C	997	TRP	CB-CG	-5.38	1.40	1.50
5	F	571	TYR	CD2-CE2	-5.25	1.31	1.39
3	D	165	TYR	CD1-CE1	-5.11	1.31	1.39
3	D	375	GLU	CB-CG	5.08	1.61	1.52
7	1	40	DC	C1'-N1	5.05	1.55	1.49

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	82	ARG	NE-CZ-NH2	-9.29	115.65	120.30
2	C	821	ARG	NE-CZ-NH2	-8.77	115.92	120.30
2	C	528	ARG	NE-CZ-NH1	8.54	124.57	120.30
3	D	1206	ARG	NE-CZ-NH1	7.84	124.22	120.30
2	C	680	LEU	CA-CB-CG	7.81	133.26	115.30
2	C	384	LEU	CA-CB-CG	7.69	132.98	115.30
3	D	1206	ARG	NE-CZ-NH2	-7.60	116.50	120.30
7	1	51	DC	O4'-C1'-N1	7.44	113.21	108.00
5	F	332	ASP	CB-CG-OD1	7.38	124.94	118.30
5	F	554	ARG	NE-CZ-NH1	6.88	123.74	120.30
7	1	53	DT	O4'-C4'-C3'	-6.58	101.87	104.50
2	C	528	ARG	NE-CZ-NH2	-6.54	117.03	120.30
3	D	799	ARG	NE-CZ-NH1	6.40	123.50	120.30
7	1	54	DC	O4'-C1'-C2'	-6.38	100.80	105.90
6	G	185	ARG	NE-CZ-NH1	6.33	123.46	120.30
7	1	23	DT	C6-C5-C7	-6.22	119.17	122.90
2	C	241	LEU	CA-CB-CG	5.98	129.04	115.30
7	1	52	DA	O4'-C1'-N9	5.94	112.16	108.00
2	C	511	LEU	CA-CB-CG	5.89	128.85	115.30
7	1	23	DT	C4-C5-C7	5.82	122.49	119.00
7	1	51	DC	O4'-C4'-C3'	-5.69	102.22	104.50
6	G	82	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	177	TYR	CB-CG-CD2	-5.51	117.69	121.00
2	C	101	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	C	246	LEU	CA-CB-CG	5.41	127.75	115.30
7	1	59	DT	N3-C4-O4	5.33	123.10	119.90
1	A	147	GLN	C-N-CA	5.25	134.81	121.70
1	A	177	TYR	CB-CG-CD1	5.18	124.11	121.00
8	2	35	DA	P-O3'-C3'	5.16	125.89	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	D	883	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	82	LEU	CA-CB-CG	5.15	127.15	115.30
2	C	719	LYS	CD-CE-NZ	-5.07	100.05	111.70
2	C	821	ARG	NE-CZ-NH1	5.03	122.81	120.30

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	149	GLY	Peptide
1	A	153	VAL	Peptide
1	A	176	CYS	Peptide
1	A	177	TYR	Peptide
1	A	191	ARG	Peptide
1	A	207	THR	Peptide
1	A	51	MET	Peptide
1	A	55	ALA	Peptide
1	A	68	TYR	Peptide
1	A	77	ASP	Peptide
1	B	191	ARG	Peptide
2	C	1004	ASP	Peptide
2	C	1034	ARG	Sidechain
2	C	1292	THR	Peptide
2	C	150	HIS	Peptide
2	C	153	PRO	Peptide
2	C	185	ASP	Peptide
2	C	186	PHE	Peptide
2	C	207	THR	Peptide
2	C	226	GLU	Peptide
2	C	234	ASP	Peptide
2	C	282	VAL	Peptide
2	C	395	TYR	Peptide
2	C	396	ASP	Peptide
2	C	449	GLY	Peptide
2	C	455	SER	Peptide
2	C	830	THR	Peptide
2	C	856	ASN	Peptide
2	C	859	GLU	Peptide
2	C	860	ALA	Peptide
2	C	872	TYR	Peptide
3	D	1046	ILE	Peptide

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Mol	Chain	Res	Type	Group
3	D	1150	PRO	Peptide
3	D	1154	ALA	Peptide
3	D	120	LEU	Peptide
3	D	121	PRO	Peptide
3	D	1357	ILE	Peptide
3	D	180	MET	Peptide
3	D	612	LEU	Peptide
3	D	673	VAL	Peptide
3	D	701	LEU	Peptide
3	D	94	GLN	Peptide
5	F	143	TYR	Peptide
5	F	165	PHE	Peptide
5	F	261	LEU	Peptide
5	F	262	VAL	Peptide
5	F	263	PRO	Peptide
5	F	395	THR	Peptide
5	F	480	PRO	Peptide
5	F	505	ILE	Peptide
5	F	601	PRO	Peptide
6	H	159	HIS	Peptide
6	H	167	ILE	Peptide
6	H	17	HIS	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	65	0
1	B	1767	1789	1789	81	0
2	C	10522	10532	10533	358	0
3	D	10396	10616	10616	273	0
4	E	627	634	634	19	0
5	F	3917	3975	3977	75	0
6	G	1556	1598	1600	51	0
6	H	1556	1599	1600	24	0
7	1	1591	889	891	17	0
8	2	1612	874	876	10	0
9	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	D	1	0	0	0	0
11	G	22	11	11	2	0
11	H	22	11	11	5	0
All	All	35377	34341	34351	884	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (884) 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)
11:H:301:CMP:H2	11:H:301:CMP:C2	0.97	1.50
11:G:301:CMP:H2	11:G:301:CMP:C2	0.97	1.48
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.44	0.90
1:A:16:ILE:HD11	1:A:214:GLU:HB2	1.58	0.84
2:C:563:THR:OG1	2:C:572:ILE:O	1.97	0.83
2:C:1122:LYS:NZ	2:C:1126:ASP:OD1	2.10	0.83
3:D:214:ARG:NH1	3:D:218:THR:OG1	2.12	0.82
1:B:113:ALA:N	1:B:126:PRO:O	2.13	0.82
1:B:58:GLU:OE1	1:B:170:ARG:NH2	2.13	0.81
1:A:101:THR:HG1	1:A:116:THR:HG1	1.11	0.80
2:C:853:ASP:OD2	6:G:22:LYS:NZ	2.15	0.79
2:C:954:LYS:NZ	6:G:18:CYS:O	2.16	0.79
2:C:684:ASN:O	2:C:688:GLN:NE2	2.15	0.79
2:C:247:ARG:N	2:C:249:GLU:OE1	2.15	0.79
2:C:841:ARG:NH1	2:C:843:THR:OG1	2.16	0.78
2:C:1080:ASN:ND2	2:C:1085:MET:SD	2.56	0.78
3:D:848:VAL:HG11	3:D:880:VAL:HG23	1.64	0.78
5:F:278:ASP:O	5:F:282:THR:OG1	2.01	0.78
2:C:869:GLY:O	2:C:872:TYR:N	2.17	0.78
3:D:814:CYS:HG	3:D:816:THR:HG1	1.22	0.78
1:B:218:ARG:NH1	1:B:222:THR:OG1	2.16	0.77
3:D:826:ILE:HG22	3:D:831:VAL:HA	1.65	0.77
2:C:411:ARG:O	2:C:584:TYR:OH	2.03	0.77
1:A:6:THR:OG1	1:B:226:GLU:OE2	2.02	0.77
1:B:131:CYS:SG	1:B:132:HIS:N	2.58	0.77
3:D:1034:PHE:N	3:D:1081:VAL:O	2.18	0.77
2:C:955:GLN:NE2	2:C:959:ASP:OD2	2.17	0.76
3:D:954:ASN:OD1	3:D:992:LYS:NZ	2.13	0.76
3:D:842:ARG:NH2	3:D:898:CYS:O	2.18	0.76
3:D:1290:ARG:NH2	3:D:1300:ALA:O	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:138:VAL:HG22	3:D:145:VAL:HG21	1.66	0.76
2:C:93:SER:OG	2:C:126:GLU:OE1	2.02	0.76
2:C:557:ARG:NH2	2:C:606:LEU:O	2.19	0.76
2:C:621:SER:OG	2:C:653:MET:SD	2.44	0.75
3:D:1062:LEU:O	3:D:1067:ARG:NH2	2.19	0.75
6:G:147:LEU:HD21	6:G:172:ILE:HD11	1.67	0.75
3:D:1310:THR:O	3:D:1313:SER:OG	2.03	0.75
2:C:592:ARG:N	2:C:653:MET:O	2.20	0.74
2:C:269:ILE:HG22	2:C:274:ILE:HG13	1.69	0.74
1:A:168:ILE:HD11	2:C:872:TYR:HB3	1.68	0.74
3:D:556:GLU:O	3:D:564:VAL:N	2.20	0.73
1:A:38:THR:HG23	1:B:42:ALA:HB1	1.70	0.73
1:A:190:ALA:N	1:A:198:LEU:O	2.19	0.73
3:D:1058:SER:OG	3:D:1109:LEU:O	2.06	0.73
2:C:1331:ARG:NH1	3:D:102:MET:SD	2.62	0.73
3:D:827:GLU:O	3:D:1242:ARG:NH1	2.22	0.73
3:D:1154:ALA:HB2	3:D:1190:ILE:HG23	1.70	0.73
2:C:402:ARG:NH1	2:C:424:ASP:OD2	2.22	0.73
3:D:99:ARG:NH2	3:D:248:ASP:OD2	2.22	0.73
2:C:300:ASP:OD1	2:C:313:ALA:N	2.21	0.72
3:D:827:GLU:OE1	3:D:983:LYS:NZ	2.22	0.72
2:C:805:MET:O	2:C:811:ASN:ND2	2.21	0.72
2:C:701:GLY:N	2:C:1182:ILE:O	2.22	0.72
6:G:182:THR:HG21	7:1:38:DA:OP2	1.89	0.72
2:C:1330:ILE:HG23	2:C:1337:ILE:HG21	1.72	0.72
3:D:631:TYR:O	3:D:635:SER:N	2.22	0.72
2:C:255:ILE:N	2:C:263:VAL:O	2.24	0.71
1:B:218:ARG:O	1:B:222:THR:OG1	2.04	0.71
2:C:232:ILE:HD11	2:C:322:LEU:HD11	1.71	0.71
5:F:130:VAL:HG13	5:F:365:MET:HG2	1.71	0.71
3:D:202:ARG:NH2	3:D:225:GLU:OE1	2.24	0.71
5:F:154:GLU:OE1	5:F:157:ARG:NE	2.24	0.71
3:D:738:ARG:O	3:D:742:GLY:N	2.24	0.70
3:D:1078:LEU:HD12	3:D:1107:VAL:HG21	1.73	0.70
5:F:143:TYR:O	5:F:146:GLU:N	2.24	0.70
5:F:279:ARG:NH2	5:F:351:THR:HG21	2.05	0.70
2:C:251:ALA:O	2:C:266:GLY:N	2.25	0.70
1:B:79:LEU:HD23	1:B:82:LEU:HD12	1.74	0.70
3:D:740:LEU:O	3:D:762:ASN:ND2	2.25	0.70
2:C:210:LEU:HD11	2:C:223:LEU:HD11	1.72	0.70
2:C:59:ILE:HG21	2:C:479:LEU:HD13	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:418:GLU:OE2	4:E:3:ARG:NE	2.24	0.69
2:C:138:ILE:O	2:C:141:THR:OG1	2.10	0.69
3:D:225:GLU:OE2	3:D:229:GLN:NE2	2.25	0.69
3:D:108:ALA:HB3	3:D:279:LEU:HD23	1.73	0.69
5:F:386:LEU:N	7:1:70:DT:O2	2.26	0.69
3:D:1164:SER:O	3:D:1176:VAL:N	2.25	0.69
2:C:443:ASP:OD1	2:C:451:ARG:NH1	2.25	0.69
1:A:90:VAL:HG11	1:A:146:VAL:HG11	1.76	0.68
3:D:884:SER:N	3:D:887:SER:OG	2.26	0.68
1:A:39:LEU:HD22	1:B:228:LEU:HD21	1.74	0.68
3:D:70:CYS:SG	3:D:74:LYS:N	2.67	0.68
3:D:474:LEU:HD21	4:E:27:ALA:HB3	1.75	0.68
1:A:158:ARG:O	1:A:161:SER:OG	2.06	0.68
3:D:1330:ARG:O	3:D:1333:THR:OG1	2.12	0.68
5:F:465:ARG:NH1	8:2:27:DG:OP2	2.27	0.68
6:G:129:GLU:OE2	6:G:145:GLN:NE2	2.26	0.68
2:C:148:GLN:NE2	2:C:535:PRO:O	2.27	0.67
3:D:884:SER:O	3:D:888:CYS:N	2.27	0.67
6:H:83:SER:OG	11:H:301:CMP:O1P	2.02	0.67
2:C:1245:ALA:HB3	3:D:372:MET:SD	2.35	0.67
2:C:1248:THR:OG1	3:D:348:ASP:OD1	2.10	0.66
3:D:885:VAL:CG1	3:D:894:VAL:HG11	2.24	0.66
1:B:74:VAL:HG22	1:B:133:LEU:HD23	1.76	0.66
2:C:950:GLU:OE2	6:G:20:ILE:N	2.28	0.66
3:D:1368:ASP:OD1	3:D:1371:ARG:NH1	2.29	0.66
2:C:524:ILE:O	2:C:528:ARG:N	2.28	0.66
3:D:885:VAL:HG13	3:D:894:VAL:HG11	1.78	0.66
5:F:234:THR:OG1	5:F:248:GLU:OE1	2.08	0.66
5:F:279:ARG:HE	5:F:347:ILE:HG23	1.61	0.66
2:C:956:ALA:HB1	2:C:1032:LYS:NZ	2.11	0.66
2:C:1326:LEU:O	2:C:1330:ILE:HG22	1.96	0.66
3:D:888:CYS:SG	3:D:895:CYS:N	2.69	0.66
2:C:1002:LEU:HD12	2:C:1007:LYS:HD2	1.78	0.66
5:F:139:GLU:O	5:F:142:THR:OG1	2.13	0.66
1:B:12:ARG:N	1:B:29:GLU:O	2.28	0.65
2:C:801:ARG:NH2	2:C:1229:TYR:OH	2.29	0.65
6:G:9:PRO:N	6:G:12:GLU:HG2	2.11	0.65
2:C:860:ALA:O	2:C:862:LEU:N	2.29	0.65
7:1:21:DC:N4	8:2:69:DG:O6	2.29	0.65
1:A:131:CYS:SG	1:A:132:HIS:N	2.69	0.65
1:B:98:VAL:HG11	1:B:121:VAL:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:201:LEU:CD2	3:D:217:LEU:HD22	2.27	0.65
2:C:36:GLN:O	2:C:40:GLU:N	2.29	0.65
2:C:700:VAL:HG21	2:C:1114:GLU:HG3	1.78	0.65
2:C:1327:LEU:HD22	2:C:1337:ILE:HG12	1.78	0.65
2:C:241:LEU:HD22	2:C:277:LEU:HD11	1.79	0.65
2:C:624:ASP:N	2:C:628:HIS:O	2.29	0.65
2:C:663:VAL:O	2:C:666:SER:OG	2.07	0.65
3:D:510:LEU:HD13	3:D:631:TYR:OH	1.97	0.65
5:F:348:GLU:O	5:F:352:GLY:N	2.28	0.65
3:D:579:LEU:HD22	3:D:582:ILE:HD12	1.78	0.64
5:F:600:HIS:O	5:F:602:SER:N	2.31	0.64
1:A:55:ALA:O	1:A:56:VAL:HG23	1.97	0.64
5:F:471:LEU:HD23	5:F:471:LEU:O	1.98	0.64
2:C:14:ASP:OD2	2:C:1156:ARG:NH2	2.26	0.64
3:D:275:ARG:NH1	3:D:298:MET:O	2.31	0.64
2:C:302:ILE:O	2:C:330:HIS:NE2	2.31	0.64
2:C:811:ASN:O	2:C:1099:ASN:ND2	2.30	0.64
2:C:1313:HIS:O	4:E:28:ARG:NH2	2.31	0.64
2:C:1223:ARG:NH1	3:D:721:SER:OG	2.31	0.64
3:D:1157:ALA:N	3:D:1208:ASP:O	2.27	0.64
2:C:1102:GLY:O	2:C:1106:ARG:N	2.31	0.64
3:D:482:ALA:CB	4:E:6:VAL:HG11	2.28	0.64
3:D:1057:SER:N	3:D:1108:GLN:O	2.31	0.64
2:C:528:ARG:NH2	2:C:576:SER:O	2.31	0.63
2:C:888:THR:O	2:C:914:LYS:N	2.31	0.63
6:H:82:ARG:NH1	11:H:301:CMP:O2P	2.31	0.63
2:C:1326:LEU:HD22	3:D:331:ILE:HG23	1.79	0.63
2:C:1033:ARG:HD2	6:G:12:GLU:HB3	1.78	0.63
5:F:380:VAL:HG22	5:F:416:VAL:HG21	1.79	0.63
1:A:9:LEU:HD21	1:A:30:PRO:HG2	1.80	0.63
2:C:63:SER:O	2:C:107:ARG:NH1	2.32	0.63
2:C:933:VAL:HG22	2:C:1050:VAL:HG13	1.81	0.63
2:C:950:GLU:OE2	6:G:19:HIS:HA	1.98	0.63
3:D:1357:ILE:HG22	3:D:1358:PRO:HD3	1.81	0.63
2:C:450:ASN:HB3	2:C:453:ILE:HD12	1.81	0.62
6:G:181:GLU:OE2	7:1:40:DC:N4	2.27	0.62
3:D:147:ILE:HG23	3:D:184:ALA:HA	1.81	0.62
5:F:456:MET:O	5:F:459:THR:OG1	2.17	0.62
2:C:699:LEU:O	2:C:1182:ILE:N	2.31	0.62
3:D:214:ARG:O	3:D:218:THR:OG1	2.17	0.62
2:C:956:ALA:HB1	2:C:1032:LYS:CE	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:VAL:HG12	1:A:147:GLN:H	1.65	0.62
2:C:565:GLU:CG	3:D:783:LEU:HD21	2.29	0.62
2:C:851:THR:HG23	2:C:945:ALA:HB2	1.82	0.62
3:D:1333:THR:O	3:D:1337:VAL:HG13	1.99	0.61
2:C:1003:THR:O	2:C:1008:GLN:NE2	2.33	0.61
2:C:1291:LEU:HD11	3:D:1351:VAL:HG13	1.82	0.61
2:C:411:ARG:NE	2:C:413:GLU:OE1	2.33	0.61
2:C:1280:ALA:HB1	3:D:918:ILE:CD1	2.31	0.61
3:D:986:ASP:OD1	3:D:990:ARG:N	2.33	0.61
5:F:242:HIS:O	5:F:246:GLN:N	2.29	0.61
2:C:246:LEU:HG	2:C:269:ILE:HG21	1.82	0.61
2:C:563:THR:OG1	2:C:569:ILE:O	2.18	0.61
5:F:385:ARG:HA	5:F:388:ILE:HG22	1.82	0.61
1:A:100:LEU:HD12	1:A:146:VAL:HG21	1.83	0.61
2:C:756:TYR:O	2:C:757:THR:OG1	2.16	0.61
2:C:1280:ALA:HB1	3:D:918:ILE:HD13	1.83	0.61
1:B:61:ILE:HG23	1:B:142:MET:HB3	1.81	0.61
3:D:85:CYS:O	3:D:89:GLY:N	2.34	0.61
3:D:1045:THR:O	3:D:1067:ARG:NE	2.34	0.60
2:C:145:ILE:HG21	2:C:456:VAL:HB	1.83	0.60
5:F:379:MET:CG	5:F:416:VAL:HG22	2.31	0.60
5:F:541:ARG:HH21	5:F:565:ILE:HG23	1.65	0.60
2:C:521:LEU:O	2:C:525:THR:HG22	2.02	0.60
2:C:1222:GLU:N	2:C:1222:GLU:OE1	2.35	0.60
3:D:136:GLU:O	3:D:140:TYR:N	2.31	0.60
3:D:261:ALA:HB1	5:F:507:MET:HE2	1.84	0.60
1:B:158:ARG:O	1:B:162:GLU:N	2.31	0.60
1:B:158:ARG:HD2	1:B:172:LEU:HD11	1.84	0.60
1:B:96:ASP:O	1:B:148:ARG:N	2.35	0.60
2:C:246:LEU:O	2:C:274:ILE:HD11	2.02	0.60
3:D:115:TRP:HB3	3:D:1333:THR:HG22	1.85	0.59
2:C:768:MET:O	2:C:785:ASP:N	2.32	0.59
1:B:112:ALA:N	1:B:128:HIS:O	2.35	0.59
2:C:598:VAL:HG22	2:C:627:GLY:O	2.01	0.59
1:A:51:MET:CG	1:A:180:VAL:HG11	2.33	0.59
2:C:820:GLU:N	2:C:1080:ASN:O	2.34	0.59
1:B:84:ASN:O	1:B:128:HIS:NE2	2.32	0.59
5:F:108:VAL:HG11	5:F:381:GLU:HB3	1.84	0.59
1:B:106:GLY:O	1:B:133:LEU:HD12	2.03	0.59
2:C:618:GLN:O	2:C:621:SER:OG	2.21	0.59
1:B:92:VAL:O	1:B:148:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:525:THR:HG21	2:C:687:ARG:CD	2.33	0.59
2:C:1223:ARG:NH2	3:D:719:PHE:O	2.36	0.59
3:D:857:LEU:HD12	3:D:858:VAL:HG13	1.84	0.59
2:C:448:LEU:O	2:C:450:ASN:ND2	2.36	0.59
3:D:370:LYS:HG2	3:D:441:LEU:HD22	1.85	0.59
4:E:10:VAL:O	4:E:14:GLY:N	2.35	0.59
2:C:851:THR:CG2	2:C:945:ALA:HB2	2.33	0.58
3:D:649:LYS:HE3	3:D:696:ALA:HB2	1.85	0.58
2:C:68:LEU:HD11	2:C:492:MET:CE	2.33	0.58
2:C:247:ARG:HA	2:C:274:ILE:HD11	1.85	0.58
2:C:821:ARG:NH2	2:C:1095:ASP:OD1	2.36	0.58
3:D:930:LEU:HD13	3:D:1246:VAL:HG22	1.86	0.58
6:G:122:ARG:NH2	6:H:77:GLU:OE1	2.37	0.58
2:C:257:ALA:N	2:C:260:LYS:O	2.35	0.58
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.83	0.58
3:D:672:LEU:O	3:D:674:THR:N	2.36	0.58
2:C:360:LEU:HD11	2:C:378:ARG:HD2	1.85	0.58
2:C:1043:ALA:HB3	2:C:1046:VAL:HB	1.84	0.58
2:C:525:THR:HG21	2:C:687:ARG:HD3	1.86	0.58
5:F:110:LEU:HD21	7:1:70:DT:C2	2.39	0.57
2:C:232:ILE:HD11	2:C:322:LEU:CD1	2.33	0.57
2:C:658:GLN:O	2:C:661:VAL:HG22	2.03	0.57
2:C:1333:LEU:HD12	2:C:1335:ILE:HD12	1.86	0.57
2:C:246:LEU:HD21	2:C:277:LEU:HD21	1.85	0.57
2:C:878:THR:N	2:C:881:ASP:OD2	2.34	0.57
6:H:163:MET:O	6:H:204:VAL:N	2.37	0.57
1:B:166:ARG:NH2	1:B:172:LEU:HD22	2.19	0.57
2:C:821:ARG:NH2	2:C:1093:PRO:O	2.37	0.57
3:D:198:CYS:SG	3:D:202:ARG:NH1	2.78	0.57
3:D:475:GLU:OE1	4:E:28:ARG:NH2	2.36	0.57
3:D:953:LYS:HB2	3:D:984:LEU:HD23	1.87	0.57
1:A:12:ARG:N	1:A:29:GLU:O	2.38	0.57
2:C:176:ILE:HD11	2:C:429:MET:SD	2.44	0.57
2:C:1304:MET:O	2:C:1308:ILE:HG23	2.05	0.57
2:C:65:ASN:OD1	2:C:66:SER:N	2.37	0.57
2:C:974:ARG:O	2:C:978:VAL:HG23	2.05	0.57
3:D:816:THR:HG21	3:D:889:ASP:HB2	1.85	0.57
2:C:367:TYR:O	2:C:371:ARG:N	2.33	0.57
3:D:218:THR:HA	3:D:221:ILE:HD12	1.86	0.57
3:D:1040:MET:SD	3:D:1078:LEU:N	2.78	0.57
1:A:58:GLU:OE1	1:A:170:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD23	1:B:82:LEU:CD1	2.34	0.56
1:B:158:ARG:HD2	1:B:172:LEU:HD21	1.86	0.56
2:C:565:GLU:HG3	3:D:783:LEU:HD21	1.87	0.56
2:C:1033:ARG:HD2	6:G:12:GLU:CB	2.35	0.56
1:B:147:GLN:NE2	1:B:148:ARG:O	2.37	0.56
2:C:697:LYS:NZ	2:C:699:LEU:HD23	2.20	0.56
3:D:1154:ALA:HB3	3:D:1211:SER:OG	2.05	0.56
2:C:184:LEU:HD13	2:C:198:ILE:HA	1.87	0.56
2:C:403:MET:O	2:C:406:ASN:N	2.37	0.56
3:D:133:ARG:NH1	3:D:136:GLU:OE1	2.38	0.56
5:F:551:LEU:HD11	5:F:598:LEU:HD21	1.88	0.56
2:C:263:VAL:HG22	2:C:273:HIS:CD2	2.40	0.56
3:D:624:ILE:HA	3:D:627:THR:HG22	1.86	0.56
5:F:466:ILE:HG21	5:F:487:MET:HA	1.88	0.56
5:F:379:MET:HG2	5:F:416:VAL:HG22	1.87	0.56
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	1.88	0.56
2:C:1116:HIS:HB3	2:C:1195:ILE:HG21	1.86	0.56
2:C:1280:ALA:HB2	3:D:917:VAL:HB	1.88	0.56
3:D:902:ASP:N	3:D:907:HIS:O	2.37	0.56
2:C:246:LEU:HD23	2:C:246:LEU:H	1.71	0.56
2:C:1064:ASP:HB2	2:C:1076:ILE:HD12	1.87	0.56
3:D:160:LEU:HD12	3:D:178:ALA:CB	2.36	0.56
3:D:261:ALA:HB1	5:F:507:MET:CE	2.36	0.56
2:C:261:VAL:HG11	2:C:264:GLU:OE2	2.06	0.56
3:D:140:TYR:O	3:D:297:ARG:NH2	2.39	0.56
5:F:279:ARG:HH21	5:F:351:THR:HG21	1.71	0.56
1:B:9:LEU:HD21	1:B:30:PRO:HG2	1.88	0.56
3:D:848:VAL:HG11	3:D:880:VAL:CG2	2.35	0.56
6:H:28:THR:HG23	6:H:87:ARG:HG2	1.88	0.56
3:D:366:CYS:O	3:D:440:VAL:N	2.39	0.55
3:D:814:CYS:SG	3:D:816:THR:OG1	2.44	0.55
5:F:234:THR:O	5:F:245:ALA:HB2	2.05	0.55
1:B:26:VAL:N	1:B:203:ILE:O	2.38	0.55
2:C:146:VAL:HG12	2:C:511:LEU:HD13	1.86	0.55
2:C:636:CYS:SG	2:C:650:VAL:HG22	2.47	0.55
1:B:84:ASN:HB3	1:B:130:ILE:HA	1.87	0.55
2:C:409:LEU:HD22	2:C:411:ARG:HB2	1.87	0.55
3:D:146:VAL:HA	3:D:178:ALA:HA	1.87	0.55
2:C:1285:TYR:HB2	3:D:1361:THR:HG21	1.88	0.55
2:C:1291:LEU:CD1	3:D:1351:VAL:HG13	2.37	0.55
3:D:664:ILE:HG23	3:D:678:ARG:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1026:GLU:O	2:C:1030:GLU:HG2	2.07	0.55
3:D:201:LEU:HB3	3:D:221:ILE:HD11	1.88	0.55
2:C:13:LYS:O	2:C:1183:ALA:N	2.36	0.55
3:D:482:ALA:HB2	4:E:6:VAL:HG11	1.86	0.55
1:B:90:VAL:HG11	1:B:146:VAL:HG21	1.89	0.55
1:A:39:LEU:CD2	1:B:228:LEU:HD21	2.37	0.55
1:B:158:ARG:CD	1:B:172:LEU:HD11	2.37	0.55
1:A:45:ARG:NH1	2:C:1216:ARG:O	2.40	0.54
3:D:801:VAL:HG13	3:D:917:VAL:HG22	1.89	0.54
3:D:1034:PHE:HB2	3:D:1081:VAL:HG23	1.88	0.54
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.06	0.54
2:C:404:LYS:HG3	2:C:452:ARG:HD2	1.89	0.54
3:D:114:ILE:HG23	3:D:115:TRP:CD1	2.43	0.54
3:D:552:ILE:O	3:D:567:THR:OG1	2.10	0.54
2:C:301:TYR:OH	2:C:334:GLU:N	2.40	0.54
3:D:416:ILE:HD13	3:D:441:LEU:HD21	1.87	0.54
3:D:799:ARG:NH2	3:D:1146:GLU:OE1	2.39	0.54
3:D:1060:VAL:HG22	3:D:1106:ILE:HG23	1.88	0.54
3:D:1287:ILE:HG22	3:D:1290:ARG:NH2	2.23	0.54
2:C:548:ARG:NH1	2:C:567:PRO:O	2.40	0.54
5:F:117:ILE:HG23	5:F:421:TYR:CG	2.41	0.54
6:G:43:VAL:CG2	6:G:95:ALA:HB2	2.37	0.54
3:D:138:VAL:HG22	3:D:145:VAL:CG2	2.36	0.54
3:D:226:ALA:O	3:D:230:SER:OG	2.15	0.54
3:D:965:SER:OG	3:D:973:LEU:HD11	2.07	0.54
5:F:161:LEU:HD11	5:F:165:PHE:CE1	2.42	0.54
1:B:104:LYS:HG2	1:B:133:LEU:HD11	1.89	0.54
2:C:197:ARG:NH2	8:2:5:DG:OP1	2.41	0.54
2:C:1303:LYS:O	2:C:1307:ASN:ND2	2.41	0.54
2:C:989:LEU:O	2:C:997:TRP:NE1	2.41	0.54
3:D:1220:ILE:O	3:D:1224:ARG:N	2.41	0.54
1:B:71:LYS:HD3	1:B:74:VAL:HG21	1.89	0.54
2:C:678:ARG:NH2	2:C:1071:GLY:O	2.41	0.54
3:D:515:ARG:NH2	3:D:717:VAL:HG21	2.23	0.54
3:D:674:THR:HG23	3:D:675:ALA:H	1.73	0.54
2:C:68:LEU:HD11	2:C:492:MET:HE3	1.89	0.53
2:C:478:ARG:NH2	2:C:492:MET:O	2.42	0.53
2:C:617:ALA:N	2:C:652:TYR:O	2.31	0.53
2:C:958:LYS:O	2:C:962:GLU:HG3	2.08	0.53
2:C:998:LEU:HD21	2:C:1014:LEU:CD2	2.38	0.53
1:B:22:THR:OG1	1:B:207:THR:O	2.25	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:209:ILE:O	2:C:213:LEU:N	2.41	0.53
5:F:132:CYS:O	5:F:135:ALA:N	2.40	0.53
5:F:322:MET:SD	5:F:323:ASN:N	2.80	0.53
6:H:77:GLU:OE1	6:H:80:GLN:NE2	2.42	0.53
2:C:359:ARG:O	2:C:362:ALA:HB3	2.09	0.53
3:D:183:GLU:OE2	3:D:186:GLN:NE2	2.42	0.53
2:C:397:LEU:HD22	2:C:419:ILE:HA	1.90	0.53
2:C:633:LEU:HD23	2:C:644:LEU:HB3	1.91	0.53
5:F:383:ASN:HB2	5:F:412:LEU:HD21	1.89	0.53
2:C:788:SER:O	2:C:795:ALA:N	2.40	0.53
3:D:1154:ALA:HB3	3:D:1211:SER:CB	2.38	0.53
2:C:1329:GLU:OE1	3:D:331:ILE:HD11	2.09	0.53
3:D:19:ALA:HB2	3:D:1343:GLU:OE2	2.08	0.53
2:C:696:ASP:OD2	2:C:827:ARG:NH2	2.41	0.53
2:C:1155:VAL:HG12	2:C:1157:GLN:H	1.72	0.53
3:D:1029:THR:O	3:D:1118:GLY:N	2.40	0.53
1:A:74:VAL:HG13	1:A:131:CYS:SG	2.48	0.53
1:A:60:GLU:O	1:A:143:ARG:N	2.39	0.53
2:C:964:LEU:HD11	2:C:1025:PHE:CD1	2.44	0.53
2:C:990:ASP:OD1	2:C:991:LYS:N	2.40	0.53
3:D:412:LEU:HG	3:D:416:ILE:HD12	1.91	0.53
2:C:934:PHE:HB2	2:C:1051:LYS:HE3	1.91	0.52
1:A:16:ILE:HG12	1:A:26:VAL:HG22	1.91	0.52
1:B:74:VAL:HG22	1:B:132:HIS:O	2.09	0.52
2:C:1293:VAL:HG23	2:C:1294:LYS:HG3	1.91	0.52
1:A:86:LYS:NZ	2:C:824:GLN:O	2.37	0.52
2:C:629:PHE:CE2	2:C:650:VAL:HG21	2.43	0.52
2:C:802:VAL:HG22	2:C:1096:ILE:HD11	1.92	0.52
1:B:155:ALA:HB2	1:B:173:VAL:CA	2.39	0.52
2:C:360:LEU:HD13	2:C:360:LEU:O	2.08	0.52
5:F:124:GLU:OE1	5:F:128:ASN:ND2	2.42	0.52
2:C:1066:MET:SD	2:C:1076:ILE:HD11	2.49	0.52
3:D:169:LEU:O	3:D:173:GLY:N	2.42	0.52
2:C:263:VAL:HG21	2:C:269:ILE:HG13	1.91	0.52
5:F:428:SER:O	5:F:432:THR:OG1	2.17	0.52
1:A:51:MET:HG3	1:A:180:VAL:HG11	1.91	0.52
2:C:189:ASP:OD1	2:C:193:ASN:N	2.43	0.52
2:C:887:VAL:HB	2:C:913:VAL:HG12	1.92	0.52
2:C:1333:LEU:O	2:C:1333:LEU:HD13	2.10	0.52
3:D:134:ASP:O	3:D:138:VAL:HG23	2.09	0.52
3:D:1279:GLN:NE2	3:D:1281:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:479:THR:O	5:F:481:GLU:N	2.41	0.52
1:A:76:GLU:OE2	1:A:132:HIS:ND1	2.38	0.52
1:A:190:ALA:HB3	1:A:198:LEU:CB	2.40	0.52
1:A:191:ARG:NH1	1:A:196:THR:O	2.43	0.52
1:B:98:VAL:HG11	1:B:121:VAL:CG2	2.40	0.52
2:C:325:LEU:O	2:C:328:SER:OG	2.25	0.52
3:D:487:THR:HG21	4:E:4:VAL:HG12	1.92	0.52
6:G:83:SER:OG	11:G:301:CMP:O2P	2.24	0.52
1:B:93:GLN:N	1:B:120:ASP:O	2.41	0.52
2:C:69:GLN:N	2:C:101:ARG:O	2.39	0.52
3:D:64:PRO:O	3:D:98:ARG:NH1	2.43	0.52
3:D:649:LYS:CE	3:D:696:ALA:HB2	2.40	0.52
2:C:987:GLU:N	2:C:987:GLU:OE1	2.43	0.51
2:C:1329:GLU:CD	3:D:331:ILE:HD11	2.31	0.51
6:H:70:ILE:HG21	6:H:86:VAL:HG11	1.91	0.51
3:D:1319:PHE:O	3:D:1323:ALA:N	2.42	0.51
3:D:194:LEU:HD22	3:D:224:LEU:HD23	1.92	0.51
3:D:416:ILE:CD1	3:D:441:LEU:HD21	2.40	0.51
3:D:429:LEU:HD13	3:D:925:GLU:HG2	1.92	0.51
6:G:30:ILE:HG23	6:G:82:ARG:HH11	1.74	0.51
5:F:562:ARG:NH1	5:F:571:TYR:O	2.43	0.51
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.92	0.51
2:C:1017:GLN:O	2:C:1021:LEU:HD23	2.10	0.51
3:D:113:HIS:ND1	3:D:237:MET:O	2.43	0.51
3:D:678:ARG:O	3:D:682:VAL:HG23	2.09	0.51
3:D:1051:ASP:OD1	3:D:1106:ILE:HG21	2.10	0.51
3:D:1197:ASN:N	3:D:1210:ILE:O	2.42	0.51
1:A:31:LEU:N	1:A:199:ASP:O	2.40	0.51
2:C:483:ASP:OD1	2:C:484:LEU:N	2.44	0.51
2:C:893:THR:O	2:C:895:LEU:HD23	2.11	0.51
2:C:1251:TYR:OH	2:C:1301:ARG:NH1	2.44	0.51
5:F:385:ARG:NH2	7:1:71:DG:N7	2.58	0.51
2:C:802:VAL:HG13	2:C:1096:ILE:HD11	1.93	0.51
2:C:869:GLY:O	2:C:871:VAL:N	2.44	0.51
2:C:953:LEU:HB2	2:C:1036:ILE:HG21	1.93	0.51
3:D:201:LEU:HD22	3:D:217:LEU:HD22	1.92	0.51
2:C:979:LEU:HD11	2:C:1014:LEU:HD11	1.93	0.50
3:D:502:PRO:O	3:D:598:LYS:NZ	2.35	0.50
1:B:91:ARG:O	1:B:122:GLU:N	2.44	0.50
2:C:65:ASN:O	2:C:104:ILE:HG23	2.11	0.50
3:D:438:GLU:OE2	4:E:3:ARG:NH2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:GLU:O	1:B:25:LYS:N	2.39	0.50
1:B:64:VAL:HG13	1:B:169:GLY:HA2	1.94	0.50
2:C:59:ILE:CG2	2:C:479:LEU:HD13	2.41	0.50
2:C:400:VAL:O	2:C:404:LYS:HB2	2.11	0.50
2:C:734:ILE:HG23	2:C:749:ASP:HB2	1.94	0.50
3:D:902:ASP:O	3:D:906:GLY:N	2.43	0.50
3:D:952:VAL:HG13	3:D:1011:VAL:HG22	1.92	0.50
4:E:18:ASP:O	4:E:22:VAL:HG23	2.11	0.50
6:G:138:ASP:O	6:G:142:ARG:N	2.43	0.50
1:B:205:MET:SD	1:B:205:MET:N	2.85	0.50
2:C:725:GLN:N	2:C:733:VAL:O	2.43	0.50
7:1:56:DT:O4	8:2:34:DA:N6	2.44	0.50
1:A:17:GLU:OE2	1:A:27:THR:HG23	2.12	0.50
3:D:506:VAL:HG21	3:D:625:MET:HA	1.93	0.50
3:D:515:ARG:O	3:D:573:THR:HG21	2.11	0.50
6:G:41:TYR:O	6:G:95:ALA:N	2.39	0.50
2:C:728:ASP:OD1	2:C:729:ALA:N	2.44	0.50
2:C:1253:LEU:HD22	3:D:253:VAL:HG22	1.92	0.50
5:F:412:LEU:O	5:F:416:VAL:HG23	2.12	0.50
3:D:483:LEU:HD21	4:E:16:ARG:CB	2.42	0.50
2:C:985:GLU:HB2	2:C:989:LEU:HB2	1.92	0.49
4:E:19:LEU:CD1	4:E:54:ILE:HG21	2.42	0.49
6:G:75:LEU:HD21	6:G:102:PHE:CE2	2.46	0.49
1:A:58:GLU:O	1:A:145:LYS:N	2.44	0.49
5:F:228:TYR:CE1	5:F:252:LEU:HD11	2.48	0.49
6:G:15:LEU:HD22	6:G:43:VAL:HG22	1.93	0.49
6:G:181:GLU:CD	7:1:40:DC:H41	2.14	0.49
2:C:210:LEU:HD13	2:C:220:ILE:HG12	1.94	0.49
2:C:1312:ASN:OD1	4:E:28:ARG:NH1	2.45	0.49
5:F:541:ARG:NH2	5:F:565:ILE:HG23	2.27	0.49
2:C:1005:GLU:N	2:C:1005:GLU:OE1	2.43	0.49
6:H:55:GLU:N	6:H:55:GLU:OE1	2.46	0.49
6:H:84:ALA:HB3	11:H:301:CMP:H5'1	1.94	0.49
1:A:13:LEU:HD11	1:A:26:VAL:HG13	1.94	0.49
2:C:835:GLU:OE1	2:C:835:GLU:N	2.46	0.49
2:C:851:THR:O	2:C:887:VAL:HG13	2.13	0.49
3:D:818:GLU:CB	3:D:845:ALA:HB1	2.43	0.49
1:A:174:ASP:OD1	2:C:1059:ARG:NH1	2.46	0.49
2:C:208:ILE:HG23	2:C:209:ILE:H	1.78	0.49
2:C:757:THR:O	2:C:765:ILE:N	2.43	0.49
5:F:558:VAL:O	5:F:562:ARG:CB	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD23	1:B:101:THR:N	2.26	0.49
2:C:59:ILE:HG21	2:C:479:LEU:CD1	2.42	0.49
2:C:956:ALA:HB1	2:C:1032:LYS:HE2	1.95	0.49
3:D:973:LEU:HB3	3:D:1003:LEU:HD12	1.95	0.49
1:A:13:LEU:HD12	1:A:14:VAL:H	1.78	0.49
1:B:15:ASP:OD1	1:B:16:ILE:N	2.45	0.49
2:C:210:LEU:HD21	2:C:223:LEU:HD21	1.94	0.49
5:F:505:ILE:HG22	5:F:505:ILE:O	2.12	0.49
1:B:31:LEU:N	1:B:199:ASP:O	2.38	0.48
2:C:295:LYS:O	2:C:317:LEU:N	2.43	0.48
2:C:617:ALA:HB2	2:C:650:VAL:CG1	2.42	0.48
3:D:836:ARG:NE	3:D:870:ASP:OD1	2.41	0.48
5:F:571:TYR:HE2	5:F:576:VAL:HG22	1.78	0.48
2:C:217:THR:CG2	2:C:347:ILE:HG21	2.43	0.48
2:C:729:ALA:HB1	2:C:769:PRO:HD3	1.95	0.48
6:G:57:LYS:HG2	6:G:58:GLU:H	1.78	0.48
7:1:51:DC:H41	8:2:40:DG:H21	1.59	0.48
1:B:211:ILE:HG21	1:B:216:ALA:HB2	1.95	0.48
2:C:719:LYS:NZ	2:C:750:ILE:O	2.29	0.48
3:D:490:ILE:HG22	3:D:490:ILE:O	2.11	0.48
6:G:147:LEU:HD21	6:G:172:ILE:CD1	2.42	0.48
7:1:51:DC:N4	8:2:40:DG:H21	2.11	0.48
2:C:557:ARG:NH1	2:C:611:GLU:OE1	2.46	0.48
2:C:1040:ASP:OD1	2:C:1048:LYS:NZ	2.34	0.48
2:C:42:ASP:OD2	2:C:47:TYR:N	2.46	0.48
2:C:292:ILE:HD13	2:C:322:LEU:HD13	1.95	0.48
2:C:1151:LEU:HD11	2:C:1201:LEU:HD22	1.96	0.48
2:C:1261:GLY:O	2:C:1266:GLY:N	2.46	0.48
3:D:1333:THR:OG1	3:D:1334:GLU:N	2.47	0.48
6:G:173:GLY:O	6:G:177:GLY:N	2.37	0.48
2:C:176:ILE:N	2:C:208:ILE:HD11	2.29	0.48
7:1:33:DT:H3	8:2:58:DA:H61	1.60	0.48
2:C:693:LEU:HD22	2:C:1057:LYS:NZ	2.28	0.48
3:D:1058:SER:HB2	3:D:1107:VAL:HB	1.95	0.48
1:A:71:LYS:NZ	2:C:928:VAL:O	2.28	0.48
1:B:54:CYS:HB2	1:B:91:ARG:HA	1.96	0.48
1:B:65:LEU:O	1:B:171:LEU:HD21	2.14	0.48
2:C:565:GLU:HG2	3:D:783:LEU:HD21	1.95	0.48
3:D:211:GLU:O	3:D:214:ARG:N	2.46	0.48
5:F:471:LEU:HD12	5:F:478:PRO:HD3	1.94	0.48
6:G:196:ILE:HD12	6:G:204:VAL:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:555:TYR:OH	2:C:654:ASP:OD2	2.23	0.47
2:C:950:GLU:OE2	6:G:19:HIS:CA	2.61	0.47
3:D:204:GLU:OE2	3:D:217:LEU:HD13	2.13	0.47
3:D:259:ARG:HG2	5:F:505:ILE:HD12	1.95	0.47
6:G:43:VAL:N	6:G:93:GLU:O	2.47	0.47
2:C:461:GLU:N	2:C:461:GLU:OE1	2.47	0.47
3:D:535:ARG:O	3:D:539:SER:OG	2.32	0.47
3:D:603:LYS:O	3:D:607:THR:HG23	2.14	0.47
5:F:124:GLU:O	5:F:128:ASN:ND2	2.48	0.47
2:C:562:GLU:OE2	2:C:687:ARG:NE	2.47	0.47
2:C:759:SER:OG	2:C:763:THR:N	2.42	0.47
2:C:921:PRO:O	2:C:924:VAL:HG23	2.15	0.47
5:F:380:VAL:CG2	5:F:416:VAL:HG21	2.43	0.47
2:C:942:ASP:O	2:C:945:ALA:HB3	2.14	0.47
3:D:844:THR:HG21	3:D:858:VAL:HG11	1.96	0.47
2:C:243:PRO:HG3	2:C:283:LYS:HZ1	1.80	0.47
2:C:944:ARG:HA	2:C:947:GLU:HB2	1.97	0.47
3:D:172:PHE:O	3:D:174:ASP:N	2.47	0.47
3:D:579:LEU:CD2	3:D:582:ILE:HD12	2.43	0.47
3:D:1292:LEU:O	3:D:1294:ALA:N	2.48	0.47
3:D:574:VAL:HG12	3:D:578:ILE:HD12	1.97	0.47
3:D:1076:PRO:O	3:D:1101:LEU:N	2.47	0.47
3:D:1320:ILE:HG22	3:D:1352:ILE:HD12	1.96	0.47
5:F:330:LEU:HD12	5:F:330:LEU:O	2.14	0.47
6:G:47:VAL:HG21	6:G:86:VAL:HG12	1.95	0.47
2:C:128:PRO:HB3	2:C:138:ILE:HD11	1.96	0.47
2:C:243:PRO:CB	2:C:274:ILE:HG23	2.45	0.47
2:C:263:VAL:HG21	2:C:269:ILE:CG1	2.45	0.47
2:C:344:GLY:O	2:C:346:TYR:N	2.46	0.47
2:C:818:VAL:HG23	2:C:1096:ILE:HG22	1.96	0.47
2:C:1033:ARG:HE	6:G:12:GLU:CD	2.17	0.47
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.97	0.47
5:F:164:GLY:HA2	5:F:263:PRO:HD2	1.97	0.47
6:H:39:LEU:N	6:H:97:ILE:O	2.44	0.47
1:A:97:GLU:HA	1:A:148:ARG:HB3	1.97	0.47
1:A:167:PRO:O	1:A:168:ILE:HG23	2.14	0.47
1:B:10:LYS:O	1:B:12:ARG:NH1	2.48	0.47
2:C:68:LEU:HD13	2:C:489:PRO:HB3	1.96	0.47
2:C:1311:GLY:HA3	4:E:32:VAL:HG22	1.97	0.47
3:D:820:ILE:HG23	3:D:884:SER:HB2	1.95	0.47
1:B:104:LYS:HB3	1:B:140:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:310:ILE:HG23	2:C:324:LYS:HD3	1.97	0.47
1:A:133:LEU:HD21	1:A:140:ILE:HB	1.96	0.47
2:C:1238:LEU:O	2:C:1241:ASP:N	2.48	0.47
3:D:1318:SER:OG	3:D:1342:ASP:OD2	2.20	0.47
5:F:441:ARG:NH1	7:1:63:DG:N7	2.63	0.47
1:A:16:ILE:HG23	1:A:213:PRO:HG3	1.97	0.46
2:C:184:LEU:HG	2:C:208:ILE:HG13	1.97	0.46
2:C:773:LEU:HD13	2:C:774:GLY:N	2.31	0.46
5:F:558:VAL:HG11	5:F:587:ILE:CG2	2.45	0.46
2:C:436:ARG:NH1	2:C:437:ASN:OD1	2.48	0.46
2:C:1333:LEU:HD22	3:D:307:LEU:HD22	1.97	0.46
1:B:179:PRO:O	1:B:207:THR:OG1	2.30	0.46
2:C:241:LEU:H	2:C:283:LYS:HB3	1.80	0.46
1:A:45:ARG:NE	1:B:38:THR:OG1	2.47	0.46
2:C:95:PRO:HA	2:C:126:GLU:HA	1.96	0.46
2:C:823:VAL:HG22	2:C:1060:ILE:HD11	1.98	0.46
3:D:301:GLU:OE2	3:D:312:ARG:NH2	2.48	0.46
3:D:1040:MET:HE3	3:D:1061:VAL:HG22	1.97	0.46
3:D:1077:ALA:HB2	3:D:1100:PHE:HA	1.97	0.46
6:H:50:LEU:HD21	6:H:87:ARG:HD3	1.97	0.46
2:C:700:VAL:HG12	2:C:1117:LEU:HD23	1.97	0.46
3:D:497:GLU:OE1	3:D:497:GLU:N	2.48	0.46
1:A:203:ILE:HG23	1:A:203:ILE:O	2.15	0.46
1:B:133:LEU:HD13	1:B:138:ALA:O	2.15	0.46
2:C:360:LEU:HD21	2:C:378:ARG:CD	2.45	0.46
3:D:495:ASN:OD1	3:D:495:ASN:N	2.47	0.46
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.98	0.46
1:A:59:VAL:HG21	1:A:82:LEU:CD2	2.46	0.46
2:C:149:LEU:HD13	2:C:450:ASN:HA	1.97	0.46
2:C:674:ASP:OD2	2:C:1070:HIS:ND1	2.49	0.46
2:C:1160:ASP:OD1	2:C:1161:LEU:N	2.49	0.46
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.97	0.46
3:D:646:ILE:HG23	3:D:646:ILE:O	2.15	0.46
2:C:24:VAL:HG12	2:C:578:TYR:HE1	1.79	0.46
2:C:1333:LEU:CD2	3:D:307:LEU:HD22	2.45	0.46
5:F:400:GLN:O	5:F:404:LEU:HD13	2.16	0.46
1:B:155:ALA:HB2	1:B:173:VAL:N	2.30	0.46
2:C:394:ARG:O	2:C:396:ASP:N	2.49	0.46
6:H:36:ALA:HB2	6:H:82:ARG:NE	2.31	0.46
1:A:51:MET:HG2	1:A:180:VAL:HG11	1.97	0.46
1:A:190:ALA:HB2	1:A:200:LYS:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1308:ILE:HG22	2:C:1313:HIS:HD2	1.81	0.46
3:D:597:GLY:O	3:D:600:ALA:HB3	2.16	0.46
1:A:15:ASP:OD1	1:A:16:ILE:N	2.49	0.45
1:B:155:ALA:HB2	1:B:173:VAL:C	2.36	0.45
2:C:577:VAL:N	2:C:661:VAL:O	2.49	0.45
3:D:124:ILE:HD11	3:D:189:LEU:HD21	1.98	0.45
3:D:1072:LYS:HG2	3:D:1169:THR:HG21	1.98	0.45
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.98	0.45
3:D:1342:ASP:OD1	3:D:1343:GLU:N	2.49	0.45
2:C:318:SER:OG	2:C:320:ASP:OD1	2.28	0.45
2:C:460:ALA:HB2	2:C:506:PHE:HZ	1.81	0.45
3:D:527:LEU:HD13	3:D:550:VAL:HG12	1.98	0.45
4:E:6:VAL:HG12	4:E:6:VAL:O	2.16	0.45
6:G:49:VAL:HG23	6:G:64:LEU:HD13	1.98	0.45
6:G:196:ILE:HD11	6:G:202:THR:CG2	2.47	0.45
6:H:50:LEU:HD11	6:H:87:ARG:HD3	1.98	0.45
2:C:243:PRO:HA	2:C:246:LEU:HD21	1.97	0.45
3:D:580:TRP:CE3	3:D:583:VAL:HG21	2.52	0.45
4:E:42:GLU:OE1	4:E:52:ARG:NH1	2.49	0.45
5:F:387:VAL:HG23	5:F:412:LEU:HD22	1.97	0.45
6:H:60:ILE:HD13	6:H:174:GLN:HA	1.97	0.45
1:B:110:VAL:O	1:B:130:ILE:N	2.50	0.45
2:C:210:LEU:O	2:C:214:ASN:N	2.50	0.45
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.98	0.45
3:D:1229:VAL:O	3:D:1233:ILE:HD12	2.16	0.45
6:G:47:VAL:CG2	6:G:86:VAL:HG12	2.47	0.45
1:A:168:ILE:HD12	2:C:876:GLU:C	2.37	0.45
1:A:207:THR:OG1	1:A:208:ASN:O	2.21	0.45
2:C:60:GLN:HB3	2:C:67:GLU:HB3	1.99	0.45
3:D:142:GLU:HB3	3:D:159:ILE:HD13	1.99	0.45
5:F:265:GLN:O	5:F:269:LEU:HD13	2.16	0.45
6:G:75:LEU:HD11	6:G:102:PHE:HD2	1.81	0.45
1:B:152:TYR:OH	1:B:180:VAL:O	2.35	0.45
2:C:164:THR:OG1	2:C:167:SER:OG	1.99	0.45
3:D:482:ALA:HA	4:E:6:VAL:HG21	1.98	0.45
3:D:950:ILE:O	3:D:1017:VAL:HG21	2.16	0.45
1:B:104:LYS:NZ	1:B:131:CYS:SG	2.89	0.45
2:C:30:ILE:HD12	2:C:455:SER:HB3	1.97	0.45
2:C:411:ARG:HE	2:C:412:GLU:H	1.63	0.45
2:C:699:LEU:HD22	2:C:1121:ALA:HB1	1.99	0.45
3:D:331:ILE:HD12	3:D:331:ILE:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:559:ALA:O	3:D:561:GLY:N	2.49	0.45
5:F:559:LEU:HD11	5:F:594:ALA:CB	2.47	0.45
6:H:145:GLN:O	6:H:149:ASN:ND2	2.49	0.45
1:A:100:LEU:HD12	1:A:146:VAL:CG2	2.47	0.45
2:C:378:ARG:HA	2:C:378:ARG:NE	2.32	0.45
5:F:379:MET:HG3	5:F:416:VAL:HG22	1.99	0.45
1:A:69:SER:H	2:C:927:THR:HG23	1.81	0.45
1:B:207:THR:OG1	1:B:208:ASN:N	2.50	0.45
2:C:146:VAL:HG12	2:C:511:LEU:HD22	1.98	0.45
2:C:155:VAL:HB	2:C:436:ARG:HD2	1.99	0.45
2:C:599:VAL:CG2	2:C:623:LEU:HD13	2.46	0.45
3:D:320:ASN:OD1	3:D:321:LYS:N	2.50	0.45
3:D:608:CYS:SG	3:D:612:LEU:HD12	2.57	0.45
5:F:119:ILE:HG22	5:F:123:ILE:HD12	1.97	0.45
5:F:320:ILE:HG22	5:F:320:ILE:O	2.17	0.45
3:D:147:ILE:N	3:D:177:ASP:O	2.50	0.45
3:D:690:ASN:HB2	3:D:743:MET:SD	2.57	0.45
3:D:845:ALA:HA	3:D:883:ARG:HG3	1.98	0.45
1:B:103:ASN:HA	1:B:141:SER:HA	1.98	0.44
2:C:82:VAL:HG22	2:C:137:VAL:HG21	1.98	0.44
2:C:296:VAL:HG11	2:C:336:LEU:HD11	1.99	0.44
2:C:360:LEU:HD21	2:C:378:ARG:HD3	1.99	0.44
2:C:848:GLU:HG2	2:C:888:THR:HG22	1.98	0.44
2:C:950:GLU:OE1	6:G:20:ILE:HG13	2.17	0.44
2:C:1002:LEU:HD13	2:C:1011:LEU:HD11	1.98	0.44
5:F:437:GLN:HG2	7:1:65:DT:H73	1.99	0.44
1:A:16:ILE:HD11	1:A:214:GLU:CB	2.40	0.44
1:B:178:SER:OG	1:B:180:VAL:HG22	2.17	0.44
2:C:186:PHE:CG	2:C:194:LEU:HD11	2.52	0.44
2:C:196:VAL:HG11	2:C:206:ALA:HB3	1.99	0.44
2:C:1276:TRP:CG	3:D:801:VAL:HG11	2.52	0.44
3:D:675:ALA:O	3:D:679:TYR:N	2.37	0.44
3:D:953:LYS:HB2	3:D:984:LEU:HB3	1.98	0.44
3:D:1290:ARG:NH2	3:D:1291:GLU:OE2	2.50	0.44
5:F:141:ILE:HD11	5:F:269:LEU:HG	1.99	0.44
6:H:146:THR:OG1	6:H:176:VAL:HG21	2.17	0.44
1:A:55:ALA:HB1	1:A:147:GLN:HB2	1.99	0.44
2:C:448:LEU:HB2	2:C:558:VAL:HG22	1.99	0.44
2:C:465:ARG:HG2	2:C:468:LEU:HD12	1.99	0.44
2:C:934:PHE:N	2:C:1049:ILE:O	2.49	0.44
3:D:124:ILE:HD11	3:D:189:LEU:HD11	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:156:ARG:CD	3:D:188:LEU:HD12	2.48	0.44
3:D:840:LEU:HD22	3:D:866:GLU:OE2	2.17	0.44
1:B:74:VAL:HG13	1:B:132:HIS:O	2.17	0.44
2:C:759:SER:N	2:C:763:THR:O	2.50	0.44
3:D:123:ARG:HG3	3:D:1337:VAL:HG11	2.00	0.44
3:D:256:ASP:OD1	3:D:257:GLY:N	2.49	0.44
3:D:690:ASN:HB2	3:D:743:MET:HG3	1.99	0.44
5:F:415:ALA:HB2	5:F:431:ALA:HA	1.98	0.44
6:G:20:ILE:HD13	6:G:43:VAL:HG21	1.98	0.44
1:B:85:LEU:HD21	1:B:130:ILE:HG23	2.00	0.44
2:C:617:ALA:HB2	2:C:650:VAL:HG11	1.98	0.44
3:D:97:VAL:O	3:D:101:ARG:N	2.42	0.44
6:G:133:ASN:OD1	6:G:137:LEU:HD22	2.18	0.44
6:G:147:LEU:HD22	6:G:204:VAL:HG21	1.99	0.44
3:D:137:ARG:C	3:D:159:ILE:HD11	2.37	0.44
1:B:135:ASP:OD1	1:B:136:GLU:N	2.51	0.44
2:C:122:VAL:HG22	2:C:490:GLN:HB2	2.00	0.44
3:D:813:ASP:OD1	3:D:883:ARG:NH2	2.50	0.44
5:F:428:SER:OG	7:1:70:DT:O4	2.33	0.44
5:F:562:ARG:HA	5:F:571:TYR:HB3	1.99	0.44
3:D:614:LEU:HD23	3:D:614:LEU:H	1.83	0.44
6:G:60:ILE:HD13	6:G:63:TYR:CE1	2.52	0.44
1:A:67:GLU:OE1	2:C:876:GLU:HA	2.18	0.44
1:B:111:THR:HG22	1:B:127:GLN:O	2.18	0.44
2:C:277:LEU:HG	2:C:283:LYS:NZ	2.33	0.44
2:C:805:MET:N	2:C:1098:LEU:O	2.48	0.44
2:C:998:LEU:HD21	2:C:1014:LEU:HD22	2.00	0.44
3:D:768:ASN:OD1	3:D:769:VAL:N	2.50	0.44
1:B:210:THR:O	1:B:211:ILE:HD13	2.18	0.43
3:D:716:GLN:HE21	3:D:717:VAL:HG22	1.82	0.43
3:D:1027:VAL:HG12	3:D:1099:TYR:CD2	2.53	0.43
3:D:1111:ASP:OD1	3:D:1112:GLY:N	2.51	0.43
3:D:1306:LEU:O	3:D:1307:LEU:HB2	2.18	0.43
1:B:12:ARG:O	1:B:14:VAL:HG23	2.18	0.43
2:C:303:ASP:HA	2:C:328:SER:HB2	2.00	0.43
2:C:599:VAL:HG23	2:C:623:LEU:HD13	2.00	0.43
1:A:179:PRO:O	1:A:207:THR:HG22	2.18	0.43
2:C:42:ASP:O	2:C:46:GLN:NE2	2.44	0.43
2:C:109:ALA:HB1	2:C:110:PRO:HD2	2.01	0.43
3:D:20:ILE:HB	3:D:1341:ARG:HG2	2.00	0.43
3:D:826:ILE:HG22	3:D:831:VAL:CA	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:902:ASP:HB2	3:D:909:ILE:HA	2.00	0.43
3:D:1241:TYR:CD1	3:D:1246:VAL:HG11	2.52	0.43
2:C:66:SER:CB	2:C:484:LEU:HB3	2.48	0.43
2:C:256:GLU:HA	2:C:261:VAL:HA	2.00	0.43
2:C:838:CYS:HB3	2:C:1050:VAL:HB	2.00	0.43
2:C:1067:ALA:O	2:C:1233:LEU:N	2.41	0.43
2:C:1101:LEU:HD11	3:D:504:GLN:CD	2.39	0.43
3:D:679:TYR:CE2	3:D:756:GLU:HB2	2.54	0.43
3:D:1047:THR:OG1	3:D:1062:LEU:HD11	2.17	0.43
3:D:1226:VAL:O	3:D:1230:THR:HG22	2.18	0.43
2:C:230:PHE:HB2	2:C:333:ILE:HB	2.00	0.43
2:C:320:ASP:OD1	2:C:321:LEU:N	2.51	0.43
2:C:594:VAL:HG22	2:C:599:VAL:HG22	1.99	0.43
2:C:621:SER:HB2	2:C:629:PHE:HD1	1.83	0.43
2:C:1033:ARG:NE	6:G:12:GLU:HG3	2.33	0.43
3:D:483:LEU:HD21	4:E:16:ARG:HB2	1.99	0.43
6:G:50:LEU:O	6:G:84:ALA:HB1	2.18	0.43
6:G:167:ILE:HG22	6:G:202:THR:HB	2.01	0.43
2:C:552:PRO:HA	2:C:554:HIS:HD1	1.84	0.43
4:E:44:ASP:OD2	4:E:48:VAL:HG11	2.18	0.43
1:B:155:ALA:HB1	1:B:172:LEU:HD23	1.99	0.43
2:C:946:LEU:O	2:C:950:GLU:HG2	2.18	0.43
3:D:115:TRP:CZ2	3:D:1329:THR:HG23	2.54	0.43
3:D:915:ILE:HD12	3:D:916:GLY:N	2.33	0.43
1:A:74:VAL:HG12	1:A:76:GLU:N	2.34	0.43
2:C:124:MET:HB3	2:C:493:ILE:HG21	2.01	0.43
2:C:676:ALA:O	2:C:680:LEU:HB2	2.19	0.43
2:C:871:VAL:HG12	2:C:871:VAL:O	2.18	0.43
3:D:527:LEU:HB2	3:D:550:VAL:HG12	2.00	0.43
3:D:1004:ALA:N	3:D:1017:VAL:O	2.44	0.43
3:D:1164:SER:N	3:D:1176:VAL:O	2.45	0.43
5:F:471:LEU:O	5:F:475:GLY:N	2.45	0.43
7:1:53:DT:H2'	7:1:54:DC:O4'	2.18	0.43
1:B:61:ILE:O	1:B:64:VAL:HG12	2.19	0.43
2:C:547:VAL:HG12	2:C:547:VAL:O	2.19	0.43
2:C:979:LEU:N	2:C:979:LEU:HD12	2.33	0.43
3:D:212:THR:HA	3:D:215:LYS:HG3	2.00	0.43
3:D:531:LYS:O	3:D:534:GLU:HG3	2.19	0.43
3:D:864:LEU:HD22	3:D:868:TRP:HB3	2.01	0.43
5:F:562:ARG:NH1	5:F:562:ARG:O	2.43	0.43
5:F:576:VAL:HG11	5:F:587:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:138:ASP:OD1	6:G:139:VAL:N	2.47	0.43
6:H:29:LEU:N	6:H:86:VAL:O	2.47	0.43
1:B:158:ARG:O	1:B:161:SER:OG	2.13	0.43
2:C:816:ILE:HD11	2:C:1074:GLY:HA3	2.01	0.43
2:C:1033:ARG:NH2	2:C:1034:ARG:NH2	2.66	0.43
2:C:1116:HIS:CB	2:C:1195:ILE:HG21	2.47	0.43
3:D:884:SER:N	3:D:887:SER:HG	2.17	0.43
3:D:1234:VAL:HA	3:D:1237:VAL:HG12	2.01	0.43
1:B:133:LEU:HD22	1:B:138:ALA:HB1	2.00	0.42
2:C:10:ARG:HA	2:C:1176:LEU:HD21	2.01	0.42
2:C:91:THR:HG23	2:C:138:ILE:HD12	2.00	0.42
2:C:676:ALA:HA	3:D:772:TYR:CZ	2.54	0.42
3:D:612:LEU:HD13	3:D:616:PRO:HB2	2.01	0.42
3:D:951:GLN:HB3	3:D:984:LEU:HD11	2.00	0.42
5:F:138:PRO:HB3	5:F:353:LEU:HD13	2.01	0.42
2:C:210:LEU:O	2:C:215:TYR:N	2.52	0.42
2:C:257:ALA:HB1	2:C:282:VAL:HG21	2.01	0.42
2:C:616:ILE:HG22	2:C:617:ALA:O	2.19	0.42
2:C:673:HIS:O	2:C:1110:GLY:N	2.52	0.42
2:C:1066:MET:O	2:C:1074:GLY:N	2.52	0.42
2:C:1068:GLY:N	2:C:1072:ASN:OD1	2.51	0.42
2:C:1068:GLY:HA2	2:C:1232:MET:HA	2.01	0.42
2:C:1253:LEU:O	2:C:1256:GLN:NE2	2.52	0.42
3:D:816:THR:HG21	3:D:889:ASP:CB	2.49	0.42
1:A:35:PHE:HD1	1:B:224:LEU:HD13	1.84	0.42
2:C:137:VAL:O	2:C:138:ILE:HD13	2.20	0.42
2:C:371:ARG:HB3	2:C:374:GLU:HB3	2.01	0.42
3:D:808:VAL:HG13	3:D:911:LYS:HD3	2.02	0.42
6:G:75:LEU:HD11	6:G:102:PHE:CD2	2.54	0.42
1:B:76:GLU:OE1	1:B:132:HIS:N	2.52	0.42
2:C:131:THR:OG1	2:C:135:THR:N	2.53	0.42
2:C:519:ASN:ND2	2:C:686:GLN:O	2.52	0.42
2:C:770:CYS:HB2	2:C:791:LEU:HD23	2.01	0.42
2:C:786:GLY:N	2:C:789:THR:OG1	2.53	0.42
2:C:798:GLN:NE2	2:C:827:ARG:O	2.52	0.42
3:D:1329:THR:O	3:D:1333:THR:HG23	2.19	0.42
5:F:276:MET:O	5:F:279:ARG:NH1	2.47	0.42
1:A:91:ARG:HG3	1:A:210:THR:HG23	2.01	0.42
1:B:20:SER:OG	1:B:21:SER:N	2.52	0.42
2:C:843:THR:HB	2:C:846:GLY:O	2.19	0.42
2:C:964:LEU:HD11	2:C:1025:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1322:SER:O	2:C:1326:LEU:HG	2.19	0.42
3:D:1107:VAL:HG22	3:D:1121:LEU:C	2.40	0.42
3:D:1155:ILE:HD13	3:D:1158:GLU:OE2	2.19	0.42
6:G:15:LEU:CD2	6:G:43:VAL:HG22	2.50	0.42
6:G:142:ARG:HB3	6:G:176:VAL:HG13	2.02	0.42
6:H:30:ILE:HD12	6:H:86:VAL:HG21	2.02	0.42
3:D:24:LEU:HD13	3:D:237:MET:N	2.35	0.42
3:D:1046:ILE:HG22	3:D:1061:VAL:HA	2.02	0.42
6:G:49:VAL:HG12	6:G:50:LEU:N	2.34	0.42
6:H:147:LEU:HD23	6:H:150:LEU:HD12	2.02	0.42
1:A:153:VAL:HG22	1:A:154:PRO:HD3	2.01	0.42
1:B:159:ILE:HD12	1:B:166:ARG:NH2	2.35	0.42
2:C:122:VAL:HG13	2:C:490:GLN:CG	2.50	0.42
2:C:428:VAL:O	2:C:432:LEU:HD13	2.20	0.42
6:H:84:ALA:HB3	11:H:301:CMP:C5'	2.50	0.42
1:B:211:ILE:HG22	1:B:212:ASP:O	2.20	0.42
2:C:269:ILE:HG23	2:C:273:HIS:HB3	2.01	0.42
3:D:34:SER:HG	3:D:104:HIS:CG	2.33	0.42
3:D:103:GLY:O	3:D:244:VAL:N	2.47	0.42
6:G:188:LYS:NZ	6:G:191:GLU:OE2	2.41	0.42
1:A:25:LYS:HG2	1:A:26:VAL:N	2.35	0.42
1:A:79:LEU:HD12	2:C:1057:LYS:HG2	2.02	0.42
1:B:201:LEU:HD21	1:B:203:ILE:HD11	2.01	0.42
1:A:146:VAL:CG1	1:A:147:GLN:H	2.32	0.41
2:C:243:PRO:HB3	2:C:274:ILE:HG23	2.02	0.41
2:C:401:GLY:O	2:C:404:LYS:N	2.52	0.41
2:C:577:VAL:HG23	2:C:661:VAL:HG23	2.02	0.41
2:C:1033:ARG:NE	6:G:12:GLU:CG	2.83	0.41
3:D:736:GLN:O	3:D:740:LEU:HD13	2.20	0.41
5:F:576:VAL:HG21	5:F:587:ILE:HG21	2.02	0.41
2:C:733:VAL:HG22	2:C:750:ILE:HG13	2.02	0.41
5:F:117:ILE:HG23	5:F:421:TYR:CB	2.50	0.41
2:C:966:ILE:HG13	2:C:967:LEU:N	2.36	0.41
2:C:1101:LEU:HD11	3:D:504:GLN:NE2	2.35	0.41
2:C:1258:PRO:O	3:D:346:ARG:NH1	2.52	0.41
1:B:100:LEU:HD21	1:B:115:ILE:HB	2.02	0.41
1:B:185:TYR:HB2	1:B:201:LEU:HD11	2.01	0.41
3:D:132:LEU:O	3:D:135:ILE:N	2.53	0.41
3:D:226:ALA:O	3:D:230:SER:CB	2.68	0.41
3:D:1297:LYS:HZ1	3:D:1301:THR:HG23	1.86	0.41
2:C:516:ASP:OD2	2:C:522:SER:OG	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:932:GLN:CG	2:C:1051:LYS:HD2	2.51	0.41
2:C:1146:GLN:NE2	2:C:1150:ASP:OD2	2.54	0.41
3:D:357:VAL:HG22	3:D:461:PHE:CE2	2.55	0.41
5:F:279:ARG:HG2	5:F:280:VAL:HG23	2.03	0.41
6:H:46:SER:OG	6:H:65:ASN:ND2	2.53	0.41
1:A:152:TYR:OH	2:C:1083:GLU:OE2	2.38	0.41
2:C:102:LEU:HG	2:C:104:ILE:HD11	2.02	0.41
2:C:853:ASP:OD1	2:C:854:ILE:N	2.54	0.41
2:C:1322:SER:OG	3:D:342:LEU:HD13	2.20	0.41
2:C:1335:ILE:HG21	3:D:1336:ALA:HB1	2.03	0.41
3:D:839:VAL:HG13	3:D:864:LEU:HD12	2.03	0.41
3:D:1157:ALA:HA	3:D:1210:ILE:HD11	2.02	0.41
5:F:526:THR:O	5:F:526:THR:HG23	2.21	0.41
6:H:196:ILE:CD1	6:H:204:VAL:HG22	2.50	0.41
2:C:296:VAL:HG21	2:C:338:THR:HB	2.03	0.41
2:C:525:THR:HA	2:C:528:ARG:HB2	2.03	0.41
2:C:1103:VAL:HG22	2:C:1111:GLN:HE22	1.86	0.41
3:D:209:ASN:HA	3:D:214:ARG:HG3	2.03	0.41
3:D:1088:VAL:O	3:D:1097:ALA:HB3	2.21	0.41
7:1:24:DA:C2	8:2:68:DA:C2	3.09	0.41
2:C:67:GLU:O	2:C:102:LEU:HD12	2.21	0.41
2:C:310:ILE:O	2:C:321:LEU:HD22	2.20	0.41
2:C:935:THR:HG23	2:C:1042:LEU:HD11	2.02	0.41
3:D:214:ARG:HH12	3:D:218:THR:HG23	1.85	0.41
3:D:371:LYS:HG2	3:D:372:MET:HE2	2.03	0.41
3:D:1157:ALA:CA	3:D:1210:ILE:HD11	2.51	0.41
5:F:390:ILE:HD12	5:F:435:ILE:HD13	2.03	0.41
8:2:22:DT:C2	8:2:23:DT:H73	2.56	0.41
1:A:6:THR:HG22	1:A:7:GLU:N	2.36	0.41
1:A:84:ASN:O	1:A:128:HIS:NE2	2.54	0.41
1:A:190:ALA:HB3	1:A:198:LEU:HB2	2.02	0.41
2:C:629:PHE:CD2	2:C:650:VAL:HG21	2.55	0.41
3:D:48:THR:O	3:D:50:LYS:N	2.53	0.41
3:D:68:TYR:OH	3:D:81:ARG:NH1	2.54	0.41
3:D:950:ILE:C	3:D:1017:VAL:HG21	2.41	0.41
3:D:1029:THR:N	3:D:1119:ASP:O	2.46	0.41
3:D:1241:TYR:HD1	3:D:1246:VAL:HG11	1.86	0.41
3:D:1320:ILE:HD12	3:D:1342:ASP:OD2	2.21	0.41
6:G:72:GLU:O	6:G:75:LEU:HB3	2.21	0.41
6:G:114:MET:SD	6:H:103:ARG:NH1	2.94	0.41
6:G:180:ARG:HG3	6:G:181:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:HD12	1:B:140:ILE:HA	2.01	0.41
2:C:700:VAL:HG23	2:C:1069:ARG:NH2	2.35	0.41
2:C:1291:LEU:HD23	3:D:342:LEU:O	2.21	0.41
3:D:156:ARG:HG2	3:D:157:GLN:N	2.36	0.41
2:C:100:LEU:HD12	2:C:122:VAL:HG21	2.02	0.40
2:C:445:ILE:HD12	2:C:445:ILE:H	1.86	0.40
2:C:621:SER:HB2	2:C:629:PHE:CD1	2.55	0.40
3:D:1080:ILE:HD11	3:D:1121:LEU:HD21	2.03	0.40
3:D:1140:ARG:NH2	3:D:1236:GLU:OE2	2.54	0.40
3:D:1234:VAL:HG12	3:D:1253:ILE:HG22	2.03	0.40
1:B:54:CYS:HA	1:B:148:ARG:HA	2.03	0.40
1:B:65:LEU:HA	1:B:168:ILE:HG22	2.03	0.40
2:C:624:ASP:CB	2:C:630:VAL:HG22	2.51	0.40
2:C:845:LEU:HD13	2:C:890:LYS:C	2.41	0.40
3:D:97:VAL:HG21	3:D:101:ARG:CZ	2.51	0.40
3:D:138:VAL:HG13	3:D:145:VAL:HG21	2.03	0.40
3:D:707:ILE:N	3:D:714:GLU:O	2.49	0.40
3:D:950:ILE:HD12	3:D:1003:LEU:HD11	2.03	0.40
3:D:975:ILE:O	3:D:1000:GLY:N	2.50	0.40
2:C:86:GLN:HA	2:C:140:GLY:HA2	2.03	0.40
2:C:297:VAL:HB	2:C:317:LEU:HD21	2.03	0.40
2:C:617:ALA:HA	2:C:636:CYS:HA	2.03	0.40
2:C:808:ASN:OD1	2:C:1216:ARG:NH2	2.54	0.40
3:D:513:MET:O	3:D:515:ARG:N	2.52	0.40
6:H:36:ALA:HB2	6:H:82:ARG:HE	1.85	0.40
7:1:21:DC:H2"	7:1:22:DC:C6	2.56	0.40
3:D:1034:PHE:O	3:D:1081:VAL:N	2.38	0.40
1:A:153:VAL:HG13	1:A:154:PRO:CD	2.52	0.40
2:C:56:VAL:HG11	2:C:472:GLU:OE2	2.22	0.40
2:C:246:LEU:HD12	2:C:269:ILE:HG12	2.02	0.40
2:C:616:ILE:O	2:C:637:ARG:N	2.55	0.40
3:D:574:VAL:HG12	3:D:578:ILE:CD1	2.50	0.40
5:F:558:VAL:HG11	5:F:587:ILE:HG23	2.03	0.40
6:G:185:ARG:NH2	8:2:51:DG:N7	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	192 (84%)	30 (13%)	6 (3%)	5	34
1	B	226/329 (69%)	205 (91%)	21 (9%)	0	100	100
2	C	1330/1342 (99%)	1158 (87%)	161 (12%)	11 (1%)	19	60
3	D	1331/1407 (95%)	1155 (87%)	170 (13%)	6 (0%)	29	68
4	E	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	478/628 (76%)	418 (87%)	56 (12%)	4 (1%)	19	60
6	G	195/210 (93%)	181 (93%)	14 (7%)	0	100	100
6	H	195/210 (93%)	178 (91%)	16 (8%)	1 (0%)	29	68
All	All	4060/4546 (89%)	3561 (88%)	471 (12%)	28 (1%)	26	62

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	SER
2	C	339	ASN
2	C	860	ALA
2	C	861	ALA
2	C	872	TYR
3	D	673	VAL
5	F	262	VAL
2	C	870	ILE
5	F	263	PRO
6	H	168	THR
1	A	147	GLN
1	A	153	VAL
1	A	167	PRO
2	C	151	ARG
2	C	208	ILE
1	A	148	ARG
3	D	121	PRO

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Mol	Chain	Res	Type
3	D	1307	LEU
5	F	566	ASP
1	A	149	GLY
2	C	857	VAL
3	D	212	THR
3	D	514	THR
3	D	674	THR
5	F	507	MET
2	C	404	LYS
2	C	855	PRO
2	C	873	ILE

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%)	196 (100%)	0	100	100
2	C	1150/1157 (99%)	1134 (99%)	16 (1%)	67	81
3	D	1120/1168 (96%)	1106 (99%)	14 (1%)	69	82
4	E	67/75 (89%)	66 (98%)	1 (2%)	65	80
5	F	428/554 (77%)	421 (98%)	7 (2%)	62	79
6	G	170/181 (94%)	167 (98%)	3 (2%)	59	77
6	H	170/181 (94%)	169 (99%)	1 (1%)	86	92
All	All	3499/3888 (90%)	3454 (99%)	45 (1%)	70	82

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	33	ARG
1	A	179	PRO
2	C	130	MET

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Mol	Chain	Res	Type
2	C	239	MET
2	C	258	ASN
2	C	339	ASN
2	C	622	ASN
2	C	677	ASN
2	C	697	LYS
2	C	766	ASN
2	C	841	ARG
2	C	944	ARG
2	C	994	ARG
2	C	1022	LYS
2	C	1034	ARG
2	C	1090	ASN
2	C	1147	ARG
2	C	1299	ASN
3	D	96	LYS
3	D	214	ARG
3	D	215	LYS
3	D	322	ARG
3	D	378	LYS
3	D	400	MET
3	D	521	LYS
3	D	749	LYS
3	D	795	TYR
3	D	1149	ARG
3	D	1206	ARG
3	D	1247	LYS
3	D	1357	ILE
3	D	1372	ARG
4	E	35	LYS
5	F	105	MET
5	F	220	LYS
5	F	263	PRO
5	F	281	ARG
5	F	400	GLN
5	F	502	LYS
5	F	557	LYS
6	G	103	ARG
6	G	122	ARG
6	G	166	LYS
6	H	194	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	B	23	HIS
1	B	37	HIS
2	C	219	GLN
2	C	258	ASN
2	C	339	ASN
2	C	622	ASN
2	C	686	GLN
2	C	688	GLN
2	C	766	ASN
2	C	1017	GLN
2	C	1237	HIS
2	C	1244	HIS
2	C	1288	GLN
2	C	1307	ASN
2	C	1313	HIS
2	C	1314	GLN
3	D	489	ASN
3	D	702	GLN
3	D	817	HIS
3	D	1218	HIS
3	D	1279	GLN
5	F	362	ASN
6	G	80	GLN
6	H	65	ASN
6	H	80	GLN
6	H	149	ASN
6	H	194	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CMP	G	301	-	22,25,25	1.49	4 (18%)	24,39,39	1.51	4 (16%)
11	CMP	H	301	-	22,25,25	1.59	5 (22%)	24,39,39	1.79	7 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CMP	G	301	-	-	0/0/31/31	0/4/4/4
11	CMP	H	301	-	-	0/0/31/31	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	301	CMP	P-O3'	3.77	1.64	1.57
11	G	301	CMP	P-O3'	3.57	1.63	1.57
11	H	301	CMP	P-O5'	3.52	1.61	1.57
11	G	301	CMP	P-O5'	3.11	1.61	1.57
11	H	301	CMP	O5'-C5'	-2.71	1.42	1.46
11	G	301	CMP	O3'-C3'	-2.38	1.40	1.44
11	G	301	CMP	C5-C4	2.20	1.46	1.40
11	H	301	CMP	C5-C4	2.07	1.46	1.40
11	H	301	CMP	O3'-C3'	-2.06	1.41	1.44

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	301	CMP	N3-C2-N1	-3.83	122.69	128.68
11	H	301	CMP	O3'-C3'-C2'	3.67	119.20	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	G	301	CMP	N3-C2-N1	-3.23	123.62	128.68
11	H	301	CMP	O2P-P-O3'	2.83	113.63	107.04
11	G	301	CMP	O5'-P-O3'	2.68	109.37	105.68
11	G	301	CMP	C4-C5-N7	-2.68	106.61	109.40
11	H	301	CMP	O5'-P-O1P	-2.64	104.35	110.44
11	G	301	CMP	O2P-P-O1P	2.63	116.97	108.73
11	H	301	CMP	O5'-P-O3'	2.58	109.23	105.68
11	H	301	CMP	C4-C5-N7	-2.42	106.88	109.40
11	H	301	CMP	C1'-N9-C4	-2.39	122.44	126.64

There are no chirality outliers.

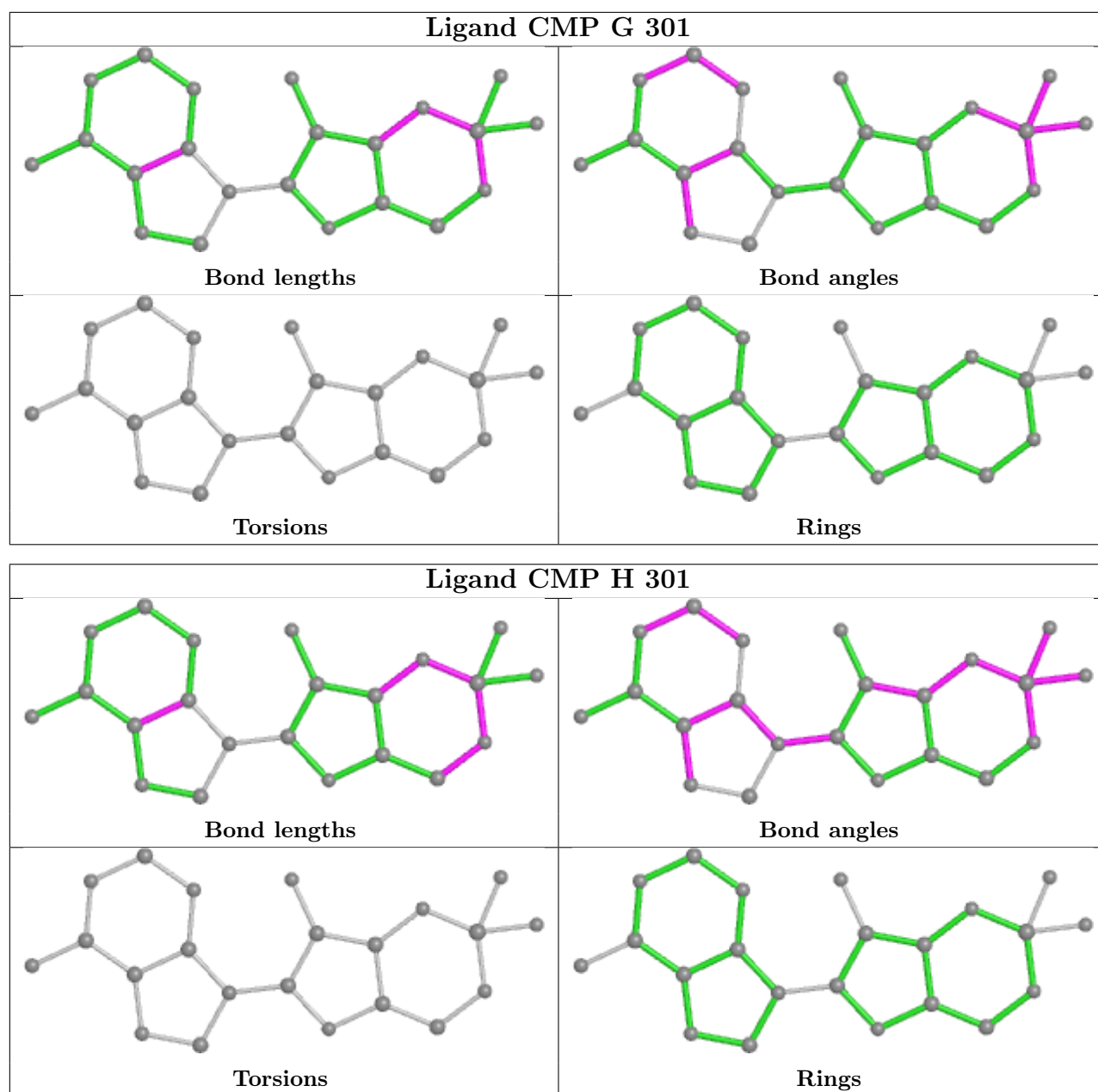
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	301	CMP	2	0
11	H	301	CMP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

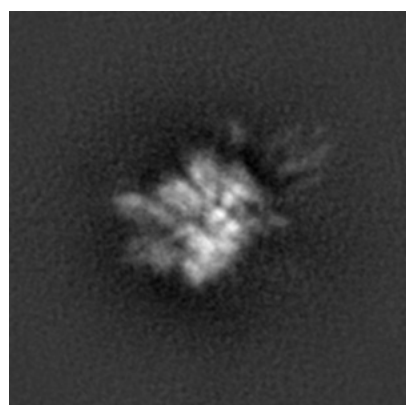
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20287. These allow visual inspection of the internal detail of the map and identification of artifacts.

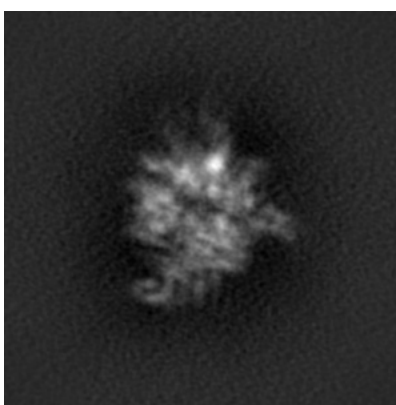
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

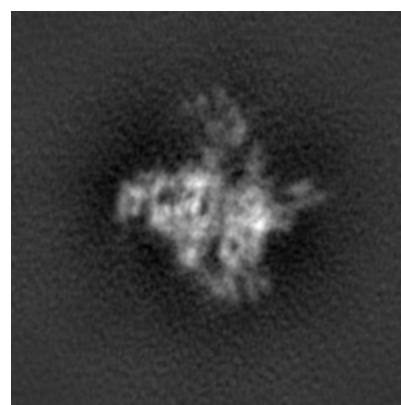
6.1.1 Primary map



X



Y

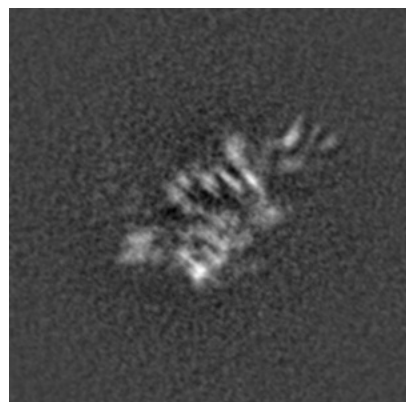


Z

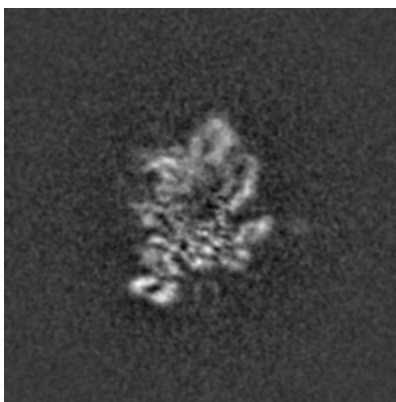
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

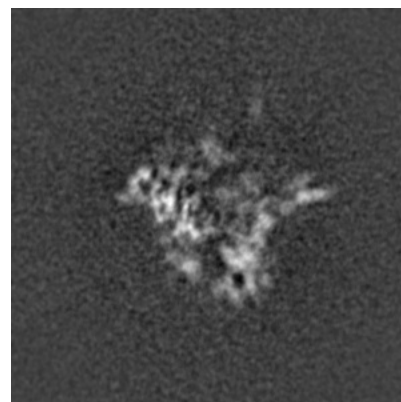
6.2.1 Primary map



X Index: 192



Y Index: 192

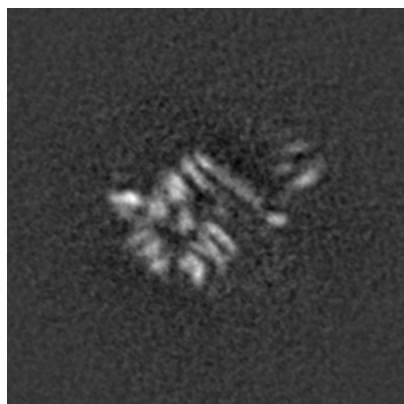


Z Index: 192

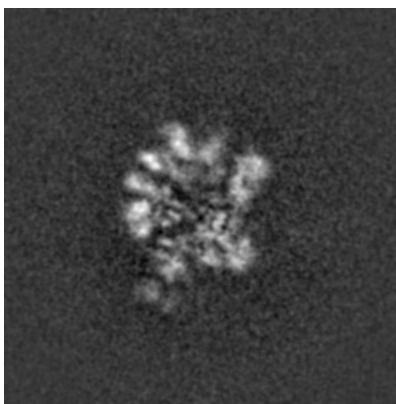
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

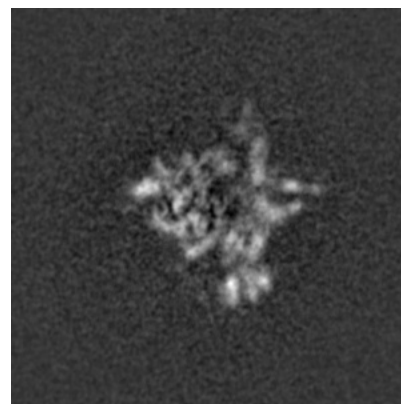
6.3.1 Primary map



X Index: 211



Y Index: 180



Z Index: 203

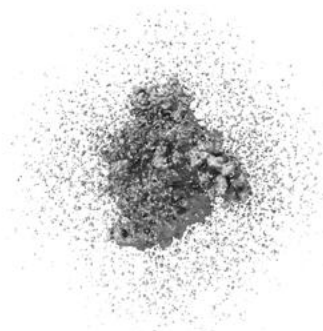
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

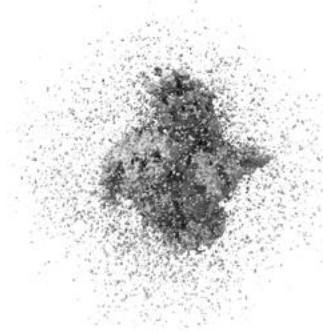
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

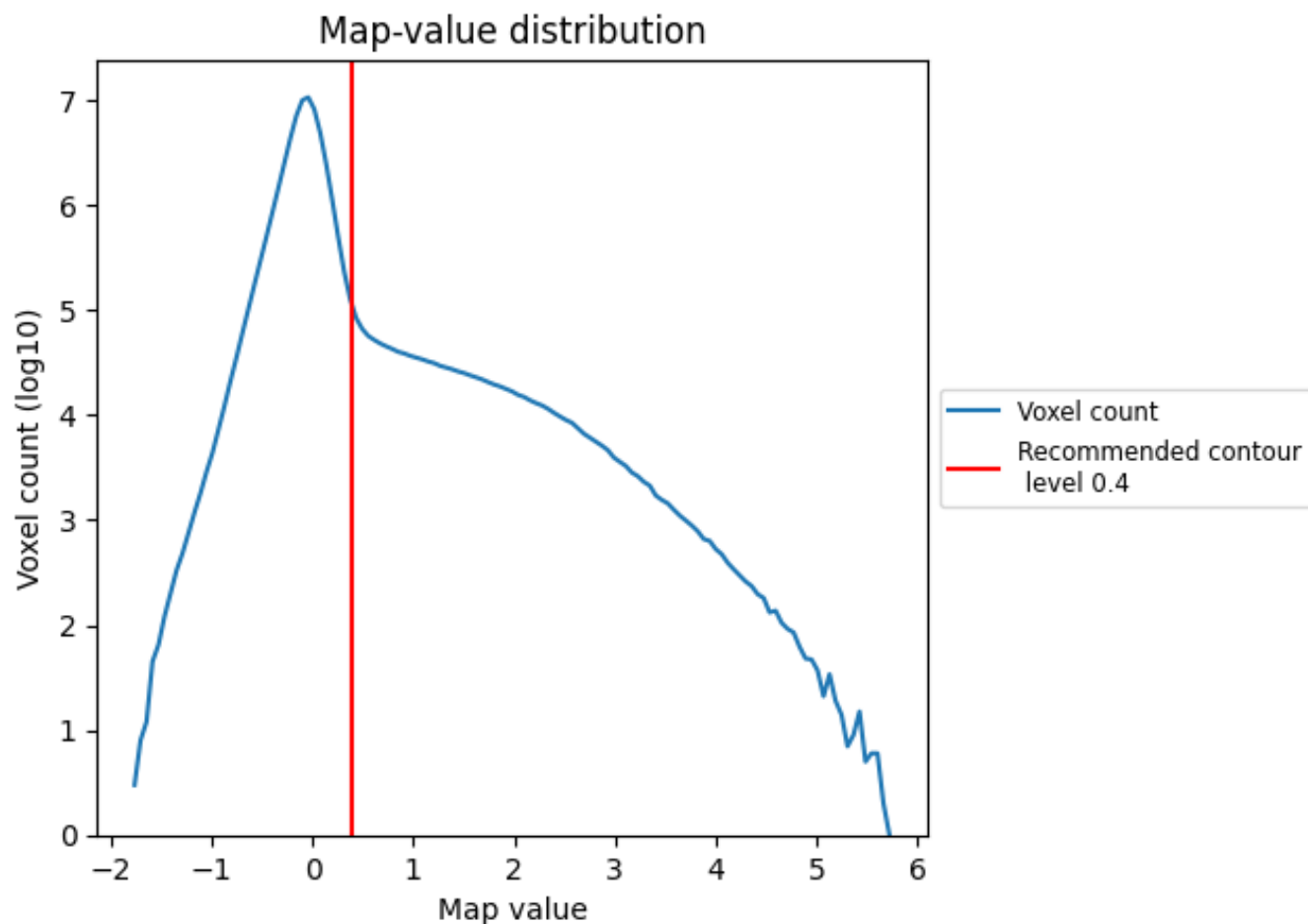
6.5 Mask visualisation

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

7 Map analysis [i](#)

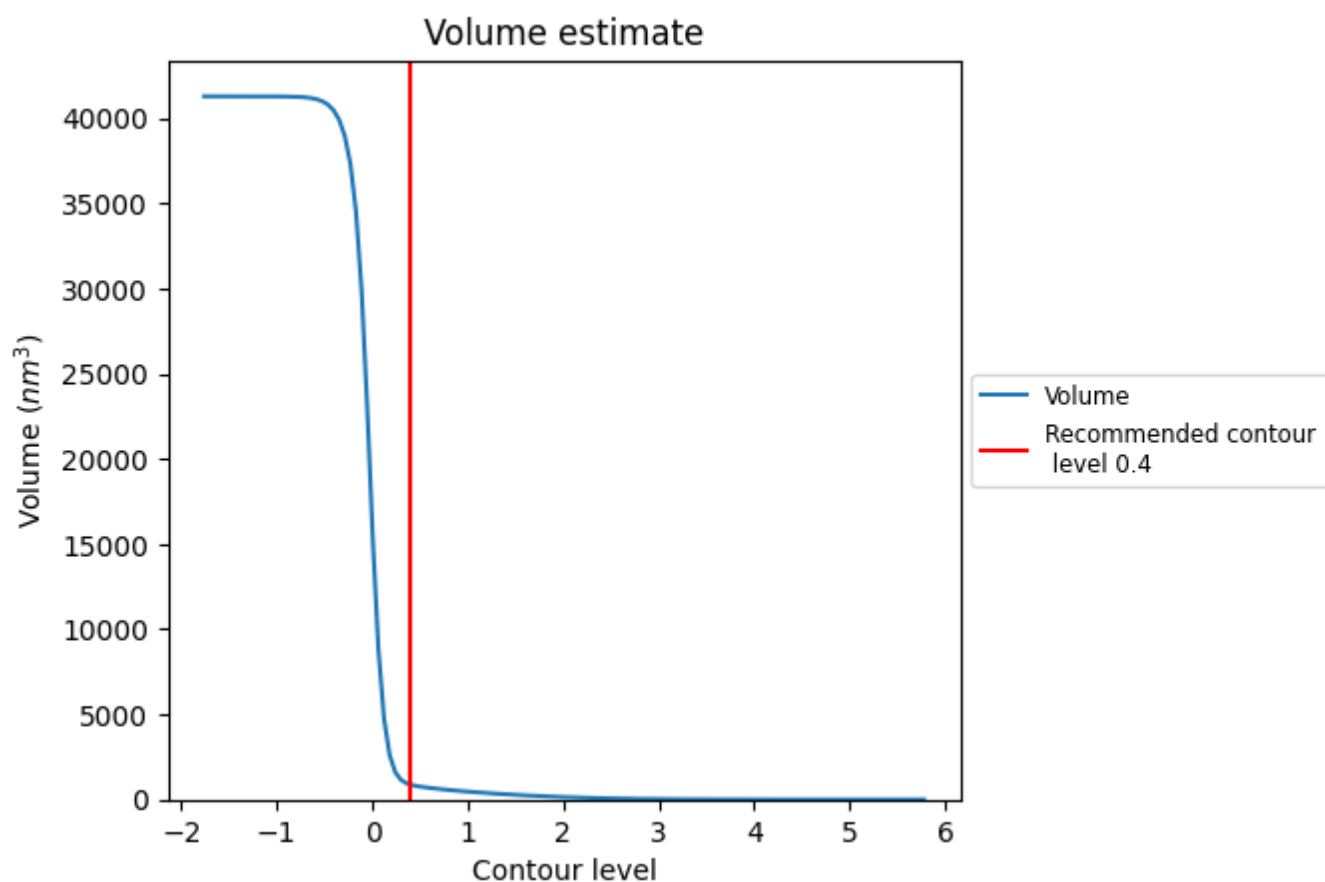
This section contains the results of statistical analysis of the map.

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.

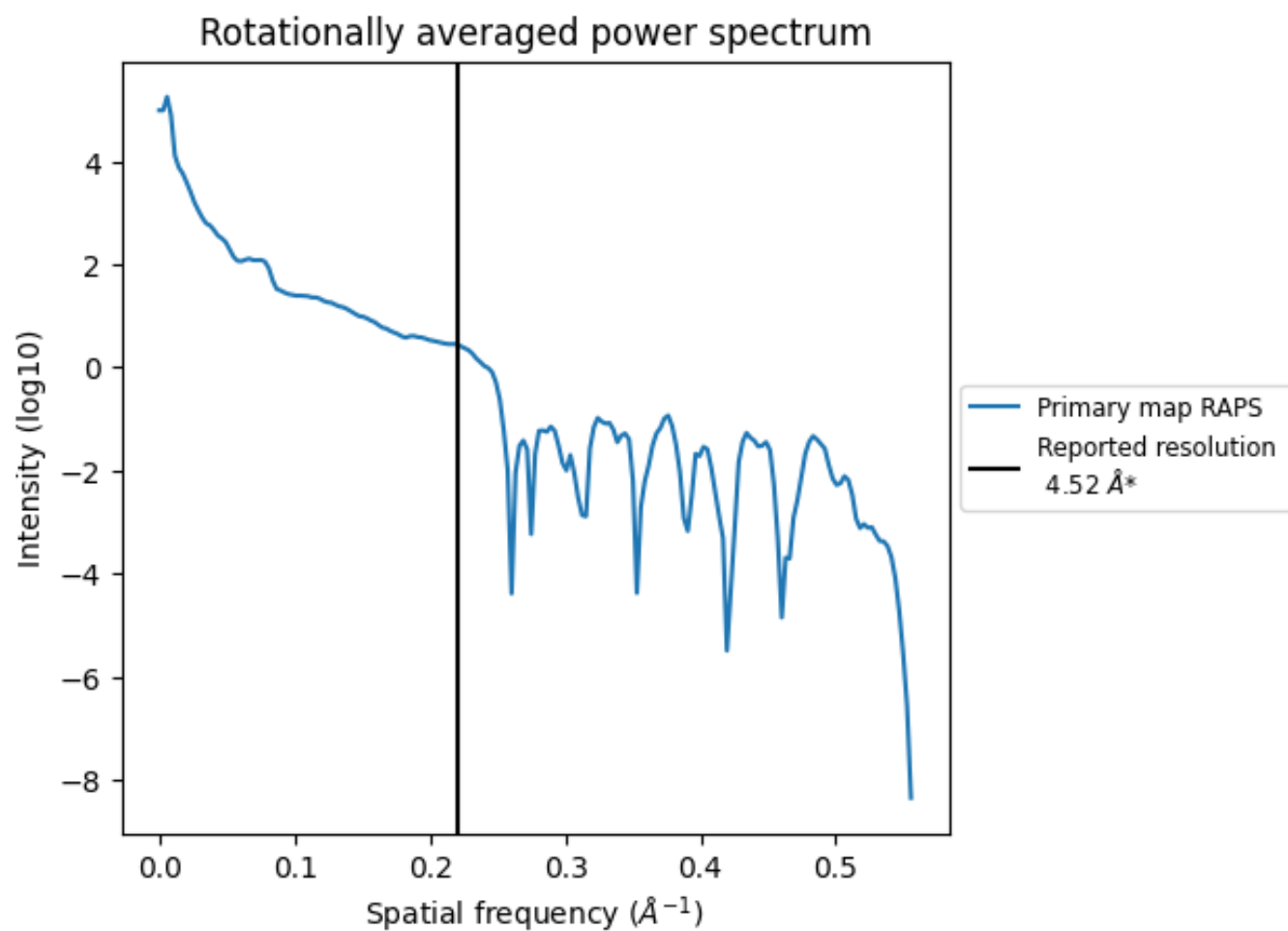
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 881 nm³; this corresponds to an approximate mass of 796 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 0.221 Å⁻¹

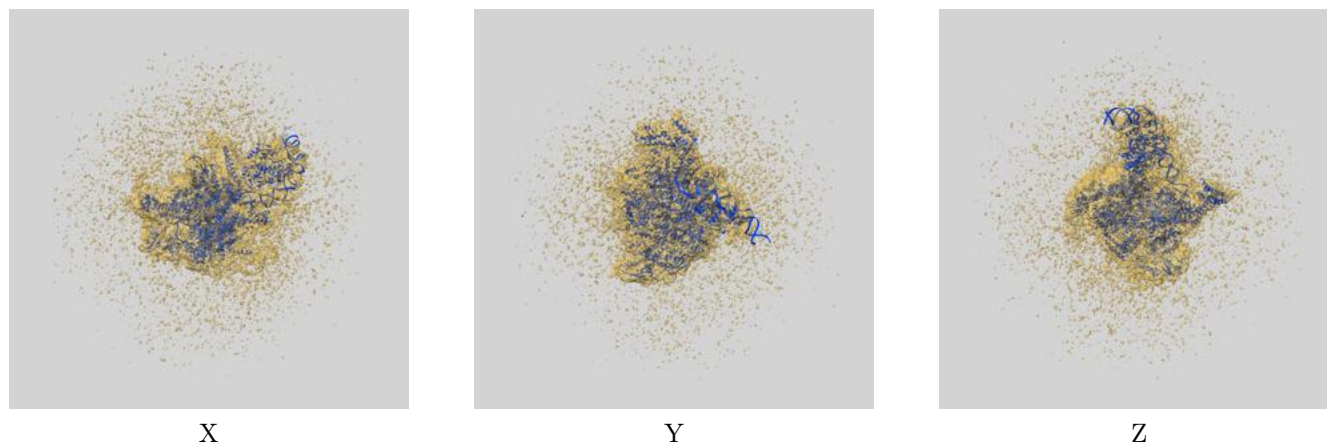
8 Fourier-Shell correlation

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-20287 and PDB model 6PB5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



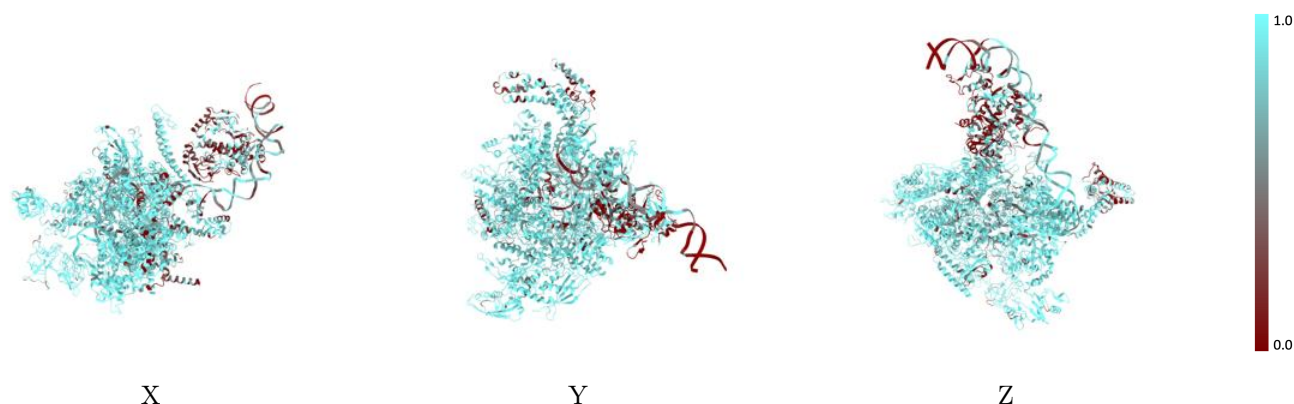
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



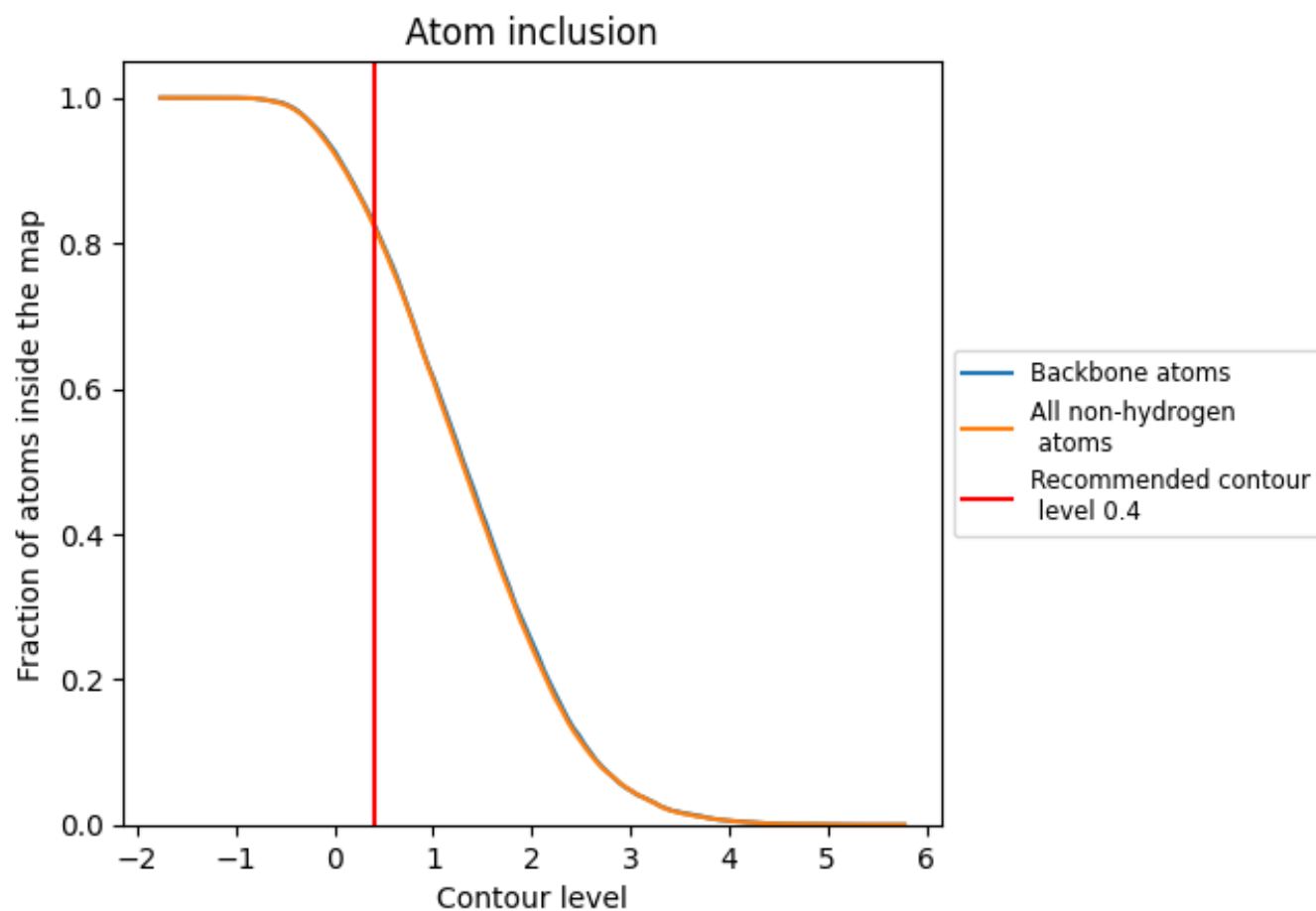
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8246	<div></div> 0.0820
1	<div></div> 0.6530	<div></div> 0.0640
2	<div></div> 0.6135	<div></div> 0.0680
A	<div></div> 0.9405	<div></div> 0.0860
B	<div></div> 0.9382	<div></div> 0.1250
C	<div></div> 0.8973	<div></div> 0.0740
D	<div></div> 0.9452	<div></div> 0.1100
E	<div></div> 0.6268	<div></div> 0.0430
F	<div></div> 0.7192	<div></div> 0.0700
G	<div></div> 0.3578	<div></div> 0.0280
H	<div></div> 0.4384	<div></div> 0.0200

