Full wwPDB EM Validation Report (i)

May 5, 2024 – 08:26 PM EDT

PDB ID	:	6PB6
EMDB ID	:	EMD-20288
Title	:	The E. coli class-II CAP-dependent transcription activation complex at the state 2
Authors	:	Liu, B.; Shi, W.
Deposited on	:	2019-06-13
Resolution	:	4.29 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 (i) 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 (1)) were used in the production of this report:

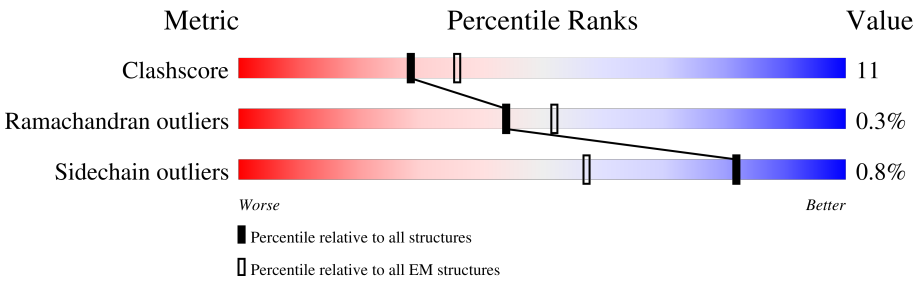
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.29 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 <=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	53% 16% • 30%
1	B	329	• 50% 19% 31%
2	C	1342	• 74% 25%
3	D	1407	• 70% 25% 5%
4	E	91	70% 70% 16% 13%
5	F	628	8% 56% 20% • 23%
6	G	210	9% 70% 23% 6%
6	H	210	7% 68% 26% 6%

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Mol	Chain	Length	Quality of chain
7	1	78	9% 79% 21%
8	2	78	18% 68% 29% •

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 69846 atoms, of which 34410 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	230	3599	1112	1813	317	351	6	0	0
1	B	228	3556	1100	1789	312	349	6	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	F	483	7917	2455	3989	704	746	23	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	initiating methionine	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
			Total	C	H	N	O	S		
6	G	197	3156	986	1600	273	288	9	0	0
6	H	197	3156	986	1600	273	288	9	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
7	1	78	2482	765	891	264	484	78	0	0

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

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
8	2	78	2488	767	876	313	454	78	0	0

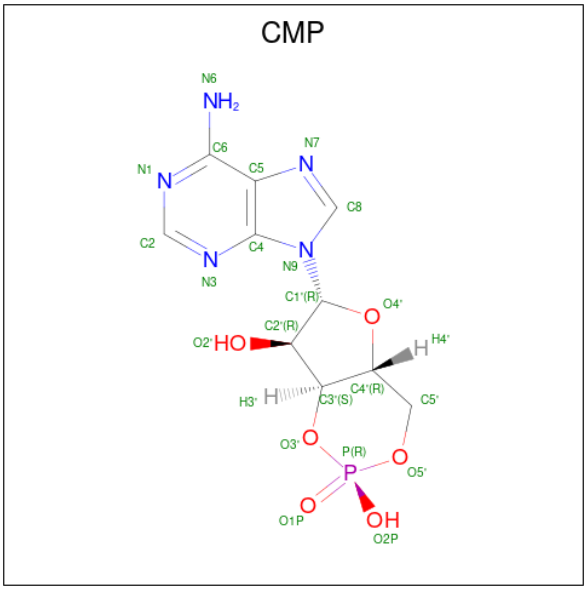
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

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

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

- Molecule 11 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: $C_{10}H_{12}N_5O_6P$) (labeled as "Ligand of Interest" by depositor).



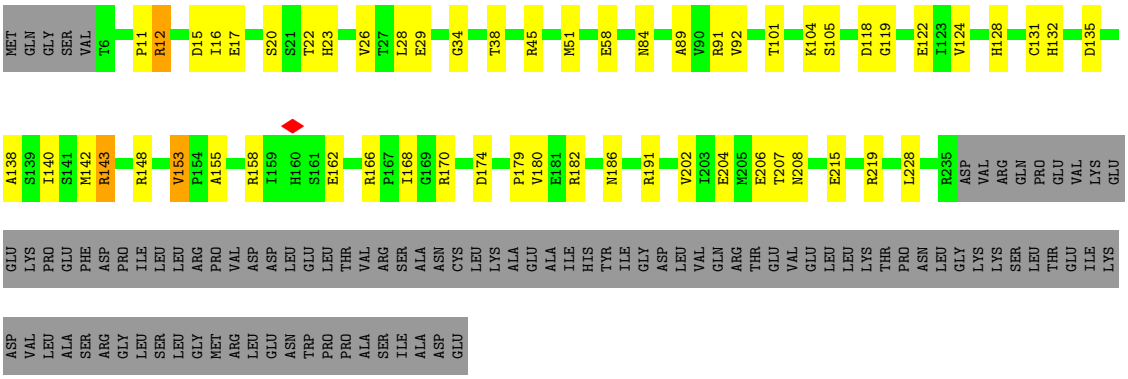
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
11	G	1	33	10	11	5	6	1	0
			Total	C	H	N	O	P	
11	H	1	33	10	11	5	6	1	0

3 Residue-property plots (i)

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.

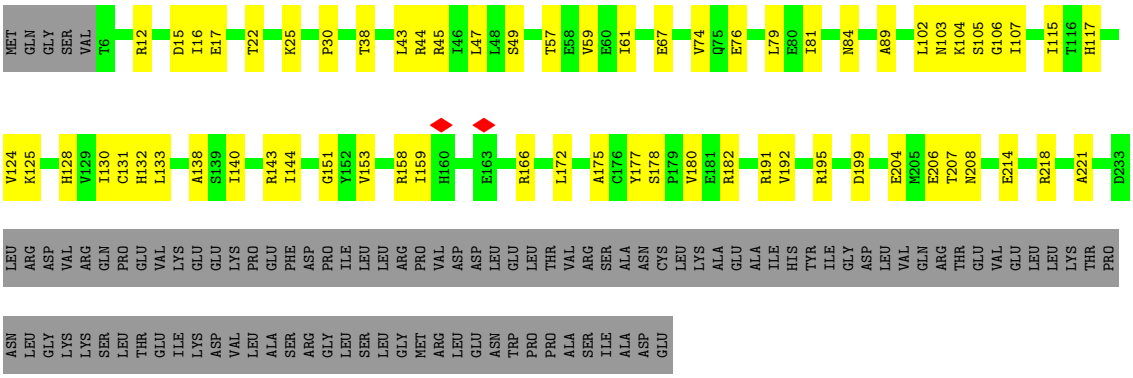
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



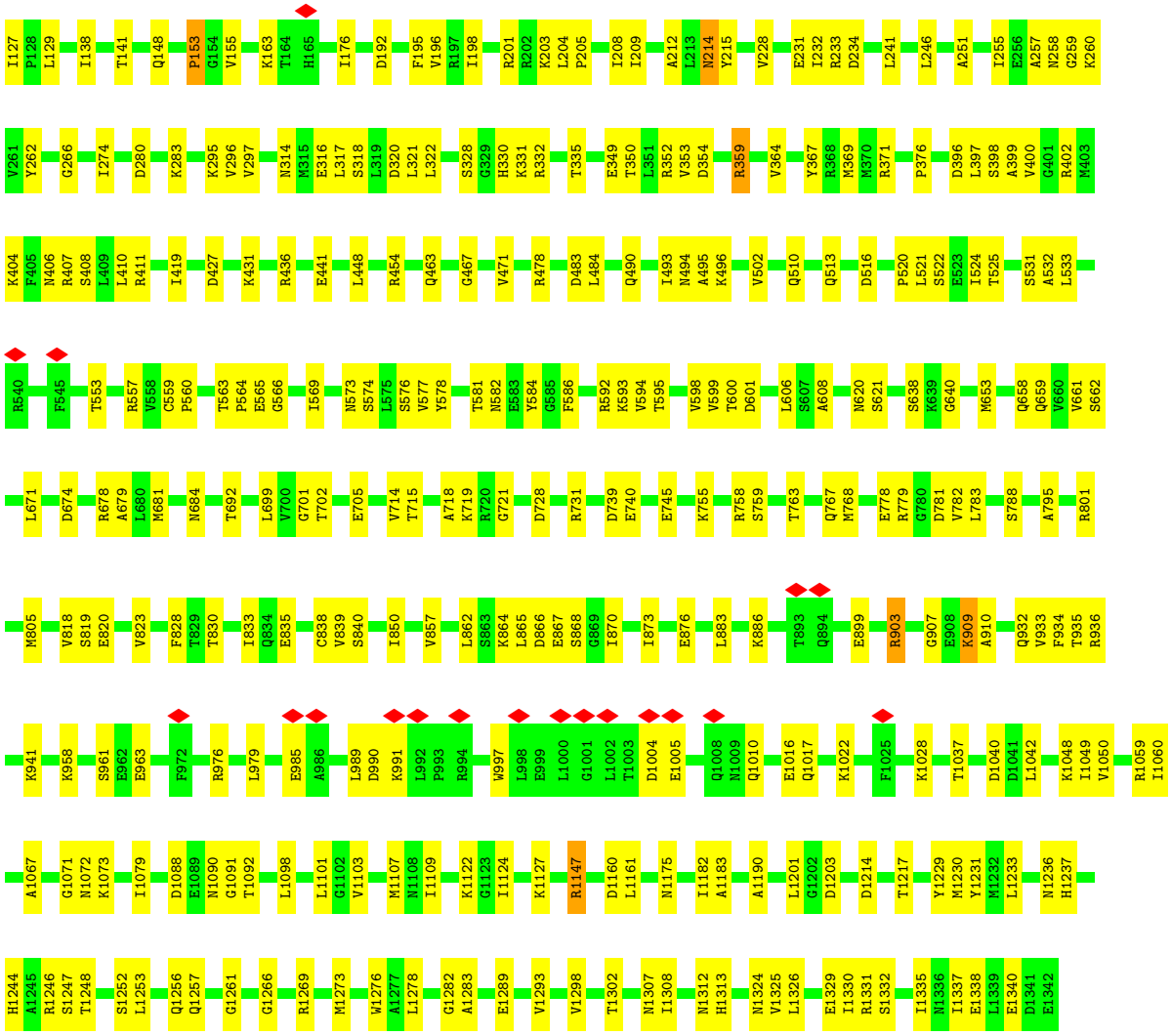
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain B:



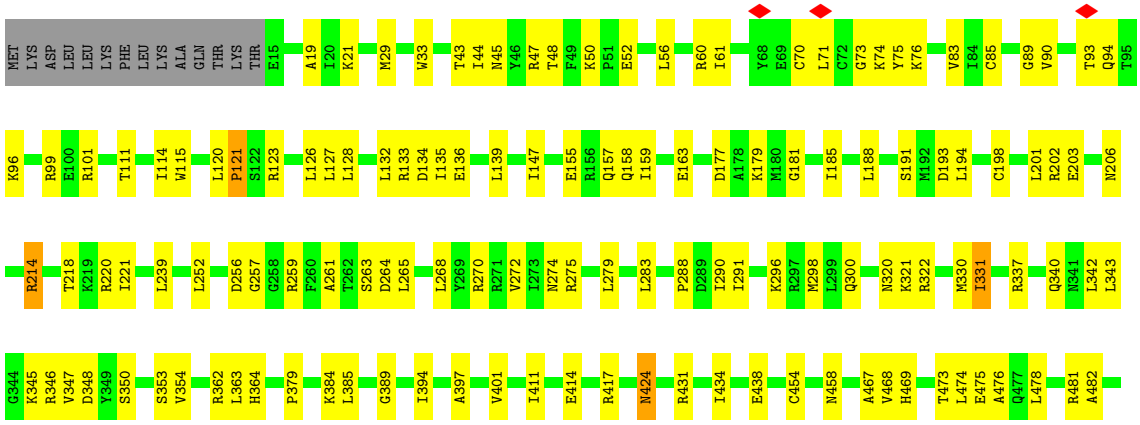
• Molecule 2: DNA-directed RNA polymerase subunit beta

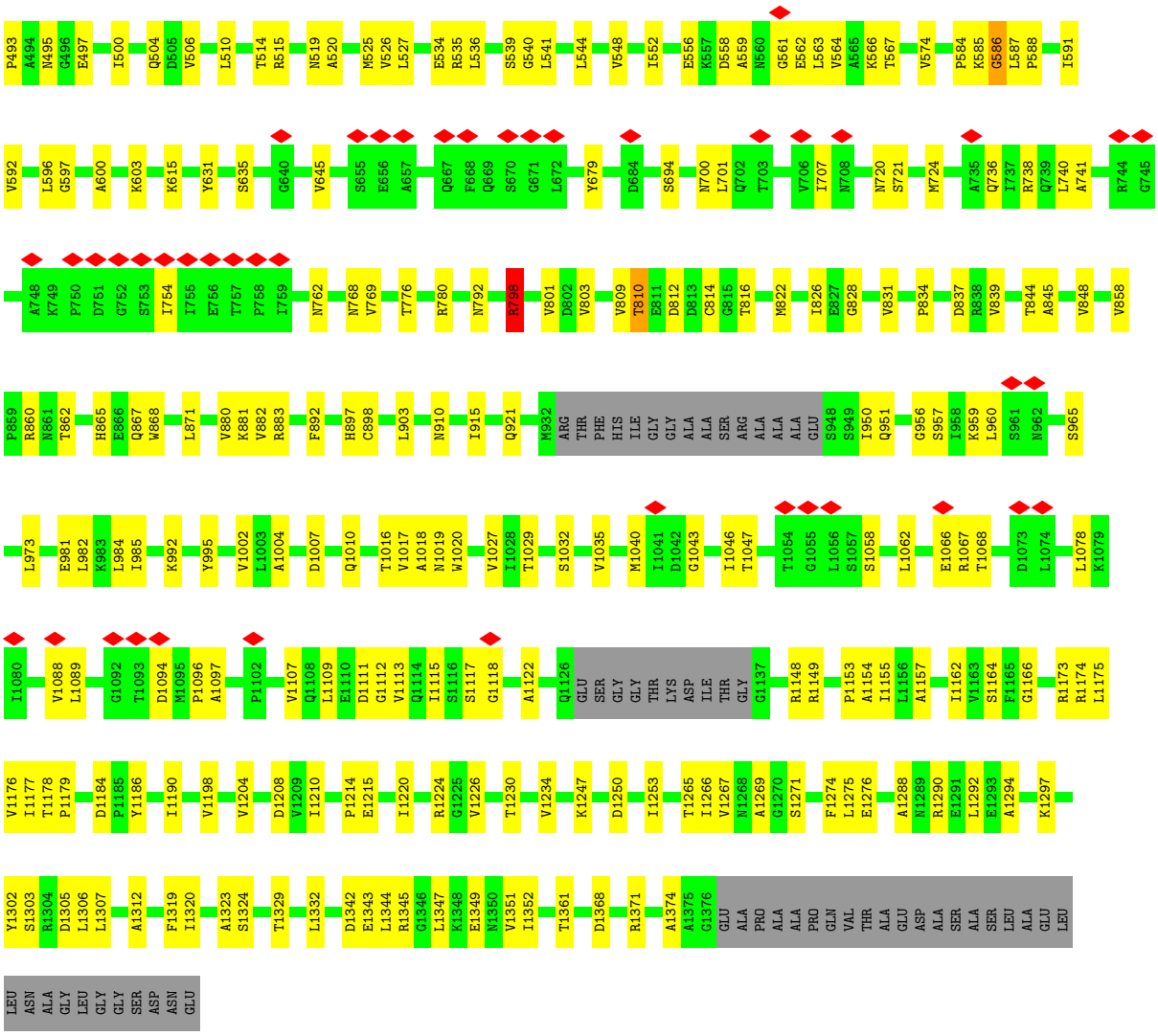
Chain C:



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

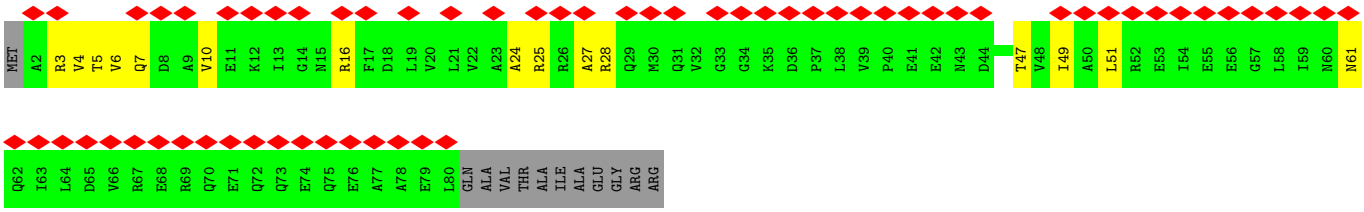
Chain D:





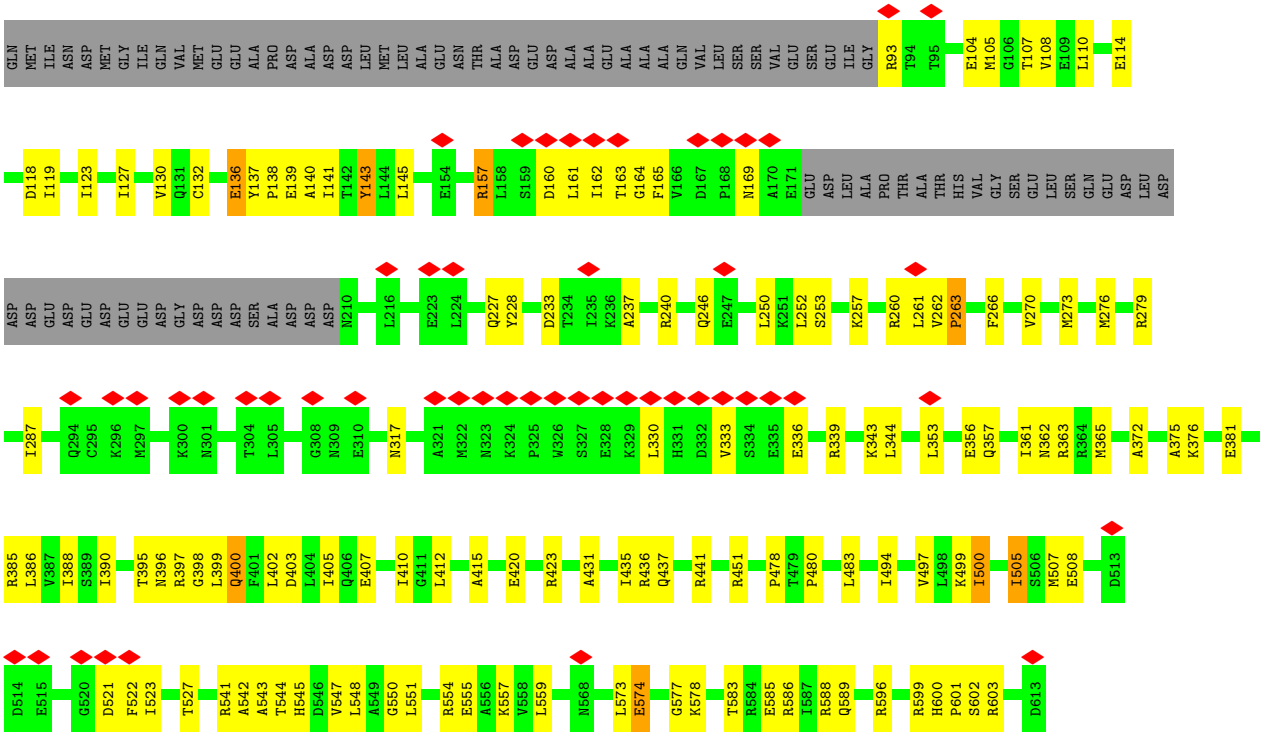
• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:



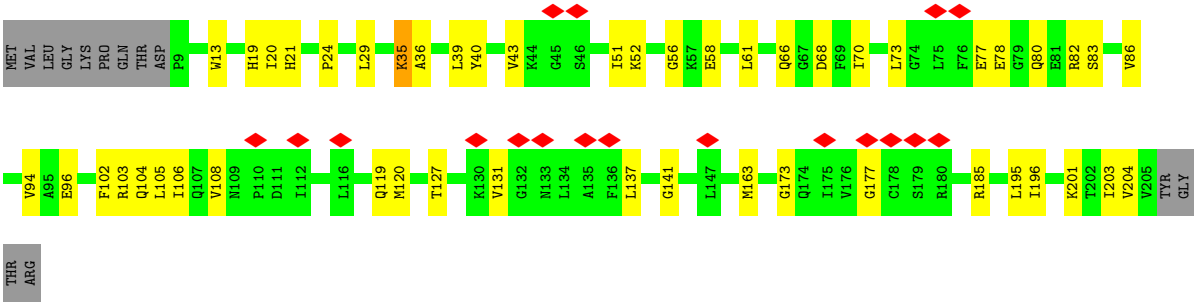
• Molecule 5: RNA polymerase sigma factor RpoD

Chain F:



• Molecule 6: cAMP-activated global transcriptional regulator CRP

Chain G:

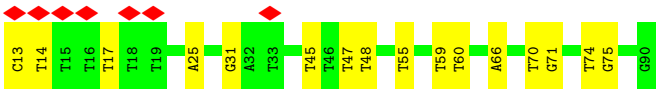


• Molecule 6: cAMP-activated global transcriptional regulator CRP

Chain H:

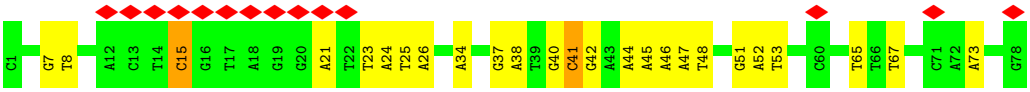
• Molecule 7: SYNTHETIC NONTEMPLATE STRAND DNA (78-MER)

Chain 1:



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

Chain 2:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37456	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 ($e^-/Å^2$)	45	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	6.817	Depositor
Minimum map value	-3.021	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.337	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	345.59998, 345.59998, 345.59998	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8999999, 0.8999999, 0.8999999	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.43	0/1808	0.67	0/2450
1	B	0.41	0/1789	0.69	0/2425
2	C	0.51	1/10739 (0.0%)	0.68	1/14489 (0.0%)
3	D	0.47	0/10553	0.69	3/14248 (0.0%)
4	E	0.34	0/629	0.61	0/847
5	F	0.43	0/3982	0.71	2/5354 (0.0%)
6	G	0.40	0/1580	0.64	0/2127
6	H	0.41	0/1580	0.71	0/2127
7	1	0.99	0/1777	1.24	3/2741 (0.1%)
8	2	1.03	3/1815 (0.2%)	1.13	4/2800 (0.1%)
All	All	0.54	4/36252 (0.0%)	0.76	13/49608 (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	A	0	1
1	B	0	1
2	C	0	3
3	D	0	10
5	F	0	8
6	H	0	1
All	All	0	24

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	42	DG	C3'-O3'	9.14	1.55	1.44
2	C	215	TYR	CD2-CE2	-5.76	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	2	67	DT	C3'-O3'	5.55	1.51	1.44
8	2	34	DA	C3'-O3'	5.43	1.51	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	2	42	DG	O4'-C1'-N9	14.09	117.86	108.00
8	2	42	DG	C1'-O4'-C4'	-8.84	101.26	110.10
7	1	31	DG	O4'-C1'-N9	7.50	113.25	108.00
8	2	41	DC	OP1-P-OP2	-7.25	108.72	119.60
5	F	157	ARG	NE-CZ-NH1	5.77	123.18	120.30
8	2	15	DC	O5'-P-OP1	-5.75	100.52	105.70
7	1	48	DT	C1'-O4'-C4'	-5.42	104.68	110.10
5	F	143	TYR	CA-CB-CG	5.24	123.35	113.40
7	1	55	DT	P-O3'-C3'	5.21	125.95	119.70
3	D	362	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	C	359	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	D	798	ARG	NE-CZ-NH1	5.10	122.85	120.30
3	D	871	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (24) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	153	VAL	Peptide
1	B	191	ARG	Peptide
2	C	214	ASN	Peptide
2	C	581	THR	Peptide
2	C	909	LYS	Peptide
3	D	1046	ILE	Peptide
3	D	1184	ASP	Peptide
3	D	120	LEU	Peptide
3	D	1297	LYS	Peptide
3	D	331	ILE	Peptide
3	D	584	PRO	Peptide
3	D	586	GLY	Peptide
3	D	803	VAL	Peptide
3	D	810	THR	Peptide
3	D	839	VAL	Peptide
5	F	136	GLU	Peptide
5	F	165	PHE	Peptide
5	F	263	PRO	Peptide

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Mol	Chain	Res	Type	Group
5	F	353	LEU	Peptide
5	F	395	THR	Peptide
5	F	500	ILE	Peptide
5	F	505	ILE	Peptide
5	F	527	THR	Peptide
6	H	167	ILE	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1786	1813	1813	37	0
1	B	1767	1789	1789	46	0
2	C	10570	10582	10582	235	0
3	D	10396	10614	10614	249	0
4	E	627	634	634	21	0
5	F	3928	3989	3990	85	0
6	G	1556	1600	1600	50	0
6	H	1556	1600	1600	38	0
7	1	1591	891	891	12	0
8	2	1612	876	876	20	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	G	22	11	11	4	0
11	H	22	11	11	2	0
All	All	35436	34410	34411	727	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 (727) 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:G:301:CMP:H2	11:G:301:CMP:C2	0.97	1.49
11:H:301:CMP:H2	11:H:301:CMP:C2	0.97	1.46
6:G:52:LYS:HA	6:G:58:GLU:HG3	1.27	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:40:TYR:CD1	6:G:96:GLU:HG2	1.86	1.09
6:G:52:LYS:CA	6:G:58:GLU:HG3	1.94	0.96
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.50	0.93
6:G:94:VAL:HG12	6:G:96:GLU:HG3	1.51	0.91
6:G:185:ARG:NH2	8:2:51:DG:N7	2.23	0.87
3:D:566:LYS:NZ	3:D:567:THR:O	2.08	0.86
2:C:839:VAL:O	2:C:886:LYS:NZ	2.08	0.86
7:1:47:DT:O4	8:2:44:DA:N6	2.12	0.83
3:D:1058:SER:OG	3:D:1109:LEU:O	1.97	0.81
3:D:814:CYS:SG	3:D:883:ARG:NH2	2.54	0.81
3:D:951:GLN:OE1	3:D:1016:THR:OG1	1.97	0.81
5:F:397:ARG:NH2	7:1:75:DG:OP1	2.13	0.81
6:G:40:TYR:CD1	6:G:96:GLU:CG	2.64	0.81
3:D:473:THR:OG1	4:E:28:ARG:NH2	2.13	0.80
6:G:40:TYR:CE1	6:G:96:GLU:CD	2.54	0.80
3:D:296:LYS:O	3:D:300:GLN:NE2	2.15	0.80
5:F:574:GLU:OE1	5:F:578:LYS:NZ	2.14	0.80
3:D:330:MET:O	3:D:337:ARG:NH1	2.14	0.79
2:C:234:ASP:OD1	2:C:331:LYS:NZ	2.13	0.78
2:C:592:ARG:NH2	2:C:601:ASP:OD1	2.17	0.78
1:A:182:ARG:NH1	2:C:1090:ASN:O	2.16	0.78
2:C:963:GLU:OE1	2:C:1028:LYS:NZ	2.17	0.78
3:D:514:THR:HG21	3:D:596:LEU:HD12	1.66	0.78
2:C:478:ARG:NH2	8:2:25:DT:OP1	2.17	0.77
6:G:43:VAL:O	6:G:66:GLN:NE2	2.18	0.77
5:F:437:GLN:OE1	8:2:26:DA:N6	2.17	0.76
2:C:406:ASN:O	2:C:410:LEU:N	2.19	0.76
1:A:84:ASN:O	1:A:128:HIS:NE2	2.18	0.76
3:D:346:ARG:NH1	8:2:15:DC:OP1	2.18	0.75
6:G:40:TYR:HD1	6:G:96:GLU:HG2	1.50	0.75
3:D:556:GLU:O	3:D:564:VAL:N	2.20	0.75
3:D:73:GLY:O	3:D:76:LYS:NZ	2.20	0.75
3:D:121:PRO:O	3:D:123:ARG:NH1	2.20	0.74
3:D:552:ILE:O	3:D:567:THR:OG1	2.02	0.74
2:C:1282:GLY:O	3:D:1361:THR:OG1	2.00	0.74
5:F:276:MET:SD	5:F:279:ARG:NH1	2.61	0.74
3:D:495:ASN:ND2	3:D:1247:LYS:O	2.20	0.74
2:C:678:ARG:NH1	2:C:681:MET:SD	2.61	0.73
3:D:85:CYS:O	3:D:89:GLY:N	2.21	0.73
2:C:674:ASP:OD1	2:C:1109:ILE:N	2.21	0.73
2:C:560:PRO:O	3:D:780:ARG:NH2	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:163:MET:O	6:G:204:VAL:N	2.22	0.72
2:C:936:ARG:HG3	2:C:1042:LEU:HD12	1.71	0.72
3:D:1148:ARG:NH1	3:D:1149:ARG:O	2.22	0.72
6:G:35:LYS:O	6:G:82:ARG:NH1	2.21	0.72
2:C:54:ARG:NH2	2:C:57:PHE:O	2.21	0.72
3:D:198:CYS:SG	3:D:202:ARG:NH1	2.62	0.72
3:D:270:ARG:O	3:D:274:ASN:ND2	2.23	0.72
2:C:864:LYS:NZ	2:C:876:GLU:O	2.23	0.72
2:C:557:ARG:NH2	2:C:606:LEU:O	2.23	0.72
5:F:136:GLU:O	5:F:357:GLN:NE2	2.23	0.72
2:C:18:ARG:NH2	2:C:620:ASN:O	2.23	0.71
2:C:865:LEU:O	6:G:19:HIS:NE2	2.23	0.71
3:D:1043:GLY:O	3:D:1068:THR:OG1	2.09	0.71
3:D:1062:LEU:O	3:D:1067:ARG:NH2	2.23	0.71
3:D:60:ARG:NE	3:D:89:GLY:O	2.24	0.71
5:F:253:SER:O	5:F:257:LYS:N	2.23	0.71
2:C:367:TYR:O	2:C:371:ARG:N	2.24	0.71
5:F:137:TYR:OH	5:F:273:MET:SD	2.43	0.70
1:A:38:THR:OG1	1:B:45:ARG:NE	2.24	0.70
1:A:215:GLU:OE2	1:A:219:ARG:NH2	2.24	0.70
2:C:13:LYS:O	2:C:1183:ALA:N	2.24	0.70
2:C:494:ASN:ND2	8:2:24:DA:OP1	2.24	0.70
2:C:93:SER:OG	2:C:126:GLU:OE1	2.08	0.70
3:D:29:MET:SD	3:D:33:TRP:NE1	2.65	0.70
3:D:809:VAL:HG23	3:D:915:ILE:HD11	1.74	0.70
1:A:58:GLU:OE1	1:A:170:ARG:NH2	2.24	0.70
3:D:536:LEU:O	3:D:540:GLY:N	2.25	0.70
3:D:828:GLY:O	3:D:995:TYR:OH	2.06	0.70
6:H:170:GLN:O	6:H:180:ARG:NH2	2.25	0.69
2:C:262:TYR:OH	2:C:280:ASP:OD2	2.11	0.69
1:A:22:THR:OG1	1:A:207:THR:O	2.04	0.69
5:F:596:ARG:NH1	6:G:56:GLY:O	2.25	0.69
6:G:40:TYR:CE1	6:G:96:GLU:OE2	2.45	0.69
6:H:78:GLU:OE2	6:H:103:ARG:NH1	2.25	0.69
2:C:719:LYS:O	2:C:779:ARG:NE	2.26	0.69
3:D:515:ARG:NH1	3:D:724:MET:SD	2.66	0.69
3:D:70:CYS:SG	3:D:74:LYS:N	2.66	0.69
2:C:1214:ASP:OD2	2:C:1217:THR:N	2.25	0.68
2:C:1329:GLU:O	2:C:1332:SER:OG	2.06	0.68
6:G:52:LYS:CB	6:G:58:GLU:HG3	2.23	0.68
1:A:207:THR:HG23	1:A:208:ASN:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:414:GLU:O	3:D:417:ARG:NH1	2.27	0.68
2:C:835:GLU:OE1	2:C:835:GLU:N	2.26	0.68
2:C:46:GLN:OE1	2:C:46:GLN:N	2.27	0.68
5:F:402:LEU:HD23	5:F:405:ILE:HD12	1.76	0.68
2:C:94:ALA:CB	2:C:129:LEU:HD11	2.24	0.68
1:B:89:ALA:HB1	1:B:124:VAL:HB	1.74	0.68
6:H:169:ARG:NH2	6:H:180:ARG:O	2.26	0.68
5:F:596:ARG:O	5:F:600:HIS:ND1	2.27	0.68
2:C:295:LYS:O	2:C:317:LEU:N	2.27	0.67
2:C:408:SER:O	2:C:431:LYS:NZ	2.20	0.67
3:D:519:ASN:OD1	3:D:520:ALA:N	2.28	0.67
3:D:214:ARG:NH1	3:D:218:THR:OG1	2.27	0.67
1:B:153:VAL:O	1:B:175:ALA:N	2.28	0.67
3:D:810:THR:OG1	3:D:892:PHE:O	2.13	0.67
5:F:541:ARG:O	5:F:544:THR:OG1	2.12	0.67
2:C:759:SER:OG	2:C:763:THR:N	2.29	0.66
1:B:151:GLY:O	1:B:178:SER:N	2.29	0.66
2:C:755:LYS:NZ	2:C:767:GLN:O	2.28	0.66
2:C:903:ARG:O	2:C:907:GLY:N	2.27	0.66
3:D:1154:ALA:N	3:D:1214:PRO:O	2.29	0.66
2:C:805:MET:N	2:C:1098:LEU:O	2.28	0.66
5:F:114:GLU:O	5:F:118:ASP:N	2.29	0.66
1:A:142:MET:SD	1:A:142:MET:N	2.69	0.66
3:D:47:ARG:HH22	5:F:500:ILE:HD11	1.61	0.66
2:C:153:PRO:O	2:C:404:LYS:NZ	2.28	0.66
3:D:188:LEU:O	3:D:191:SER:OG	2.05	0.66
6:G:94:VAL:CG1	6:G:96:GLU:HG3	2.24	0.66
3:D:1175:LEU:HB3	3:D:1190:ILE:HD11	1.77	0.65
3:D:1275:LEU:HD12	3:D:1276:GLU:HA	1.77	0.65
3:D:473:THR:HG23	3:D:476:ALA:H	1.61	0.65
3:D:679:TYR:OH	3:D:754:ILE:O	2.14	0.65
2:C:9:LYS:O	2:C:1175:ASN:ND2	2.29	0.65
3:D:631:TYR:O	3:D:635:SER:N	2.30	0.65
5:F:104:GLU:O	5:F:107:THR:OG1	2.09	0.65
6:H:39:LEU:N	6:H:97:ILE:O	2.29	0.65
2:C:297:VAL:HB	2:C:317:LEU:HD21	1.77	0.65
2:C:559:CYS:SG	2:C:662:SER:N	2.69	0.65
6:G:68:ASP:OD1	6:G:119:GLN:NE2	2.29	0.65
2:C:257:ALA:N	2:C:260:LYS:O	2.30	0.64
3:D:1164:SER:O	3:D:1176:VAL:N	2.29	0.64
6:H:111:ASP:OD2	6:H:115:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:18:ARG:NH1	2:C:621:SER:O	2.31	0.64
2:C:1016:GLU:OE1	2:C:1017:GLN:NE2	2.30	0.64
3:D:43:THR:O	3:D:52:GLU:N	2.31	0.64
1:B:207:THR:HG23	1:B:208:ASN:O	1.98	0.64
2:C:577:VAL:HG23	2:C:661:VAL:O	1.97	0.64
3:D:960:LEU:HD11	3:D:982:LEU:HG	1.80	0.64
3:D:1035:VAL:N	3:D:1113:VAL:O	2.31	0.64
2:C:516:ASP:OD2	2:C:522:SER:OG	2.14	0.64
6:G:83:SER:OG	11:G:301:CMP:O2P	2.14	0.64
1:B:45:ARG:O	1:B:49:SER:OG	2.12	0.64
2:C:398:SER:O	2:C:400:VAL:N	2.31	0.64
2:C:718:ALA:N	2:C:781:ASP:O	2.31	0.64
2:C:801:ARG:NH2	2:C:1229:TYR:OH	2.31	0.63
3:D:438:GLU:OE2	4:E:3:ARG:NH2	2.30	0.63
2:C:4:SER:OG	2:C:778:GLU:OE2	2.09	0.63
2:C:867:GLU:HG2	2:C:868:SER:N	2.14	0.63
3:D:1344:LEU:HD23	3:D:1349:GLU:HB3	1.80	0.63
3:D:865:HIS:ND1	3:D:867:GLN:OE1	2.30	0.63
3:D:1027:VAL:HG21	3:D:1122:ALA:HB3	1.81	0.63
1:B:107:ILE:HG23	1:B:133:LEU:O	1.99	0.63
2:C:989:LEU:O	2:C:997:TRP:NE1	2.31	0.63
2:C:840:SER:OG	2:C:1048:LYS:N	2.32	0.63
3:D:1271:SER:OG	3:D:1290:ARG:NH1	2.32	0.63
2:C:702:THR:OG1	2:C:705:GLU:OE2	2.14	0.62
2:C:936:ARG:CG	2:C:1042:LEU:HD12	2.29	0.62
2:C:1338:GLU:OE2	3:D:21:LYS:NZ	2.22	0.62
6:H:187:LEU:HD12	6:H:196:ILE:HG21	1.80	0.62
2:C:510:GLN:O	2:C:513:GLN:NE2	2.32	0.62
1:A:158:ARG:O	1:A:162:GLU:N	2.32	0.62
3:D:1288:ALA:O	3:D:1292:LEU:HD22	1.99	0.62
5:F:497:VAL:HA	5:F:500:ILE:HD12	1.79	0.62
2:C:592:ARG:O	2:C:653:MET:N	2.33	0.62
3:D:350:SER:OG	3:D:469:HIS:ND1	2.32	0.62
2:C:658:GLN:O	2:C:661:VAL:HG22	1.99	0.62
1:A:104:LYS:NZ	1:A:105:SER:O	2.29	0.62
1:A:182:ARG:NH1	2:C:1090:ASN:OD1	2.33	0.62
3:D:1004:ALA:N	3:D:1017:VAL:O	2.33	0.62
5:F:160:ASP:O	5:F:163:THR:OG1	2.16	0.62
1:A:45:ARG:NE	1:B:38:THR:OG1	2.33	0.61
2:C:318:SER:OG	2:C:320:ASP:OD1	2.12	0.61
2:C:1313:HIS:O	4:E:28:ARG:NE	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:721:GLY:N	2:C:740:GLU:OE1	2.33	0.61
6:G:94:VAL:HG12	6:G:96:GLU:CG	2.27	0.61
2:C:840:SER:HG	2:C:1048:LYS:H	1.46	0.61
2:C:1307:ASN:O	2:C:1312:ASN:N	2.34	0.61
3:D:60:ARG:HG2	3:D:90:VAL:HG22	1.82	0.61
3:D:475:GLU:OE1	4:E:28:ARG:NH2	2.33	0.61
6:G:52:LYS:HA	6:G:58:GLU:CG	2.18	0.61
2:C:496:LYS:NZ	8:2:23:DT:OP2	2.33	0.61
2:C:941:LYS:NZ	2:C:1037:THR:O	2.27	0.61
5:F:436:ARG:NH2	8:2:26:DA:O4'	2.34	0.61
3:D:1220:ILE:O	3:D:1224:ARG:N	2.33	0.61
2:C:411:ARG:NH2	2:C:427:ASP:OD2	2.33	0.61
2:C:1088:ASP:OD1	2:C:1091:GLY:N	2.34	0.61
5:F:330:LEU:O	5:F:333:VAL:HG12	2.00	0.60
5:F:132:CYS:SG	5:F:257:LYS:NZ	2.71	0.60
5:F:169:ASN:ND2	5:F:420:GLU:OE2	2.34	0.60
5:F:266:PHE:O	5:F:270:VAL:HG23	2.01	0.60
2:C:1127:LYS:NZ	2:C:1203:ASP:OD2	2.34	0.60
3:D:454:CYS:O	3:D:458:ASN:N	2.34	0.60
3:D:474:LEU:HD21	4:E:27:ALA:HB3	1.84	0.60
2:C:111:GLU:O	2:C:113:THR:N	2.35	0.60
2:C:839:VAL:HA	2:C:1049:ILE:HG22	1.84	0.60
3:D:1029:THR:O	3:D:1118:GLY:N	2.34	0.60
5:F:554:ARG:NE	5:F:555:GLU:OE2	2.33	0.60
1:B:180:VAL:O	3:D:535:ARG:NE	2.34	0.59
3:D:127:LEU:O	3:D:220:ARG:NH2	2.34	0.59
1:B:158:ARG:HD2	1:B:172:LEU:HD11	1.85	0.59
5:F:548:LEU:HA	5:F:551:LEU:HD13	1.84	0.59
2:C:396:ASP:OD1	2:C:397:LEU:N	2.35	0.59
5:F:141:ILE:O	5:F:143:TYR:N	2.35	0.59
3:D:139:LEU:HD21	3:D:185:ILE:HD13	1.84	0.59
5:F:157:ARG:O	5:F:162:ILE:HD12	2.02	0.59
3:D:510:LEU:O	3:D:514:THR:HG22	2.01	0.59
3:D:1173:ARG:O	3:D:1190:ILE:N	2.35	0.59
1:B:102:LEU:HD23	1:B:103:ASN:N	2.18	0.59
2:C:1160:ASP:OD1	2:C:1161:LEU:N	2.36	0.59
2:C:565:GLU:OE1	2:C:684:ASN:ND2	2.36	0.59
3:D:1234:VAL:HG12	3:D:1253:ILE:HG21	1.85	0.59
2:C:205:PRO:O	2:C:208:ILE:HG22	2.02	0.59
5:F:110:LEU:HD21	7:1:70:DT:C2	2.37	0.59
2:C:935:THR:N	2:C:1040:ASP:OD2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:144:ALA:O	6:H:147:LEU:HD23	2.03	0.58
6:H:39:LEU:O	6:H:97:ILE:N	2.34	0.58
5:F:287:ILE:HD13	5:F:344:LEU:HD12	1.84	0.58
6:H:51:ILE:O	6:H:59:MET:N	2.36	0.58
3:D:591:ILE:HG23	3:D:592:VAL:HG13	1.86	0.58
5:F:250:LEU:O	5:F:253:SER:OG	2.18	0.58
5:F:407:GLU:HA	5:F:410:ILE:HD12	1.84	0.58
3:D:1267:VAL:HG23	3:D:1302:TYR:CA	2.34	0.58
2:C:823:VAL:O	2:C:1059:ARG:NH2	2.37	0.57
2:C:148:GLN:O	2:C:454:ARG:N	2.36	0.57
2:C:1276:TRP:CZ2	3:D:801:VAL:HG11	2.39	0.57
2:C:1252:SER:OG	2:C:1256:GLN:N	2.37	0.57
3:D:1166:GLY:N	3:D:1174:ARG:O	2.37	0.57
2:C:148:GLN:NE2	2:C:533:LEU:O	2.36	0.57
6:H:13:TRP:O	6:H:16:SER:OG	2.10	0.57
3:D:981:GLU:OE1	3:D:995:TYR:N	2.38	0.57
5:F:588:ARG:NH2	5:F:589:GLN:OE1	2.38	0.57
3:D:320:ASN:OD1	3:D:321:LYS:N	2.37	0.57
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.38	0.57
1:B:84:ASN:O	1:B:128:HIS:NE2	2.36	0.57
5:F:108:VAL:HG11	5:F:381:GLU:HB3	1.86	0.57
2:C:148:GLN:OE1	2:C:454:ARG:NH2	2.38	0.56
2:C:397:LEU:O	2:C:398:SER:OG	2.23	0.56
3:D:535:ARG:O	3:D:539:SER:OG	2.16	0.56
1:A:17:GLU:N	1:A:17:GLU:OE1	2.38	0.56
1:B:131:CYS:SG	1:B:132:HIS:N	2.78	0.56
2:C:1331:ARG:NH2	2:C:1337:ILE:O	2.39	0.56
6:H:198:ALA:HB1	6:H:202:THR:HG22	1.87	0.56
2:C:592:ARG:N	2:C:653:MET:O	2.36	0.56
3:D:424:ASN:HA	3:D:434:ILE:HG22	1.87	0.56
3:D:826:ILE:HG22	3:D:831:VAL:HG23	1.87	0.56
2:C:593:LYS:O	2:C:600:THR:N	2.39	0.56
2:C:701:GLY:N	2:C:1182:ILE:O	2.39	0.56
3:D:960:LEU:N	3:D:1007:ASP:OD1	2.39	0.56
8:2:47:DA:H5”	8:2:48:DT:H72	1.87	0.55
3:D:475:GLU:OE1	3:D:475:GLU:N	2.38	0.55
2:C:246:LEU:O	2:C:274:ILE:HD11	2.06	0.55
1:B:15:ASP:OD1	1:B:16:ILE:N	2.40	0.55
2:C:976:ARG:NH2	2:C:979:LEU:HD22	2.22	0.55
2:C:1088:ASP:OD1	2:C:1092:THR:N	2.39	0.55
3:D:481:ARG:HE	4:E:47:THR:HG21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLY:O	1:B:45:ARG:NH2	2.39	0.55
2:C:576:SER:OG	2:C:577:VAL:N	2.39	0.55
2:C:483:ASP:OD1	2:C:484:LEU:N	2.40	0.55
1:A:92:VAL:O	1:A:148:ARG:NH2	2.39	0.55
2:C:198:ILE:O	2:C:201:ARG:N	2.40	0.55
2:C:820:GLU:HG2	2:C:1079:ILE:HD13	1.88	0.55
3:D:694:SER:OG	3:D:738:ARG:NH2	2.39	0.55
6:G:29:LEU:N	6:G:86:VAL:O	2.40	0.55
2:C:932:GLN:NE2	2:C:933:VAL:O	2.40	0.55
3:D:397:ALA:O	3:D:401:VAL:HG23	2.06	0.55
3:D:1269:ALA:HB2	3:D:1274:PHE:HA	1.89	0.55
2:C:899:GLU:N	2:C:899:GLU:OE1	2.40	0.54
2:C:1103:VAL:O	2:C:1107:MET:N	2.40	0.54
2:C:1252:SER:N	2:C:1257:GLN:O	2.39	0.54
1:A:15:ASP:O	1:A:26:VAL:HG13	2.08	0.54
6:G:173:GLY:O	6:G:177:GLY:N	2.40	0.54
3:D:163:GLU:N	3:D:163:GLU:OE1	2.39	0.54
1:B:159:ILE:HD12	1:B:166:ARG:NH2	2.22	0.54
2:C:42:ASP:OD2	2:C:45:GLY:N	2.41	0.54
2:C:758:ARG:NH1	2:C:833:ILE:O	2.40	0.54
2:C:1330:ILE:CG2	2:C:1335:ILE:HD11	2.38	0.54
2:C:1273:MET:SD	2:C:1273:MET:N	2.80	0.54
3:D:1320:ILE:HD12	3:D:1342:ASP:OD2	2.08	0.54
5:F:137:TYR:CE1	5:F:361:ILE:HG21	2.43	0.54
1:B:104:LYS:NZ	1:B:105:SER:O	2.37	0.54
2:C:407:ARG:NH2	2:C:411:ARG:O	2.40	0.54
3:D:826:ILE:HG22	3:D:831:VAL:HA	1.89	0.54
1:B:74:VAL:HG22	1:B:133:LEU:HD23	1.90	0.53
2:C:1071:GLY:O	2:C:1073:LYS:N	2.41	0.53
3:D:1267:VAL:HG23	3:D:1302:TYR:HA	1.90	0.53
7:1:74:DT:OP1	7:1:75:DG:N2	2.41	0.53
3:D:193:ASP:OD1	3:D:194:LEU:N	2.41	0.53
3:D:858:VAL:HG12	3:D:862:THR:OG1	2.07	0.53
2:C:38:PHE:O	2:C:49:LEU:HD22	2.09	0.53
2:C:15:PHE:CG	2:C:1190:ALA:HB2	2.44	0.53
2:C:196:VAL:O	2:C:204:LEU:N	2.42	0.53
3:D:959:LYS:C	3:D:960:LEU:HD12	2.28	0.53
3:D:139:LEU:HD21	3:D:185:ILE:CD1	2.39	0.53
3:D:1345:ARG:N	3:D:1349:GLU:OE1	2.42	0.53
2:C:866:ASP:OD1	2:C:870:ILE:N	2.41	0.53
3:D:956:GLY:N	3:D:1010:GLN:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ARG:NH2	3:D:534:GLU:OE2	2.42	0.53
1:B:115:ILE:HD13	1:B:117:HIS:HB3	1.91	0.53
2:C:65:ASN:OD1	2:C:66:SER:N	2.42	0.52
4:E:25:ARG:NH1	4:E:61:ASN:OD1	2.43	0.52
5:F:555:GLU:O	5:F:559:LEU:HD13	2.08	0.52
6:G:137:LEU:HD23	6:G:141:GLY:C	2.29	0.52
1:B:17:GLU:N	1:B:25:LYS:O	2.43	0.52
2:C:553:THR:HG21	2:C:608:ALA:HB1	1.90	0.52
3:D:957:SER:N	3:D:985:ILE:O	2.42	0.52
6:H:131:VAL:HA	6:H:134:LEU:HD12	1.90	0.52
5:F:130:VAL:HG22	5:F:365:MET:HA	1.91	0.52
5:F:402:LEU:HA	5:F:405:ILE:HD12	1.92	0.52
2:C:448:LEU:HD23	2:C:553:THR:HB	1.91	0.52
3:D:1111:ASP:OD1	3:D:1112:GLY:N	2.42	0.52
2:C:595:THR:O	2:C:598:VAL:N	2.43	0.52
2:C:958:LYS:O	2:C:961:SER:OG	2.21	0.52
3:D:812:ASP:O	3:D:897:HIS:ND1	2.40	0.52
1:B:182:ARG:NH1	1:B:204:GLU:OE1	2.42	0.52
3:D:1004:ALA:HB3	3:D:1017:VAL:HA	1.91	0.52
1:B:153:VAL:H	1:B:175:ALA:HB3	1.74	0.52
2:C:74:ARG:NH2	2:C:121:GLU:OE2	2.41	0.52
3:D:478:LEU:CD2	4:E:47:THR:HG23	2.40	0.52
2:C:714:VAL:HG13	2:C:715:THR:HG23	1.92	0.51
3:D:71:LEU:HG	3:D:90:VAL:HG21	1.90	0.51
6:G:195:LEU:O	6:G:196:ILE:HD13	2.10	0.51
6:G:94:VAL:CG1	6:G:96:GLU:CG	2.87	0.51
3:D:75:TYR:CE1	3:D:83:VAL:HG11	2.45	0.51
5:F:554:ARG:O	5:F:557:LYS:NZ	2.42	0.51
7:1:45:DT:H3	8:2:46:DA:H61	1.59	0.51
1:A:131:CYS:SG	1:A:132:HIS:N	2.80	0.51
2:C:349:GLU:O	2:C:353:VAL:HG23	2.11	0.51
6:H:49:VAL:HG22	6:H:86:VAL:HG22	1.93	0.51
1:B:192:VAL:HB	1:B:195:ARG:HB2	1.91	0.51
5:F:585:GLU:O	5:F:589:GLN:NE2	2.44	0.51
2:C:857:VAL:HG11	6:G:21:HIS:CE1	2.46	0.51
3:D:1089:LEU:HD22	3:D:1094:ASP:O	2.11	0.51
2:C:758:ARG:NH2	2:C:835:GLU:OE1	2.44	0.51
6:H:133:ASN:HD22	6:H:137:LEU:HD12	1.76	0.51
5:F:362:ASN:OD1	5:F:363:ARG:N	2.42	0.51
1:A:155:ALA:HB3	1:A:174:ASP:HA	1.93	0.51
5:F:573:LEU:HD21	8:2:45:DA:H5'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1265:THR:N	3:D:1303:SER:O	2.44	0.50
4:E:10:VAL:HG11	4:E:16:ARG:NH1	2.26	0.50
2:C:1060:ILE:HD12	2:C:1060:ILE:H	1.76	0.50
2:C:1340:GLU:N	3:D:19:ALA:O	2.44	0.50
3:D:60:ARG:CG	3:D:90:VAL:HG22	2.42	0.50
3:D:61:ILE:O	3:D:101:ARG:NH1	2.43	0.50
2:C:214:ASN:H	2:C:359:ARG:HE	1.60	0.50
2:C:320:ASP:OD1	2:C:321:LEU:N	2.44	0.50
2:C:1308:ILE:HG21	3:D:379:PRO:HG2	1.93	0.50
1:B:182:ARG:NH2	1:B:204:GLU:OE2	2.44	0.50
5:F:385:ARG:NH2	7:1:71:DG:N7	2.60	0.50
3:D:385:LEU:O	3:D:389:GLY:N	2.40	0.50
5:F:260:ARG:HB2	5:F:262:VAL:HG13	1.94	0.50
2:C:1236:ASN:OD1	2:C:1237:HIS:N	2.44	0.50
6:G:104:GLN:O	6:G:108:VAL:HG23	2.12	0.50
1:A:186:ASN:ND2	1:A:204:GLU:OE2	2.44	0.50
2:C:1122:LYS:NZ	2:C:1229:TYR:OH	2.45	0.50
1:B:84:ASN:HB3	1:B:130:ILE:HA	1.94	0.50
2:C:862:LEU:HD11	6:G:19:HIS:CB	2.41	0.50
3:D:1265:THR:OG1	3:D:1305:ASP:OD2	2.20	0.50
6:G:40:TYR:CD1	6:G:96:GLU:CD	2.85	0.50
3:D:384:LYS:HD3	3:D:411:ILE:HG23	1.94	0.50
2:C:138:ILE:O	2:C:141:THR:OG1	2.05	0.49
5:F:240:ARG:NH1	5:F:246:GLN:OE1	2.42	0.49
6:G:120:MET:SD	6:H:124:LEU:HD11	2.52	0.49
2:C:91:THR:HG23	2:C:138:ILE:HD13	1.93	0.49
2:C:934:PHE:HD2	2:C:1049:ILE:HD11	1.77	0.49
3:D:1029:THR:HB	3:D:1115:ILE:HD13	1.93	0.49
7:1:17:DT:O4	8:2:73:DA:N6	2.45	0.49
1:A:168:ILE:HD13	2:C:873:ILE:O	2.12	0.49
2:C:788:SER:O	2:C:795:ALA:N	2.45	0.49
2:C:1324:ASN:OD1	2:C:1325:VAL:N	2.45	0.49
3:D:478:LEU:HD23	4:E:47:THR:HG23	1.92	0.49
3:D:965:SER:HB2	3:D:973:LEU:HD11	1.93	0.49
3:D:1371:ARG:HA	3:D:1374:ALA:HB3	1.94	0.49
5:F:396:ASN:O	5:F:398:GLY:N	2.44	0.49
3:D:500:ILE:HG22	3:D:500:ILE:O	2.12	0.49
1:A:12:ARG:N	1:A:29:GLU:O	2.46	0.49
1:A:91:ARG:HB3	1:A:122:GLU:HB3	1.95	0.49
2:C:990:ASP:OD1	2:C:991:LYS:N	2.46	0.49
3:D:883:ARG:NH1	3:D:898:CYS:SG	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:127:ILE:HG23	5:F:261:LEU:HD22	1.94	0.49
6:H:127:THR:HG23	6:H:130:LYS:HE3	1.95	0.49
6:H:138:ASP:OD1	6:H:140:THR:OG1	2.16	0.49
2:C:251:ALA:O	2:C:266:GLY:N	2.41	0.49
2:C:400:VAL:HG22	2:C:584:TYR:HD1	1.77	0.49
1:B:43:LEU:O	1:B:47:LEU:HD23	2.13	0.49
2:C:328:SER:OG	2:C:330:HIS:ND1	2.45	0.49
6:G:77:GLU:OE2	6:H:122:ARG:NH2	2.46	0.49
6:H:140:THR:OG1	6:H:141:GLY:N	2.45	0.49
1:B:214:GLU:OE2	1:B:218:ARG:NH2	2.46	0.48
2:C:126:GLU:C	2:C:127:ILE:HD12	2.34	0.48
3:D:331:ILE:HD12	3:D:331:ILE:N	2.28	0.48
3:D:481:ARG:O	4:E:6:VAL:HG21	2.13	0.48
3:D:558:ASP:HB3	3:D:564:VAL:HG21	1.95	0.48
5:F:412:LEU:HA	5:F:435:ILE:HD11	1.93	0.48
3:D:43:THR:HB	3:D:56:LEU:HD21	1.96	0.48
5:F:385:ARG:HA	5:F:388:ILE:HG22	1.95	0.48
2:C:594:VAL:HG22	2:C:599:VAL:HG13	1.95	0.48
2:C:1335:ILE:HD12	2:C:1337:ILE:N	2.27	0.48
3:D:363:LEU:HD21	4:E:4:VAL:HG11	1.94	0.48
6:H:47:VAL:HG21	6:H:86:VAL:HG12	1.94	0.48
2:C:228:VAL:N	2:C:335:THR:O	2.42	0.48
2:C:350:THR:O	2:C:354:ASP:N	2.45	0.48
2:C:745:GLU:OE1	2:C:745:GLU:N	2.47	0.48
3:D:265:LEU:O	3:D:268:LEU:N	2.39	0.48
6:H:83:SER:OG	11:H:301:CMP:O1P	2.18	0.48
2:C:819:SER:OG	2:C:820:GLU:N	2.46	0.48
2:C:1079:ILE:HD12	2:C:1079:ILE:O	2.14	0.48
3:D:353:SER:OG	3:D:354:VAL:O	2.17	0.48
2:C:1107:MET:HG2	3:D:740:LEU:HD11	1.95	0.48
2:C:1253:LEU:HD13	5:F:523:ILE:HD13	1.94	0.48
3:D:1157:ALA:N	3:D:1208:ASP:O	2.46	0.48
2:C:22:LEU:HD23	2:C:578:TYR:CE1	2.48	0.48
2:C:490:GLN:HA	2:C:493:ILE:HD12	1.96	0.48
5:F:547:VAL:HG13	5:F:603:ARG:CD	2.43	0.48
5:F:600:HIS:O	5:F:602:SER:N	2.46	0.48
6:G:78:GLU:OE2	6:G:103:ARG:NH2	2.47	0.48
6:H:103:ARG:HA	6:H:106:ILE:HD12	1.94	0.48
3:D:559:ALA:HB3	3:D:562:GLU:HB3	1.94	0.48
3:D:256:ASP:OD1	3:D:257:GLY:N	2.46	0.48
5:F:119:ILE:HG23	5:F:375:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:65:ASN:O	2:C:105:TYR:N	2.46	0.48
3:D:588:PRO:O	3:D:591:ILE:HG22	2.13	0.48
3:D:822:MET:N	3:D:880:VAL:O	2.41	0.48
1:B:182:ARG:N	1:B:206:GLU:O	2.45	0.47
2:C:251:ALA:HB1	2:C:255:ILE:HD12	1.96	0.47
2:C:1010:GLN:OE1	2:C:1010:GLN:N	2.44	0.47
5:F:542:ALA:O	5:F:545:HIS:ND1	2.47	0.47
2:C:883:LEU:H	2:C:883:LEU:HD23	1.79	0.47
3:D:132:LEU:O	3:D:135:ILE:N	2.48	0.47
3:D:597:GLY:O	3:D:600:ALA:HB3	2.14	0.47
3:D:75:TYR:CD1	3:D:83:VAL:HG11	2.49	0.47
3:D:1319:PHE:O	3:D:1323:ALA:N	2.48	0.47
5:F:399:LEU:HD23	5:F:400:GLN:CB	2.44	0.47
2:C:862:LEU:HD11	6:G:19:HIS:HB2	1.95	0.47
5:F:547:VAL:HG13	5:F:603:ARG:HD3	1.94	0.47
6:G:40:TYR:CZ	6:G:96:GLU:OE2	2.67	0.47
3:D:252:LEU:HD22	3:D:261:ALA:O	2.14	0.47
1:A:15:ASP:OD1	1:A:16:ILE:N	2.47	0.47
1:A:38:THR:HG23	1:B:45:ARG:HD3	1.96	0.47
3:D:481:ARG:NE	4:E:47:THR:HG21	2.29	0.47
2:C:1261:GLY:O	2:C:1266:GLY:N	2.47	0.47
3:D:93:THR:HG22	3:D:94:GLN:N	2.29	0.47
3:D:1062:LEU:HD13	3:D:1066:GLU:HG2	1.97	0.47
5:F:227:GLN:HB3	5:F:252:LEU:HD13	1.97	0.47
3:D:44:ILE:HD12	3:D:45:ASN:C	2.34	0.47
3:D:155:GLU:N	3:D:158:GLN:OE1	2.46	0.47
3:D:848:VAL:HG22	3:D:858:VAL:HG22	1.97	0.47
5:F:386:LEU:HD11	5:F:390:ILE:HD11	1.97	0.47
1:B:89:ALA:HB3	1:B:125:LYS:N	2.30	0.47
2:C:155:VAL:HG23	2:C:176:ILE:HG22	1.97	0.47
2:C:228:VAL:O	2:C:335:THR:N	2.48	0.47
3:D:203:GLU:O	3:D:206:ASN:N	2.47	0.47
5:F:336:GLU:OE2	5:F:339:ARG:NH2	2.47	0.47
3:D:134:ASP:HB3	3:D:159:ILE:HD11	1.96	0.47
2:C:699:LEU:O	2:C:1182:ILE:N	2.40	0.46
3:D:342:LEU:O	3:D:345:LYS:NZ	2.39	0.46
3:D:48:THR:HG22	3:D:50:LYS:HD3	1.97	0.46
3:D:526:VAL:C	3:D:527:LEU:HD12	2.35	0.46
3:D:1035:VAL:HG11	3:D:1109:LEU:HD11	1.97	0.46
3:D:1266:ILE:N	3:D:1275:LEU:O	2.37	0.46
4:E:7:GLN:O	4:E:10:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:262:VAL:HB	5:F:263:PRO:CD	2.45	0.46
5:F:431:ALA:HB1	5:F:435:ILE:CD1	2.45	0.46
1:A:118:ASP:OD1	1:A:119:GLY:N	2.46	0.46
3:D:128:LEU:O	3:D:157:GLN:NE2	2.46	0.46
3:D:798:ARG:HA	3:D:801:VAL:HG12	1.98	0.46
1:B:81:ILE:HG23	1:B:130:ILE:HG22	1.98	0.46
1:B:207:THR:OG1	1:B:208:ASN:N	2.48	0.46
2:C:201:ARG:NE	2:C:369:MET:O	2.48	0.46
2:C:582:ASN:N	2:C:586:PHE:O	2.48	0.46
3:D:957:SER:O	3:D:985:ILE:N	2.44	0.46
5:F:543:ALA:O	5:F:547:VAL:HG23	2.16	0.46
2:C:196:VAL:N	2:C:204:LEU:O	2.46	0.46
3:D:478:LEU:HD12	4:E:24:ALA:HB2	1.97	0.46
3:D:506:VAL:O	3:D:510:LEU:HD23	2.15	0.46
5:F:372:ALA:HB1	5:F:376:LYS:NZ	2.31	0.46
2:C:14:ASP:OD1	2:C:15:PHE:N	2.49	0.46
2:C:402:ARG:NH2	2:C:419:ILE:O	2.43	0.46
3:D:343:LEU:HD21	3:D:1352:ILE:HD11	1.97	0.46
3:D:559:ALA:O	3:D:561:GLY:N	2.49	0.46
3:D:1215:GLU:N	3:D:1215:GLU:OE1	2.49	0.46
3:D:1347:LEU:O	3:D:1351:VAL:HG23	2.16	0.46
2:C:296:VAL:HG22	2:C:316:GLU:HA	1.97	0.46
3:D:1062:LEU:HD12	3:D:1067:ARG:HA	1.98	0.46
6:H:133:ASN:ND2	6:H:137:LEU:HD12	2.31	0.46
2:C:935:THR:HG23	2:C:1048:LYS:HE2	1.97	0.45
2:C:1326:LEU:O	2:C:1329:GLU:N	2.49	0.45
3:D:111:THR:O	3:D:239:LEU:HD23	2.17	0.45
3:D:275:ARG:NH1	3:D:298:MET:O	2.49	0.45
5:F:412:LEU:O	5:F:415:ALA:N	2.48	0.45
1:B:17:GLU:O	1:B:25:LYS:N	2.43	0.45
2:C:49:LEU:HD23	2:C:50:GLU:H	1.80	0.45
2:C:521:LEU:O	2:C:525:THR:HG22	2.16	0.45
2:C:564:PRO:O	2:C:566:GLY:N	2.49	0.45
2:C:1230:MET:SD	2:C:1231:TYR:N	2.89	0.45
2:C:1278:LEU:HD12	2:C:1283:ALA:HB3	1.99	0.45
1:B:61:ILE:CG2	1:B:140:ILE:HD11	2.47	0.45
2:C:560:PRO:HB2	3:D:776:THR:HG21	1.98	0.45
2:C:909:LYS:HG2	2:C:910:ALA:HB2	1.99	0.45
2:C:1124:ILE:HD12	2:C:1124:ILE:H	1.80	0.45
3:D:85:CYS:N	3:D:90:VAL:O	2.45	0.45
3:D:865:HIS:O	3:D:868:TRP:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:36:ALA:N	6:G:80:GLN:O	2.45	0.45
6:G:73:LEU:HD22	11:G:301:CMP:H3'	1.99	0.45
2:C:828:PHE:O	2:C:1060:ILE:HD11	2.17	0.45
3:D:147:ILE:HD11	3:D:179:LYS:HB2	1.98	0.45
3:D:268:LEU:O	3:D:272:VAL:HG23	2.17	0.45
3:D:1250:ASP:O	3:D:1253:ILE:N	2.43	0.45
5:F:550:GLY:C	5:F:551:LEU:HD12	2.37	0.45
2:C:463:GLN:HE22	2:C:502:VAL:HG22	1.80	0.45
3:D:1088:VAL:O	3:D:1097:ALA:HB3	2.17	0.45
3:D:1226:VAL:O	3:D:1230:THR:OG1	2.18	0.45
3:D:816:THR:O	3:D:860:ARG:NH2	2.50	0.45
3:D:1234:VAL:HG12	3:D:1253:ILE:CG2	2.47	0.45
6:H:139:VAL:HG13	6:H:142:ARG:NH2	2.31	0.45
7:1:25:DA:N6	8:2:65:DT:O4	2.50	0.45
3:D:844:THR:CG2	3:D:858:VAL:HG11	2.46	0.44
5:F:137:TYR:CD1	5:F:361:ILE:HD13	2.52	0.44
2:C:258:ASN:OD1	2:C:259:GLY:N	2.44	0.44
3:D:320:ASN:ND2	3:D:322:ARG:O	2.50	0.44
3:D:1029:THR:CB	3:D:1115:ILE:HD13	2.47	0.44
3:D:1198:VAL:HG12	3:D:1210:ILE:HG23	1.98	0.44
2:C:251:ALA:CB	2:C:255:ILE:HD12	2.47	0.44
3:D:431:ARG:N	3:D:921:GLN:OE1	2.50	0.44
3:D:1177:ILE:HD12	3:D:1186:TYR:O	2.17	0.44
5:F:478:PRO:HG2	5:F:483:LEU:HD11	1.98	0.44
6:G:127:THR:O	6:G:131:VAL:HG23	2.17	0.44
2:C:232:ILE:HD11	2:C:322:LEU:HD12	1.98	0.44
2:C:985:GLU:O	2:C:989:LEU:N	2.46	0.44
4:E:5:THR:HG22	4:E:7:GLN:H	1.82	0.44
6:H:30:ILE:HD12	6:H:86:VAL:CG2	2.48	0.44
2:C:573:ASN:OD1	2:C:574:SER:N	2.51	0.44
2:C:1329:GLU:OE2	3:D:331:ILE:HD11	2.18	0.44
3:D:768:ASN:OD1	3:D:769:VAL:N	2.50	0.44
3:D:320:ASN:HA	8:2:21:DA:H61	1.83	0.44
6:H:70:ILE:O	6:H:72:GLU:N	2.50	0.44
1:B:74:VAL:HG12	1:B:76:GLU:H	1.83	0.44
3:D:201:LEU:HD13	3:D:221:ILE:HG13	1.99	0.44
3:D:960:LEU:HD11	3:D:982:LEU:CG	2.47	0.44
3:D:984:LEU:O	3:D:992:LYS:N	2.43	0.44
2:C:241:LEU:N	2:C:283:LYS:O	2.51	0.44
3:D:147:ILE:HD12	3:D:177:ASP:HB3	1.99	0.44
7:1:45:DT:O4	8:2:46:DA:N6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:467:GLY:O	2:C:471:VAL:HG23	2.18	0.44
2:C:782:VAL:C	2:C:783:LEU:HD22	2.38	0.44
2:C:1101:LEU:HD13	3:D:504:GLN:HB3	2.00	0.44
3:D:519:ASN:HD22	3:D:707:ILE:HD13	1.83	0.44
2:C:49:LEU:HD11	2:C:73:TYR:CZ	2.53	0.43
2:C:857:VAL:HG11	6:G:21:HIS:HE1	1.82	0.43
2:C:15:PHE:CB	2:C:1190:ALA:HB2	2.49	0.43
2:C:531:SER:OG	2:C:532:ALA:N	2.50	0.43
2:C:840:SER:OG	2:C:1048:LYS:O	2.36	0.43
4:E:6:VAL:HG12	4:E:6:VAL:O	2.18	0.43
5:F:161:LEU:O	5:F:164:GLY:N	2.49	0.43
5:F:287:ILE:CD1	5:F:344:LEU:HD12	2.48	0.43
2:C:1124:ILE:HD12	2:C:1124:ILE:N	2.34	0.43
2:C:1335:ILE:HD12	2:C:1337:ILE:H	1.80	0.43
3:D:45:ASN:HB3	3:D:48:THR:HB	2.00	0.43
3:D:288:PRO:HB2	3:D:290:ILE:HG22	2.00	0.43
3:D:1306:LEU:HD23	3:D:1307:LEU:N	2.32	0.43
5:F:145:LEU:HD21	5:F:228:TYR:CD2	2.53	0.43
6:G:51:ILE:HG12	6:G:61:LEU:HD21	2.00	0.43
1:B:22:THR:OG1	1:B:207:THR:O	2.32	0.43
3:D:563:LEU:HD21	3:D:585:LYS:O	2.18	0.43
3:D:1078:LEU:HD12	3:D:1107:VAL:HG21	1.99	0.43
3:D:544:LEU:HA	3:D:574:VAL:HB	1.99	0.43
5:F:240:ARG:HE	5:F:357:GLN:HE22	1.65	0.43
6:G:201:LYS:HD2	6:G:203:ILE:HD11	2.01	0.43
1:B:59:VAL:HG22	1:B:144:ILE:HG23	2.01	0.43
2:C:1147:ARG:NH2	2:C:1201:LEU:HD13	2.33	0.43
3:D:1019:ASN:OD1	3:D:1020:TRP:N	2.51	0.43
3:D:1342:ASP:OD1	3:D:1343:GLU:N	2.49	0.43
6:G:73:LEU:HD13	11:G:301:CMP:O3'	2.19	0.43
6:H:30:ILE:HD12	6:H:86:VAL:HG21	2.00	0.43
1:A:11:PRO:HB2	1:A:28:LEU:HD11	2.00	0.43
1:A:101:THR:HG22	1:A:143:ARG:HG3	2.00	0.43
2:C:314:ASN:O	2:C:352:ARG:NH1	2.51	0.43
2:C:1067:ALA:O	2:C:1233:LEU:N	2.47	0.43
3:D:96:LYS:HA	3:D:99:ARG:NH1	2.33	0.43
3:D:347:VAL:HG12	3:D:348:ASP:O	2.17	0.43
5:F:119:ILE:HG22	5:F:123:ILE:HD12	2.00	0.43
6:H:142:ARG:NH1	6:H:143:ILE:HD11	2.34	0.43
1:B:106:GLY:O	1:B:133:LEU:HD12	2.19	0.43
2:C:828:PHE:C	2:C:1060:ILE:HD11	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:482:ALA:HA	4:E:6:VAL:HG21	1.99	0.43
3:D:834:PRO:O	3:D:837:ASP:N	2.51	0.43
3:D:1032:SER:OG	3:D:1117:SER:N	2.52	0.43
1:A:182:ARG:O	1:A:206:GLU:N	2.52	0.43
3:D:741:ALA:O	3:D:762:ASN:ND2	2.51	0.43
3:D:123:ARG:HA	3:D:126:LEU:HD23	1.99	0.43
3:D:497:GLU:OE1	3:D:497:GLU:N	2.50	0.43
3:D:1157:ALA:HB3	3:D:1208:ASP:H	1.84	0.43
2:C:873:ILE:HD12	2:C:873:ILE:H	1.84	0.42
3:D:1329:THR:HA	3:D:1332:LEU:HD12	2.01	0.42
5:F:227:GLN:CB	5:F:252:LEU:HD13	2.49	0.42
5:F:521:ASP:OD1	5:F:522:PHE:N	2.52	0.42
5:F:574:GLU:O	5:F:577:GLY:N	2.52	0.42
8:2:40:DG:H4'	8:2:41:DC:OP1	2.19	0.42
2:C:1244:HIS:NE2	2:C:1266:GLY:O	2.51	0.42
3:D:48:THR:O	3:D:50:LYS:N	2.52	0.42
4:E:49:ILE:HD12	4:E:49:ILE:H	1.83	0.42
5:F:399:LEU:HD22	5:F:403:ASP:HB2	2.00	0.42
6:G:39:LEU:HD12	6:G:70:ILE:O	2.18	0.42
2:C:692:THR:HA	2:C:830:THR:HG22	2.01	0.42
2:C:1247:SER:OG	2:C:1248:THR:N	2.52	0.42
3:D:600:ALA:O	3:D:603:LYS:HG2	2.19	0.42
3:D:1307:LEU:CB	3:D:1312:ALA:HB2	2.49	0.42
4:E:10:VAL:HG11	4:E:16:ARG:HH12	1.83	0.42
2:C:520:PRO:O	2:C:524:ILE:HG22	2.19	0.42
2:C:563:THR:HG21	2:C:569:ILE:O	2.18	0.42
2:C:576:SER:OG	2:C:659:GLN:O	2.37	0.42
3:D:259:ARG:NH1	5:F:499:LYS:O	2.50	0.42
3:D:1089:LEU:HD23	3:D:1096:PRO:HA	2.02	0.42
6:H:51:ILE:HD13	6:H:61:LEU:HD21	2.01	0.42
2:C:441:GLU:OE1	2:C:441:GLU:N	2.52	0.42
3:D:514:THR:HG23	3:D:514:THR:O	2.19	0.42
5:F:361:ILE:HG22	5:F:365:MET:CE	2.49	0.42
6:H:47:VAL:HG23	6:H:88:ALA:HA	2.01	0.42
1:B:151:GLY:O	1:B:177:TYR:N	2.53	0.42
2:C:1298:VAL:O	2:C:1302:THR:HG23	2.19	0.42
3:D:290:ILE:HG23	3:D:291:ILE:HG13	2.01	0.42
3:D:845:ALA:HB2	3:D:882:VAL:N	2.35	0.42
3:D:1157:ALA:HB2	3:D:1204:VAL:HG21	2.02	0.42
5:F:583:THR:HG23	5:F:586:ARG:CZ	2.49	0.42
2:C:1049:ILE:O	2:C:1049:ILE:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1182:ILE:HG22	2:C:1183:ALA:N	2.35	0.42
3:D:645:VAL:HB	3:D:701:LEU:HD21	2.02	0.42
5:F:412:LEU:CA	5:F:435:ILE:HD11	2.49	0.42
6:H:28:THR:HG23	6:H:87:ARG:HE	1.85	0.42
2:C:516:ASP:OD1	2:C:516:ASP:N	2.48	0.42
2:C:840:SER:HB3	2:C:850:ILE:HD11	2.02	0.42
2:C:231:GLU:OE1	2:C:233:ARG:NH2	2.52	0.42
3:D:720:ASN:OD1	3:D:721:SER:N	2.53	0.42
6:G:13:TRP:CH2	6:G:105:LEU:HD22	2.55	0.42
6:G:20:ILE:HD12	6:G:20:ILE:H	1.84	0.42
6:G:131:VAL:HG22	6:H:131:VAL:CG2	2.49	0.42
8:2:52:DA:H2'	8:2:53:DT:H72	2.02	0.42
1:A:89:ALA:HB3	1:A:124:VAL:HB	2.01	0.42
1:A:135:ASP:HB3	1:A:138:ALA:HB2	2.01	0.42
1:B:67:GLU:OE2	1:B:79:LEU:HD22	2.20	0.42
2:C:739:ASP:OD1	2:C:740:GLU:N	2.52	0.42
3:D:43:THR:CB	3:D:56:LEU:HD21	2.50	0.42
3:D:384:LYS:CD	3:D:411:ILE:HG23	2.49	0.42
3:D:1288:ALA:HA	3:D:1292:LEU:HD13	2.00	0.42
2:C:818:VAL:HG22	2:C:819:SER:N	2.34	0.41
3:D:1002:VAL:O	3:D:1019:ASN:N	2.45	0.41
5:F:356:GLU:OE1	5:F:356:GLU:N	2.45	0.41
6:H:33:GLY:N	6:H:81:GLU:OE1	2.52	0.41
2:C:867:GLU:HG2	2:C:868:SER:H	1.82	0.41
2:C:1269:ARG:NH2	3:D:340:GLN:O	2.50	0.41
2:C:1331:ARG:HE	2:C:1337:ILE:CG2	2.32	0.41
3:D:135:ILE:HG22	3:D:139:LEU:HD12	2.03	0.41
3:D:525:MET:H	3:D:548:VAL:HG13	1.85	0.41
3:D:1153:PRO:HB2	3:D:1155:ILE:HG23	2.02	0.41
5:F:599:ARG:O	5:F:599:ARG:NH1	2.49	0.41
6:G:102:PHE:O	6:G:106:ILE:HG22	2.20	0.41
7:1:59:DT:H2'	7:1:60:DT:H72	2.03	0.41
8:2:7:DG:H2"	8:2:8:DT:H71	2.02	0.41
2:C:124:MET:HB2	2:C:495:ALA:HB2	2.02	0.41
2:C:910:ALA:HB3	6:G:24:PRO:HG3	2.00	0.41
3:D:139:LEU:HD23	3:D:181:GLY:HA2	2.02	0.41
3:D:331:ILE:HG22	3:D:331:ILE:O	2.20	0.41
3:D:536:LEU:HD23	3:D:541:LEU:HD12	2.01	0.41
1:A:140:ILE:HB	1:A:142:MET:HE1	2.02	0.41
2:C:209:ILE:O	2:C:212:ALA:HB3	2.20	0.41
2:C:400:VAL:HG22	2:C:584:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:HG2	1:A:180:VAL:HG23	2.02	0.41
1:A:186:ASN:N	1:A:202:VAL:O	2.53	0.41
1:A:228:LEU:HD11	1:B:221:ALA:HB1	2.02	0.41
2:C:104:ILE:HG22	2:C:105:TYR:N	2.35	0.41
3:D:493:PRO:O	3:D:903:LEU:HD22	2.19	0.41
3:D:1047:THR:HB	3:D:1062:LEU:HD11	2.02	0.41
6:H:60:ILE:HD12	6:H:60:ILE:N	2.35	0.41
7:1:13:DC:C2'	7:1:14:DT:H72	2.50	0.41
3:D:816:THR:OG1	3:D:883:ARG:NH2	2.54	0.41
3:D:1040:MET:SD	3:D:1078:LEU:N	2.94	0.41
5:F:423:ARG:NH1	7:1:66:DA:N7	2.68	0.41
2:C:195:PHE:HB3	2:C:203:LYS:HG3	2.03	0.41
3:D:71:LEU:CG	3:D:90:VAL:HG21	2.50	0.41
3:D:1320:ILE:O	3:D:1324:SER:OG	2.33	0.41
5:F:480:PRO:HB3	5:F:494:ILE:HG21	2.03	0.41
2:C:232:ILE:HD11	2:C:322:LEU:CD1	2.50	0.41
2:C:910:ALA:HB3	6:G:24:PRO:CG	2.51	0.41
3:D:44:ILE:HG22	3:D:50:LYS:C	2.41	0.41
1:A:20:SER:N	1:A:23:HIS:O	2.47	0.41
1:B:57:THR:O	1:B:172:LEU:HD12	2.21	0.41
1:B:199:ASP:OD1	1:B:199:ASP:N	2.54	0.41
2:C:82:VAL:HG23	2:C:83:GLN:N	2.35	0.41
2:C:101:ARG:HG2	2:C:103:VAL:HG23	2.02	0.41
2:C:638:SER:O	2:C:640:GLY:N	2.54	0.41
2:C:1004:ASP:OD1	2:C:1005:GLU:N	2.53	0.41
2:C:1331:ARG:HE	2:C:1337:ILE:HG23	1.86	0.41
3:D:279:LEU:CD1	3:D:283:LEU:HD11	2.51	0.41
3:D:586:GLY:CA	3:D:587:LEU:HD22	2.50	0.41
3:D:844:THR:OG1	3:D:858:VAL:HG21	2.20	0.41
3:D:1292:LEU:O	3:D:1294:ALA:N	2.54	0.41
5:F:505:ILE:HG22	5:F:505:ILE:O	2.21	0.41
6:H:198:ALA:CB	6:H:202:THR:HG22	2.51	0.41
8:2:7:DG:C2'	8:2:8:DT:H71	2.51	0.41
2:C:933:VAL:CG2	2:C:1050:VAL:HG23	2.51	0.41
3:D:136:GLU:O	3:D:139:LEU:N	2.53	0.41
3:D:481:ARG:HD2	4:E:51:LEU:HD11	2.03	0.41
3:D:495:ASN:OD1	3:D:495:ASN:N	2.53	0.41
5:F:508:GLU:OE1	5:F:508:GLU:N	2.54	0.41
1:B:12:ARG:HE	1:B:30:PRO:HD2	1.86	0.40
2:C:910:ALA:HB3	6:G:24:PRO:CB	2.51	0.40
3:D:394:ILE:O	3:D:397:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:950:ILE:HB	3:D:1018:ALA:HB3	2.03	0.40
3:D:1162:ILE:HG23	3:D:1178:THR:HB	2.02	0.40
6:H:179:SER:O	6:H:183:VAL:HG23	2.20	0.40
3:D:468:VAL:HG12	3:D:469:HIS:N	2.36	0.40
3:D:880:VAL:HG12	3:D:881:LYS:N	2.36	0.40
5:F:583:THR:HG23	5:F:586:ARG:NE	2.36	0.40
6:G:51:ILE:HG21	6:G:61:LEU:HD11	2.02	0.40
1:A:51:MET:HG3	1:A:180:VAL:HG21	2.03	0.40
2:C:671:LEU:HD11	2:C:679:ALA:HB2	2.03	0.40
2:C:1289:GLU:O	2:C:1293:VAL:HG22	2.21	0.40
3:D:114:ILE:HG23	3:D:115:TRP:HD1	1.87	0.40
3:D:263:SER:OG	3:D:264:ASP:N	2.54	0.40
3:D:424:ASN:N	3:D:467:ALA:O	2.54	0.40
3:D:736:GLN:O	3:D:740:LEU:HD12	2.20	0.40
6:H:11:LEU:HD21	6:H:43:VAL:HG22	2.04	0.40
1:A:166:ARG:HD2	1:A:170:ARG:HE	1.87	0.40
2:C:364:VAL:HG13	2:C:376:PRO:HG3	2.02	0.40
3:D:364:HIS:ND1	3:D:438:GLU:OE1	2.54	0.40
6:H:97:ILE:HG23	6:H:101:LYS:NZ	2.36	0.40
8:2:37:DG:H2'	8:2:38:DA:C8	2.57	0.40
1:B:133:LEU:HD13	1:B:138:ALA:O	2.22	0.40
2:C:192:ASP:OD1	2:C:436:ARG:NH2	2.55	0.40
2:C:728:ASP:N	2:C:731:ARG:O	2.54	0.40
2:C:838:CYS:SG	2:C:839:VAL:N	2.94	0.40
3:D:519:ASN:CB	3:D:707:ILE:HG21	2.51	0.40
3:D:1177:ILE:HG22	3:D:1179:PRO:HD3	2.03	0.40
5:F:233:ASP:O	5:F:237:ALA:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	228/329 (69%)	201 (88%)	26 (11%)	1 (0%)	34	72
1	B	226/329 (69%)	204 (90%)	22 (10%)	0	100	100
2	C	1338/1342 (100%)	1202 (90%)	132 (10%)	4 (0%)	41	76
3	D	1331/1407 (95%)	1185 (89%)	145 (11%)	1 (0%)	51	85
4	E	77/91 (85%)	71 (92%)	6 (8%)	0	100	100
5	F	479/628 (76%)	404 (84%)	69 (14%)	6 (1%)	12	48
6	G	195/210 (93%)	183 (94%)	12 (6%)	0	100	100
6	H	195/210 (93%)	176 (90%)	19 (10%)	0	100	100
All	All	4069/4546 (90%)	3626 (89%)	431 (11%)	12 (0%)	44	76

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	399	ALA
5	F	139	GLU
2	C	1072	ASN
3	D	121	PRO
5	F	140	ALA
5	F	507	MET
5	F	574	GLU
2	C	153	PRO
5	F	601	PRO
5	F	138	PRO
1	A	153	VAL
2	C	112	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	198/286 (69%)	195 (98%)	3 (2%)	65	80
1	B	196/286 (68%)	195 (100%)	1 (0%)	88	93
2	C	1155/1157 (100%)	1147 (99%)	8 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	1120/1168 (96%)	1112 (99%)	8 (1%)	84	90
4	E	67/75 (89%)	67 (100%)	0	100	100
5	F	429/554 (77%)	422 (98%)	7 (2%)	62	79
6	G	170/181 (94%)	169 (99%)	1 (1%)	86	92
6	H	170/181 (94%)	169 (99%)	1 (1%)	86	92
All	All	3505/3888 (90%)	3476 (99%)	29 (1%)	82	89

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	143	ARG
1	A	191	ARG
1	B	143	ARG
2	C	97	ARG
2	C	163	LYS
2	C	332	ARG
2	C	768	MET
2	C	903	ARG
2	C	1022	LYS
2	C	1147	ARG
2	C	1246	ARG
3	D	133	ARG
3	D	214	ARG
3	D	424	ASN
3	D	615	LYS
3	D	700	ASN
3	D	792	ASN
3	D	798	ARG
3	D	910	ASN
5	F	93	ARG
5	F	105	MET
5	F	317	ASN
5	F	343	LYS
5	F	400	GLN
5	F	441	ARG
5	F	451	ARG
6	G	35	LYS
6	H	201	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	120	GLN
2	C	684	ASN
2	C	766	ASN
3	D	274	ASN
3	D	424	ASN
3	D	792	ASN
5	F	169	ASN
5	F	383	ASN
5	F	464	ASN
6	G	149	ASN
6	H	133	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	1.50	5 (22%)	24,39,39	1.55	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	CMP	H	301	-	22,25,25	1.40	4 (18%)	24,39,39	1.54	4 (16%)

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	G	301	CMP	P-O3'	3.29	1.63	1.57
11	H	301	CMP	P-O5'	3.09	1.61	1.57
11	G	301	CMP	P-O5'	2.96	1.61	1.57
11	H	301	CMP	P-O3'	2.66	1.62	1.57
11	H	301	CMP	C5-C4	2.47	1.47	1.40
11	G	301	CMP	O5'-C5'	-2.34	1.42	1.46
11	G	301	CMP	C5-C4	2.24	1.46	1.40
11	H	301	CMP	O3'-C3'	-2.19	1.41	1.44
11	G	301	CMP	O3'-C3'	-2.06	1.41	1.44

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	301	CMP	C4-C5-N7	-3.61	105.64	109.40
11	H	301	CMP	N3-C2-N1	-3.53	123.16	128.68
11	G	301	CMP	O5'-P-O3'	3.34	110.28	105.68
11	G	301	CMP	N3-C2-N1	-3.03	123.94	128.68
11	H	301	CMP	C4-C5-N7	-2.95	106.32	109.40
11	G	301	CMP	O2P-P-O1P	2.89	117.77	108.73
11	H	301	CMP	O2P-P-O1P	2.81	117.54	108.73
11	H	301	CMP	O3'-P-O1P	-2.28	105.50	110.39

There are no chirality outliers.

There are no torsion outliers.

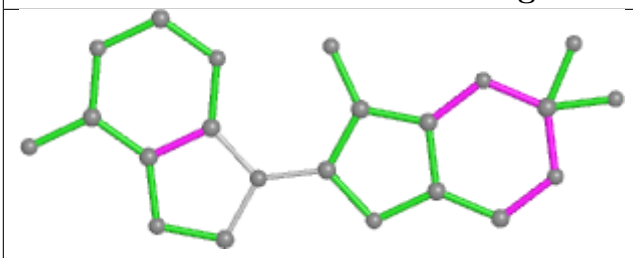
There are no ring outliers.

2 monomers are involved in 6 short contacts:

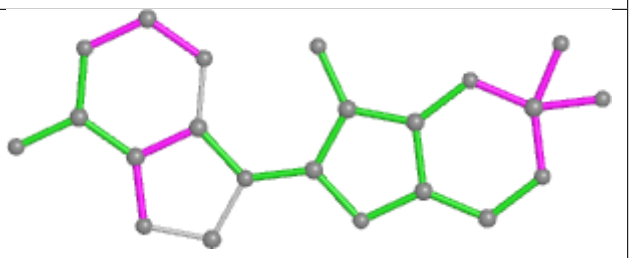
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	301	CMP	4	0
11	H	301	CMP	2	0

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 then 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.

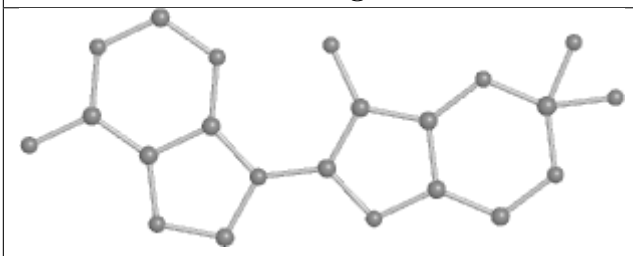
Ligand CMP G 301



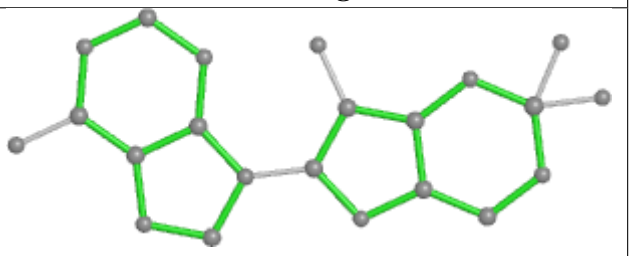
Bond lengths



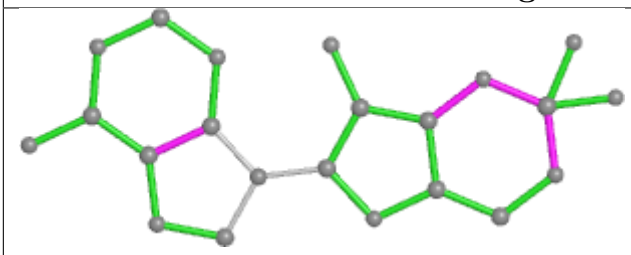
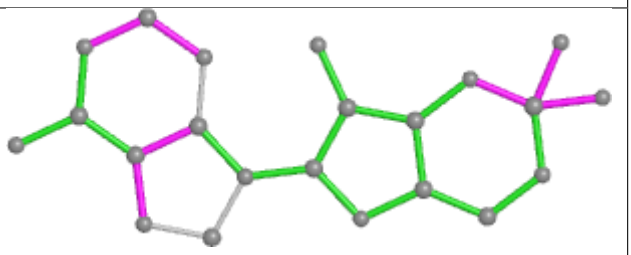
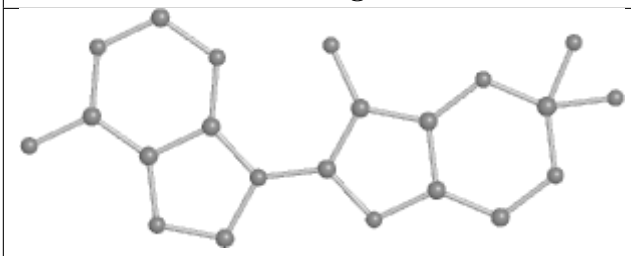
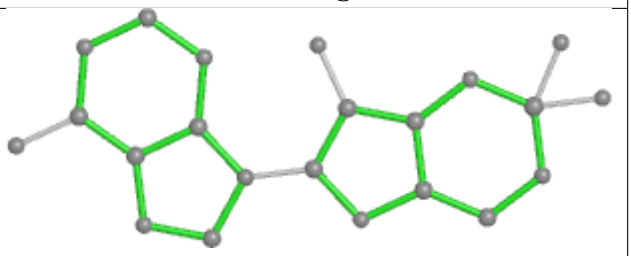
Bond angles



Torsions



Rings

Ligand CMP H 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

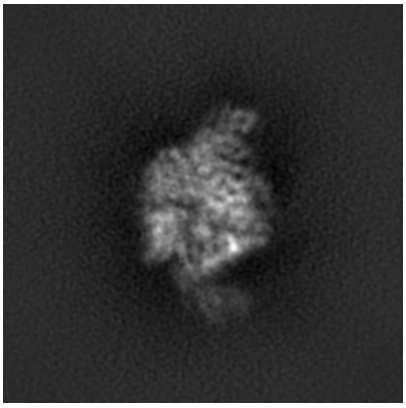
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20288. These allow visual inspection of the internal detail of the map and identification of artifacts.

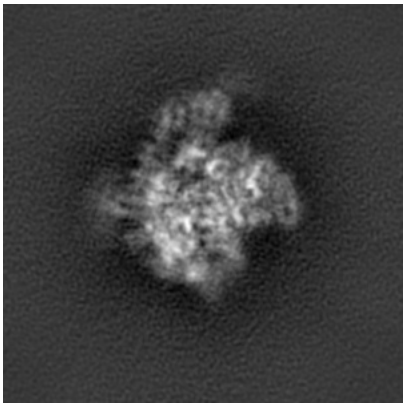
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

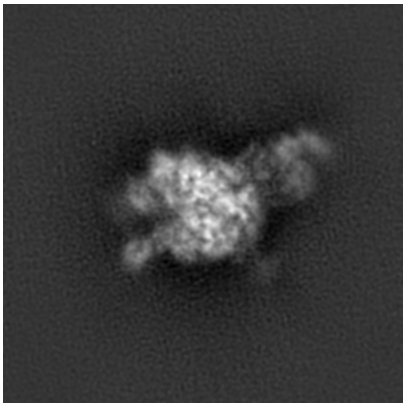
6.1.1 Primary map



X



Y

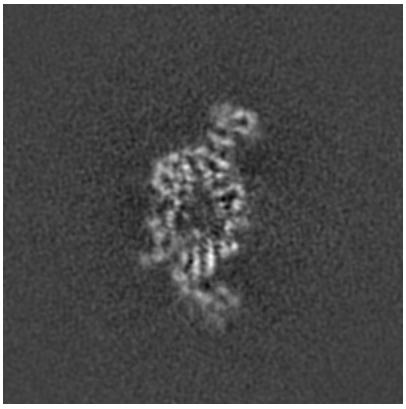


Z

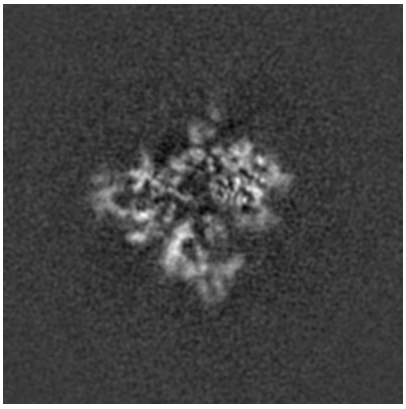
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

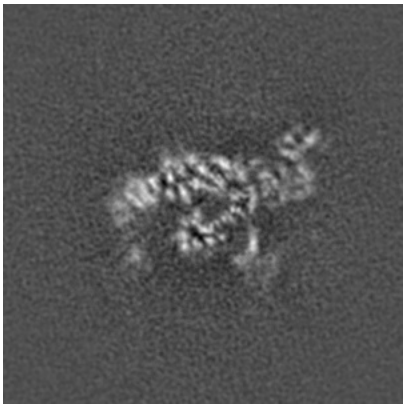
6.2.1 Primary map



X Index: 192



Y Index: 192

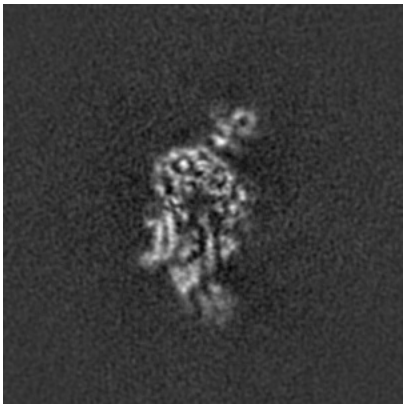


Z Index: 192

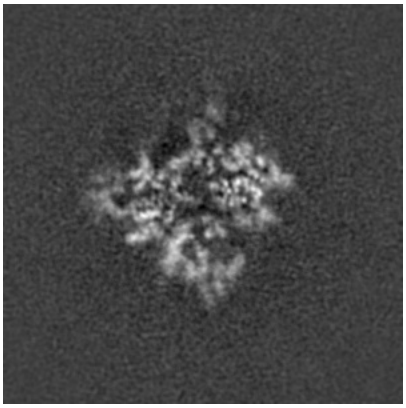
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

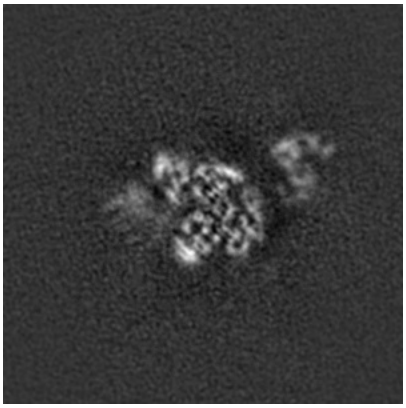
6.3.1 Primary map



X Index: 196



Y Index: 194

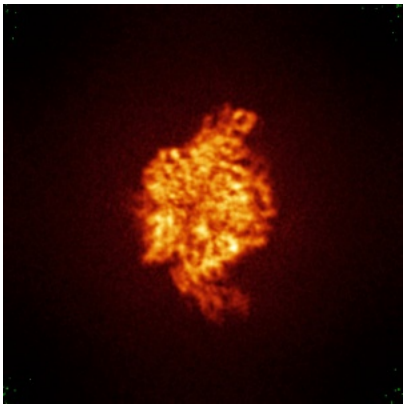


Z Index: 209

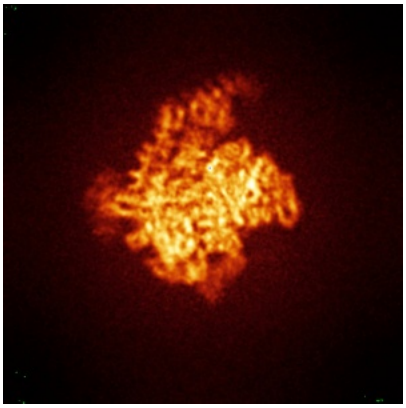
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

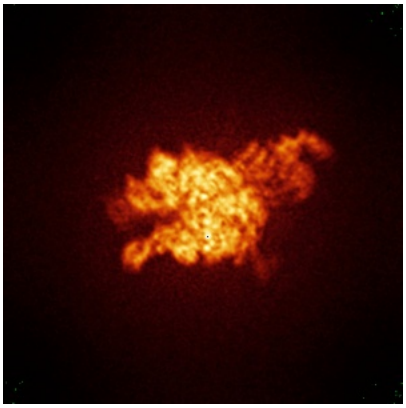
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

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.

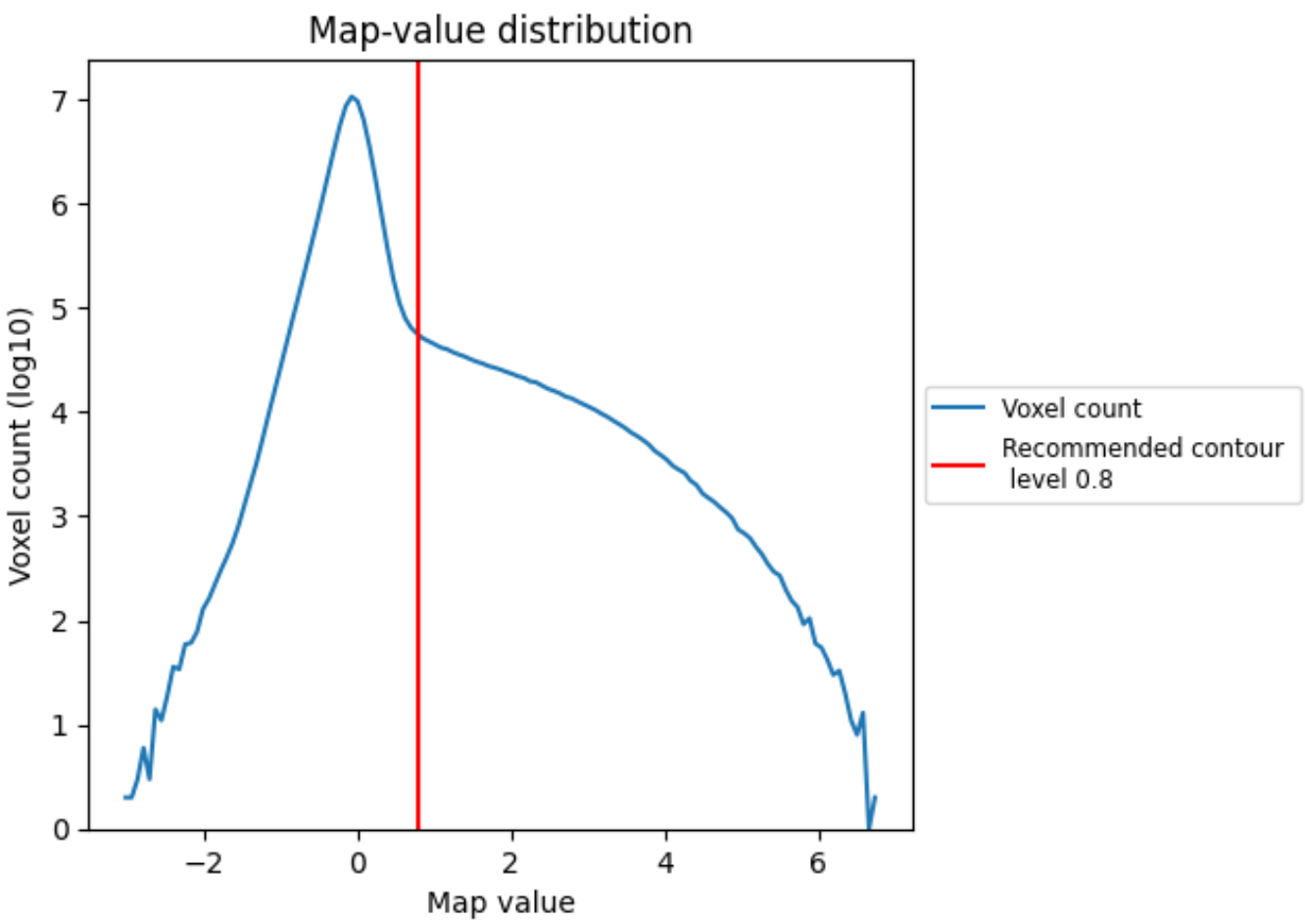
6.6 Mask visualisation (i)

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

7 Map analysis (i)

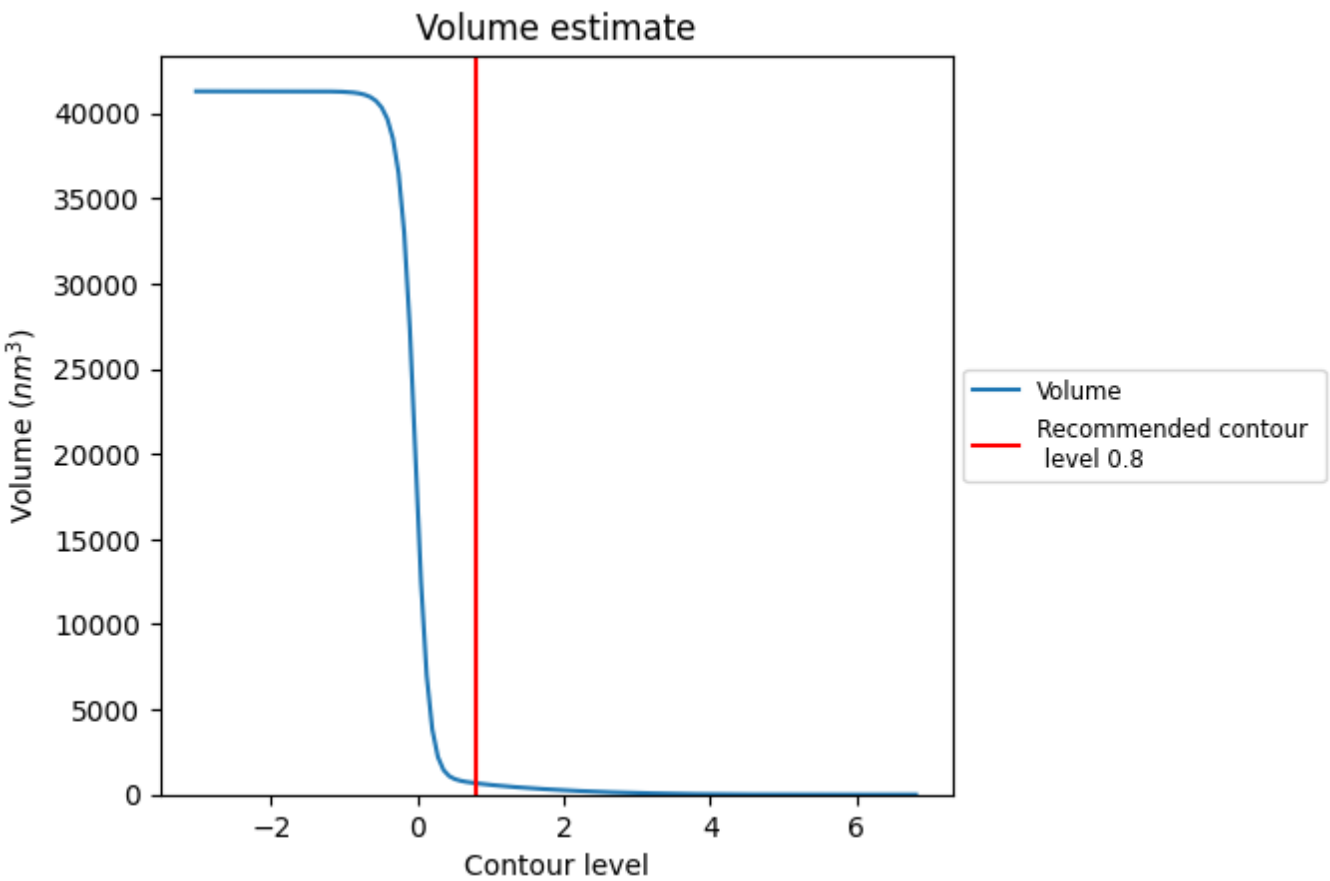
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

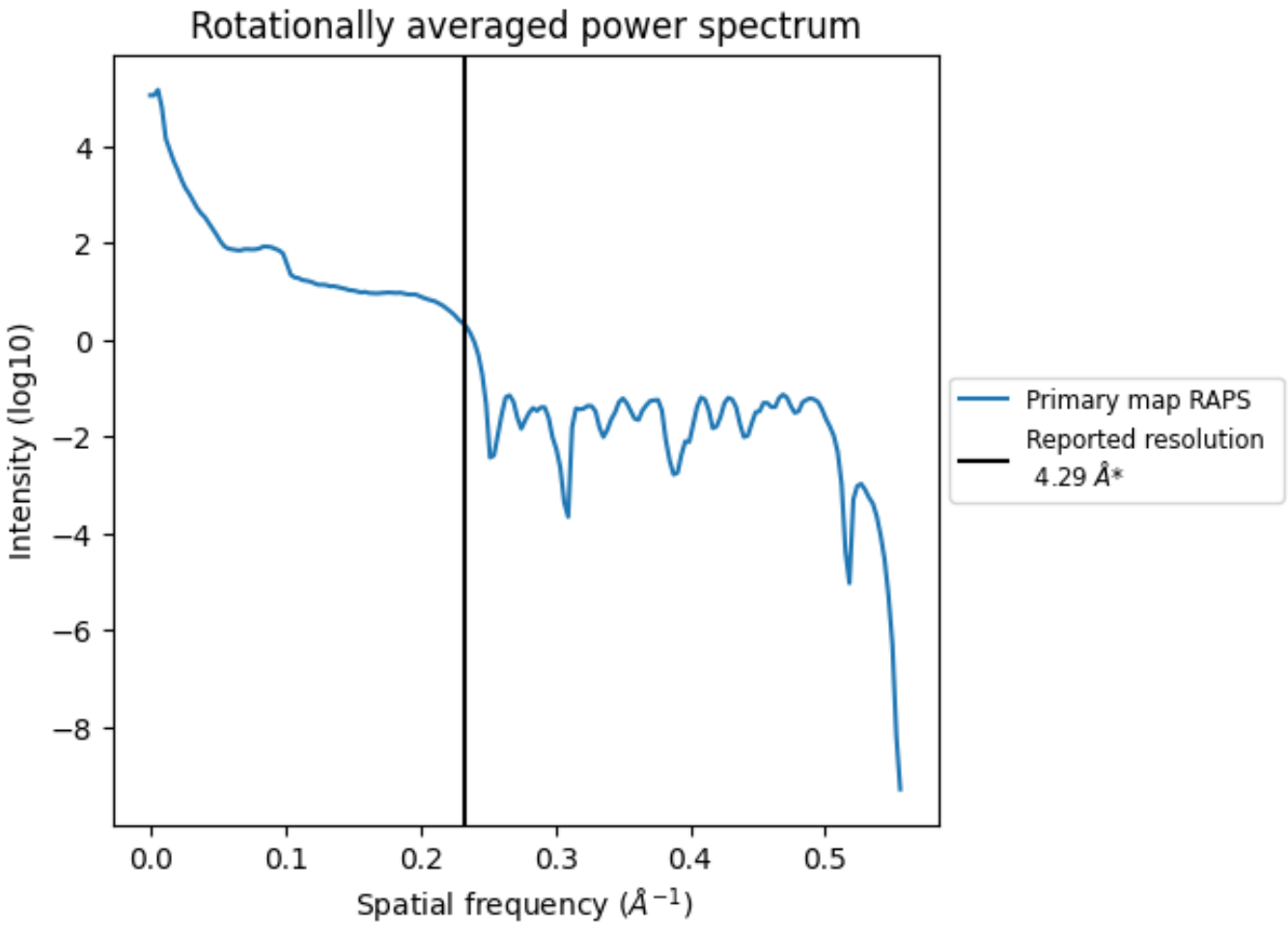
7.2 Volume estimate (i)



The volume at the recommended contour level is 667 nm^3; this corresponds to an approximate mass of 602 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.233 Å^{-1}

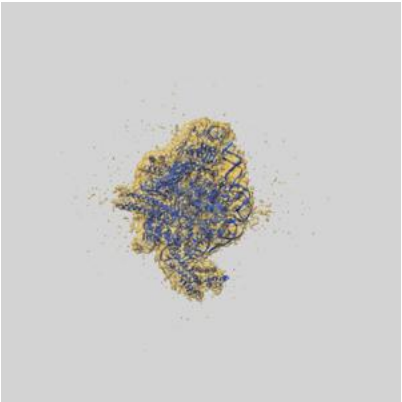
8 Fourier-Shell correlation (i)

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

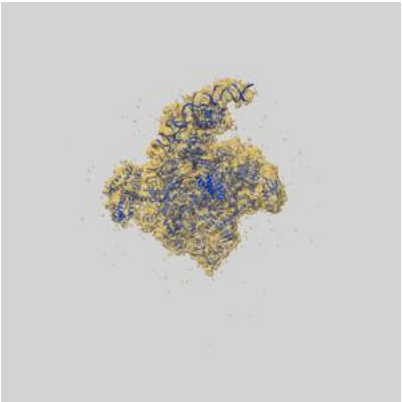
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20288 and PDB model 6PB6. Per-residue inclusion information can be found in section 3 on page 7.

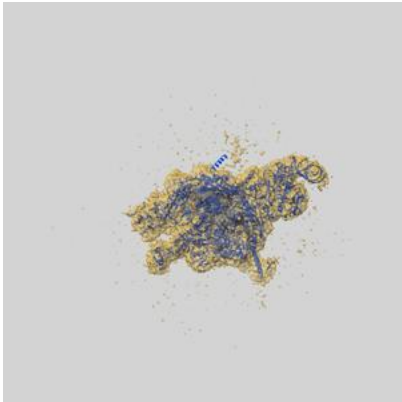
9.1 Map-model overlay (i)



X



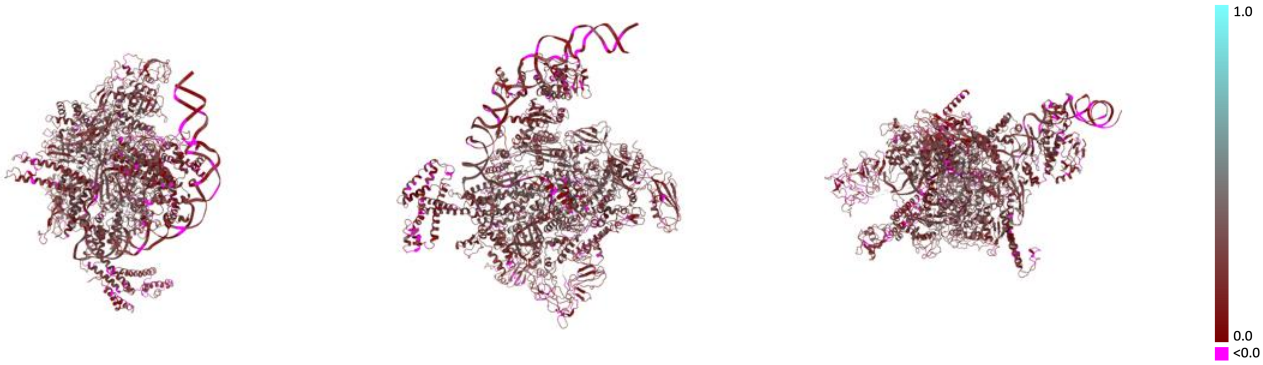
Y



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.

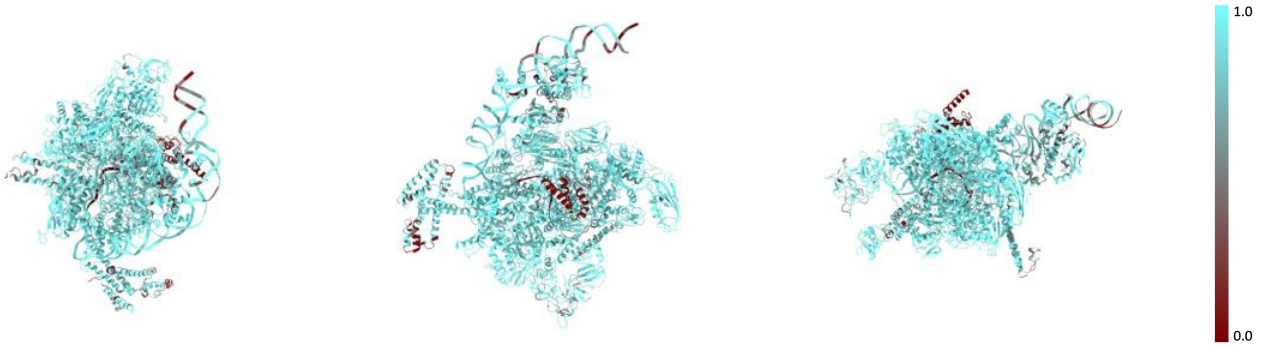
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

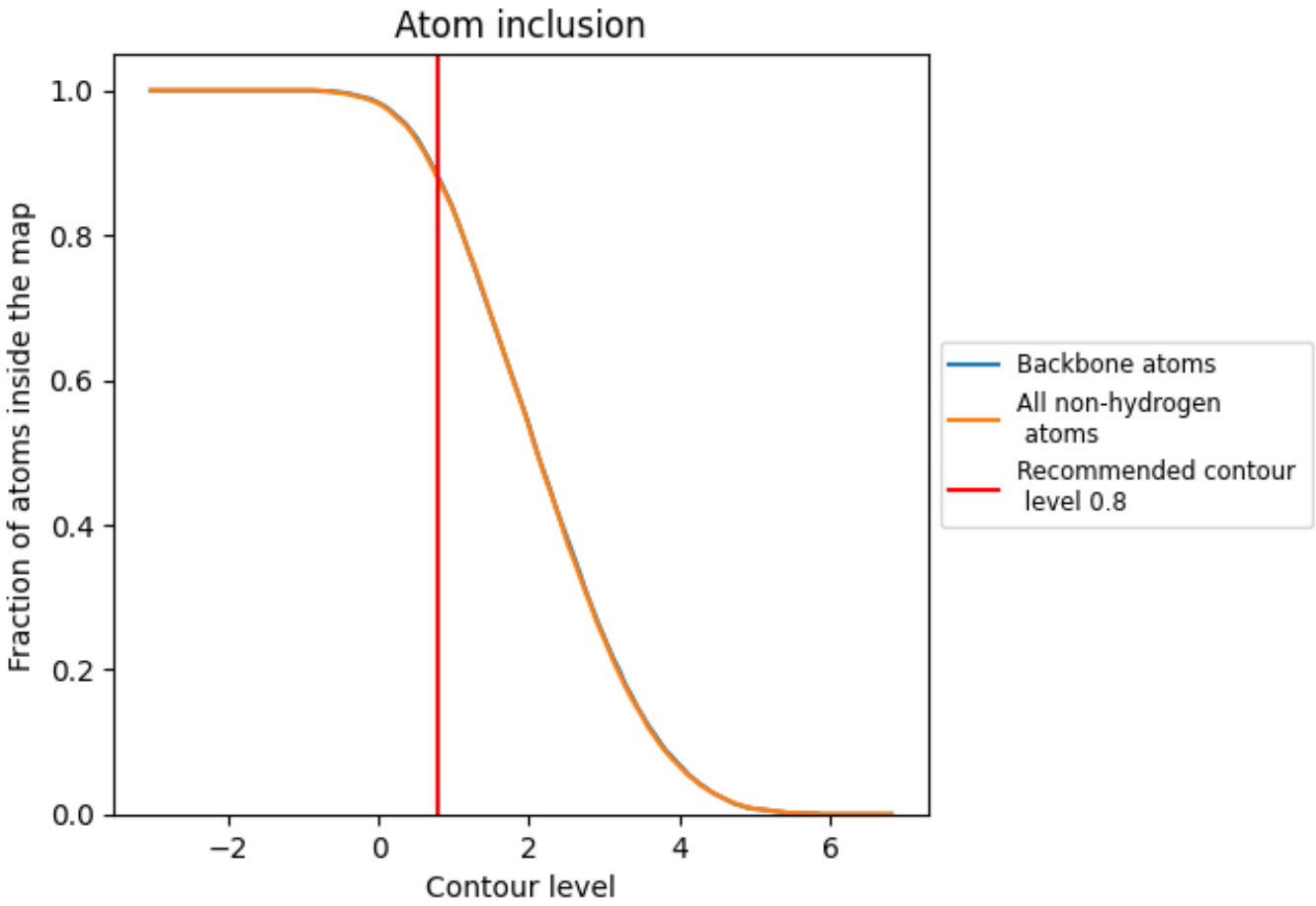
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 88% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.8760	0.2230
1	0.8440	0.1860
2	0.7320	0.1580
A	0.9710	0.2410
B	0.9450	0.2140
C	0.9450	0.2560
D	0.9120	0.2340
E	0.1590	0.0970
F	0.8190	0.1890
G	0.7960	0.2010
H	0.8050	0.1770