

Feb 24, 2024 – 01:39 PM EST

PDB ID	:	7K1N
EMDB ID	:	EMD-22626
Title	:	CryoEM structure of inactivated-form DNA-PK (Complex V)
Authors	:	Chen, X.; Gellert, M.; Yang, W.
Deposited on	:	2020-09-08
Resolution	:	3.90 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.dev70
MolProbity	:	4.02b-467
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

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 3.90 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 $(\#Entries)$	${ m EM} { m structures} \ (\#{ m Entries})$
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	А	4128	74%	13%	12%
2	В	609	6 6% 14%	•	20%
3	С	732	17%	17%	11%
4	D	24	88%		12%
4	F	24	8%		12%
5	Е	16	6% 69% 12%	Ď	19%
5	G	16	100%		



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 39521 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

• Molecule 1 is a protein called DNA-dependent protein kinase catalytic subunit.

Mol	Chain	Residues		Α	toms			AltConf	Trace
1	А	3634	Total 28808	C 18485	N 4884	O 5252	S 187	0	0

• Molecule 2 is a protein called X-ray repair cross-complementing protein 6.

Mol	Chain	Residues		At	oms			AltConf	Trace
2	В	490	Total 3954	C 2533	N 671	0 733	S 17	0	0

• Molecule 3 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues		At	oms			AltConf	Trace
3	С	655	Total 5251	C 3359	N 877	O 989	S 26	0	0

• Molecule 4 is a DNA chain called DNA (5'-D(P*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP *CP*TP*GP*CP*TP*CP*GP*AP*TP*AP*TP*CP*G)-3').

Mol	Chain	Residues		At	oms			AltConf	Trace
4	Л	24	Total	С	Ν	0	Р	0	0
4	D	24	484	233	82	146	23	0	0
4	Б	-91	Total	С	Ν	0	Р	0	0
4	Г	21	425	204	69	131	21	0	0

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

Mol	Chain	Residues		Ate	oms			AltConf	Trace
5	F	12	Total	С	Ν	0	Р	0	0
0		10	269	128	58	71	12	0	0
5	С	16	Total	С	Ν	0	Р	0	0
0	G	10	330	157	68	90	15		U



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-dependent protein kinase catalytic subunit











• Molecule 4: DNA (5'-D(P*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*T P*CP*GP*AP*TP*CP*G)-3')

Chain D:	88%	12%
61 14 120 624 624		

• Molecule 4: DNA (5'-D(P*GP*CP*AP*TP*GP*CP*TP*CP*TP*AP*CP*TP*GP*CP*TP*T P*CP*GP*AP*TP*CP*G)-3')

8%			
Chain F:	88%	12%	I
••			
DG DA T4 G5 G24 G24			
• Molecule 5:	DNA (5'-D(P*AP*AP*GP*CP*AP*GP*	*TP*AP*GP*AP*G	P*CP*A)-3')
6%			

Chain E:	69%	12%	19%
A25 C28 A29 D1 D1 D1 D1			

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

Chain G:

100%

There are no outlier residues recorded for this chain.



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138985	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT $(4k \ge 4k)$	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.055	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (Å)	408.31998, 408.31998, 408.31998	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.16, 1.16, 1.16	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Mol Chain		ond lengths	Bond angles		
	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	А	0.37	1/29394~(0.0%)	0.59	11/39755~(0.0%)	
2	В	0.36	0/4031	0.60	2/5429~(0.0%)	
3	С	0.32	0/5351	0.60	2/7213~(0.0%)	
4	D	0.80	0/540	1.06	0/831	
4	F	0.77	0/473	1.05	0/727	
5	Е	0.60	0/304	0.87	0/468	
5	G	0.77	0/372	0.90	0/573	
All	All	0.39	1/40465~(0.0%)	0.62	15/54996~(0.0%)	

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	А	1195	VAL	C-N	5.33	1.44	1.34

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	3311	ASN	N-CA-C	-8.40	88.33	111.00
3	С	671	LEU	CA-CB-CG	7.85	133.36	115.30
1	А	2887	PRO	CB-CA-C	7.76	131.41	112.00
1	А	1984	LEU	CA-CB-CG	6.89	131.15	115.30
2	В	497	LEU	N-CA-C	-5.85	95.20	111.00
1	А	2545	LEU	CA-CB-CG	5.58	128.13	115.30
2	В	356	LEU	CA-CB-CG	5.55	128.07	115.30
1	А	1524	LEU	CA-CB-CG	5.53	128.03	115.30
3	С	194	LEU	CA-CB-CG	5.50	127.96	115.30
1	А	765	LEU	CA-CB-CG	5.48	127.89	115.30
1	А	444	ASP	CB-CG-OD2	5.45	123.20	118.30
1	А	3918	LEU	CA-CB-CG	5.17	127.19	115.30
1	А	975	ASP	CB-CG-OD2	5.17	122.95	118.30
1	А	2528	GLU	C-N-CA	5.12	134.50	121.70
1	А	1044	ILE	C-N-CA	5.06	134.36	121.70

All (15) bond angle outliers are listed below:



There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	28808	0	29022	330	0
2	В	3954	0	4042	66	0
3	С	5251	0	5269	78	0
4	D	484	0	274	2	0
4	F	425	0	240	0	0
5	Е	269	0	146	1	0
5	G	330	0	180	0	0
All	All	39521	0	39173	460	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 6.

All (460) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:3352:GLU:HG3	1:A:3355:LYS:HG3	1.38	1.00
1:A:7:GLY:N	1:A:10:CYS:HG	1.69	0.90
1:A:3352:GLU:HG3	1:A:3355:LYS:CG	2.13	0.77
1:A:1416:GLU:O	1:A:1420:ARG:HB2	1.86	0.74
2:B:495:LEU:HB3	2:B:497:LEU:CD2	2.24	0.68
2:B:165:ARG:HA	2:B:199:PHE:O	1.94	0.68
2:B:495:LEU:HB3	2:B:497:LEU:HD23	1.76	0.68
1:A:1151:ARG:HD2	1:A:1163:LEU:H	1.60	0.66
1:A:3586:LYS:HG2	1:A:3667:LEU:HD21	1.78	0.66
3:C:387:LEU:HB3	3:C:389:MET:HG2	1.78	0.66
1:A:3647:GLY:HA2	1:A:3651:LEU:HB2	1.78	0.65
1:A:1206:LEU:O	1:A:1210:ASP:HB2	1.95	0.65
2:B:264:ASN:HD22	3:C:530:LEU:HD13	1.62	0.65
1:A:3630:ARG:HG2	1:A:3632:PHE:H	1.63	0.64
1:A:4028:ILE:HG22	1:A:4029:GLN:HG2	1.81	0.63
1:A:1356:TRP:HE1	1:A:1409:SER:HB2	1.63	0.62



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:C:408:ALA:HA	3:C:420:VAL:O	1.99	0.62
2:B:35:ARG:NH2	2:B:80:ARG:O	2.34	0.61
3:C:409:PHE:HB2	3:C:420:VAL:HG22	1.84	0.60
1:A:1178:ARG:NH1	1:A:1183:CYS:SG	2.75	0.60
1:A:54:GLN:HA	1:A:57:LEU:HB3	1.84	0.60
2:B:36:ASP:OD1	2:B:36:ASP:N	2.35	0.59
2:B:368:VAL:HG13	2:B:434:LEU:HD11	1.84	0.59
1:A:1375:THR:HA	1:A:1379:PRO:HB3	1.84	0.59
1:A:3648:GLY:O	1:A:3653:ARG:NH1	2.36	0.59
1:A:2524:PHE:O	1:A:2530:ARG:NH2	2.36	0.59
2:B:204:HIS:O	2:B:237:SER:N	2.36	0.59
1:A:215:PRO:HD3	3:C:550:ALA:HB2	1.85	0.59
1:A:1704:GLY:HA2	1:A:1707:LEU:HB3	1.85	0.59
1:A:859:LEU:O	1:A:867:ASN:ND2	2.36	0.59
1:A:791:ASP:OD1	1:A:791:ASP:N	2.36	0.59
3:C:466:LYS:HA	3:C:473:LEU:HA	1.85	0.59
3:C:684:THR:HG21	3:C:705:LEU:HD21	1.84	0.59
1:A:1266:CYS:SG	1:A:1267:TYR:N	2.75	0.58
1:A:3959:MET:SD	1:A:3959:MET:N	2.73	0.58
2:B:413:LEU:HB3	2:B:432:PHE:HD2	1.68	0.58
1:A:3755:GLY:HA2	1:A:3799:ARG:HB2	1.86	0.58
3:C:11:VAL:HB	3:C:132:ILE:HG12	1.85	0.58
2:B:241:ASP:OD1	2:B:241:ASP:N	2.37	0.58
1:A:3831:ASP:HB3	1:A:3834:ALA:HB2	1.86	0.58
1:A:1684:LEU:HB3	1:A:1688:LEU:HB2	1.86	0.58
1:A:1969:GLU:HB2	1:A:1975:LEU:HB3	1.85	0.58
1:A:3050:LYS:O	1:A:3054:GLN:NE2	2.37	0.57
1:A:3327:ASN:HB2	1:A:3388:ALA:HB2	1.86	0.57
1:A:72:SER:O	1:A:82:ARG:NH1	2.37	0.57
3:C:131:HIS:NE2	3:C:133:GLU:OE2	2.38	0.57
1:A:1274:ARG:NH1	1:A:1351:THR:OG1	2.38	0.57
1:A:3515:GLN:NE2	1:A:3551:ASN:OD1	2.38	0.57
3:C:407:VAL:O	3:C:421:TYR:HA	2.05	0.57
1:A:998:ASN:HA	1:A:1001:PHE:HB2	1.87	0.57
2:B:245:LYS:O	2:B:245:LYS:HG3	2.05	0.57
1:A:1190:LEU:O	1:A:1194:PHE:HB2	2.05	0.56
1:A:3119:VAL:O	1:A:3125:ARG:NH2	2.38	0.56
1:A:3289:ARG:NH1	1:A:3993:SER:OG	2.38	0.56
1:A:1261:LEU:HD13	1:A:1337:VAL:HG12	1.88	0.56
1:A:3595:GLU:OE2	1:A:3602:ASN:ND2	2.37	0.56
2:B:48:MET:SD	2:B:48:MET:N	2.77	0.56



	h a c	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:76:ASN:ND2	3:C:103:GLN:O	2.38	0.56
1:A:1829:TRP:O	1:A:1883:ARG:NH2	2.38	0.56
1:A:2177:ASN:HB3	1:A:2182:ILE:HG12	1.86	0.56
1:A:3299:THR:HA	1:A:3302:LYS:HE3	1.87	0.56
1:A:2458:VAL:HG11	1:A:2476:ILE:HD11	1.86	0.56
3:C:265:LYS:NZ	3:C:360:GLN:OE1	2.37	0.56
1:A:1681:ASP:HB3	1:A:1683:LYS:HE3	1.87	0.56
1:A:1751:GLU:O	1:A:1788:ARG:NH2	2.39	0.56
1:A:2143:ARG:HG2	1:A:2171:LEU:HD21	1.88	0.56
1:A:3314:SER:O	1:A:3318:LYS:NZ	2.39	0.56
2:B:144:SER:HB3	2:B:186:ALA:HA	1.88	0.56
2:B:399:ARG:NH2	3:C:516:LEU:O	2.38	0.56
1:A:723:ASP:OD1	1:A:723:ASP:N	2.37	0.56
1:A:657:SER:HA	1:A:660:LEU:HB2	1.88	0.56
1:A:901:MET:SD	1:A:2535:THR:OG1	2.63	0.56
1:A:3190:LEU:HD22	1:A:3231:ILE:HG23	1.88	0.56
1:A:3352:GLU:HB3	1:A:3355:LYS:HB2	1.87	0.56
1:A:2963:SER:OG	1:A:3251:ASN:ND2	2.39	0.55
1:A:1104:LEU:HD12	1:A:1134:LEU:HD23	1.88	0.55
1:A:10:CYS:SG	1:A:14:ARG:NH2	2.73	0.55
1:A:4083:GLY:HA3	1:A:4091:ALA:HB2	1.87	0.55
1:A:210:SER:HB2	2:B:332:GLU:HG3	1.88	0.55
1:A:1021:VAL:O	1:A:1021:VAL:HG13	2.06	0.55
1:A:1833:LEU:HB3	1:A:1836:LEU:HB2	1.88	0.55
1:A:2810:SER:HG	1:A:2857:CYS:HG	1.53	0.55
1:A:3360:LEU:HG	1:A:3373:VAL:HG11	1.88	0.55
1:A:1129:ASP:O	1:A:1133:HIS:ND1	2.40	0.55
1:A:3573:ASN:HB3	1:A:3627:ALA:HB2	1.89	0.55
2:B:495:LEU:CB	2:B:497:LEU:HD21	2.37	0.55
3:C:137:ASP:HA	3:C:166:PRO:HD3	1.89	0.55
1:A:442:GLN:NE2	1:A:457:CYS:SG	2.79	0.55
1:A:2230:VAL:O	1:A:2234:ASN:ND2	2.40	0.55
1:A:3484:THR:HG22	1:A:3513:ALA:HA	1.88	0.55
3:C:66:ASN:ND2	3:C:68:LEU:O	2.38	0.55
1:A:1228:GLY:HA3	1:A:1259:LEU:HD13	1.89	0.55
3:C:371:GLU:HB2	3:C:374:ALA:HB3	1.87	0.55
1:A:3253:SER:O	1:A:3257:LYS:NZ	2.39	0.54
3:C:57:VAL:HG22	3:C:79:VAL:HG12	1.89	0.54
1:A:1071:ASN:O	1:A:1075:ARG:NH1	2.41	0.54
1:A:1075:ARG:NH2	1:A:1117:ASP:OD1	2.38	0.54
5:E:28:DC:H2"	5:E:29:DA:C8	2.42	0.54



	h a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:74:LYS:HE2	2:B:83:LEU:HD11	1.89	0.54
1:A:2376:ASP:OD1	1:A:2404:ARG:NH2	2.41	0.54
1:A:526:ASP:OD1	1:A:526:ASP:N	2.39	0.54
1:A:1590:THR:HG1	1:A:1632:TRP:HE1	1.54	0.54
1:A:3378:TYR:OH	1:A:3426:LYS:NZ	2.40	0.54
1:A:4088:ASN:ND2	1:A:4113:ASP:OD2	2.39	0.54
1:A:414:LEU:HD12	1:A:464:VAL:HG21	1.88	0.54
1:A:621:SER:O	1:A:625:ASN:ND2	2.40	0.54
2:B:219:ASP:OD1	2:B:219:ASP:N	2.40	0.54
1:A:7:GLY:N	1:A:10:CYS:SG	2.76	0.54
1:A:3813:LYS:HB2	1:A:3925:LEU:HB3	1.89	0.54
2:B:95:ASN:HD21	2:B:99:PHE:HB2	1.73	0.54
1:A:1400:VAL:HG11	1:A:1460:ARG:HG2	1.90	0.54
1:A:14:ARG:HA	1:A:17:GLU:HB2	1.90	0.54
1:A:1414:ILE:O	1:A:1418:HIS:ND1	2.36	0.54
3:C:219:ASP:OD1	3:C:219:ASP:N	2.35	0.54
1:A:212:VAL:HG12	1:A:213:ARG:HB2	1.88	0.53
1:A:3714:GLU:O	1:A:3718:ARG:NH1	2.42	0.53
1:A:76:ILE:O	1:A:79:ARG:NH1	2.42	0.53
2:B:249:LYS:NZ	2:B:250:GLU:O	2.42	0.53
1:A:1143:VAL:HG23	1:A:1197:LEU:HD21	1.90	0.53
1:A:4006:VAL:HA	1:A:4011:PHE:HZ	1.73	0.53
1:A:1100:VAL:HA	1:A:1103:ALA:HB3	1.90	0.53
1:A:2034:SER:N	1:A:2037:SER:HG	2.05	0.53
1:A:4049:ARG:NH2	1:A:4062:ASP:OD2	2.38	0.53
3:C:111:LEU:HD11	3:C:150:ILE:HD12	1.91	0.53
1:A:2962:ARG:NH1	1:A:4101:GLU:OE2	2.42	0.53
2:B:95:ASN:OD1	2:B:95:ASN:N	2.41	0.53
1:A:1267:TYR:HE2	1:A:1290:LEU:HD13	1.73	0.53
1:A:1820:VAL:HG23	1:A:1824:LEU:HD11	1.90	0.52
2:B:143:LEU:HD23	2:B:182:LYS:HE3	1.90	0.52
3:C:687:THR:HG22	3:C:701:ALA:HB2	1.90	0.52
1:A:2103:HIS:O	1:A:2107:SER:CB	2.58	0.52
1:A:572:VAL:HG23	1:A:626:LEU:HD11	1.92	0.52
1:A:2978:LYS:NZ	1:A:2985:GLU:OE2	2.43	0.52
2:B:49:PHE:O	2:B:128:GLN:NE2	2.42	0.52
1:A:1169:VAL:HA	1:A:1172:LEU:HD12	1.92	0.52
1:A:60:SER:OG	1:A:63:PHE:O	2.26	0.52
1:A:278:HIS:HB3	1:A:281:GLN:HG3	1.92	0.52
1:A:3652:LEU:HD22	1:A:3653:ARG:HH21	1.75	0.51
1:A:2384:PHE:O	1:A:2388:LYS:NZ	2.43	0.51



	h i o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:4010:SER:O	1:A:4015:ASN:ND2	2.43	0.51
3:C:250:ARG:HH21	3:C:252:THR:HG21	1.75	0.51
1:A:9:ARG:HA	1:A:12:LEU:HD13	1.92	0.51
1:A:603:ILE:HG13	1:A:1083:ASN:HB3	1.91	0.51
1:A:2254:ARG:HA	1:A:2257:PHE:HB3	1.92	0.51
1:A:2493:ASN:HA	1:A:2496:GLN:HE21	1.74	0.51
1:A:3602:ASN:N	1:A:3602:ASN:OD1	2.42	0.51
2:B:55:ASP:OD1	2:B:55:ASP:N	2.43	0.51
1:A:142:ARG:HE	1:A:143:LEU:H	1.58	0.51
1:A:1634:ALA:O	1:A:1642:LYS:NZ	2.43	0.51
1:A:1440:ASP:OD1	1:A:1440:ASP:N	2.35	0.51
1:A:3048:LYS:HB3	1:A:3061:LEU:HD22	1.92	0.51
1:A:3147:LYS:HB3	1:A:3150:ASN:HB2	1.93	0.51
2:B:505:ASP:OD2	3:C:333:TYR:OH	2.28	0.51
1:A:739:ASN:OD1	1:A:739:ASN:N	2.44	0.51
1:A:3137:GLU:OE2	1:A:3167:ARG:NH2	2.42	0.51
2:B:52:GLN:HE22	2:B:207:LYS:HA	1.74	0.51
3:C:624:LEU:HD12	3:C:665:LYS:HE2	1.92	0.51
1:A:3026:ASP:N	1:A:3026:ASP:OD1	2.44	0.51
1:A:1206:LEU:O	1:A:1210:ASP:CB	2.58	0.51
1:A:1685:ASP:H	1:A:1688:LEU:HD12	1.75	0.51
1:A:1726:SER:OG	1:A:1727:ARG:N	2.44	0.51
1:A:1986:ARG:NH2	1:A:1988:TYR:OH	2.43	0.51
2:B:480:ASN:O	2:B:484:GLN:HB2	2.11	0.51
3:C:223:GLU:OE2	3:C:239:LYS:NZ	2.43	0.50
1:A:1407:LYS:NZ	1:A:1462:GLY:O	2.44	0.50
1:A:2131:GLY:O	1:A:2135:ASN:ND2	2.44	0.50
3:C:6:ASN:ND2	3:C:128:GLU:OE1	2.43	0.50
1:A:1019:ASP:OD1	1:A:1019:ASP:N	2.43	0.50
1:A:2824:LYS:O	1:A:2829:LYS:NZ	2.38	0.50
1:A:3354:ASP:OD1	1:A:3354:ASP:N	2.44	0.50
1:A:1836:LEU:HD21	1:A:1839:PHE:HB3	1.93	0.50
3:C:17:GLY:O	3:C:20:MET:HB3	2.11	0.50
1:A:189:MET:HG2	1:A:192:ASN:HD21	1.77	0.50
1:A:738:HIS:ND1	1:A:741:ILE:O	2.44	0.50
1:A:2507:ILE:HG21	1:A:2547:SER:HB3	1.93	0.50
2:B:266:ASP:OD1	2:B:266:ASP:N	2.43	0.50
1:A:1418:HIS:O	1:A:1422:LYS:NZ	2.36	0.50
1:A:1888:ASP:OD1	1:A:1888:ASP:N	2.42	0.50
2:B:245:LYS:O	2:B:246:VAL:HG22	2.11	0.50
2:B:288:LEU:HB3	3:C:311:ILE:HG13	1.93	0.50



	t i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:16:GLN:NE2	1:A:62:ASP:O	2.45	0.49
1:A:889:GLU:O	1:A:891:ARG:NH1	2.45	0.49
1:A:2897:LEU:HD11	1:A:2922:ARG:HB3	1.94	0.49
1:A:3588:TRP:NE1	1:A:3609:MET:SD	2.80	0.49
2:B:35:ARG:HH22	2:B:80:ARG:HB2	1.77	0.49
2:B:86:VAL:HG13	2:B:104:VAL:HG12	1.93	0.49
3:C:63:GLY:O	3:C:78:THR:OG1	2.30	0.49
1:A:66:LEU:HD11	1:A:110:THR:HG21	1.94	0.49
1:A:399:GLN:HG3	1:A:400:THR:HG23	1.94	0.49
1:A:2428:ASP:O	1:A:2432:GLN:NE2	2.44	0.49
1:A:3140:GLU:OE2	1:A:3164:TRP:NE1	2.45	0.49
2:B:194:ARG:NH1	2:B:219:ASP:O	2.46	0.49
2:B:202:LEU:HG	2:B:221:ILE:HD12	1.94	0.49
1:A:1068:LEU:HD21	1:A:1106:ILE:HD11	1.95	0.49
1:A:1178:ARG:HG2	1:A:1180:GLN:H	1.77	0.49
1:A:1588:ASP:N	1:A:1588:ASP:OD1	2.46	0.49
1:A:2290:PRO:HB3	1:A:2295:GLN:HA	1.94	0.49
1:A:1503:LEU:HD13	1:A:1508:LYS:HE2	1.94	0.48
2:B:507:THR:OG1	3:C:394:ARG:NH1	2.45	0.48
1:A:2551:GLU:OE2	1:A:2849:SER:OG	2.30	0.48
1:A:2990:GLU:HA	1:A:2993:PHE:HB3	1.95	0.48
1:A:3468:LEU:HA	1:A:3471:ILE:HG22	1.95	0.48
1:A:3700:GLU:OE2	1:A:3716:HIS:ND1	2.36	0.48
2:B:107:GLU:O	2:B:115:ARG:NH1	2.37	0.48
3:C:199:GLU:HA	3:C:202:LYS:HD2	1.95	0.48
1:A:1455:CYS:HA	1:A:1458:LEU:HD12	1.95	0.48
1:A:535:LEU:O	1:A:561:ASN:ND2	2.46	0.48
1:A:1440:ASP:O	1:A:1445:ARG:NH1	2.46	0.48
2:B:326:GLN:HE21	2:B:328:ILE:HD11	1.77	0.48
1:A:100:ILE:HG22	1:A:103:TYR:HB2	1.96	0.48
1:A:737:PRO:O	1:A:739:ASN:OD1	2.32	0.48
1:A:1853:SER:OG	1:A:1866:GLN:NE2	2.46	0.48
1:A:2859:GLN:NE2	1:A:2880:CYS:SG	2.77	0.48
1:A:333:MET:SD	1:A:333:MET:N	2.76	0.48
1:A:1045:THR:OG1	1:A:1048:GLN:NE2	2.46	0.48
1:A:1265:GLU:OE2	1:A:1340:ARG:NE	2.42	0.48
1:A:268:PRO:HB2	1:A:308:LEU:HD11	1.96	0.48
1:A:4011:PHE:HA	1:A:4015:ASN:HD22	1.78	0.48
1:A:1359:LEU:HB3	1:A:1363:LEU:HD21	1.95	0.48
1:A:2103:HIS:O	1:A:2107:SER:HB3	2.13	0.48
1:A:2265:PRO:HB3	1:A:2309:PHE:CG	2.49	0.48



	h i a	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:3590:ASN:HA	1:A:3593:ARG:HG2	1.94	0.48
1:A:2162:LYS:HA	1:A:2200:ALA:HB2	1.96	0.48
1:A:1167:ASP:OD1	1:A:1167:ASP:N	2.44	0.48
2:B:416:GLN:NE2	2:B:433:GLN:OE1	2.40	0.48
1:A:191:ASN:OD1	1:A:191:ASN:N	2.47	0.47
3:C:636:ILE:HA	3:C:639:ILE:HG12	1.95	0.47
1:A:1250:LEU:O	1:A:1253:THR:OG1	2.28	0.47
1:A:2290:PRO:HD3	1:A:2296:SER:HB3	1.95	0.47
1:A:2540:LEU:HD11	1:A:2835:LYS:HD2	1.95	0.47
1:A:2555:LEU:HD21	1:A:2854:PHE:HD1	1.79	0.47
1:A:3069:MET:O	1:A:3070:HIS:ND1	2.48	0.47
2:B:495:LEU:HD22	2:B:497:LEU:HD21	1.97	0.47
1:A:3448:GLU:HG2	1:A:3482:LEU:HD11	1.95	0.47
1:A:3471:ILE:O	1:A:3475:TYR:HB2	2.13	0.47
1:A:3751:LEU:HB3	1:A:3803:ILE:HG23	1.95	0.47
1:A:671:SER:HA	1:A:674:VAL:HG12	1.97	0.47
1:A:2149:LEU:O	1:A:2153:THR:OG1	2.29	0.47
1:A:3457:ASN:OD1	1:A:3494:GLN:NE2	2.47	0.47
1:A:2937:ASP:OD1	1:A:3784:ARG:NH2	2.46	0.47
1:A:3786:LEU:HD22	1:A:3910:LEU:HD22	1.97	0.47
3:C:351:VAL:HG21	3:C:407:VAL:HG21	1.97	0.47
1:A:2103:HIS:O	1:A:2107:SER:OG	2.32	0.47
1:A:2459:VAL:HB	1:A:2505:VAL:HG21	1.96	0.47
2:B:375:VAL:HG12	3:C:541:GLU:HB2	1.96	0.47
1:A:1407:LYS:HD3	1:A:1463:LEU:HD12	1.96	0.47
3:C:309:ASP:OD1	3:C:309:ASP:N	2.39	0.47
3:C:365:PHE:CD2	3:C:366:ALA:N	2.83	0.47
3:C:672:ASN:HA	3:C:675:TRP:HB2	1.96	0.47
1:A:583:LEU:HA	1:A:614:PRO:HA	1.97	0.46
1:A:1071:ASN:HD22	1:A:1074:LYS:HG3	1.80	0.46
1:A:1762:MET:HA	1:A:1765:VAL:HG12	1.97	0.46
1:A:2327:LEU:HD11	1:A:2345:VAL:HG11	1.96	0.46
1:A:3620:PRO:HG2	1:A:3621:LYS:HE2	1.96	0.46
1:A:3761:ASP:HA	1:A:3764:VAL:HG22	1.97	0.46
1:A:1782:PHE:HA	1:A:1785:ILE:HD12	1.96	0.46
1:A:3658:ASP:OD1	1:A:3658:ASP:N	2.47	0.46
1:A:4044:ILE:O	1:A:4048:LYS:HB2	2.15	0.46
3:C:11:VAL:O	3:C:132:ILE:HA	2.15	0.46
3:C:666:VAL:O	3:C:675:TRP:NE1	2.40	0.46
1:A:2184:TYR:HA	1:A:2187:VAL:HG22	1.97	0.46
1:A:4099:SER:O	1:A:4103:GLN:HB2	2.15	0.46



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:962:TYR:HA	1:A:965:THR:HG22	1.97	0.46
1:A:1686:LEU:HB3	1:A:1738:ASN:HD21	1.80	0.46
1:A:2837:LEU:O	1:A:2841:ASN:ND2	2.35	0.46
1:A:211:ALA:HB2	3:C:551:GLN:HE21	1.81	0.46
3:C:39:THR:O	3:C:43:GLN:HB2	2.15	0.46
1:A:96:MET:SD	1:A:96:MET:N	2.89	0.46
1:A:3492:CYS:SG	1:A:3524:ASN:ND2	2.88	0.46
1:A:704:PHE:HD1	1:A:704:PHE:O	1.99	0.46
1:A:873:VAL:HG13	1:A:874:THR:H	1.80	0.46
1:A:1896:ILE:HD12	1:A:1908:GLY:HA2	1.97	0.46
1:A:3508:LYS:NZ	1:A:3509:ASP:O	2.44	0.46
1:A:3289:ARG:NH1	1:A:3993:SER:O	2.49	0.46
3:C:6:ASN:HB3	3:C:7:LYS:H	1.58	0.46
1:A:263:LYS:HA	1:A:263:LYS:HD2	1.76	0.46
1:A:2169:LEU:HD21	1:A:2193:ILE:HG21	1.98	0.46
2:B:140:ASP:OD1	2:B:140:ASP:N	2.42	0.46
2:B:263:LEU:HB2	2:B:267:ILE:HG13	1.97	0.46
2:B:407:PRO:HG2	3:C:486:ARG:HD2	1.97	0.46
1:A:3530:VAL:HG11	1:A:3568:ILE:HG21	1.99	0.45
1:A:3885:ARG:HA	1:A:3888:VAL:HG12	1.98	0.45
2:B:160:LYS:HB2	2:B:160:LYS:HE3	1.78	0.45
1:A:2927:ALA:HB2	1:A:2942:ILE:HD11	1.98	0.45
1:A:3883:LEU:HB3	1:A:3970:LEU:HD13	1.98	0.45
2:B:83:LEU:HD12	2:B:111:PRO:HD3	1.99	0.45
3:C:686:ILE:HD12	3:C:690:GLU:HB2	1.99	0.45
1:A:1917:LYS:O	1:A:1917:LYS:NZ	2.46	0.45
1:A:2126:MET:HG3	1:A:2164:TRP:HE1	1.80	0.45
1:A:976:VAL:O	1:A:981:ARG:NH1	2.49	0.45
1:A:300:TRP:HD1	1:A:303:HIS:HD2	1.64	0.45
3:C:528:ILE:HG23	3:C:529:PRO:HD3	1.98	0.45
3:C:666:VAL:HA	3:C:671:LEU:HD21	1.99	0.45
1:A:317:GLU:OE2	1:A:364:ARG:NE	2.42	0.45
1:A:1856:THR:HG22	1:A:1858:LEU:HD22	1.97	0.45
2:B:93:ASP:HB3	2:B:101:ASN:H	1.82	0.45
3:C:69:SER:HA	3:C:74:TYR:HB2	1.99	0.45
1:A:1507:CYS:SG	1:A:1508:LYS:N	2.90	0.45
1:A:2338:GLU:O	1:A:2342:CYS:CB	2.65	0.45
1:A:4115:ASN:OD1	1:A:4119:ARG:NH2	2.49	0.45
1:A:1623:LEU:HA	1:A:1626:TRP:HD1	1.82	0.45
3:C:464:ALA:HA	3:C:475:ASP:HA	1.99	0.45
2:B:495:LEU:CB	2:B:497:LEU:CD2	2.90	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:169:THR:OG1	4:D:14:DC:OP1	2.30	0.44
1:A:532:ARG:O	1:A:536:SER:OG	2.32	0.44
1:A:704:PHE:O	1:A:704:PHE:CD1	2.70	0.44
1:A:1212:LEU:HD13	1:A:1220:LEU:HB2	1.99	0.44
1:A:1633:TRP:HA	1:A:1642:LYS:HZ2	1.81	0.44
1:A:3680:LEU:HD22	1:A:3724:GLU:HG2	1.99	0.44
1:A:3772:ASN:HA	1:A:3775:LEU:HB2	1.98	0.44
3:C:356:PHE:HD2	3:C:422:VAL:HG11	1.81	0.44
1:A:65:LEU:HD11	1:A:89:LEU:HD21	1.98	0.44
1:A:1816:ARG:HA	1:A:1816:ARG:HD2	1.80	0.44
1:A:1892:LYS:HD2	1:A:1896:ILE:HD11	1.99	0.44
1:A:3095:ASP:N	1:A:3095:ASP:OD1	2.50	0.44
1:A:3447:VAL:HG22	1:A:3468:LEU:HD22	1.99	0.44
1:A:3958:LEU:O	1:A:4110:GLN:NE2	2.50	0.44
1:A:4029:GLN:HB3	1:A:4030:GLU:H	1.47	0.44
2:B:363:ARG:HH11	3:C:269:GLN:HE22	1.65	0.44
1:A:1697:PRO:HG3	1:A:1752:LEU:HD21	2.00	0.44
2:B:342:ASP:OD1	2:B:342:ASP:N	2.50	0.44
1:A:2043:PHE:O	1:A:2047:THR:OG1	2.31	0.44
1:A:238:MET:SD	1:A:283:SER:N	2.91	0.44
1:A:1386:ILE:HG23	1:A:1392:MET:HG3	2.00	0.44
1:A:2842:ARG:O	1:A:2846:THR:OG1	2.31	0.44
1:A:215:PRO:HG2	3:C:553:ILE:HG21	2.00	0.44
1:A:678:LYS:HD2	1:A:737:PRO:HA	1.99	0.44
1:A:1850:VAL:HA	1:A:1853:SER:HB3	1.98	0.44
1:A:9:ARG:HB3	1:A:63:PHE:HE2	1.83	0.44
1:A:68:PHE:HA	1:A:71:LYS:HG2	2.00	0.44
1:A:1869:LYS:HE3	1:A:1869:LYS:HB2	1.87	0.44
1:A:1964:GLY:O	1:A:1968:SER:OG	2.36	0.44
3:C:365:PHE:HB3	3:C:418:CYS:SG	2.57	0.44
1:A:2492:ASP:O	1:A:2496:GLN:NE2	2.51	0.43
1:A:2788:SER:O	1:A:2792:THR:OG1	2.34	0.43
1:A:3531:TYR:HB3	1:A:3796:MET:HA	2.00	0.43
2:B:207:LYS:HB2	2:B:213:ILE:HD11	2.00	0.43
2:B:237:SER:OG	2:B:238:LYS:N	2.51	0.43
1:A:436:GLU:HA	1:A:439:VAL:HG12	2.00	0.43
1:A:2512:ASP:OD1	1:A:2512:ASP:N	2.48	0.43
1:A:3629:ARG:HH12	1:A:3634:GLN:HG3	1.84	0.43
1:A:3767:LEU:HD13	1:A:3918:LEU:HD22	2.00	0.43
3:C:363:LYS:HG2	3:C:420:VAL:HG12	1.99	0.43
2:B:485:GLN:NE2	3:C:332:LYS:O	2.39	0.43



	jus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:C:16:VAL:HG13	3:C:58:LEU:HD11	2.01	0.43
3:C:602:VAL:HA	3:C:606:LYS:HD2	2.00	0.43
1:A:93:LEU:HD12	1:A:100:ILE:HD13	2.00	0.43
1:A:335:LYS:HE2	1:A:376:ILE:HD11	1.99	0.43
1:A:913:ARG:HH22	1:A:2803:ILE:HG13	1.83	0.43
1:A:1525:CYS:SG	1:A:1574:ASN:ND2	2.91	0.43
1:A:1989:ASN:OD1	1:A:1989:ASN:N	2.45	0.43
1:A:2383:PHE:HE2	1:A:2408:MET:HE1	1.84	0.43
1:A:67:VAL:HA	1:A:70:ARG:HB2	2.00	0.43
1:A:485:GLN:HE22	1:A:2040:MET:HA	1.84	0.43
1:A:1082:PHE:HA	1:A:1085:ILE:HG12	2.01	0.43
1:A:1632:TRP:HB3	1:A:1645:VAL:HG21	2.00	0.43
1:A:3876:SER:O	1:A:3876:SER:OG	2.35	0.43
1:A:1729:PHE:HB2	1:A:1736:PHE:HB2	1.99	0.43
1:A:2784:GLN:HB3	1:A:2785:ILE:H	1.61	0.43
2:B:410:PHE:HB2	2:B:439:PHE:HE1	1.84	0.43
2:B:497:LEU:H	2:B:497:LEU:HG	1.59	0.43
3:C:61:THR:OG1	3:C:62:ASP:N	2.50	0.43
1:A:851:ILE:HD13	1:A:851:ILE:HA	1.89	0.42
1:A:1190:LEU:HA	1:A:1193:LYS:HG2	2.00	0.42
1:A:2387:PRO:O	2:B:158:GLN:NE2	2.46	0.42
1:A:3098:ARG:HE	1:A:3102:TYR:HE2	1.65	0.42
1:A:3138:ILE:HG12	1:A:3189:PHE:HZ	1.84	0.42
1:A:3686:TRP:HH2	1:A:3699:LEU:HD11	1.84	0.42
2:B:143:LEU:O	2:B:145:GLU:N	2.52	0.42
1:A:95:LYS:HA	1:A:834:LEU:HD11	2.00	0.42
1:A:782:ARG:NH1	1:A:3166:ASN:OD1	2.52	0.42
1:A:3011:LEU:HD23	1:A:3047:SER:HB2	2.01	0.42
1:A:3554:PHE:HD1	1:A:3557:ARG:HH21	1.66	0.42
1:A:3829:LEU:HD23	1:A:3829:LEU:HA	1.87	0.42
1:A:346:TYR:HA	1:A:349:ILE:HG22	2.01	0.42
1:A:3623:PRO:HG3	1:A:3633:ILE:HG12	2.02	0.42
2:B:240:GLU:HA	2:B:243:LEU:HD12	2.01	0.42
2:B:245:LYS:O	2:B:246:VAL:CG2	2.67	0.42
1:A:2980:ASP:OD1	1:A:2980:ASP:N	2.46	0.42
2:B:262:LYS:HA	2:B:268:VAL:HG12	2.01	0.42
3:C:116:ASP:O	3:C:120:HIS:ND1	2.49	0.42
1:A:2036:LEU:O	1:A:2040:MET:HB2	2.19	0.42
2:B:51:SER:O	2:B:51:SER:OG	2.38	0.42
3:C:12:LEU:HD13	3:C:38:ILE:HD11	2.02	0.42
1:A:485:GLN:HE21	1:A:2040:MET:HG3	1.85	0.42



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:1900:PHE:HD1	1:A:1900:PHE:HA	1.76	0.42
1:A:1864:ASP:HA	1:A:1867:ILE:HD12	2.01	0.42
1:A:2190:VAL:HA	1:A:2193:ILE:HG22	2.02	0.42
1:A:3883:LEU:HD13	1:A:3970:LEU:HD22	2.01	0.42
3:C:413:LYS:HD3	3:C:413:LYS:HA	1.87	0.42
3:C:606:LYS:NZ	3:C:608:SER:O	2.53	0.42
1:A:2955:SER:O	1:A:2971:GLN:NE2	2.52	0.42
1:A:3733:ARG:HH22	1:A:4022:LYS:HD2	1.85	0.41
3:C:331:MET:HE3	3:C:331:MET:HB2	1.81	0.41
1:A:3351:ILE:O	1:A:3352:GLU:HB2	2.19	0.41
3:C:353:ARG:HA	3:C:356:PHE:HE1	1.85	0.41
3:C:726:ASP:HA	3:C:729:LEU:HG	2.01	0.41
1:A:205:LYS:O	1:A:209:THR:OG1	2.34	0.41
1:A:680:ILE:HD12	1:A:680:ILE:HA	1.95	0.41
1:A:2286:PRO:HB3	1:A:2329:TYR:CE2	2.56	0.41
1:A:2464:HIS:ND1	1:A:2469:CYS:SG	2.93	0.41
3:C:45:GLN:HE21	3:C:237:PHE:HE1	1.68	0.41
3:C:132:ILE:O	3:C:161:LEU:HA	2.21	0.41
1:A:848:LEU:HD12	1:A:848:LEU:HA	1.91	0.41
1:A:863:GLY:HA2	1:A:3167:ARG:HG3	2.01	0.41
1:A:1137:ILE:HD12	1:A:1137:ILE:HA	1.94	0.41
1:A:1590:THR:OG1	1:A:1632:TRP:NE1	2.46	0.41
1:A:1811:ARG:HE	3:C:626:THR:HG23	1.86	0.41
2:B:346:MET:HB2	2:B:346:MET:HE3	1.66	0.41
3:C:108:LEU:HD13	3:C:147:LEU:HD21	2.03	0.41
3:C:372:ALA:HA	3:C:375:VAL:HG12	2.02	0.41
1:A:12:LEU:HD23	1:A:64:GLY:HA2	2.01	0.41
1:A:473:PRO:HA	1:A:476:ARG:HG2	2.01	0.41
1:A:1532:LEU:HD23	1:A:1532:LEU:HA	1.86	0.41
2:B:422:ASP:N	2:B:422:ASP:OD2	2.53	0.41
3:C:155:LYS:NZ	3:C:215:LEU:O	2.49	0.41
3:C:614:ASN:OD1	3:C:614:ASN:N	2.53	0.41
1:A:214:GLU:HA	1:A:215:PRO:HD2	1.73	0.41
1:A:1141:LYS:HD3	1:A:1141:LYS:HA	1.93	0.41
3:C:339:CYS:O	3:C:395:TYR:HA	2.21	0.41
1:A:117:LYS:HE2	1:A:117:LYS:HB2	1.80	0.41
1:A:862:LEU:HD12	1:A:862:LEU:HA	1.94	0.41
1:A:1605:PHE:O	1:A:1608:ARG:NH2	2.45	0.41
1:A:3489:SER:O	1:A:3489:SER:OG	2.34	0.41
3:C:617:ILE:HA	3:C:620:ILE:HG12	2.01	0.41
1:A:790:LYS:HE2	1:A:790:LYS:HB3	1.88	0.41



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:879:MET:H	1:A:879:MET:HG2	1.66	0.41
1:A:1774:MET:HB3	1:A:1777:LEU:HD21	2.02	0.41
1:A:2801:ASP:N	1:A:2801:ASP:OD1	2.54	0.41
1:A:3620:PRO:HG3	1:A:3638:LYS:HD3	2.03	0.41
1:A:3753:LYS:HE2	1:A:3803:ILE:HG21	2.01	0.41
3:C:247:TRP:HB3	3:C:263:ALA:HB3	2.03	0.41
1:A:1246:GLY:HA2	1:A:1247:PRO:HD3	1.95	0.41
1:A:1474:ASP:OD1	1:A:1474:ASP:N	2.52	0.41
1:A:2256:ILE:H	1:A:2256:ILE:HG12	1.64	0.41
1:A:2352:HIS:HB3	1:A:2360:PHE:HB2	2.03	0.41
3:C:324:SER:OG	3:C:325:LYS:N	2.53	0.41
1:A:2328:ARG:NH1	1:A:2332:GLU:OE2	2.55	0.40
3:C:138:LEU:HD23	3:C:138:LEU:HA	1.95	0.40
1:A:96:MET:HB2	1:A:100:ILE:HD11	2.04	0.40
1:A:3582:GLU:OE2	1:A:3671:ASN:ND2	2.55	0.40
1:A:3975:LYS:HA	1:A:3975:LYS:HD3	1.89	0.40
4:D:19:DA:H2'	4:D:20:DT:H71	2.04	0.40
1:A:76:ILE:HD13	1:A:76:ILE:HA	1.96	0.40
1:A:2834:GLN:HE21	1:A:2834:GLN:HB2	1.59	0.40
1:A:3714:GLU:H	1:A:3714:GLU:HG2	1.79	0.40
1:A:3772:ASN:HD22	1:A:3788:LEU:HB2	1.86	0.40
1:A:3972:LEU:HD23	1:A:3972:LEU:HA	1.91	0.40
2:B:94:LYS:HB3	2:B:103:TYR:CD1	2.57	0.40
3:C:322:PRO:HB2	3:C:323:PHE:H	1.65	0.40
1:A:919:LEU:HD11	1:A:968:VAL:HG23	2.03	0.40
1:A:1484:LEU:HD22	1:A:1524:LEU:HD21	2.03	0.40
1:A:1725:GLN:HG2	3:C:622:GLN:HG3	2.04	0.40
1:A:3962:ARG:NH1	1:A:4128:MET:O	2.55	0.40
2:B:238:LYS:HZ3	2:B:238:LYS:HG2	1.75	0.40
1:A:181:LEU:HB3	1:A:189:MET:HE1	2.03	0.40
1:A:663:ILE:HD13	1:A:663:ILE:HA	1.93	0.40
2:B:358:LYS:HD2	2:B:358:LYS:HA	1.84	0.40
2:B:510:LYS:HE2	2:B:510:LYS:HB2	1.97	0.40
3:C:666:VAL:HB	3:C:675:TRP:CD1	2.56	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	Perce	entiles
1	А	3594/4128~(87%)	3123 (87%)	459 (13%)	12 (0%)	41	75
2	В	486/609~(80%)	409 (84%)	74 (15%)	3 (1%)	25	63
3	С	645/732~(88%)	549 (85%)	92 (14%)	4 (1%)	25	63
All	All	4725/5469 (86%)	4081 (86%)	625 (13%)	19 (0%)	38	71

All (19) Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	1476	HIS
1	А	2826	LEU
1	А	3352	GLU
2	В	144	SER
1	А	215	PRO
1	А	3058	ASP
1	А	3311	ASN
2	В	245	LYS
3	С	299	ASP
3	С	322	PRO
1	А	1021	VAL
1	А	3028	ASN
1	А	3083	SER
3	С	300	ASP
1	А	661	PRO
1	А	2548	PRO
1	А	2547	SER
3	С	193	PRO
2	В	499	GLU



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	3174/3671~(86%)	3146~(99%)	28 (1%)	78 87
2	В	444/548 (81%)	436 (98%)	8 (2%)	59 77
3	С	587/649~(90%)	586 (100%)	1 (0%)	93 96
All	All	4205/4868~(86%)	4168 (99%)	37 (1%)	79 87

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	57	LEU
1	А	100	ILE
1	А	215	PRO
1	А	284	THR
1	А	364	ARG
1	А	396	PHE
1	А	739	ASN
1	А	789	TYR
1	А	1051	LYS
1	А	1213	LYS
1	А	1639	LEU
1	А	1735	ARG
1	А	1752	LEU
1	А	1837	ARG
1	А	2183	HIS
1	А	2214	ARG
1	А	3058	ASP
1	А	3301	LEU
1	A	3310	ASN
1	А	3335	ARG
1	A	3352	GLU
1	А	3642	LYS
1	А	3650	LYS
1	А	3653	ARG
1	А	3696	ARG
1	А	3743	HIS



Mol	Chain	Res	Type
1	А	4023	LYS
1	А	4036	LYS
2	В	36	ASP
2	В	217	TYR
2	В	292	THR
2	В	368	VAL
2	В	409	TYR
2	В	470	ARG
2	В	493	LEU
2	В	497	LEU
3	С	365	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	109	ASN
1	А	192	ASN
1	А	303	HIS
1	А	442	GLN
1	А	485	GLN
1	А	720	GLN
1	А	867	ASN
1	А	1048	GLN
1	А	1115	HIS
1	А	1598	ASN
1	А	1610	ASN
1	А	1624	GLN
1	А	1772	HIS
1	А	1866	GLN
1	А	2103	HIS
1	А	2135	ASN
1	А	2222	HIS
1	А	2283	ASN
1	А	2365	ASN
1	А	2432	GLN
1	А	2496	GLN
1	А	2834	GLN
1	А	2885	GLN
1	А	3112	GLN
1	А	3122	HIS
1	А	3251	ASN
1	А	3379	GLN



Mol	Chain	Res	Type
1	А	3383	GLN
1	А	3524	ASN
1	А	3573	ASN
1	А	3760	GLN
1	А	3772	ASN
1	А	3822	GLN
1	А	4110	GLN
2	В	52	GLN
2	В	152	ASN
2	В	264	ASN
2	В	326	GLN
2	В	360	HIS
3	С	269	GLN
3	С	411	HIS
3	С	511	HIS
3	С	551	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.



5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22626. 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



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

6.2 Central slices (i)

6.2.1 Primary map



X Index: 176

Y Index: 176



Z Index: 176

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: 187

Y Index: 149

Z Index: 199

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



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



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.013. 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 378 $\rm nm^3;$ this corresponds to an approximate mass of 341 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 0.256 ${\rm \AA^{-1}}$



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-22626 and PDB model 7K1N. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.013 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 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 (0.013).



9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 84% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8350	0.4170
А	0.8590	0.4300
В	0.8490	0.4160
С	0.6850	0.3710
D	0.8930	0.3510
Е	0.7580	0.2840
F	0.8590	0.3510
G	0.9000	0.3430

