

Jan 23, 2024 - 08:07 PM JST

PDB ID	:	8HWH
EMDB ID	:	EMD-35058
Title	:	Cryo-EM Structure of D5 Apo-ssDNA form
Authors	:	Li, Y.N.; Zhu, J.; Guo, Y.Y.; Yan, R.H.
Deposited on	:	2022-12-29
Resolution	:	3.60 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	:	FAILED
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
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 3.60 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
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%

Mol	Chain	Length	Quality of chain			
1	А	785	34%	11%	55%	
1	В	785	33%	12%	55%	
1	С	785	36%	9%	54%	
1	D	785	33%	13% •	54%	
1	Е	785	30%	11%	58%	
1	F	785	28%	12% •	60%	
2	S	6	17%		83%	



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16948 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.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	Δ	353	Total	С	Ν	Ο	\mathbf{S}	0	0
1	Л	000	2858	1828	485	529	16	0	0
1	Р	357	Total	С	Ν	Ο	S	0	0
	D		2887	1845	489	537	16	0	0
1	C	261	Total	С	Ν	0	S	0	0
	501	2920	1868	495	541	16	0	0	
1	П	262	Total	С	Ν	0	S	0	0
1	D	505	2940	1881	497	546	16	0	
1	F	320	Total	С	Ν	Ο	\mathbf{S}	0	0
1	Ľ	529	2662	1697	455	495	15	0	0
1	F	316	Total	C	N	0	S	0	0
	Ľ	510	2561	1636	434	477	14	0	U

• Molecule 1 is a protein called Primase D5.

• Molecule 2 is a DNA chain called DNA (5'-D(P*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms			AltConf	Trace		
2	S	6	Total 120	C 60	N 12	O 42	Р 6	0	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. 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. 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: Primase D5







• Molecule 1: Primase D5









• Molecule 2: DNA (5'-D(P*TP*TP*TP*TP*TP*T)-3')

Chain S: 17%

<mark>11</mark> 12 15 16 16 83%

DB

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56953	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 $(e^-/\text{\AA}^2)$	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	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 Chain		Bond	lengths	Bond angles	
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.25	0/2918	0.53	0/3940
1	В	0.25	0/2947	0.53	0/3979
1	С	0.25	0/2980	0.52	0/4022
1	D	0.26	0/3001	0.52	0/4051
1	Е	0.25	0/2714	0.52	0/3660
1	F	0.25	0/2610	0.52	0/3521
2	S	0.67	0/131	1.44	0/200
All	All	0.26	0/17301	0.54	0/23373

There are no bond length outliers.

There are no bond angle outliers.

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	2858	0	2885	50	0
1	В	2887	0	2909	66	0
1	С	2920	0	2955	50	0
1	D	2940	0	2968	68	0
1	Е	2662	0	2691	63	0
1	F	2561	0	2591	64	0
2	S	120	0	73	8	0
All	All	16948	0	17072	351	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (351) 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:F:421:ASP:O	1:F:425:GLY:HA2	1.83	0.77
1:E:336:THR:HG1	1:E:338:SER:HG	1.32	0.75
1:D:389:ARG:NH1	1:E:398:ASP:OD2	2.20	0.74
1:A:510:SER:HB2	1:A:514:ARG:HH21	1.53	0.73
1:B:693:ILE:HB	1:B:696:PHE:HB2	1.71	0.72
1:A:411:ASP:OD1	1:A:412:LYS:NZ	2.23	0.72
1:A:389:ARG:NH1	1:B:398:ASP:OD2	2.24	0.70
1:E:462:MET:HA	1:E:465:ILE:HG22	1.73	0.70
1:C:532:LEU:HB3	1:C:569:ILE:HG23	1.73	0.70
1:C:677:LYS:HA	1:C:681:ILE:HD11	1.75	0.68
1:D:578:THR:HG21	1:D:620:ARG:HE	1.58	0.67
1:F:421:ASP:O	1:F:425:GLY:CA	2.42	0.67
1:F:485:THR:HG21	1:F:499:THR:HG21	1.77	0.67
1:B:385:CYS:SG	1:B:387:ARG:NH1	2.68	0.67
1:E:413:LEU:HD11	1:E:490:LEU:HD22	1.78	0.66
1:F:351:ILE:HD11	1:F:367:LEU:HA	1.76	0.66
1:B:340:LEU:HD13	1:B:404:VAL:HG21	1.78	0.66
1:E:529:GLN:NE2	1:E:557:GLU:O	2.29	0.65
1:A:500:PHE:HB2	1:A:623:VAL:HG22	1.79	0.65
1:E:535:VAL:HB	1:E:538:LYS:HG2	1.79	0.65
1:C:421:ASP:O	1:C:425:GLY:HA2	1.97	0.64
1:B:504:GLU:OE2	1:B:504:GLU:N	2.28	0.64
1:F:469:GLN:OE1	1:F:475:ASN:ND2	2.30	0.64
1:B:386:PRO:HG3	1:C:391:THR:HG23	1.79	0.63
1:B:500:PHE:HB2	1:B:623:VAL:HG22	1.81	0.63
1:E:460:GLU:O	1:E:464:ILE:HG13	1.99	0.63
1:E:389:ARG:NH1	1:F:398:ASP:OD2	2.31	0.63
1:A:511:THR:O	1:A:515:LEU:HG	1.99	0.62
1:D:469:GLN:OE1	1:D:475:ASN:ND2	2.32	0.62
1:E:421:ASP:O	1:E:425:GLY:N	2.32	0.62
1:B:411:ASP:OD2	1:B:412:LYS:NZ	2.31	0.62
1:E:500:PHE:HB2	1:E:623:VAL:HG22	1.81	0.62
1:E:579:GLU:HG3	1:E:581:CYS:H	1.65	0.62
1:D:536:LEU:HD23	1:D:536:LEU:H	1.65	0.62
1:D:542:PRO:O	1:D:546:ASN:ND2	2.33	0.62
1:A:553:VAL:HG22	1:A:600:ILE:HG22	1.82	0.61
1:E:349:VAL:HG23	1:E:367:LEU:HD22	1.82	0.61



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:540:PRO:HG3	2:S:4:DT:OP1	2.00	0.61
1:B:619:ARG:HA	1:B:688:PRO:HG3	1.83	0.61
1:B:536:LEU:HD23	1:B:573:ASN:HD22	1.63	0.61
1:C:569:ILE:H	1:C:569:ILE:HD12	1.66	0.60
1:B:348:ILE:HG22	1:B:357:PHE:HB3	1.82	0.60
1:D:426:MET:SD	1:D:426:MET:N	2.74	0.60
1:E:462:MET:O	1:E:466:ASN:ND2	2.35	0.60
1:F:536:LEU:HD13	1:F:576:LYS:HG2	1.83	0.60
1:A:348:ILE:HG22	1:A:357:PHE:HB3	1.83	0.59
1:A:495:LYS:NZ	1:A:597:HIS:O	2.33	0.59
1:C:389:ARG:NH1	1:D:398:ASP:OD2	2.35	0.59
1:A:501:PHE:HB2	1:A:603:ASP:HA	1.84	0.59
1:E:472:THR:O	1:E:479:ARG:NH2	2.35	0.59
1:E:572:ASP:O	1:E:576:LYS:HG3	2.03	0.59
1:B:498:LEU:HD22	1:B:600:ILE:HB	1.84	0.58
1:D:600:ILE:HD12	1:D:600:ILE:H	1.68	0.58
1:B:534:ASP:OD1	1:B:535:VAL:N	2.36	0.58
1:A:658:LYS:HG3	1:A:664:TYR:CE2	2.39	0.58
1:B:413:LEU:HD22	1:B:490:LEU:HD23	1.86	0.58
1:D:460:GLU:O	1:D:464:ILE:HG13	2.03	0.58
1:D:504:GLU:O	1:D:507:THR:OG1	2.20	0.58
1:F:462:MET:O	1:F:466:ASN:ND2	2.37	0.58
1:E:421:ASP:O	1:E:425:GLY:CA	2.51	0.58
1:A:569:ILE:HB	1:A:610:PHE:HA	1.85	0.57
1:E:490:LEU:O	1:E:551:ARG:NH1	2.38	0.57
1:E:495:LYS:HD3	1:E:599:THR:HG22	1.87	0.57
1:F:329:ILE:HD11	1:F:379:TYR:HB3	1.87	0.57
1:D:579:GLU:N	1:D:579:GLU:OE2	2.38	0.56
1:A:507:THR:HG21	1:A:626:PHE:HB3	1.86	0.56
1:A:570:ARG:HA	1:A:611:ASP:HB2	1.88	0.56
1:C:421:ASP:O	1:C:425:GLY:CA	2.53	0.56
1:E:360:GLU:OE1	1:E:360:GLU:N	2.27	0.56
1:B:455:SER:OG	1:B:457:GLU:OE1	2.23	0.56
1:A:670:TYR:O	1:A:674:LYS:HG2	2.06	0.56
1:D:561:PHE:HD1	1:D:609:VAL:HB	1.71	0.55
1:B:547:MET:HG3	1:B:547:MET:O	2.06	0.55
1:D:490:LEU:O	1:D:551:ARG:NH1	2.39	0.55
1:B:389:ARG:NH1	1:C:398:ASP:OD2	2.40	0.55
1:E:333:ILE:HG12	1:E:371:ILE:HG21	1.89	0.55
1:E:421:ASP:O	1:E:425:GLY:HA2	2.07	0.55
1:E:509:LYS:NZ	1:E:605:ASN:OD1	2.37	0.55



	to us page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:340:LEU:HD13	1:C:404:VAL:HG21	1.87	0.55
1:C:682:PRO:O	1:C:683:ILE:HD13	2.06	0.54
1:F:453:GLU:O	1:F:458:MET:HG2	2.08	0.54
1:C:606:TYR:OH	1:D:612:ARG:NH1	2.39	0.54
1:C:496:GLY:HA2	1:C:578:THR:HB	1.88	0.54
1:D:498:LEU:HD22	1:D:600:ILE:HB	1.90	0.54
1:A:555:CYS:HB3	1:A:602:ILE:HD12	1.90	0.54
1:C:490:LEU:HD11	1:C:672:LEU:HB3	1.90	0.54
1:D:543:PHE:HD1	1:D:543:PHE:H	1.56	0.54
1:F:349:VAL:HG21	1:F:363:LEU:HB2	1.90	0.53
1:A:349:VAL:HB	1:A:367:LEU:HD12	1.91	0.53
1:C:657:GLY:O	1:C:661:ASN:ND2	2.39	0.53
1:A:529:GLN:NE2	1:A:556:SER:O	2.42	0.53
1:E:458:MET:SD	1:E:459:GLU:N	2.82	0.53
1:B:526:GLU:OE1	1:B:526:GLU:N	2.41	0.52
1:D:571:SER:OG	1:D:612:ARG:NH2	2.34	0.52
1:B:578:THR:HG21	1:B:620:ARG:HD3	1.92	0.52
1:C:516:LEU:O	1:C:520:ILE:HG12	2.10	0.52
1:A:556:SER:HB3	1:A:603:ASP:HB3	1.91	0.52
1:E:503:GLY:O	1:E:509:LYS:NZ	2.33	0.52
1:F:428:TYR:HB2	1:F:433:ALA:HB2	1.92	0.52
1:B:475:ASN:O	1:B:475:ASN:ND2	2.43	0.51
1:C:348:ILE:HG22	1:C:357:PHE:HB3	1.92	0.51
1:D:334:LEU:HD11	1:D:400:LEU:HD21	1.91	0.51
1:D:571:SER:HB2	1:D:617:LEU:HD21	1.91	0.51
1:D:470:PRO:HB2	1:D:472:THR:HG23	1.93	0.51
1:E:656:ASP:N	1:E:656:ASP:OD1	2.40	0.51
1:C:395:ASN:O	1:C:399:MET:HG3	2.10	0.51
1:C:525:VAL:HG23	1:C:553:VAL:HG23	1.92	0.51
1:A:393:GLU:OE2	1:A:397:ARG:NH2	2.43	0.51
1:A:529:GLN:NE2	1:A:557:GLU:O	2.43	0.51
1:A:658:LYS:HG3	1:A:664:TYR:HE2	1.75	0.51
1:B:460:GLU:O	1:B:464:ILE:HG12	2.11	0.51
1:F:346:ASP:OD1	1:F:359:SER:OG	2.28	0.51
1:E:532:LEU:HD13	1:E:569:ILE:HD12	1.93	0.51
1:B:477:LYS:O	1:B:480:GLU:HG3	2.11	0.50
1:C:652:ASP:HB3	1:C:655:LEU:HB2	1.93	0.50
1:B:658:LYS:HB2	1:B:663:ARG:HD3	1.92	0.50
1:E:464:ILE:O	1:E:468:ILE:HG12	2.11	0.50
1:E:478:ASN:ND2	1:E:625:ARG:O	2.43	0.50
1:B:516:LEU:O	1:B:520:ILE:HG12	2.12	0.50



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:695:ASP:OD2	1:B:696:PHE:N	2.45	0.50
1:C:658:LYS:HB2	1:C:663:ARG:HD3	1.94	0.50
1:F:480:GLU:O	1:F:484:LYS:HG3	2.12	0.50
1:A:407:ASP:HB2	1:A:595:ARG:NH2	2.26	0.50
1:D:658:LYS:HD2	1:D:663:ARG:HH11	1.77	0.50
1:E:456:PRO:HA	1:E:459:GLU:OE2	2.12	0.50
1:F:334:LEU:HD11	1:F:400:LEU:HD21	1.93	0.49
1:F:514:ARG:HA	1:F:517:LYS:HG2	1.93	0.49
1:D:479:ARG:NH1	1:D:483:GLU:OE2	2.45	0.49
1:C:466:ASN:OD1	1:C:479:ARG:NH2	2.45	0.49
1:B:456:PRO:O	1:B:460:GLU:HG3	2.12	0.49
1:C:479:ARG:NH1	1:C:483:GLU:OE2	2.45	0.49
1:F:337:ASN:OD1	1:F:340:LEU:HD21	2.13	0.49
1:B:537:ASP:N	1:B:537:ASP:OD1	2.45	0.49
1:D:586:PRO:HD2	1:D:589:SER:HB3	1.94	0.49
1:C:536:LEU:HD13	1:C:576:LYS:HE2	1.94	0.49
1:A:395:ASN:OD1	1:F:389:ARG:NH2	2.46	0.49
1:A:391:THR:HG23	1:F:386:PRO:HG2	1.94	0.48
1:F:466:ASN:OD1	1:F:479:ARG:NH2	2.45	0.48
1:A:510:SER:O	1:A:513:LYS:HG2	2.14	0.48
1:C:350:TRP:CZ2	1:C:353:ASN:HA	2.49	0.48
1:D:618:MET:HG3	1:D:696:PHE:CD2	2.48	0.48
1:D:621:ILE:HG13	1:D:696:PHE:HE2	1.78	0.48
1:C:572:ASP:O	1:C:576:LYS:HG2	2.14	0.48
1:D:389:ARG:NH2	1:E:395:ASN:OD1	2.47	0.48
1:F:542:PRO:O	1:F:546:ASN:N	2.33	0.48
1:D:447:ASP:HB2	1:D:666:PHE:HE2	1.79	0.48
1:F:385:CYS:HB3	1:F:388:LYS:HG3	1.95	0.48
1:D:348:ILE:HG22	1:D:357:PHE:HB3	1.95	0.48
1:D:625:ARG:HH12	1:D:627:ARG:HD2	1.77	0.48
1:E:614:ASP:N	1:E:614:ASP:OD1	2.47	0.48
1:F:364:ILE:O	1:F:368:ILE:HG13	2.14	0.48
1:D:599:THR:HG22	1:D:599:THR:O	2.13	0.48
1:F:406:THR:OG1	1:F:407:ASP:OD2	2.25	0.48
1:B:536:LEU:HB2	1:B:544:ILE:HD11	1.96	0.48
1:D:525:VAL:HG23	1:D:553:VAL:HG23	1.96	0.48
1:E:489:CYS:HG	1:E:599:THR:HG1	1.60	0.48
1:F:525:VAL:HG23	1:F:553:VAL:HG22	1.96	0.48
1:B:616:ALA:O	1:B:620:ARG:NH1	2.46	0.47
1:B:554:PHE:HE2	1:B:603:ASP:HB2	1.79	0.47
1:B:681:ILE:HD12	1:B:681:ILE:H	1.79	0.47



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Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:E:470:PRO:O	1:E:479:ARG:NE	2.42	0.47
1:B:415:PHE:CZ	1:B:669:LEU:HD21	2.49	0.47
2:S:4:DT:H2"	2:S:5:DT:O4'	2.15	0.47
2:S:3:DT:H4'	2:S:4:DT:OP1	2.15	0.47
1:C:620:ARG:C	1:C:621:ILE:HD13	2.35	0.47
1:B:553:VAL:HB	1:B:600:ILE:HD13	1.96	0.47
1:E:569:ILE:O	1:E:611:ASP:N	2.41	0.47
1:F:421:ASP:O	1:F:425:GLY:N	2.48	0.47
2:S:4:DT:H2"	2:S:5:DT:O5'	2.14	0.47
1:D:415:PHE:HZ	1:D:669:LEU:HD21	1.80	0.47
1:E:386:PRO:HG3	1:F:391:THR:HG23	1.97	0.47
1:E:420:LEU:HG	1:E:422:LEU:HD23	1.96	0.47
1:C:470:PRO:HB2	1:C:472:THR:HG23	1.95	0.47
1:F:533:THR:HA	1:F:570:ARG:HH11	1.80	0.47
1:E:508:GLY:O	1:E:512:THR:HG23	2.14	0.47
1:F:614:ASP:OD1	1:F:614:ASP:N	2.47	0.47
1:C:660:GLN:N	1:C:660:GLN:OE1	2.48	0.46
1:A:584:GLY:N	1:A:592:ILE:O	2.45	0.46
1:B:532:LEU:HD11	1:B:602:ILE:HD11	1.98	0.46
1:F:325:LYS:HE3	1:F:379:TYR:CD1	2.50	0.46
1:C:529:GLN:NE2	1:C:555:CYS:SG	2.84	0.46
1:A:607:LYS:HE3	1:A:692:GLU:HG3	1.97	0.46
1:D:500:PHE:N	1:D:622:ALA:O	2.49	0.46
1:F:684:MET:H	1:F:684:MET:CE	2.29	0.46
1:C:535:VAL:HA	1:C:570:ARG:HH22	1.81	0.46
1:C:695:ASP:N	1:C:695:ASP:OD1	2.47	0.46
1:D:582:VAL:HG12	1:D:594:ASN:HB2	1.98	0.46
1:A:574:ILE:HD11	1:A:617:LEU:HG	1.98	0.46
1:D:658:LYS:HA	1:D:661:ASN:OD1	2.15	0.46
1:D:671:LEU:HD12	1:D:671:LEU:HA	1.85	0.46
1:B:422:LEU:HD23	1:B:676:TYR:CD2	2.51	0.46
1:F:414:PRO:HB3	1:F:438:CYS:SG	2.56	0.46
1:C:612:ARG:HD3	1:C:612:ARG:HA	1.73	0.46
1:E:340:LEU:HD13	1:E:404:VAL:HG21	1.98	0.46
1:E:491:CYS:SG	1:E:684:MET:HG2	2.56	0.46
1:A:514:ARG:HG3	1:A:659:ILE:HG21	1.97	0.45
1:B:585:ARG:HG2	1:B:586:PRO:O	2.16	0.45
1:F:350:TRP:CZ2	1:F:353:ASN:HA	2.51	0.45
1:D:325:LYS:NZ	1:D:382:GLU:HG2	2.31	0.45
1:D:523:LEU:HD22	1:D:551:ARG:HG2	1.99	0.45
1:D:534:ASP:N	1:D:570:ARG:HH12	2.14	0.45



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:E:358:ASN:HB2	1:E:363:LEU:HD11	1.97	0.45
1:F:458:MET:SD	1:F:462:MET:HE1	2.57	0.45
1:B:673:VAL:O	1:B:677:LYS:HG2	2.16	0.45
1:D:351:ILE:O	1:D:356:LYS:NZ	2.44	0.45
1:A:501:PHE:HA	1:A:624:VAL:HG23	1.97	0.45
1:D:350:TRP:CZ2	1:D:353:ASN:HA	2.51	0.45
1:E:356:LYS:HB2	1:E:356:LYS:HE2	1.77	0.45
1:E:671:LEU:HD21	1:E:675:TRP:CH2	2.52	0.45
1:F:600:ILE:HD12	1:F:600:ILE:HA	1.82	0.45
1:A:522:ASP:C	1:A:524:PHE:H	2.20	0.45
1:D:531:ILE:HG21	1:D:544:ILE:HD11	1.98	0.45
1:D:647:LYS:HE3	1:D:647:LYS:HB3	1.80	0.45
1:B:461:LEU:HD12	1:B:664:TYR:HB3	1.98	0.45
1:D:358:ASN:HB3	1:D:361:GLU:O	2.16	0.45
1:D:665:ARG:HG2	1:D:666:PHE:CD1	2.52	0.45
1:F:573:ASN:O	1:F:577:LEU:HG	2.16	0.45
1:A:334:LEU:HA	1:A:334:LEU:HD23	1.75	0.45
1:F:339:VAL:HG13	1:F:349:VAL:HG12	1.97	0.45
1:C:514:ARG:HB3	1:C:514:ARG:NH1	2.31	0.45
1:F:351:ILE:O	1:F:356:LYS:NZ	2.50	0.45
1:F:579:GLU:O	1:F:596:ASN:ND2	2.35	0.44
1:D:537:ASP:OD1	1:D:537:ASP:N	2.50	0.44
1:E:349:VAL:HG21	1:E:367:LEU:HB2	1.99	0.44
1:F:525:VAL:HG13	1:F:550:LYS:HE2	1.99	0.44
1:A:350:TRP:CZ2	1:A:353:ASN:HA	2.52	0.44
1:A:422:LEU:HD23	1:A:422:LEU:HA	1.84	0.44
1:C:683:ILE:HG22	1:C:685:LYS:HG2	1.99	0.44
1:D:447:ASP:HB2	1:D:666:PHE:CE2	2.52	0.44
1:D:448:ASP:OD1	1:D:448:ASP:N	2.51	0.44
1:E:661:ASN:OD1	1:E:663:ARG:HG3	2.18	0.44
1:F:667:ALA:O	1:F:671:LEU:HG	2.17	0.44
1:F:325:LYS:HE2	1:F:382:GLU:OE2	2.17	0.44
1:B:490:LEU:O	1:B:551:ARG:NH1	2.49	0.44
1:C:540:PRO:CG	2:S:4:DT:OP1	2.64	0.44
1:D:654:GLY:O	1:D:658:LYS:HG2	2.17	0.44
1:F:516:LEU:HD22	1:F:668:PHE:HE2	1.82	0.44
1:A:531:ILE:HD11	1:A:543:PHE:HB3	1.99	0.44
1:B:554:PHE:CE2	1:B:603:ASP:HB2	2.52	0.44
1:D:424:ASP:N	1:D:424:ASP:OD1	2.51	0.44
1:E:516:LEU:O	1:E:520:ILE:HG12	2.18	0.44
1:F:477:LYS:O	1:F:480:GLU:HG3	2.17	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:490:LEU:O	1:A:551:ARG:NE	2.37	0.44
1:A:569:ILE:HD13	1:A:569:ILE:HA	1.86	0.44
1:F:410:PRO:HB3	1:F:493:ALA:HB2	1.99	0.43
1:E:459:GLU:HA	1:E:462:MET:SD	2.58	0.43
1:E:509:LYS:HE2	1:E:509:LYS:HB2	1.73	0.43
1:E:533:THR:HB	1:E:567:LYS:HB3	2.01	0.43
1:F:340:LEU:HB2	1:F:348:ILE:HG13	2.00	0.43
1:F:447:ASP:O	1:F:450:LYS:NZ	2.52	0.43
1:F:662:ASN:HB3	1:F:665:ARG:HH21	1.82	0.43
1:C:553:VAL:HG12	1:C:600:ILE:HA	1.99	0.43
1:C:682:PRO:C	1:C:683:ILE:HD13	2.39	0.43
1:D:445:LYS:HE3	1:D:445:LYS:HB3	1.81	0.43
1:B:530:THR:O	1:B:534:ASP:HB3	2.17	0.43
1:D:510:SER:O	1:D:514:ARG:HG3	2.18	0.43
2:S:5:DT:H2"	2:S:6:DT:H5'	2.01	0.43
1:D:477:LYS:HA	1:D:477:LYS:HD3	1.83	0.43
1:E:517:LYS:HE3	1:E:517:LYS:HB2	1.86	0.43
1:C:685:LYS:HA	1:C:685:LYS:HD2	1.86	0.43
1:B:558:LEU:HD21	1:B:569:ILE:HD11	2.00	0.43
1:D:532:LEU:HD12	1:D:532:LEU:HA	1.79	0.43
1:D:572:ASP:N	1:D:572:ASP:OD2	2.51	0.43
1:E:550:LYS:HA	1:E:550:LYS:HD3	1.69	0.43
1:A:389:ARG:NH2	1:B:395:ASN:OD1	2.52	0.43
1:B:396:ILE:HD13	1:B:396:ILE:HA	1.83	0.43
1:D:461:LEU:O	1:D:465:ILE:HG12	2.19	0.43
1:E:456:PRO:O	1:E:460:GLU:HG3	2.19	0.43
1:B:476:LYS:HG2	1:B:477:LYS:HD2	2.01	0.42
1:E:561:PHE:CZ	1:E:568:LYS:HA	2.53	0.42
1:C:421:ASP:O	1:C:425:GLY:N	2.52	0.42
2:S:2:DT:H2"	2:S:3:DT:O5'	2.18	0.42
1:A:693:ILE:HB	1:A:696:PHE:HB2	2.00	0.42
1:B:578:THR:O	1:B:578:THR:OG1	2.32	0.42
1:C:578:THR:OG1	1:C:620:ARG:NH1	2.52	0.42
1:B:514:ARG:HB2	1:B:514:ARG:NH1	2.34	0.42
1:D:507:THR:HG23	1:D:628:THR:H	1.85	0.42
1:E:622:ALA:HB2	1:E:688:PRO:HA	2.01	0.42
1:B:536:LEU:HB2	1:B:544:ILE:CD1	2.49	0.42
1:C:486:LEU:HD22	1:C:516:LEU:HD11	2.01	0.42
1:D:490:LEU:HD11	1:D:672:LEU:HB3	2.01	0.42
1:A:401:VAL:HG21	1:F:351:ILE:HG21	2.01	0.42
1:B:556:SER:HA	1:B:603:ASP:HB3	2.02	0.42



Atom-1	Atom-2	Interatomic	Clash
	1100111 2	distance (Å)	overlap (Å)
1:E:526:GLU:OE2	1:E:556:SER:OG	2.37	0.42
1:E:607:LYS:HD3	1:E:607:LYS:HA	1.93	0.42
1:F:486:LEU:HD23	1:F:486:LEU:HA	1.81	0.42
1:D:415:PHE:HA	1:D:442:THR:OG1	2.20	0.42
1:D:453:GLU:OE1	1:D:453:GLU:N	2.46	0.42
1:F:625:ARG:HB2	1:F:625:ARG:NH1	2.35	0.42
1:A:451:PHE:HZ	1:A:673:VAL:HG11	1.85	0.42
1:D:574:ILE:HG13	1:D:575:LYS:N	2.35	0.42
1:A:407:ASP:HB2	1:A:595:ARG:HH22	1.85	0.41
1:A:509:LYS:H	1:A:509:LYS:HG3	1.68	0.41
1:B:533:THR:OG1	1:B:569:ILE:HA	2.19	0.41
1:E:503:GLY:HA3	1:E:626:PHE:HB2	2.02	0.41
1:B:618:MET:H	1:B:618:MET:HG2	1.52	0.41
1:B:377:LYS:HD2	1:B:377:LYS:O	2.20	0.41
1:B:426:MET:N	1:B:426:MET:SD	2.93	0.41
1:B:556:SER:OG	1:B:557:GLU:OE2	2.33	0.41
1:F:501:PHE:CD1	1:F:601:ILE:HD11	2.55	0.41
1:B:353:ASN:HD22	1:B:430:GLY:HA2	1.84	0.41
1:E:515:LEU:HD23	1:E:515:LEU:HA	1.92	0.41
1:F:339:VAL:C	1:F:340:LEU:HD23	2.41	0.41
1:F:348:ILE:HG22	1:F:357:PHE:HB3	2.03	0.41
1:B:507:THR:HB	1:B:626:PHE:HB3	2.01	0.41
1:F:412:LYS:O	1:F:551:ARG:NH1	2.37	0.41
1:A:398:ASP:OD2	1:F:389:ARG:NH1	2.53	0.41
1:F:340:LEU:HG	1:F:355:TRP:CH2	2.56	0.41
1:A:571:SER:O	1:A:574:ILE:HG12	2.21	0.41
1:A:682:PRO:O	1:A:683:ILE:HD13	2.20	0.41
1:C:389:ARG:NH2	1:D:395:ASN:OD1	2.54	0.41
1:C:541:ASN:ND2	1:C:544:ILE:HD12	2.35	0.41
1:D:444:PHE:CE1	1:D:665:ARG:HD3	2.56	0.41
1:E:483:GLU:HG2	1:E:675:TRP:CH2	2.56	0.41
1:B:334:LEU:HA	1:B:334:LEU:HD23	1.80	0.41
1:B:350:TRP:CZ2	1:B:353:ASN:HA	2.55	0.41
1:D:578:THR:HG21	1:D:620:ARG:NE	2.30	0.41
1:E:417:ASN:OD1	1:E:417:ASN:N	2.52	0.41
1:D:414:PRO:HB3	1:D:438:CYS:SG	2.61	0.41
1:E:413:LEU:HD23	1:E:413:LEU:HA	1.90	0.41
1:F:332:ARG:HH11	1:F:379:TYR:HE2	1.69	0.41
1:F:481:LEU:O	1:F:485:THR:OG1	2.30	0.41
1:F:500:PHE:CE1	1:F:621:ILE:HG23	2.56	0.41
1:F:510:SER:HA	1:F:513:LYS:HG2	2.03	0.41



	1 / J	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:413:LEU:HA	1:A:414:PRO:HD3	1.93	0.41
1:B:371:ILE:HG12	1:B:371:ILE:O	2.21	0.41
1:D:450:LYS:HB2	1:D:666:PHE:HD2	1.85	0.41
1:E:670:TYR:HA	1:E:673:VAL:HG12	2.03	0.41
1:F:447:ASP:HB3	1:F:450:LYS:HZ1	1.86	0.41
1:F:556:SER:OG	1:F:557:GLU:N	2.54	0.41
1:C:411:ASP:OD2	1:C:412:LYS:NZ	2.50	0.40
1:A:486:LEU:HD23	1:A:486:LEU:HA	1.81	0.40
1:A:549:LEU:HD23	1:A:595:ARG:HB2	2.03	0.40
1:B:583:ILE:HD12	1:B:583:ILE:HA	1.89	0.40
1:F:334:LEU:HD12	1:F:334:LEU:HA	1.94	0.40
1:B:364:ILE:HD12	1:B:397:ARG:HH21	1.86	0.40
1:B:415:PHE:HZ	1:B:669:LEU:HD21	1.87	0.40
1:B:419:VAL:HG11	1:B:436:TYR:HD1	1.86	0.40
1:B:460:GLU:OE2	1:B:663:ARG:NH2	2.54	0.40
1:C:499:THR:HG22	1:C:622:ALA:HB3	2.03	0.40
1:C:681:ILE:HD13	1:C:681:ILE:HA	1.92	0.40
1:D:531:ILE:H	1:D:531:ILE:HG13	1.57	0.40
1:E:532:LEU:HD23	1:E:532:LEU:HA	1.88	0.40
1:A:516:LEU:O	1:A:520:ILE:HG12	2.22	0.40
1:C:612:ARG:C	1:C:613:ILE:HD13	2.41	0.40
1:C:690:PRO:HG2	1:C:700:LEU:HD11	2.03	0.40
1:D:326:LEU:HD21	1:D:388:LYS:HB3	2.04	0.40
1:E:658:LYS:HE3	1:E:658:LYS:HB3	1.86	0.40
1:B:385:CYS:HB3	1:B:388:LYS:HG3	2.03	0.40
1:B:588:PHE:CZ	2:S:6:DT:H73	2.57	0.40
1:C:520:ILE:HD11	1:C:524:PHE:HD2	1.86	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	ntiles
1	А	349/785~(44%)	329~(94%)	19 (5%)	1 (0%)	41	75
1	В	353/785~(45%)	336~(95%)	17 (5%)	0	100	100
1	С	357/785~(46%)	344~(96%)	13 (4%)	0	100	100
1	D	359/785~(46%)	332~(92%)	26 (7%)	1 (0%)	41	75
1	Е	323/785~(41%)	310 (96%)	13 (4%)	0	100	100
1	F	308/785~(39%)	296~(96%)	12 (4%)	0	100	100
All	All	2049/4710~(44%)	1947 (95%)	100 (5%)	2(0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	532	LEU
1	А	523	LEU

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	324/725~(45%)	311~(96%)	13~(4%)	31	65
1	В	327/725~(45%)	318~(97%)	9(3%)	43	72
1	С	331/725~(46%)	318 (96%)	13 (4%)	32	65
1	D	333/725~(46%)	317~(95%)	16 (5%)	25	60
1	Е	302/725~(42%)	296 (98%)	6 (2%)	55	79
1	F	291/725~(40%)	277~(95%)	14 (5%)	25	60
All	All	1908/4350 (44%)	1837 (96%)	71 (4%)	37	66

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	377	LYS
1	А	420	LEU
1	А	462	MET



Mol	Chain	Res	Type
1	А	491	CYS
1	А	534	ASP
1	А	563	CYS
1	А	566	SER
1	А	572	ASP
1	А	585	ARG
1	А	618	MET
1	А	629	HIS
1	А	658	LYS
1	А	698	PHE
1	В	370	SER
1	В	372	ARG
1	В	431	ASP
1	В	434	LYS
1	В	479	ARG
1	В	538	LYS
1	В	554	PHE
1	В	572	ASP
1	В	594	ASN
1	С	337	ASN
1	С	353	ASN
1	С	424	ASP
1	С	474	GLU
1	С	479	ARG
1	С	510	SER
1	С	514	ARG
1	С	534	ASP
1	С	547	MET
1	С	554	PHE
1	С	581	CYS
1	С	594	ASN
1	С	615	ASN
1	D	326	LEU
1	D	335	ASP
1	D	346	ASP
1	D	370	SER
1	D	372	ARG
1	D	380	SER
1	D	431	ASP
1	D	517	LYS
1	D	531	ILE
1	D	543	PHE



Mol	Chain	Res	Type
1	D	585	ARG
1	D	606	TYR
1	D	611	ASP
1	D	612	ARG
1	D	625	ARG
1	D	684	MET
1	Е	462	MET
1	Е	476	LYS
1	Е	554	PHE
1	Е	561	PHE
1	Е	610	PHE
1	Е	627	ARG
1	F	325	LYS
1	F	357	PHE
1	F	387	ARG
1	F	426	MET
1	F	438	CYS
1	F	441	SER
1	F	479	ARG
1	F	500	PHE
1	F	554	PHE
1	F	617	LEU
1	F	618	MET
1	F	627	ARG
1	F	674	LYS
1	F	684	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	475	ASN
1	Е	475	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)

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.

