Full wwPDB EM Validation Report ⓘ

Jul 8, 2025 – 03:30 PM JST

PDB ID	:	9K9V / pdb_00009k9v
EMDB ID	:	EMD-62200
Title	:	MPXV DNA polymerase complex in editing state 2
Authors	:	Xie, Y.F.; Kuai, L.; Peng, Q.; Wang, Q.; Wang, H.; Li, X.M.; Qi, J.X.; Ding, Q.; Shi, Y.; Gao, F.
Deposited on	:	2024-10-27
Resolution	:	3.00 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

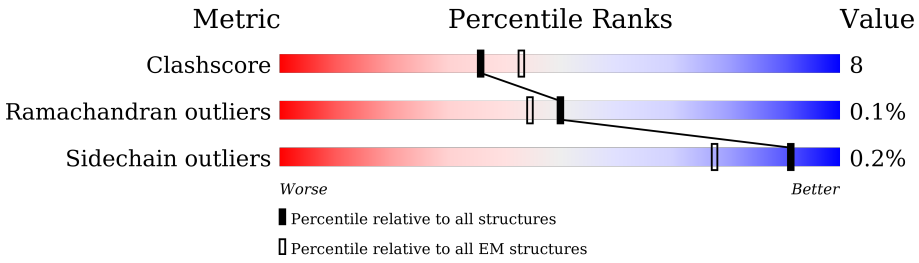
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

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 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	1031	79% 16% .
2	B	218	81% 19%
3	C	426	71% 27% .
4	P	25	60% 8% 32%
5	E	38	18% 16% 66%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13869 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.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	990	8106	5183	1357	1513	53	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP A0A7H0DN44
A	-23	TRP	-	expression tag	UNP A0A7H0DN44
A	-22	SER	-	expression tag	UNP A0A7H0DN44
A	-21	HIS	-	expression tag	UNP A0A7H0DN44
A	-20	PRO	-	expression tag	UNP A0A7H0DN44
A	-19	GLN	-	expression tag	UNP A0A7H0DN44
A	-18	PHE	-	expression tag	UNP A0A7H0DN44
A	-17	GLU	-	expression tag	UNP A0A7H0DN44
A	-16	LYS	-	expression tag	UNP A0A7H0DN44
A	-15	GLY	-	expression tag	UNP A0A7H0DN44
A	-14	SER	-	expression tag	UNP A0A7H0DN44
A	-13	GLY	-	expression tag	UNP A0A7H0DN44
A	-12	SER	-	expression tag	UNP A0A7H0DN44
A	-11	TRP	-	expression tag	UNP A0A7H0DN44
A	-10	SER	-	expression tag	UNP A0A7H0DN44
A	-9	HIS	-	expression tag	UNP A0A7H0DN44
A	-8	PRO	-	expression tag	UNP A0A7H0DN44
A	-7	GLN	-	expression tag	UNP A0A7H0DN44
A	-6	PHE	-	expression tag	UNP A0A7H0DN44
A	-5	GLU	-	expression tag	UNP A0A7H0DN44
A	-4	LYS	-	expression tag	UNP A0A7H0DN44
A	-3	GLY	-	expression tag	UNP A0A7H0DN44
A	-2	SER	-	expression tag	UNP A0A7H0DN44
A	-1	GLY	-	expression tag	UNP A0A7H0DN44
A	0	SER	-	expression tag	UNP A0A7H0DN44
A	108	PHE	LEU	conflict	UNP A0A7H0DN44
A	166	ALA	ASP	engineered mutation	UNP A0A7H0DN44
A	168	ALA	GLU	engineered mutation	UNP A0A7H0DN44

- Molecule 2 is a protein called Uracil-DNA glycosylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	218	Total	C	N	O	S	0	0
			1762	1143	289	324	6		

- Molecule 3 is a protein called DNA polymerase processivity factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	416	Total	C	N	O	S	0	0
			3389	2185	548	645	11		

- Molecule 4 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	P	17	Total	C	N	O	P	0	0
			345	167	61	101	16		

- Molecule 5 is a DNA chain called DNA (38-MER).

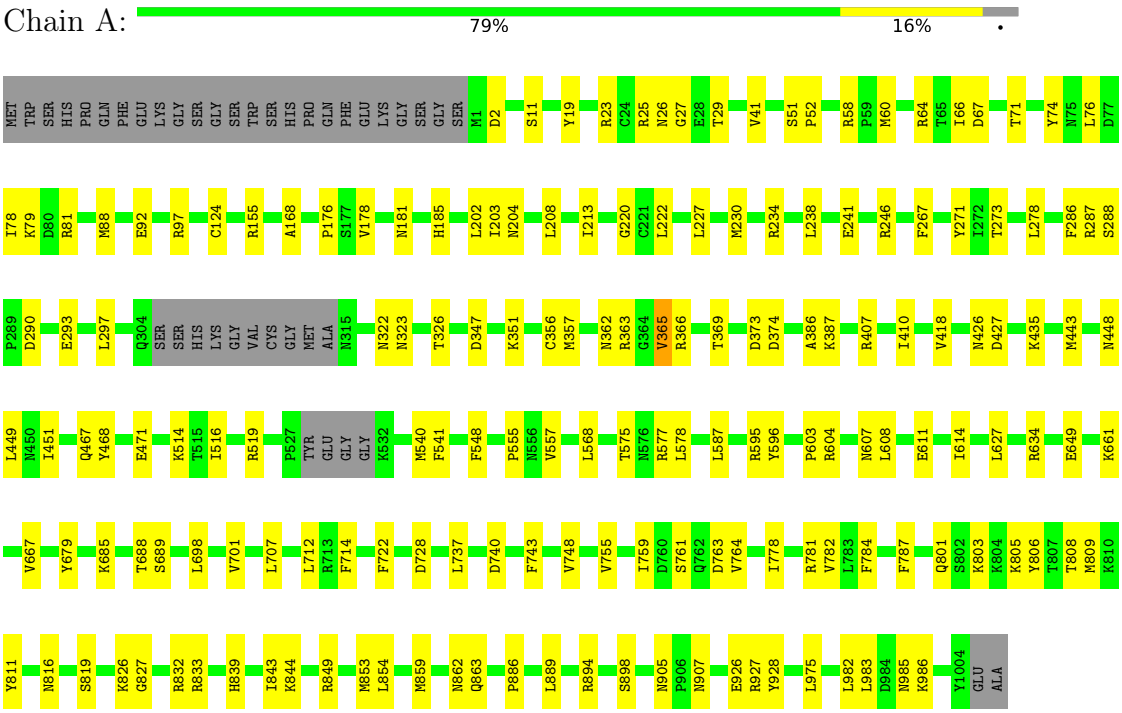
Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	13	Total	C	N	O	P	0	0
			267	128	46	80	13		

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.

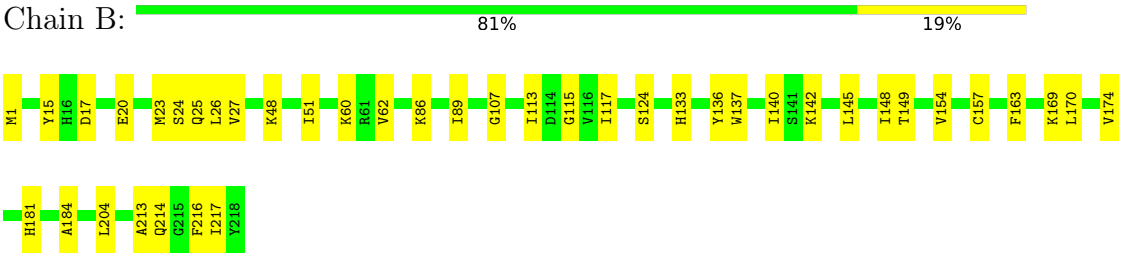
- Molecule 1: DNA polymerase

Chain A:



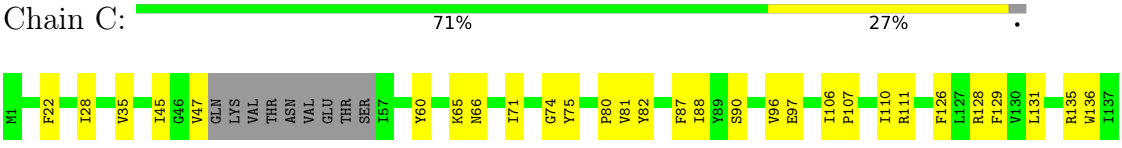
- Molecule 2: Uracil-DNA glycosylase

Chain B:



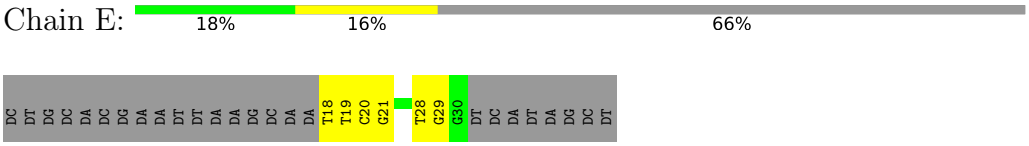
- Molecule 3: DNA polymerase processivity factor

Chain C:



• Molecule 4: DNA (25-MER)

• Molecule 5: DNA (38-MER)



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	127422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.18	0/8278	0.37	2/11177 (0.0%)
2	B	0.12	0/1812	0.33	0/2464
3	C	0.12	0/3455	0.34	0/4660
4	P	0.21	0/386	0.38	0/594
5	E	0.18	0/298	0.35	0/458
All	All	0.16	0/14229	0.36	2/19353 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	71	THR	O-C-N	-5.20	117.11	123.30
1	A	74	TYR	N-CA-C	-5.09	107.23	112.93

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	A	8106	0	8077	108	0
2	B	1762	0	1749	24	0
3	C	3389	0	3392	76	0
4	P	345	0	195	2	0
5	E	267	0	149	4	0
All	All	13869	0	13562	207	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 8.

All (207) 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)
3:C:314:ALA:HB3	3:C:318:GLN:HE22	1.50	0.76
1:A:801:GLN:HE22	1:A:982:LEU:HD23	1.51	0.73
1:A:685:LYS:O	1:A:688:THR:HG22	1.89	0.73
1:A:273:THR:HG21	1:A:297:LEU:HD22	1.72	0.71
1:A:351:LYS:HZ1	1:A:435:LYS:HG2	1.56	0.70
1:A:803:LYS:O	1:A:826:LYS:NZ	2.27	0.67
3:C:383:LYS:NZ	3:C:419:ASP:OD1	2.26	0.67
1:A:443:MET:HE3	1:A:451:ILE:HG23	1.76	0.66
1:A:322:ASN:ND2	1:A:326:THR:O	2.30	0.65
1:A:363:ARG:NH2	1:A:426:ASN:O	2.31	0.64
1:A:60:MET:O	1:A:514:LYS:NZ	2.30	0.64
3:C:87:PHE:HB2	3:C:129:PHE:HB2	1.80	0.63
4:P:19:DG:H1	5:E:20:DC:H42	1.47	0.63
3:C:375:MET:HB2	3:C:389:ILE:HA	1.79	0.63
1:A:833:ARG:HE	1:A:927:ARG:HH12	1.47	0.63
1:A:387:LYS:HG2	1:A:468:TYR:HE1	1.63	0.62
3:C:199:TYR:O	3:C:208:GLN:NE2	2.31	0.62
3:C:35:VAL:HG13	3:C:45:ILE:HD11	1.81	0.62
3:C:138:MET:HB2	3:C:163:PRO:HD3	1.82	0.61
3:C:313:ILE:O	3:C:315:GLY:N	2.34	0.61
3:C:329:ALA:N	3:C:333:GLU:OE2	2.32	0.61
3:C:216:SER:OG	3:C:268:LYS:NZ	2.32	0.61
1:A:203:ILE:HB	1:A:238:LEU:HD23	1.84	0.60
3:C:266:VAL:HG13	3:C:268:LYS:HZ2	1.67	0.60
2:B:124:SER:HB2	2:B:137:TRP:HE1	1.67	0.60
1:A:202:LEU:HD11	1:A:230:MET:HE1	1.84	0.59
1:A:155:ARG:NH2	1:A:649:GLU:OE2	2.35	0.59
1:A:26:ASN:OD1	1:A:27:GLY:N	2.35	0.59
3:C:196:SER:OG	3:C:210:VAL:O	2.21	0.59
2:B:117:ILE:HG21	2:B:148:ILE:HD11	1.84	0.59
1:A:806:TYR:HE1	1:A:826:LYS:HE3	1.68	0.58
1:A:386:ALA:HB1	1:A:410:ILE:HD12	1.86	0.58
3:C:304:ASN:HD22	3:C:364:PRO:HG3	1.68	0.58
1:A:88:MET:HE3	1:A:516:ILE:HD12	1.86	0.58
3:C:351:GLN:HE22	3:C:356:LEU:N	2.01	0.58
1:A:52:PRO:HG2	1:A:97:ARG:HH12	1.69	0.58
1:A:862:ASN:OD1	1:A:985:ASN:ND2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:VAL:HG22	1:A:366:ARG:H	1.69	0.57
1:A:728:ASP:OD2	1:A:781:ARG:NH2	2.37	0.57
1:A:2:ASP:OD2	1:A:25:ARG:NH1	2.34	0.57
2:B:181:HIS:HB3	2:B:184:ALA:HB2	1.86	0.57
2:B:24:SER:O	2:B:27:VAL:HG22	2.05	0.57
3:C:153:LYS:NZ	3:C:165:TYR:OH	2.33	0.57
3:C:177:ASP:OD1	3:C:178:ASP:N	2.35	0.57
1:A:832:ARG:HG3	4:P:21:DA:H5"	1.86	0.57
1:A:849:ARG:HG2	1:A:853:MET:HE3	1.87	0.56
3:C:409:GLN:OE1	3:C:412:SER:OG	2.23	0.56
2:B:48:LYS:HD2	2:B:51:ILE:HD13	1.88	0.56
3:C:358:ARG:HG3	3:C:363:TYR:HB2	1.88	0.56
3:C:75:TYR:HD2	3:C:202:LEU:HB2	1.71	0.55
3:C:393:ASN:OD1	3:C:394:CYS:N	2.39	0.55
5:E:18:DT:H2"	5:E:19:DT:H5"	1.89	0.55
3:C:363:TYR:CE2	3:C:403:ILE:HD12	2.42	0.55
1:A:176:PRO:HB3	1:A:181:ASN:HD22	1.71	0.55
1:A:555:PRO:HA	1:A:627:LEU:HD13	1.89	0.55
1:A:604:ARG:NH2	1:A:611:GLU:OE1	2.31	0.55
3:C:81:VAL:O	3:C:195:ILE:HG22	2.07	0.55
1:A:859:MET:HA	1:A:863:GLN:HE21	1.73	0.54
3:C:88:ILE:HG13	3:C:96:VAL:HB	1.90	0.54
3:C:395:LEU:HD23	3:C:400:ILE:HG22	1.89	0.54
3:C:396:ASN:OD1	3:C:397:ASN:N	2.40	0.54
1:A:467:GLN:NE2	1:A:471:GLU:OE2	2.41	0.54
1:A:293:GLU:OE1	1:A:323:ASN:ND2	2.38	0.54
1:A:778:ILE:HD13	1:A:782:VAL:HG21	1.91	0.53
1:A:806:TYR:CE1	1:A:826:LYS:HE3	2.43	0.53
1:A:204:ASN:ND2	1:A:241:GLU:OE2	2.35	0.53
1:A:227:LEU:HD12	1:A:246:ARG:HB3	1.89	0.53
3:C:213:PHE:HB2	3:C:267:LYS:HE2	1.89	0.53
3:C:338:ILE:O	3:C:345:LYS:NZ	2.34	0.53
1:A:519:ARG:NH2	1:A:679:TYR:O	2.40	0.52
1:A:540:MET:HE2	1:A:983:LEU:HA	1.92	0.52
3:C:90:SER:HB3	3:C:126:PHE:HB3	1.92	0.52
3:C:150:ASN:OD1	3:C:151:ILE:N	2.43	0.52
3:C:128:ARG:NH1	3:C:139:GLU:OE2	2.43	0.51
1:A:898:SER:HB3	2:B:25:GLN:HE21	1.75	0.51
2:B:60:LYS:HA	2:B:115:GLY:HA2	1.93	0.51
3:C:74:GLY:H	3:C:170:ILE:HB	1.74	0.51
3:C:397:ASN:HB3	3:C:400:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:66:ASN:HD22	3:C:213:PHE:HE1	1.59	0.51
3:C:216:SER:CB	3:C:268:LYS:HZ1	2.23	0.51
3:C:65:LYS:NZ	3:C:208:GLN:HB2	2.27	0.50
3:C:424:LEU:HD12	3:C:425:PHE:HB2	1.93	0.50
1:A:356:CYS:SG	1:A:357:MET:N	2.85	0.50
3:C:22:PHE:HA	3:C:28:ILE:HD11	1.93	0.49
3:C:75:TYR:OH	3:C:167:GLU:OE1	2.30	0.49
3:C:288:GLU:OE1	3:C:292:ARG:NH1	2.45	0.49
1:A:603:PRO:HB3	1:A:608:LEU:HB2	1.94	0.49
1:A:707:LEU:HD11	1:A:737:LEU:HD12	1.94	0.49
1:A:894:ARG:HD2	1:A:928:TYR:OH	2.12	0.49
1:A:287:ARG:HH11	1:A:287:ARG:HG2	1.78	0.49
1:A:688:THR:HG23	1:A:689:SER:N	2.28	0.49
1:A:859:MET:HA	1:A:863:GLN:NE2	2.28	0.49
3:C:149:VAL:HA	3:C:152:PHE:HD2	1.78	0.49
1:A:701:VAL:HG22	1:A:714:PHE:HD2	1.78	0.48
1:A:41:VAL:HG13	1:A:60:MET:HE1	1.95	0.48
1:A:11:SER:HB3	1:A:19:TYR:HE2	1.78	0.48
1:A:557:VAL:HG23	1:A:787:PHE:HZ	1.79	0.48
3:C:224:LYS:N	3:C:236:SER:O	2.39	0.48
1:A:373:ASP:OD1	1:A:374:ASP:N	2.42	0.48
3:C:80:PRO:HB2	3:C:82:TYR:HE2	1.78	0.48
1:A:58:ARG:NH2	1:A:92:GLU:OE1	2.47	0.48
3:C:260:GLU:HG3	3:C:261:HIS:ND1	2.29	0.47
1:A:286:PHE:HD2	1:A:322:ASN:HA	1.78	0.47
1:A:578:LEU:HD22	3:C:377:PHE:HE2	1.79	0.47
1:A:707:LEU:HD12	1:A:712:LEU:HD12	1.95	0.47
3:C:239:THR:HG21	3:C:243:LYS:HG2	1.97	0.47
1:A:362:ASN:HB3	1:A:369:THR:HB	1.96	0.47
1:A:220:GLY:O	1:A:234:ARG:NH2	2.48	0.47
1:A:23:ARG:HH21	1:A:29:THR:HG22	1.80	0.47
2:B:26:LEU:HG	2:B:140:ILE:HD12	1.97	0.47
3:C:65:LYS:HZ1	3:C:208:GLN:HB2	1.80	0.47
1:A:427:ASP:OD1	1:A:427:ASP:N	2.48	0.47
1:A:448:ASN:OD1	1:A:449:LEU:N	2.44	0.46
1:A:722:PHE:HE2	1:A:784:PHE:HZ	1.64	0.46
2:B:86:LYS:HB2	2:B:89:ILE:HG22	1.96	0.46
1:A:124:CYS:SG	1:A:155:ARG:HA	2.55	0.46
3:C:363:TYR:HE2	3:C:403:ILE:HD12	1.79	0.46
1:A:805:LYS:HG2	1:A:827:GLY:HA3	1.98	0.46
2:B:145:LEU:HA	2:B:148:ILE:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:886:PRO:HG2	1:A:889:LEU:HD13	1.97	0.46
1:A:839:HIS:O	1:A:843:ILE:HG12	2.15	0.46
5:E:20:DC:H2"	5:E:21:DG:C8	2.51	0.46
1:A:267:PHE:O	1:A:271:TYR:HB2	2.16	0.45
3:C:337:GLU:O	3:C:340:LYS:HG2	2.17	0.45
2:B:107:GLY:O	2:B:217:ILE:N	2.43	0.45
2:B:133:HIS:HA	2:B:136:TYR:HD2	1.81	0.45
3:C:255:ARG:HG3	3:C:277:ASP:OD2	2.15	0.45
1:A:839:HIS:HD2	1:A:975:LEU:HD13	1.82	0.45
1:A:985:ASN:OD1	1:A:986:LYS:N	2.49	0.45
1:A:51:SER:HB3	1:A:52:PRO:HD3	1.99	0.45
1:A:64:ARG:CZ	1:A:66:ILE:HD11	2.47	0.44
1:A:926:GLU:OE1	1:A:928:TYR:HB3	2.18	0.44
3:C:87:PHE:CE1	3:C:97:GLU:HB3	2.53	0.44
3:C:304:ASN:ND2	3:C:364:PRO:HG3	2.31	0.44
3:C:106:ILE:HB	3:C:110:ILE:HD11	1.99	0.44
3:C:335:VAL:HG22	3:C:420:VAL:HG23	1.99	0.44
1:A:168:ALA:HB3	1:A:185:HIS:HB2	1.99	0.44
1:A:222:LEU:HD22	1:A:234:ARG:HG3	1.99	0.44
2:B:149:THR:HG22	2:B:174:VAL:HG21	2.00	0.44
3:C:131:LEU:HD22	3:C:136:TRP:HE1	1.82	0.44
1:A:548:PHE:HB2	1:A:755:VAL:HG13	1.99	0.43
3:C:66:ASN:OD1	3:C:66:ASN:N	2.50	0.43
1:A:19:TYR:OH	1:A:290:ASP:OD2	2.30	0.43
1:A:801:GLN:NE2	1:A:982:LEU:HD23	2.26	0.43
3:C:60:TYR:HB3	3:C:207:ARG:CZ	2.48	0.43
3:C:156:SER:HB3	3:C:162:ILE:HD13	2.00	0.43
2:B:157:CYS:HB3	2:B:163:PHE:HD2	1.84	0.43
1:A:898:SER:HB3	2:B:25:GLN:NE2	2.33	0.43
3:C:213:PHE:CB	3:C:267:LYS:HE2	2.49	0.43
3:C:313:ILE:HG23	3:C:409:GLN:HE21	1.83	0.43
1:A:347:ASP:O	1:A:351:LYS:HG3	2.19	0.43
1:A:698:LEU:HA	1:A:701:VAL:HG12	1.99	0.43
1:A:287:ARG:HG2	1:A:287:ARG:NH1	2.32	0.43
1:A:541:PHE:CZ	1:A:748:VAL:HG11	2.54	0.43
1:A:627:LEU:HD21	1:A:667:VAL:HG21	2.00	0.43
3:C:82:TYR:HE2	3:C:194:LYS:HZ3	1.61	0.42
3:C:188:PHE:HE2	3:C:197:ILE:HD13	1.84	0.42
1:A:761:SER:OG	1:A:763:ASP:OD1	2.35	0.42
3:C:135:ARG:NH1	3:C:136:TRP:O	2.51	0.42
3:C:266:VAL:HG13	3:C:268:LYS:NZ	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:PRO:HG2	1:A:97:ARG:HH22	1.83	0.42
1:A:816:ASN:OD1	1:A:819:SER:OG	2.36	0.42
1:A:288:SER:OG	1:A:290:ASP:OD1	2.27	0.42
1:A:685:LYS:HA	1:A:688:THR:HG22	2.01	0.42
1:A:178:VAL:HG12	1:A:278:LEU:HD12	2.00	0.42
1:A:595:ARG:NH1	1:A:596:TYR:OH	2.52	0.42
1:A:844:LYS:N	1:A:844:LYS:HD2	2.33	0.42
2:B:113:ILE:HG12	2:B:214:GLN:HB2	2.00	0.42
1:A:701:VAL:HG22	1:A:714:PHE:CD2	2.55	0.42
3:C:80:PRO:HB2	3:C:82:TYR:CE2	2.54	0.42
3:C:107:PRO:O	3:C:111:ARG:HG2	2.20	0.42
1:A:743:PHE:CD2	1:A:759:ILE:HD11	2.55	0.42
3:C:371:LEU:HD13	3:C:400:ILE:HG23	2.02	0.42
2:B:17:ASP:O	2:B:20:GLU:HB3	2.20	0.42
3:C:131:LEU:HD13	3:C:136:TRP:CD1	2.54	0.42
1:A:208:LEU:O	1:A:213:ILE:HG13	2.19	0.41
1:A:854:LEU:O	1:A:859:MET:HE3	2.20	0.41
2:B:204:LEU:HD21	3:C:47:VAL:HG22	2.02	0.41
3:C:198:SER:HA	3:C:209:VAL:HA	2.01	0.41
1:A:685:LYS:O	1:A:688:THR:CG2	2.65	0.41
3:C:71:ILE:HG12	3:C:174:THR:HB	2.01	0.41
1:A:607:ASN:OD1	1:A:608:LEU:N	2.54	0.41
2:B:1:MET:HA	2:B:15:TYR:O	2.20	0.41
1:A:577:ARG:HG3	3:C:373:ASN:HA	2.03	0.41
1:A:685:LYS:C	1:A:688:THR:HG22	2.43	0.41
2:B:145:LEU:HG	2:B:170:LEU:HD21	2.02	0.41
3:C:200:ILE:HG22	3:C:207:ARG:HB2	2.01	0.41
1:A:764:VAL:HG11	1:A:811:TYR:CE1	2.55	0.41
3:C:168:ILE:HD12	3:C:184:MET:HE1	2.03	0.41
3:C:289:VAL:O	3:C:293:ILE:HG12	2.21	0.41
1:A:634:ARG:NH2	1:A:661:LYS:HD3	2.36	0.41
1:A:740:ASP:N	1:A:740:ASP:OD1	2.54	0.41
2:B:142:LYS:HE3	2:B:169:LYS:HD2	2.03	0.41
1:A:407:ARG:HG2	1:A:418:VAL:HB	2.03	0.41
1:A:467:GLN:O	1:A:471:GLU:OE1	2.39	0.41
2:B:23:MET:O	2:B:26:LEU:HB3	2.21	0.41
2:B:213:ALA:HA	2:B:216:PHE:HD2	1.85	0.41
5:E:28:DT:H2"	5:E:29:DG:C8	2.55	0.41
2:B:62:VAL:HG13	2:B:154:VAL:HG23	2.04	0.40
3:C:338:ILE:HD12	3:C:420:VAL:HG21	2.03	0.40
1:A:568:LEU:HD12	1:A:614:ILE:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:THR:HG22	1:A:608:LEU:HA	2.02	0.40
1:A:808:THR:OG1	1:A:809:MET:N	2.54	0.40
3:C:358:ARG:NH1	3:C:365:GLU:HG3	2.36	0.40
1:A:67:ASP:O	1:A:81:ARG:NH1	2.52	0.40
1:A:587:LEU:HD21	1:A:614:ILE:HD11	2.03	0.40
1:A:905:ASN:O	1:A:907:ASN:N	2.54	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	984/1031 (95%)	935 (95%)	48 (5%)	1 (0%)	48 81
2	B	216/218 (99%)	207 (96%)	9 (4%)	0	100 100
3	C	412/426 (97%)	392 (95%)	19 (5%)	1 (0%)	44 77
All	All	1612/1675 (96%)	1534 (95%)	76 (5%)	2 (0%)	50 81

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	314	ALA
1	A	365	VAL

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	915/947 (97%)	912 (100%)	3 (0%)	91 96
2	B	198/200 (99%)	198 (100%)	0	100 100
3	C	386/396 (98%)	386 (100%)	0	100 100
All	All	1499/1543 (97%)	1496 (100%)	3 (0%)	91 97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	78	ILE
1	A	79	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	ASN
1	A	442	GLN
1	A	585	GLN
1	A	665	ASN
1	A	801	GLN
1	A	841	ASN
3	C	134	ASN
3	C	318	GLN
3	C	321	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 oligosaccharides 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.