



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 4, 2018 – 10:06 AM EST

PDB ID : 6HV8
EMDB ID: : EMD-0287
Title : Cryo-EM structure of *S. cerevisiae* Polymerase epsilon deltatcat mutant
Authors : Goswami, P.; Purkiss, A.; Cheung, A.; Costa, A.
Deposited on : 2018-10-10
Resolution : 4.40 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

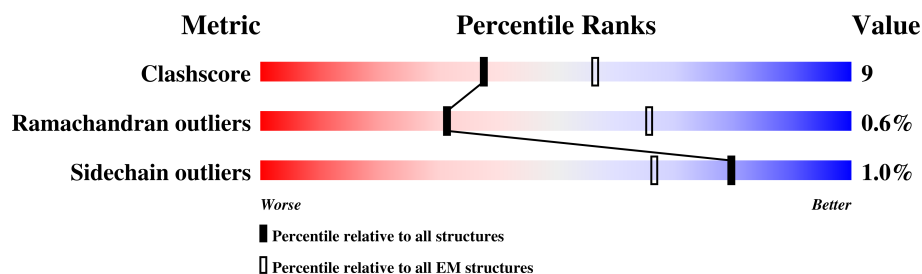
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	B	689	
2	A	914	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9206 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 polymerase epsilon subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	410	Total	C	N	O	S	0	0
			3256	2085	554	603	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	266	ASN	MET	conflict	UNP P24482

- Molecule 2 is a protein called DNA polymerase epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	774	Total	C	N	O	S	0	0
			5948	3819	992	1104	33		

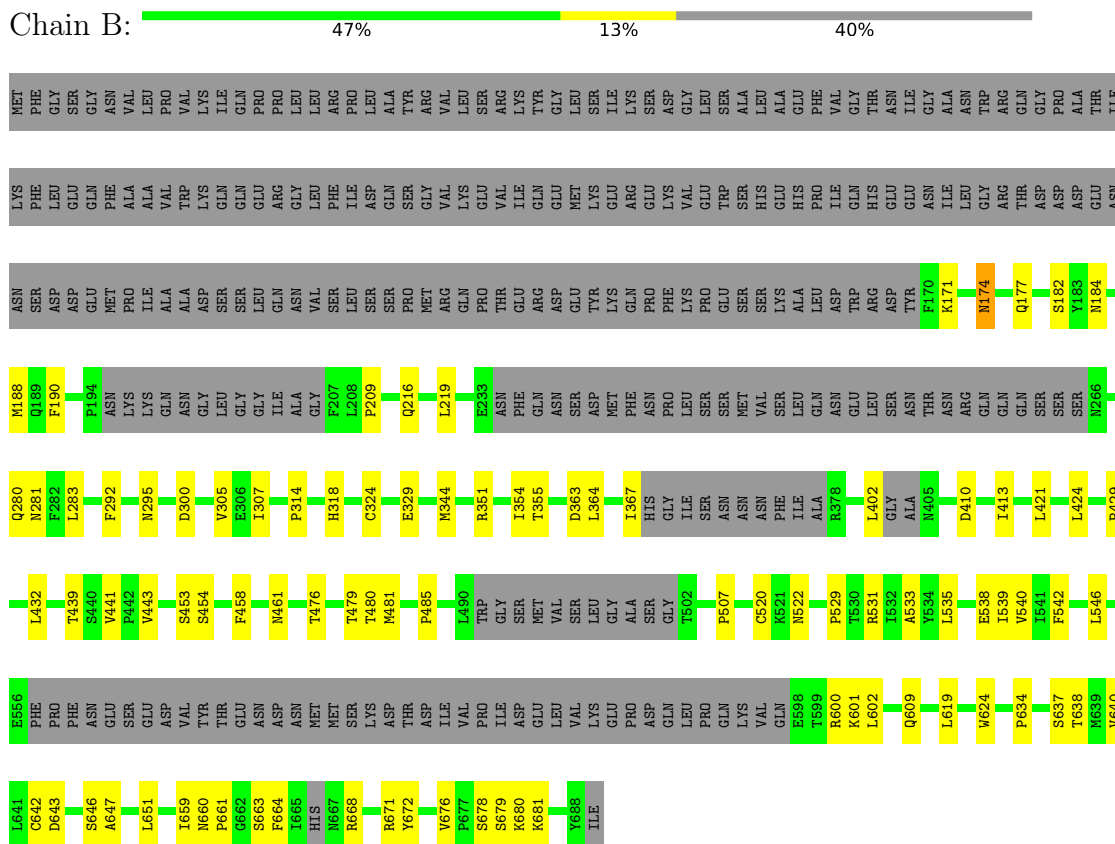
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Zn	0
			2	2	

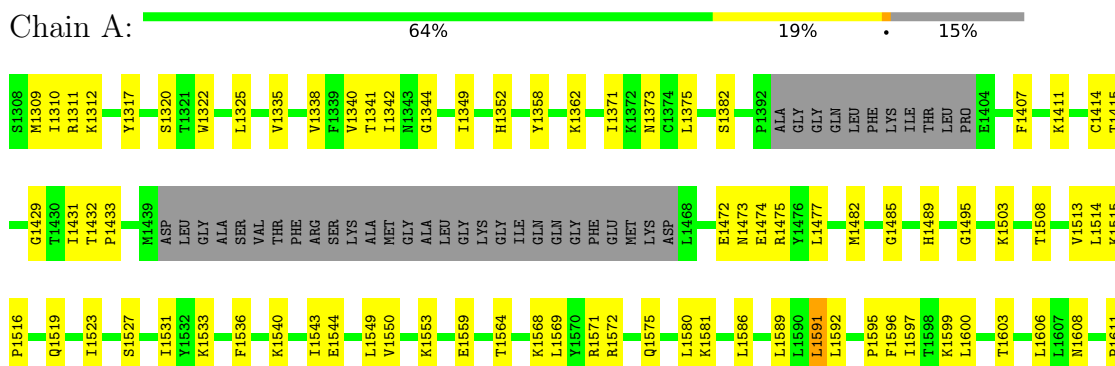
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: DNA polymerase epsilon subunit B



- Molecule 2: DNA polymerase epsilon catalytic subunit A



PRO	SER	LEU	S2100	L2101	V2102		C2108		C2111		D2118	F2119	C2120	K2121	ALA	ALA	PRO	GLU	SER	ILE	F2128	S2129		L2146		K2149		L2158		R2163	C2164	S2165	R2166	C2167	H2168		D2173		S2176		W2185		L2189	P2190	R2191		T2221												
ILE	VAL	ASN	VAL	LYS	GLN	ASP	K1993		D2029	P2030		A2034	ASP	TYR	ALA	ILE	PRO	VAL	LEU	PRO	GLY	S2043		N2046		H2060	V2061	M2062	L2063		T2068		E2071	I2072	ARG	THR	LEU	ARG	LYS	GLU	LEU	LEU	LYS	ILE	PHE	GLU	LEU	ARG	GLU	PHE	ALA	LYS	VAL	ALA	GLU	PHE	LYS	ASP	
E1850		Y1860	A1861	D1862	R1863	N1864	Q1865	I1866	L1867	K1868	T1870		P1875		Y1879		M1886		R1890		M1894	F1895	S1896	Y1897	L1898	D1899		W1906		L1909	I1910	W1911	N1916	F1917		A1921		C1922		N1930	Q1931	D1932	Y1933		V1936		P1947	I1948		N1975	SER	GLY	THR	GLN	ARG	PRO	THR	GLN	
I1612		L1622		L1745		I1646		L1649		N1657		I1660	C1661	N1662	L1663	R1664	L1665	D1666	S1667	M1668		L1675		I1685	V1686	L1687	W1688	W1689	N1690		L1695	P1696		I1701	Q1702	N1703	ASP	PHE	ASP	LEU	ASN	THR	SER	W1711	I1712		F1718	P1719	K1720	I1721		V1726	Y1727	D1728	W1729	V1730	V1731	L1732	D1733
	N1742		I1744		T1746	S1747	ALA	LEU	ILE	ASN	ASP	ALA	GLU	GLY	SER	ASP	LEU	VAL	ASN	ASN	ASN	MET	GLY	ILE	ASP	ASP	LYS	ASP	ALA	VAL	ILE	ASN	PRO	SER	GLU	PHE	VAL	HIS	ASP	ALA	PHE	S1784		G1793	M1794	L1795	K1796		K1826	L1827	F1828		L1832		V1836		T1840		

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	161376	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	B	0.44	0/3318	0.71	1/4493 (0.0%)
2	A	0.45	0/6061	0.85	17/8223 (0.2%)
All	All	0.45	0/9379	0.80	18/12716 (0.1%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1687	LEU	CA-CB-CG	7.72	133.06	115.30
2	A	1622	LEU	CA-CB-CG	7.21	131.88	115.30
2	A	2030	PRO	N-CA-CB	6.60	111.22	103.30
2	A	2063	LEU	CA-CB-CG	6.26	129.71	115.30
1	B	300	ASP	CB-CG-OD1	6.04	123.73	118.30
2	A	1591	LEU	CA-CB-CG	5.99	129.07	115.30
2	A	1640	LEU	CA-CB-CG	5.63	128.26	115.30
2	A	1477	LEU	CA-CB-CG	5.48	127.90	115.30
2	A	1675	LEU	CB-CG-CD2	-5.43	101.77	111.00
2	A	1686	VAL	CG1-CB-CG2	-5.36	102.33	110.90
2	A	1832	LEU	CA-CB-CG	5.33	127.57	115.30
2	A	1695	LEU	CA-CB-CG	-5.26	103.21	115.30
2	A	1657	ASN	N-CA-C	5.24	125.14	111.00
2	A	1886	MET	CB-CG-SD	-5.23	96.70	112.40
2	A	1911	TRP	C-N-CA	5.13	134.52	121.70
2	A	1514	LEU	CA-CB-CG	5.11	127.05	115.30
2	A	1664	ARG	CA-CB-CG	5.08	124.59	113.40
2	A	1531	ILE	CG1-CB-CG2	-5.06	100.26	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3256	0	3258	51	0
2	A	5948	0	5712	110	0
3	A	2	0	0	0	0
All	All	9206	0	8970	160	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 9.

All (160) 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)
1:B:182:SER:O	1:B:190:PHE:HA	1.76	0.85
2:A:2068:THR:HA	2:A:2071:GLU:HB3	1.59	0.84
2:A:1906:TRP:HB3	2:A:1909:LEU:HD11	1.69	0.74
2:A:1879:TYR:OH	2:A:1886:MET:SD	2.49	0.69
2:A:1712:ILE:HG12	2:A:1712:ILE:O	1.96	0.65
2:A:1549:LEU:HB3	2:A:1646:ILE:HD11	1.79	0.64
2:A:1649:LEU:HD21	2:A:1664:ARG:HG3	1.80	0.63
1:B:364:LEU:HD13	1:B:634:PRO:HD3	1.81	0.63
2:A:2062:MET:SD	2:A:2062:MET:N	2.72	0.63
1:B:676:VAL:O	1:B:680:LYS:HA	1.99	0.63
2:A:1533:LYS:HA	2:A:1536:PHE:HB3	1.81	0.62
2:A:1890:ARG:NH1	2:A:1894:MET:SD	2.73	0.62
2:A:2164:CYS:SG	2:A:2165:SER:N	2.73	0.62
1:B:647:ALA:O	1:B:660:ASN:ND2	2.33	0.61
2:A:1320:SER:HA	2:A:1341:THR:O	2.00	0.61
2:A:2108:CYS:CB	2:A:2111:CYS:SG	2.83	0.61
1:B:209:PRO:O	2:A:2191:ARG:NH2	2.33	0.61
2:A:1342:ILE:HG23	2:A:1344:GLY:H	1.65	0.61
2:A:1495:GLY:HA3	2:A:1515:LYS:HB2	1.83	0.60
2:A:1523:ILE:HG23	2:A:1527:SER:HB3	1.82	0.60
2:A:1568:LYS:HA	2:A:1571:ARG:HB3	1.83	0.60
2:A:1581:LYS:HE2	2:A:1586:LEU:HD21	1.84	0.60
2:A:2102:VAL:O	2:A:2149:LYS:NZ	2.35	0.59
1:B:531:ARG:HG2	1:B:540:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1473:ASN:OD1	2:A:1475:ARG:NH2	2.36	0.59
1:B:546:LEU:HB3	1:B:602:LEU:HD11	1.85	0.59
1:B:216:GLN:HA	1:B:219:LEU:HB2	1.86	0.57
2:A:1733:ASP:OD1	2:A:1733:ASP:N	2.35	0.57
1:B:174:ASN:HB2	1:B:177:GLN:HB2	1.86	0.57
2:A:1921:ALA:HB1	2:A:1930:ASN:HB3	1.87	0.56
1:B:174:ASN:ND2	1:B:177:GLN:OE1	2.32	0.56
2:A:1733:ASP:HB3	2:A:1906:TRP:HD1	1.70	0.56
1:B:642:CYS:HA	1:B:661:PRO:HD2	1.88	0.56
2:A:2163:ARG:NH2	2:A:2168:HIS:O	2.38	0.55
2:A:1550:VAL:HB	2:A:1553:LYS:HE3	1.88	0.55
2:A:1612:ILE:O	2:A:1664:ARG:NH2	2.39	0.55
2:A:1696:PRO:HB2	2:A:1701:ILE:HG12	1.89	0.55
2:A:2108:CYS:HB3	2:A:2111:CYS:SG	2.46	0.55
1:B:600:ARG:HE	1:B:651:LEU:HD13	1.71	0.55
2:A:1414:CYS:SG	2:A:1415:THR:N	2.79	0.54
2:A:1731:VAL:HG23	2:A:1868:ILE:HG13	1.90	0.54
1:B:184:ASN:O	1:B:188:MET:HA	2.07	0.54
1:B:643:ASP:OD2	1:B:646:SER:N	2.41	0.54
1:B:539:ILE:HG12	1:B:638:THR:HB	1.89	0.53
1:B:410:ASP:HB3	1:B:413:ILE:HG12	1.89	0.53
2:A:1362:LYS:HE2	2:A:1375:LEU:H	1.72	0.53
2:A:2119:PHE:HE2	2:A:2146:LEU:HD21	1.74	0.52
2:A:1726:VAL:HG12	2:A:1728:ASP:H	1.75	0.52
1:B:184:ASN:O	1:B:188:MET:N	2.43	0.52
2:A:1516:PRO:HB2	2:A:1519:GLN:HB2	1.91	0.52
2:A:1720:LYS:HE2	2:A:1860:TYR:HB2	1.91	0.52
2:A:1611:PRO:HB3	2:A:1660:ILE:HG23	1.92	0.51
2:A:1485:GLY:N	2:A:1589:LEU:O	2.43	0.51
2:A:1595:PRO:HG2	2:A:1612:ILE:HG23	1.93	0.51
2:A:1864:ASN:OD1	2:A:1865:GLN:NE2	2.44	0.51
2:A:1850:GLU:OE1	2:A:1890:ARG:NH2	2.43	0.51
1:B:292:PHE:H	1:B:295:ASN:HB3	1.75	0.51
1:B:351:ARG:HE	1:B:354:ILE:HG13	1.76	0.51
2:A:2176:SER:HB2	2:A:2185:TRP:HZ2	1.75	0.50
2:A:2071:GLU:HG2	2:A:2072:ILE:HG12	1.93	0.50
1:B:529:PRO:HB3	1:B:542:PHE:HD1	1.77	0.50
2:A:1581:LYS:HG3	2:A:1586:LEU:HG	1.94	0.50
1:B:174:ASN:OD1	1:B:174:ASN:N	2.45	0.50
1:B:209:PRO:HB2	1:B:624:TRP:HE3	1.76	0.50
2:A:1335:VAL:HG22	2:A:1352:HIS:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1540:LYS:O	2:A:1544:GLU:N	2.42	0.49
2:A:2043:SER:HB2	2:A:2046:ASN:HB2	1.94	0.49
2:A:1730:VAL:HG21	2:A:1869:LYS:HG2	1.94	0.49
2:A:1373:ASN:HD22	2:A:1407:PHE:HA	1.77	0.49
2:A:1543:ILE:HG12	2:A:1553:LYS:HD3	1.95	0.49
1:B:184:ASN:O	1:B:188:MET:CA	2.60	0.49
2:A:1572:ARG:NH2	2:A:1575:GLN:OE1	2.37	0.48
1:B:663:SER:OG	1:B:664:PHE:N	2.47	0.48
2:A:1732:LEU:HD23	2:A:1867:LEU:HD23	1.95	0.48
2:A:1310:ILE:HG22	2:A:1311:ARG:HG2	1.96	0.48
2:A:1595:PRO:HB2	2:A:1600:LEU:HD12	1.95	0.48
1:B:439:THR:HG22	1:B:441:VAL:H	1.79	0.48
1:B:538:GLU:O	1:B:637:SER:N	2.42	0.48
1:B:640:VAL:HG13	1:B:659:ILE:HD11	1.96	0.48
2:A:2189:LEU:HD12	2:A:2190:PRO:HD2	1.96	0.47
2:A:2164:CYS:HB3	2:A:2167:CYS:SG	2.53	0.47
2:A:1433:PRO:HD3	2:A:1689:TRP:HE1	1.79	0.47
2:A:1870:THR:HG21	2:A:1879:TYR:HB2	1.97	0.47
1:B:485:PRO:HG3	1:B:507:PRO:HA	1.97	0.47
2:A:1730:VAL:HB	2:A:1869:LYS:HA	1.96	0.47
2:A:1690:ASN:HB2	2:A:1826:LYS:HD3	1.96	0.47
1:B:480:THR:HA	1:B:522:ASN:HB3	1.96	0.47
2:A:1513:VAL:HG11	2:A:1569:LEU:HD22	1.97	0.47
2:A:1596:PHE:HA	2:A:1597:ILE:HA	1.58	0.47
2:A:1431:ILE:HD12	2:A:1687:LEU:HD11	1.97	0.46
2:A:1513:VAL:HG23	2:A:1564:THR:HA	1.97	0.46
2:A:1489:HIS:CE1	2:A:1599:LYS:HB2	2.51	0.46
2:A:1730:VAL:HG23	2:A:1732:LEU:HD11	1.98	0.46
2:A:1732:LEU:HD13	2:A:1909:LEU:HD13	1.98	0.46
2:A:2173:ASP:N	2:A:2173:ASP:OD1	2.46	0.45
1:B:280:GLN:O	1:B:281:ASN:ND2	2.41	0.45
1:B:429:PRO:HG2	1:B:479:THR:HG21	1.98	0.45
1:B:453:SER:OG	1:B:454:SER:N	2.49	0.45
2:A:1317:TYR:OH	2:A:1472:GLU:OE2	2.34	0.45
2:A:1322:TRP:HA	2:A:1340:VAL:HG12	1.98	0.45
2:A:1742:ASN:HD21	2:A:1899:ASP:HB3	1.81	0.45
1:B:324:CYS:SG	1:B:609:GLN:NE2	2.90	0.45
1:B:432:LEU:HD12	1:B:481:MET:HG2	1.98	0.45
2:A:1663:LEU:HB3	2:A:1666:ASP:HB2	1.97	0.45
2:A:1338:VAL:H	2:A:1349:ILE:HG22	1.82	0.45
2:A:1922:CYS:O	2:A:1931:GLN:NE2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:LEU:HA	1:B:672:TYR:HB2	1.98	0.45
1:B:421:LEU:HD23	1:B:424:LEU:HD12	1.99	0.45
2:A:1433:PRO:HD3	2:A:1689:TRP:NE1	2.32	0.45
2:A:1947:PRO:HA	2:A:1948:ILE:HA	1.77	0.44
2:A:1358:TYR:HB2	2:A:1429:GLY:HA2	1.99	0.44
2:A:1508:THR:OG1	2:A:1559:GLU:O	2.35	0.44
2:A:1580:LEU:HA	2:A:1580:LEU:HD13	1.73	0.44
1:B:458:PHE:HA	1:B:461:ASN:HD22	1.82	0.44
2:A:1860:TYR:OH	2:A:1862:ASP:OD2	2.28	0.44
2:A:1745:LEU:HB2	2:A:1897:TYR:CE1	2.53	0.44
1:B:668:ARG:HH21	1:B:671:ARG:HH12	1.64	0.44
2:A:2164:CYS:SG	2:A:2166:ARG:N	2.89	0.44
2:A:1503:LYS:HB2	2:A:1503:LYS:HE2	1.81	0.44
1:B:314:PRO:HB3	1:B:344:MET:H	1.82	0.44
1:B:171:LYS:H	1:B:533:ALA:HB3	1.82	0.44
2:A:1599:LYS:O	2:A:1603:THR:OG1	2.29	0.44
2:A:1695:LEU:HD13	2:A:1828:PHE:N	2.33	0.44
2:A:1860:TYR:HB3	2:A:1867:LEU:HD13	2.00	0.44
1:B:678:SER:OG	1:B:679:SER:N	2.51	0.44
2:A:1606:LEU:O	2:A:1608:ASN:ND2	2.51	0.43
2:A:1662:ASN:HB2	2:A:1664:ARG:HD2	2.00	0.43
2:A:1317:TYR:OH	2:A:1320:SER:O	2.24	0.43
2:A:1836:VAL:O	2:A:1840:THR:OG1	2.23	0.43
1:B:676:VAL:O	1:B:680:LYS:CA	2.64	0.43
2:A:1591:LEU:HD23	2:A:1611:PRO:HG3	2.01	0.43
1:B:305:VAL:HG13	1:B:307:ILE:HD11	2.00	0.43
2:A:1721:ILE:O	2:A:2060:HIS:NE2	2.52	0.42
1:B:318:HIS:HA	1:B:601:LYS:HD2	2.00	0.42
1:B:283:LEU:HD13	1:B:329:GLU:HB2	2.02	0.42
1:B:363:ASP:OD2	1:B:367:ILE:N	2.53	0.42
2:A:1474:GLU:HG2	2:A:1657:ASN:HD21	1.84	0.42
2:A:1733:ASP:HB3	2:A:1906:TRP:CD1	2.53	0.42
2:A:1382:SER:HB2	2:A:1685:ILE:HG23	2.02	0.41
1:B:619:LEU:HA	1:B:619:LEU:HD12	1.85	0.41
1:B:676:VAL:HB	1:B:681:LYS:HB2	2.02	0.41
2:A:1431:ILE:HG13	2:A:1432:THR:HG22	2.01	0.41
2:A:2118:ASP:OD1	2:A:2119:PHE:N	2.53	0.41
2:A:1917:PHE:HB2	2:A:1933:TYR:CE2	2.55	0.41
2:A:1896:SER:HA	2:A:1898:LEU:HD23	2.02	0.41
2:A:2128:PHE:HB3	2:A:2129:SER:H	1.67	0.41
2:A:1371:ILE:HG22	2:A:1373:ASN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1701:ILE:HG22	2:A:1702:GLN:HG3	2.02	0.41
2:A:1720:LYS:HE3	2:A:1911:TRP:CE3	2.56	0.41
2:A:1744:ILE:HD12	2:A:1744:ILE:HA	1.88	0.41
2:A:1718:PHE:CD1	2:A:1861:ALA:O	2.74	0.41
2:A:1503:LYS:HE3	2:A:1580:LEU:HD11	2.03	0.41
1:B:351:ARG:O	1:B:355:THR:OG1	2.36	0.41
2:A:1485:GLY:O	2:A:1591:LEU:N	2.55	0.40
2:A:1793:GLY:HA2	2:A:1796:LYS:HD2	2.04	0.40
2:A:1916:ASN:HB3	2:A:1936:VAL:O	2.21	0.40
2:A:1482:MET:N	2:A:1482:MET:SD	2.95	0.40
1:B:476:THR:HG21	1:B:520:CYS:HA	2.03	0.40
2:A:2158:LEU:HD23	2:A:2158:LEU:HA	1.84	0.40
1:B:421:LEU:HA	1:B:424:LEU:HB2	2.04	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	B	394/689 (57%)	339 (86%)	53 (14%)	2 (0%)	31	73
2	A	754/914 (82%)	548 (73%)	201 (27%)	5 (1%)	24	66
All	All	1148/1603 (72%)	887 (77%)	254 (22%)	7 (1%)	31	69

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1657	ASN
2	A	1712	ILE
1	B	443	VAL
1	B	535	LEU
2	A	1668	MET

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Mol	Chain	Res	Type
2	A	2029	ASP
2	A	1875	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	368/629 (58%)	367 (100%)	1 (0%)	93	95
2	A	627/837 (75%)	618 (99%)	9 (1%)	69	85
All	All	995/1466 (68%)	985 (99%)	10 (1%)	80	89

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	174	ASN
2	A	1309	MET
2	A	1312	LYS
2	A	1325	LEU
2	A	1411	LYS
2	A	1592	LEU
2	A	1664	ARG
2	A	1668	MET
2	A	1794	MET
2	A	2062	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	461	ASN
1	B	609	GLN
2	A	1369	GLN
2	A	1373	ASN
2	A	1608	ASN
2	A	1609	GLN

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Mol	Chain	Res	Type
2	A	1657	ASN
2	A	1742	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
2	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2060:HIS	C	2061:VAL	N	14.34
1	B	280:GLN	C	281:ASN	N	5.02