



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:54 PM GMT

PDB ID : 1MM8
Title : Crystal structure of Tn5 Transposase complexed with ME DNA
Authors : Steiniger-White, M.; Bhasin, A.; Lovell, S.; Rayment, I.; Reznikoff, W.S.
Deposited on : 2002-09-03
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

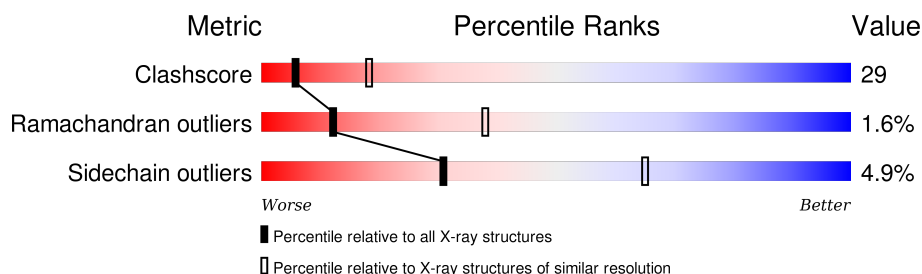
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	20	
2	C	20	
3	A	481	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4633 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA chain called ME DNA transferred strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	20	Total	C	N	O	P	0	0	0
			418	199	86	114	19			

- Molecule 2 is a DNA chain called ME DNA non-transferred strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			396	193	62	122	19			

- Molecule 3 is a protein called Tn5 Transposase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	455	Total	C	N	O	S	0	0	0
			3563	2245	654	652	12			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	LYS	GLU	ENGINEERED	UNP Q46731
A	56	ALA	MET	ENGINEERED	UNP Q46731
A	345	LYS	GLU	ENGINEERED	UNP Q46731
A	372	PRO	LEU	ENGINEERED	UNP Q46731
A	477	GLY	-	CLONING ARTIFACT	UNP Q46731

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	37	Total 37	O 37	0	0
5	C	22	Total 22	O 22	0	0
5	A	195	Total 195	O 195	0	0

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	112.50Å 112.50Å 233.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	500.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (500.00-2.80)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.217 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4633	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	B	0.53	0/472	0.87	0/729
2	C	0.54	0/440	0.81	1/675 (0.1%)
3	A	0.43	0/3633	0.61	0/4903
All	All	0.46	0/4545	0.66	1/6307 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	203	DG	C5'-C4'-C3'	-5.05	105.00	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	119	DA	Sidechain
2	C	205	DC	Sidechain

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	418	0	225	24	0
2	C	396	0	230	44	1
3	A	3563	0	3586	183	0
4	A	2	0	0	0	0
5	A	195	0	0	39	1
5	B	37	0	0	3	0
5	C	22	0	0	1	0
All	All	4633	0	4041	243	1

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 29.

All (243) 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:A:302:THR:HB	5:A:739:HOH:O	1.46	1.15
3:A:324:ARG:NH1	5:A:747:HOH:O	2.00	0.93
3:A:302:THR:HG22	3:A:304:GLU:H	1.32	0.92
3:A:287:ILE:HA	5:A:742:HOH:O	1.71	0.91
3:A:75:ARG:HD2	5:A:521:HOH:O	1.76	0.85
3:A:302:THR:HG22	3:A:304:GLU:N	1.90	0.84
3:A:131:LEU:O	3:A:132:LEU:HD23	1.76	0.84
3:A:272:LEU:HD12	3:A:277:ILE:HD11	1.59	0.83
2:C:203:DG:H2''	2:C:204:DT:H5'	1.60	0.82
3:A:24:ASP:HB3	3:A:27:ARG:HG3	1.62	0.81
3:A:302:THR:CG2	3:A:304:GLU:H	1.92	0.81
2:C:205:DC:H2'	2:C:206:DT:H72	1.61	0.81
1:B:119:DA:H2''	1:B:120:DG:O5'	1.78	0.81
3:A:208:VAL:HG22	3:A:302:THR:OG1	1.80	0.80
3:A:437:ASP:OD2	3:A:440:ARG:HA	1.81	0.80
3:A:208:VAL:HA	3:A:302:THR:OG1	1.83	0.79
3:A:265:LEU:HD11	3:A:282:VAL:CG1	2.15	0.77
3:A:371:THR:HG22	5:A:735:HOH:O	1.85	0.75
3:A:184:ILE:HD11	3:A:206:ARG:NH2	2.02	0.74
3:A:207:PHE:O	3:A:302:THR:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:DT:H2''	1:B:110:DA:H5'	1.70	0.74
3:A:218:VAL:HG22	5:A:745:HOH:O	1.87	0.74
3:A:75:ARG:HD3	3:A:145:GLN:HE21	1.53	0.73
2:C:205:DC:H2'	2:C:206:DT:C7	2.17	0.73
3:A:234:LEU:HD11	3:A:267:SER:HB3	1.69	0.72
3:A:367:ARG:HG3	3:A:449:LEU:HD12	1.70	0.72
3:A:38:LEU:HA	5:A:756:HOH:O	1.91	0.69
2:C:203:DG:H2'	2:C:204:DT:H71	1.73	0.69
3:A:313:LEU:HG	5:A:738:HOH:O	1.92	0.69
3:A:208:VAL:HA	3:A:302:THR:HG1	1.56	0.69
1:B:101:DG:HO5'	1:B:101:DG:H8	1.40	0.68
3:A:194:HIS:HA	3:A:197:LEU:HD12	1.75	0.68
3:A:81:GLN:HE21	3:A:81:GLN:HA	1.59	0.68
2:C:205:DC:C2'	2:C:206:DT:H72	2.24	0.68
3:A:302:THR:CG2	3:A:303:SER:N	2.57	0.67
3:A:425:ALA:N	5:A:729:HOH:O	2.27	0.67
2:C:217:DT:H2''	2:C:218:DC:C5'	2.24	0.67
3:A:367:ARG:HG3	3:A:449:LEU:CD1	2.25	0.66
3:A:142:LEU:HD13	5:A:570:HOH:O	1.95	0.66
3:A:20:ALA:HB3	3:A:28:THR:HG23	1.76	0.66
1:B:108:DG:H2''	1:B:109:DT:H5'	1.77	0.66
2:C:205:DC:C2'	2:C:206:DT:C7	2.74	0.65
3:A:454:GLU:HG2	5:A:640:HOH:O	1.97	0.65
1:B:114:DG:OP2	3:A:243:GLN:HG3	1.96	0.65
3:A:132:LEU:HD22	3:A:139:THR:HA	1.79	0.64
2:C:214:DA:H2''	2:C:215:DC:H5''	1.79	0.64
3:A:78:GLY:HA3	3:A:358:PHE:CE2	2.32	0.64
3:A:65:ARG:O	3:A:67:PRO:HD3	1.96	0.64
3:A:443:ILE:H	3:A:443:ILE:HD12	1.62	0.64
2:C:214:DA:C2'	2:C:215:DC:H5''	2.28	0.64
1:B:111:DT:H2'	5:A:504:HOH:O	1.97	0.63
3:A:81:GLN:NE2	3:A:81:GLN:HA	2.14	0.62
3:A:422:LEU:C	5:A:729:HOH:O	2.37	0.62
3:A:345:LYS:HA	3:A:345:LYS:NZ	2.15	0.62
2:C:217:DT:H2''	2:C:218:DC:H5''	1.82	0.62
3:A:265:LEU:HD23	5:A:738:HOH:O	1.99	0.61
1:B:116:DG:H2'	5:B:532:HOH:O	2.00	0.61
2:C:216:DA:H1'	2:C:217:DT:H5''	1.82	0.61
3:A:302:THR:HG22	3:A:303:SER:N	2.17	0.60
2:C:202:DT:H5'	3:A:298:TRP:HZ2	1.65	0.60
3:A:194:HIS:CD2	3:A:274:GLN:HG3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:214:DA:H1'	2:C:215:DC:H5''	1.85	0.59
2:C:204:DT:H2''	2:C:205:DC:O5'	2.02	0.59
3:A:414:LYS:HG2	5:A:730:HOH:O	2.01	0.59
3:A:405:LEU:HD11	3:A:428:ALA:HB1	1.84	0.59
3:A:95:ILE:HD12	3:A:322:ARG:HA	1.85	0.59
3:A:14:LYS:HG2	3:A:18:SER:OG	2.03	0.59
3:A:217:ASP:HB3	3:A:220:SER:HB3	1.83	0.59
3:A:236:GLY:HA3	5:A:744:HOH:O	2.01	0.59
2:C:215:DC:H2''	2:C:216:DA:H8	1.67	0.59
1:B:115:DA:H2''	1:B:116:DG:H5'	1.84	0.59
3:A:398:THR:OG1	3:A:401:GLU:HG2	2.03	0.58
3:A:30:ARG:O	3:A:34:VAL:HG23	2.03	0.58
3:A:399:PRO:HG2	5:A:732:HOH:O	2.02	0.58
3:A:359:VAL:O	5:A:736:HOH:O	2.17	0.58
2:C:202:DT:H2''	2:C:203:DG:OP1	2.02	0.58
3:A:38:LEU:CD2	5:A:756:HOH:O	2.51	0.57
1:B:115:DA:H1'	1:B:116:DG:H5''	1.87	0.57
3:A:194:HIS:CG	3:A:274:GLN:HG3	2.39	0.57
3:A:165:TRP:CZ3	3:A:187:CYS:HB3	2.39	0.57
1:B:109:DT:H2''	1:B:110:DA:C5'	2.34	0.57
3:A:274:GLN:H	3:A:274:GLN:CD	2.06	0.57
3:A:75:ARG:NH2	3:A:350:GLU:OE2	2.38	0.57
3:A:314:ARG:O	3:A:318:ILE:HG13	2.05	0.57
2:C:209:DT:H2''	2:C:210:DA:C5'	2.34	0.57
1:B:108:DG:H1'	1:B:109:DT:H5''	1.85	0.57
3:A:417:GLU:OE2	3:A:424:TRP:HA	2.05	0.56
1:B:116:DG:OP1	5:B:614:HOH:O	2.17	0.56
1:B:107:DT:H2''	1:B:108:DG:H5'	1.87	0.56
2:C:202:DT:O2	2:C:202:DT:C2'	2.53	0.56
1:B:102:DA:H1'	1:B:103:DG:H5'	1.87	0.56
3:A:270:ILE:HD13	3:A:281:ALA:HB2	1.88	0.55
3:A:423:GLN:C	5:A:729:HOH:O	2.44	0.55
3:A:265:LEU:HD12	3:A:266:ARG:H	1.71	0.55
3:A:188:ASP:HB2	5:A:510:HOH:O	2.06	0.55
3:A:218:VAL:HG23	3:A:271:THR:O	2.07	0.55
3:A:91:GLU:HB3	3:A:134:ALA:HB3	1.88	0.55
2:C:206:DT:C2	2:C:207:DC:C5	2.95	0.55
3:A:372:PRO:HG2	5:A:735:HOH:O	2.05	0.55
3:A:234:LEU:CD1	3:A:267:SER:HB3	2.38	0.54
3:A:38:LEU:HD23	5:A:756:HOH:O	2.07	0.54
3:A:132:LEU:HD13	5:A:747:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:147:TRP:CE3	3:A:350:GLU:HG3	2.43	0.53
3:A:345:LYS:HA	3:A:345:LYS:HZ3	1.74	0.53
3:A:265:LEU:HD11	3:A:282:VAL:HG12	1.90	0.53
3:A:467:LYS:HA	3:A:470:MET:CE	2.39	0.53
3:A:443:ILE:N	3:A:443:ILE:HD12	2.22	0.53
3:A:473:GLY:O	3:A:474:ILE:HG13	2.09	0.53
3:A:102:SER:HB2	3:A:114:LEU:CD1	2.38	0.53
3:A:93:LEU:O	3:A:131:LEU:HD23	2.09	0.52
2:C:205:DC:H2"	2:C:206:DT:C6	2.44	0.52
3:A:131:LEU:C	3:A:132:LEU:HD23	2.29	0.52
3:A:42:SER:HB2	3:A:450:TRP:CZ2	2.45	0.52
3:A:422:LEU:O	5:A:729:HOH:O	2.17	0.52
3:A:133:GLU:O	3:A:137:PHE:HA	2.10	0.52
3:A:286:GLU:OE1	3:A:289:PRO:HB3	2.10	0.52
3:A:132:LEU:HD22	5:A:747:HOH:O	2.09	0.51
3:A:265:LEU:HD11	3:A:282:VAL:HG13	1.91	0.51
2:C:217:DT:H2"	2:C:218:DC:H5'	1.90	0.51
3:A:41:TYR:O	3:A:44:LYS:HB2	2.10	0.51
3:A:405:LEU:HD11	3:A:428:ALA:CB	2.41	0.51
3:A:401:GLU:HB3	3:A:460:LEU:HD22	1.92	0.51
2:C:217:DT:C2'	2:C:218:DC:H5"	2.40	0.51
3:A:164:LYS:O	3:A:167:ALA:HB3	2.11	0.50
3:A:133:GLU:OE2	3:A:136:THR:N	2.44	0.50
3:A:194:HIS:O	3:A:198:GLN:HB2	2.12	0.50
3:A:252:LYS:C	3:A:253:ARG:HG2	2.32	0.50
1:B:116:DG:OP2	3:A:253:ARG:HD2	2.10	0.50
3:A:203:HIS:CB	3:A:205:GLU:HG3	2.41	0.50
2:C:207:DC:H1'	2:C:208:DT:H5"	1.94	0.49
3:A:147:TRP:CZ3	3:A:350:GLU:HG3	2.47	0.49
2:C:203:DG:N7	3:A:244:LYS:NZ	2.50	0.49
3:A:132:LEU:CD2	3:A:139:THR:HA	2.41	0.49
3:A:455:ALA:O	3:A:459:LYS:HD3	2.12	0.49
3:A:143:LEU:HD12	3:A:143:LEU:O	2.13	0.49
2:C:215:DC:H2"	2:C:216:DA:C8	2.48	0.48
2:C:202:DT:H5'	3:A:298:TRP:CZ2	2.48	0.48
3:A:308:SER:OG	3:A:311:GLN:HG3	2.13	0.48
3:A:45:SER:HB2	5:A:517:HOH:O	2.13	0.48
3:A:254:LYS:HB2	3:A:254:LYS:NZ	2.29	0.48
2:C:209:DT:H2"	2:C:210:DA:H5"	1.96	0.47
3:A:440:ARG:CD	5:A:504:HOH:O	2.61	0.47
3:A:33:ASN:O	3:A:37:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:64:ILE:HG21	3:A:352:MET:HG2	1.96	0.47
3:A:440:ARG:HD3	5:A:504:HOH:O	2.15	0.47
3:A:313:LEU:N	5:A:738:HOH:O	2.47	0.47
2:C:218:DC:H2'	2:C:219:DT:H72	1.95	0.47
1:B:118:DC:C2	1:B:119:DA:N7	2.83	0.47
3:A:228:LEU:O	3:A:266:ARG:HD3	2.14	0.47
3:A:274:GLN:C	3:A:276:ASN:H	2.17	0.47
3:A:286:GLU:CD	5:A:741:HOH:O	2.52	0.47
3:A:247:VAL:HA	5:A:743:HOH:O	2.14	0.46
3:A:203:HIS:HB2	3:A:205:GLU:HG3	1.96	0.46
3:A:53:SER:HB3	3:A:56:ALA:HB3	1.98	0.46
3:A:113:LYS:HD2	3:A:115:GLY:O	2.16	0.46
1:B:120:DG:N3	3:A:323:TRP:HH2	2.13	0.46
1:B:109:DT:H1'	1:B:110:DA:H5''	1.96	0.46
3:A:361:VAL:HB	5:A:639:HOH:O	2.15	0.46
3:A:66:ASN:C	3:A:68:ASN:H	2.19	0.46
3:A:434:GLY:O	3:A:436:MET:HG2	2.16	0.46
3:A:189:ARG:HB3	3:A:212:LYS:HB2	1.97	0.46
3:A:279:LEU:HD11	3:A:301:LEU:HB3	1.98	0.46
2:C:205:DC:H2''	2:C:206:DT:C7	2.46	0.46
2:C:209:DT:C2'	2:C:210:DA:H5''	2.46	0.46
3:A:41:TYR:CD1	3:A:49:SER:HA	2.51	0.46
3:A:66:ASN:ND2	3:A:68:ASN:H	2.14	0.46
3:A:289:PRO:HG3	3:A:295:PRO:HB3	1.98	0.46
2:C:208:DT:H2''	2:C:209:DT:OP2	2.16	0.45
3:A:253:ARG:HG3	3:A:253:ARG:HH11	1.82	0.45
2:C:202:DT:O2	2:C:202:DT:H2'	2.16	0.45
3:A:404:LEU:HD22	3:A:463:PHE:HB2	1.98	0.45
3:A:144:HIS:CG	3:A:145:GLN:N	2.84	0.45
3:A:265:LEU:HD12	3:A:266:ARG:N	2.32	0.45
3:A:359:VAL:HG12	3:A:359:VAL:O	2.16	0.45
2:C:209:DT:H2''	2:C:210:DA:H5'	1.99	0.45
2:C:214:DA:C1'	2:C:215:DC:H5''	2.46	0.45
3:A:75:ARG:HD3	3:A:145:GLN:NE2	2.26	0.44
3:A:238:GLN:HG2	3:A:262:SER:HA	1.98	0.44
1:B:110:DA:C8	1:B:111:DT:H72	2.52	0.44
1:B:111:DT:H2''	1:B:112:DA:H5'	1.99	0.44
3:A:8:ARG:O	3:A:9:ALA:C	2.55	0.44
1:B:102:DA:H2''	1:B:103:DG:OP2	2.15	0.44
3:A:153:ASP:OD2	3:A:155:ALA:HB3	2.18	0.44
2:C:208:DT:H1'	2:C:209:DT:H5'	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:424:TRP:N	5:A:729:HOH:O	2.51	0.44
1:B:104:DA:C8	1:B:105:DT:H72	2.53	0.44
2:C:203:DG:H5''	5:C:503:HOH:O	2.17	0.44
3:A:414:LYS:HD2	3:A:414:LYS:N	2.33	0.44
3:A:441:THR:O	3:A:443:ILE:HD12	2.18	0.44
3:A:166:LEU:HD21	3:A:196:TYR:HA	2.00	0.43
1:B:108:DG:H2''	1:B:109:DT:C5'	2.48	0.43
2:C:211:DT:H6	2:C:211:DT:H2'	1.67	0.43
3:A:116:SER:N	3:A:119:ASP:OD2	2.41	0.43
3:A:404:LEU:HD22	3:A:463:PHE:CB	2.49	0.43
3:A:216:LYS:HE3	3:A:221:GLY:O	2.19	0.43
2:C:202:DT:H73	3:A:298:TRP:CG	2.54	0.43
3:A:118:GLN:H	3:A:118:GLN:NE2	2.17	0.43
2:C:214:DA:H2''	2:C:215:DC:C5'	2.45	0.42
2:C:218:DC:C2'	2:C:219:DT:H72	2.48	0.42
3:A:291:LYS:HA	5:A:740:HOH:O	2.19	0.42
3:A:55:ALA:N	5:A:755:HOH:O	2.52	0.42
3:A:393:ALA:HB1	3:A:397:LEU:HD12	2.02	0.42
3:A:313:LEU:CA	5:A:738:HOH:O	2.67	0.42
3:A:47:THR:O	3:A:50:SER:HB2	2.20	0.42
3:A:191:ALA:O	3:A:193:ILE:N	2.52	0.42
3:A:103:TYR:HA	5:A:540:HOH:O	2.20	0.42
3:A:111:LEU:HD13	3:A:123:GLY:HA2	2.02	0.42
3:A:39:ALA:HB1	3:A:362:ARG:NH1	2.34	0.42
3:A:262:SER:HB2	3:A:287:ILE:HB	2.02	0.42
2:C:203:DG:C2'	2:C:204:DT:H71	2.47	0.42
3:A:133:GLU:OE1	3:A:138:ARG:HG2	2.20	0.42
3:A:207:PHE:CE1	3:A:302:THR:HA	2.54	0.42
3:A:6:LEU:HD21	3:A:460:LEU:HD21	2.02	0.42
3:A:458:SER:O	3:A:461:ASP:HB2	2.19	0.42
3:A:252:LYS:C	5:A:743:HOH:O	2.58	0.41
3:A:133:GLU:OE1	3:A:136:THR:HB	2.19	0.41
5:B:604:HOH:O	3:A:257:PRO:HA	2.20	0.41
2:C:202:DT:C6	3:A:298:TRP:CE2	3.07	0.41
3:A:345:LYS:HA	3:A:345:LYS:HZ2	1.85	0.41
3:A:467:LYS:HA	3:A:470:MET:HE3	2.01	0.41
3:A:337:GLY:HA3	3:A:340:ARG:NH2	2.35	0.41
3:A:170:ALA:HA	3:A:173:ARG:NH1	2.35	0.41
2:C:205:DC:H2''	2:C:206:DT:H6	1.85	0.41
3:A:246:VAL:HB	3:A:254:LYS:HG2	2.03	0.41
3:A:153:ASP:HA	3:A:154:PRO:HD2	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:248:ASP:OD1	3:A:252:LYS:N	2.52	0.41
1:B:105:DT:H2''	1:B:106:DG:OP2	2.21	0.41
3:A:158:ASP:O	3:A:159:GLU:HG2	2.21	0.41
3:A:246:VAL:HB	3:A:254:LYS:CG	2.50	0.41
3:A:12:TRP:CZ3	3:A:39:ALA:HB2	2.56	0.41
3:A:391:GLN:HB3	3:A:392:SER:H	1.61	0.41
3:A:112:GLY:O	3:A:122:ARG:HB3	2.21	0.41
3:A:98:THR:CG2	3:A:99:THR:N	2.84	0.41
3:A:437:ASP:CG	3:A:440:ARG:HA	2.41	0.41
3:A:105:HIS:O	3:A:106:GLN:C	2.59	0.41
2:C:208:DT:H1'	2:C:209:DT:C5'	2.52	0.40
3:A:28:THR:O	3:A:32:VAL:HG23	2.20	0.40
3:A:134:ALA:HB1	3:A:314:ARG:NH2	2.36	0.40
3:A:78:GLY:HA3	3:A:358:PHE:CZ	2.57	0.40
3:A:467:LYS:O	3:A:470:MET:HG2	2.21	0.40
3:A:92:LEU:HD23	3:A:133:GLU:HA	2.03	0.40
3:A:218:VAL:HG23	3:A:271:THR:HB	2.03	0.40
3:A:398:THR:HB	3:A:399:PRO:HD2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:209:DT:O5'	5:A:754:HOH:O[12_566]	2.10	0.10

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 X-ray entries followed by that with respect to entries of similar resolution.

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
3	A	451/481 (94%)	410 (91%)	34 (8%)	7 (2%)	12 38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	106	GLN
3	A	286	GLU
3	A	418	LYS
3	A	192	ASP
3	A	252	LYS
3	A	87	GLN
3	A	6	LEU

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 X-ray entries followed by that with respect to entries of similar resolution.

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
3	A	365/393 (93%)	347 (95%)	18 (5%)	31 65

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	19	SER
3	A	102	SER
3	A	118	GLN
3	A	133	GLU
3	A	135	THR
3	A	145	GLN
3	A	148	TRP
3	A	187	CYS
3	A	240	SER
3	A	254	LYS
3	A	274	GLN
3	A	279	LEU
3	A	313	LEU
3	A	343	MET
3	A	345	LYS
3	A	366	LEU
3	A	400	ASP
3	A	423	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such

sidechains are listed below:

Mol	Chain	Res	Type
3	A	57	GLN
3	A	66	ASN
3	A	68	ASN
3	A	81	GLN
3	A	87	GLN
3	A	118	GLN
3	A	145	GLN
3	A	194	HIS
3	A	231	GLN
3	A	238	GLN
3	A	321	HIS
3	A	391	GLN
3	A	403	GLN
3	A	472	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.