



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:52 AM UTC

PDB ID : 4FCY / pdb_00004fcy
Title : Crystal structure of the bacteriophage Mu transpososome
Authors : Montano, S.P.; Pigli, Y.Z.; Rice, P.A.
Deposited on : 2012-05-25
Resolution : 3.71 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

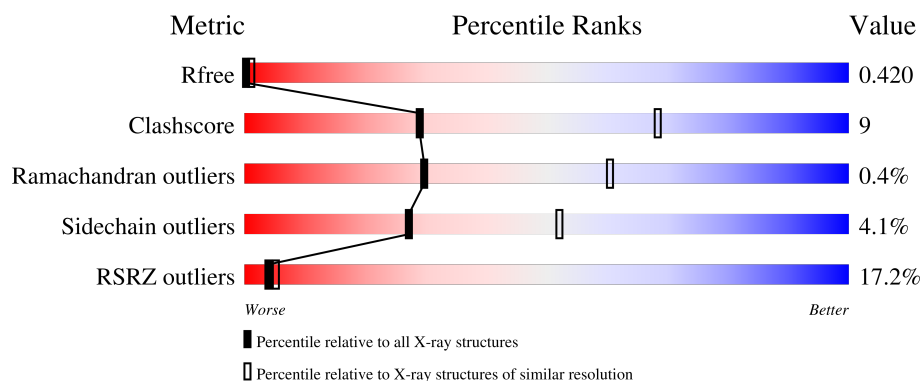
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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 of the lower 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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	529	16% 60% 22% • 16%
1	B	529	14% 69% 20% • 10%
2	C	68	16% 66% 32% •
3	E	13	69% 31%
4	D	49	14% 57% 43%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10056 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 protein called Transposase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3587	2278	640	651	18			
1	B	476	Total	C	N	O	S	0	0	0
			3810	2423	680	689	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	521	LEU	MET	engineered mutation	UNP P07636
A	525	LEU	ASN	engineered mutation	UNP P07636
B	521	LEU	MET	engineered mutation	UNP P07636
B	525	LEU	ASN	engineered mutation	UNP P07636

- Molecule 2 is a DNA chain called DNA (68-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	68	Total	C	N	O	P	0	0	0
			1384	665	226	426	67			

- Molecule 3 is a DNA chain called DNA (13-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	13	Total	C	N	O	P	0	0	0
			263	125	52	73	13			

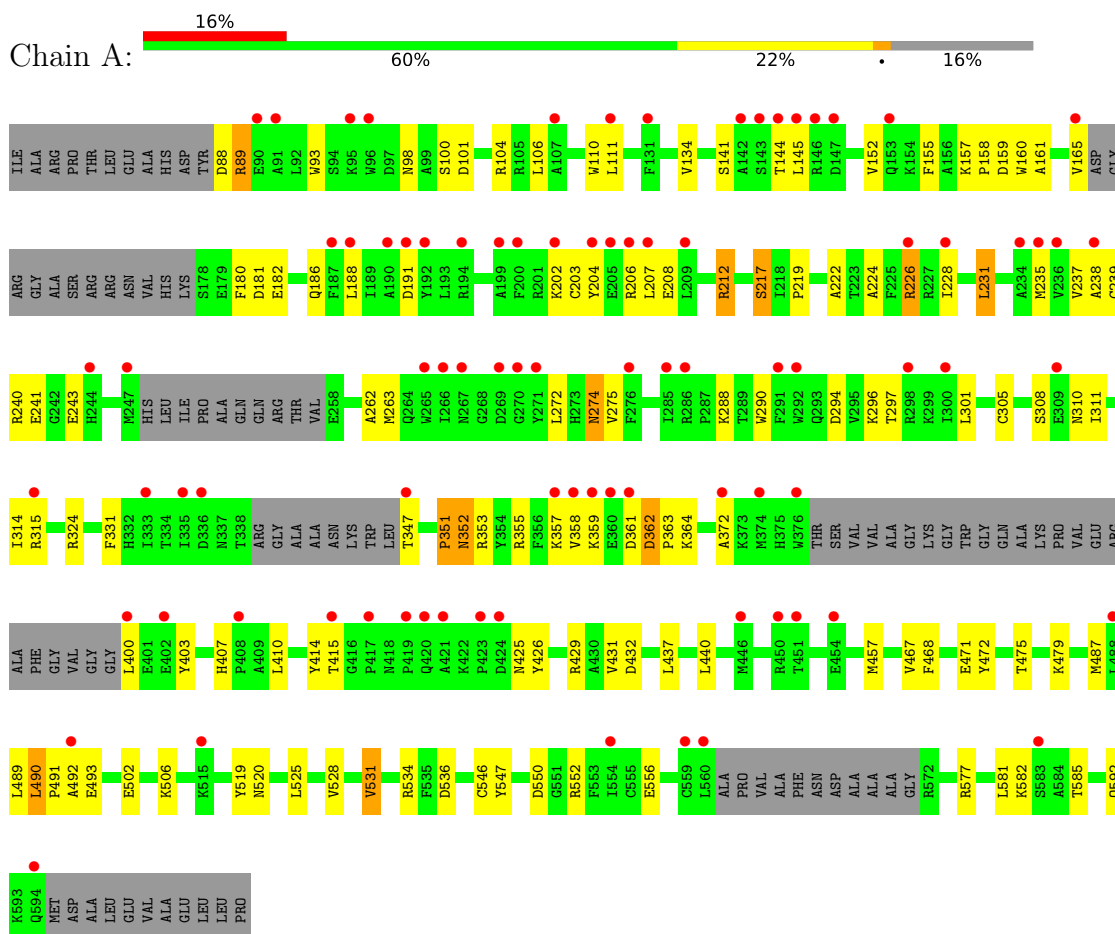
- Molecule 4 is a DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	49	Total	C	N	O	P	0	0	0
			1012	479	208	277	48			

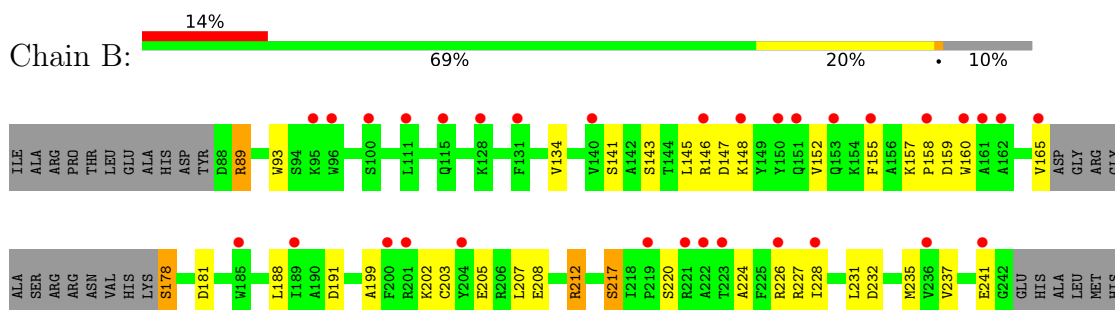
3 Residue-property plots [i](#)

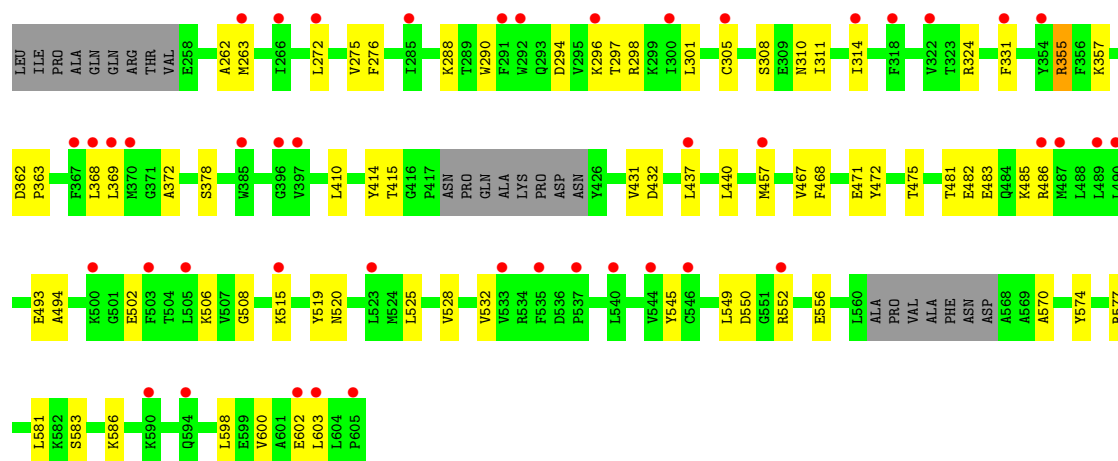
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Transposase



• Molecule 1: Transposase





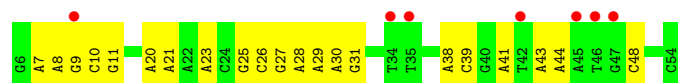
• Molecule 2: DNA (68-MER)



• Molecule 3: DNA (13-MER)



• Molecule 4: DNA (49-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	196.14Å 196.14Å 349.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 3.71 49.03 – 3.71	Depositor EDS
% Data completeness (in resolution range)	47.0 (49.03-3.71) 46.0 (49.03-3.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_847)	Depositor
R, R_{free}	0.393 , 0.437 0.381 , 0.420	Depositor DCC
R_{free} test set	939 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	144.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 184.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10056	wwPDB-VP
Average B, all atoms (Å ²)	294.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.42	0/3667	0.93	7/4945 (0.1%)
1	B	0.42	0/3895	0.88	2/5255 (0.0%)
2	C	0.27	0/1543	0.84	1/2379 (0.0%)
3	E	0.20	0/295	0.71	0/451
4	D	0.23	0/1141	0.80	0/1757
All	All	0.38	0/10541	0.88	10/14787 (0.1%)

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	A	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	ASP	CA-C-N	8.61	128.75	119.28
1	A	362	ASP	C-N-CA	8.61	128.75	119.28
1	B	362	ASP	CA-C-N	7.23	127.07	119.05
1	B	362	ASP	C-N-CA	7.23	127.07	119.05
1	A	407	HIS	CA-C-N	6.77	127.04	119.32
1	A	407	HIS	C-N-CA	6.77	127.04	119.32
1	A	240	ARG	N-CA-C	6.63	121.53	113.17
2	C	24	DG	C4'-C3'-O3'	5.51	118.26	110.00
1	A	490	LEU	N-CA-C	5.18	116.41	109.83
1	A	361	ASP	N-CA-C	5.12	114.80	108.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	PRO	Peptide

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	3587	0	3530	78	0
1	B	3810	0	3765	67	0
2	C	1384	0	779	19	0
3	E	263	0	145	3	0
4	D	1012	0	547	16	0
All	All	10056	0	8766	163	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 (163) 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:A:489:LEU:HD13	1:A:536:ASP:HB2	1.58	0.83
1:A:111:LEU:HD22	1:B:369:LEU:HD23	1.61	0.80
1:A:144:THR:OG1	4:D:25:DG:OP2	1.99	0.79
1:A:315:ARG:HH22	1:A:534:ARG:HH12	1.27	0.78
1:A:311:ILE:HD13	1:A:363:PRO:HG2	1.65	0.77
1:A:111:LEU:HD23	1:B:368:LEU:HG	1.69	0.73
4:D:27:DG:HO3'	4:D:28:DA:HO5'	1.31	0.73
1:A:315:ARG:NH2	1:A:534:ARG:HH12	1.87	0.71
1:B:272:LEU:HD13	1:B:288:LYS:HE3	1.73	0.70
1:A:272:LEU:HD13	1:A:288:LYS:HE3	1.73	0.70
1:B:600:VAL:HA	1:B:603:LEU:HD23	1.74	0.69
1:A:237:VAL:O	1:A:241:GLU:N	2.27	0.66
1:B:152:VAL:O	1:B:160:TRP:NE1	2.30	0.65
1:A:152:VAL:O	1:A:160:TRP:NE1	2.30	0.64
1:A:351:PRO:HB3	1:A:352:ASN:HB3	1.80	0.64
1:B:355:ARG:HE	1:B:508:GLY:HA3	1.62	0.64
1:A:101:ASP:OD2	1:A:104:ARG:NH2	2.31	0.63
1:B:220:SER:N	2:C:19:DG:OP2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:LYS:HD2	1:B:493:GLU:HG3	1.81	0.61
1:A:212:ARG:HH11	1:A:212:ARG:HG2	1.65	0.61
1:A:581:LEU:O	1:A:585:THR:HG23	2.01	0.61
1:A:487:MET:SD	1:A:547:TYR:OH	2.59	0.60
1:B:212:ARG:HH11	1:B:212:ARG:HG2	1.65	0.59
1:A:353:ARG:HH21	1:A:490:LEU:HD13	1.66	0.59
1:A:274:ASN:HB3	1:A:414:TYR:CE1	2.37	0.59
1:B:297:THR:HG21	1:B:468:PHE:HA	1.86	0.58
1:B:178:SER:OG	1:B:227:ARG:NH1	2.36	0.58
1:A:400:LEU:HA	1:A:403:TYR:HD2	1.69	0.57
1:B:486:ARG:HD3	1:B:545:TYR:CD2	2.39	0.57
1:A:297:THR:HG21	1:A:468:PHE:HA	1.86	0.56
1:A:410:LEU:HD22	1:A:431:VAL:HG21	1.86	0.56
2:C:33:DT:H3	4:D:23:DA:H61	1.53	0.56
1:B:147:ASP:OD2	4:D:48:DC:N4	2.40	0.54
1:B:472:TYR:O	1:B:475:THR:HG22	2.08	0.54
1:B:146:ARG:HH11	2:C:5:DT:H71	1.74	0.54
1:A:224:ALA:O	1:A:228:ILE:HG12	2.09	0.53
2:C:64:DT:O4	3:E:6:DA:N6	2.42	0.53
1:A:274:ASN:HB3	1:A:414:TYR:HE1	1.73	0.53
1:A:301:LEU:O	1:A:324:ARG:NH1	2.42	0.53
1:B:181:ASP:OD2	1:B:217:SER:N	2.39	0.53
2:C:49:DT:H3	4:D:7:DA:H61	1.54	0.53
1:A:582:LYS:O	1:A:585:THR:OG1	2.23	0.52
1:A:358:VAL:HG22	1:A:492:ALA:HA	1.90	0.52
1:B:301:LEU:O	1:B:324:ARG:NH1	2.42	0.52
1:B:532:VAL:HG23	1:B:549:LEU:HD23	1.91	0.52
1:A:237:VAL:HG13	1:A:243:GLU:H	1.75	0.52
1:A:161:ALA:HB2	1:B:369:LEU:HD22	1.91	0.51
1:A:89:ARG:HB3	1:A:93:TRP:CD1	2.45	0.51
1:A:415:THR:HG22	1:A:426:TYR:CZ	2.45	0.51
1:B:506:LYS:HD3	1:B:515:LYS:HG3	1.92	0.51
1:A:155:PHE:O	1:A:160:TRP:NE1	2.44	0.51
1:B:220:SER:HG	2:C:19:DG:H8	1.58	0.51
1:A:550:ASP:OD2	1:A:552:ARG:NH1	2.44	0.50
1:A:311:ILE:HD11	1:A:347:THR:HA	1.92	0.50
1:B:199:ALA:HB3	1:B:202:LYS:HG2	1.93	0.50
1:A:275:VAL:HG22	1:A:414:TYR:HB2	1.93	0.50
1:A:296:LYS:HE2	1:A:457:MET:SD	2.53	0.49
1:B:577:ARG:O	1:B:581:LEU:HG	2.13	0.49
4:D:38:DA:H2"	4:D:39:DC:C6	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LYS:HD3	1:B:308:SER:HA	1.95	0.49
1:A:357:LYS:HD2	1:A:493:GLU:HG3	1.94	0.49
1:A:93:TRP:O	1:B:483:GLU:HG2	2.12	0.49
1:A:288:LYS:HD3	1:A:308:SER:HA	1.95	0.49
1:B:89:ARG:HB3	1:B:93:TRP:CD1	2.47	0.49
2:C:45:DC:H2''	2:C:46:DG:C8	2.47	0.49
1:B:296:LYS:HE2	1:B:457:MET:SD	2.52	0.49
1:A:181:ASP:OD2	1:A:217:SER:N	2.42	0.48
1:A:577:ARG:O	1:A:581:LEU:HG	2.12	0.48
1:A:331:PHE:HB3	1:A:372:ALA:HA	1.95	0.48
1:A:355:ARG:HB3	1:A:506:LYS:O	2.14	0.48
1:B:155:PHE:O	1:B:160:TRP:NE1	2.44	0.48
2:C:24:DG:H4'	2:C:25:DC:OP1	2.14	0.47
1:B:331:PHE:HB3	1:B:372:ALA:HA	1.95	0.47
1:B:410:LEU:HD22	1:B:431:VAL:HG21	1.96	0.47
1:A:520:ASN:ND2	1:A:556:GLU:O	2.46	0.47
1:B:188:LEU:HB2	1:B:207:LEU:HD22	1.96	0.47
1:A:202:LYS:O	1:A:206:ARG:HG3	2.14	0.47
1:A:359:LYS:HG2	1:A:491:PRO:HB2	1.96	0.47
1:A:222:ALA:O	1:A:226:ARG:HB2	2.15	0.47
1:A:235:MET:O	1:A:238:ALA:HB3	2.15	0.47
2:C:50:DC:H2''	2:C:51:DA:H5'	1.97	0.47
3:E:9:DA:H2''	3:E:10:DA:C8	2.50	0.47
4:D:20:DA:H2''	4:D:21:DA:C8	2.49	0.47
1:A:161:ALA:CB	1:B:369:LEU:HD22	2.45	0.46
1:B:89:ARG:HB2	1:B:89:ARG:NH1	2.30	0.46
2:C:62:DT:H2''	2:C:63:DG:C8	2.51	0.46
1:B:237:VAL:O	1:B:241:GLU:HB2	2.16	0.46
1:B:275:VAL:HG22	1:B:414:TYR:HA	1.97	0.46
1:A:188:LEU:HB2	1:A:207:LEU:HD22	1.98	0.46
1:B:311:ILE:HG21	1:B:363:PRO:HG2	1.98	0.46
1:A:351:PRO:HA	1:A:357:LYS:HG3	1.98	0.46
1:B:570:ALA:O	1:B:574:TYR:HB2	2.15	0.45
1:B:355:ARG:NE	1:B:508:GLY:HA3	2.27	0.45
1:B:482:GLU:OE2	1:B:485:LYS:NZ	2.44	0.45
1:A:180:PHE:CE2	1:A:219:PRO:HB3	2.51	0.45
1:A:359:LYS:HB2	1:A:491:PRO:O	2.16	0.45
1:B:237:VAL:O	1:B:241:GLU:N	2.50	0.45
2:C:65:DT:H2''	2:C:66:DG:C8	2.51	0.45
1:B:224:ALA:O	1:B:228:ILE:HG12	2.17	0.44
4:D:43:DA:H2''	4:D:44:DA:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASN:HA	1:B:552:ARG:HG2	1.99	0.44
1:A:212:ARG:HH11	1:A:212:ARG:CG	2.29	0.44
1:A:262:ALA:O	1:A:263:MET:HB2	2.18	0.44
4:D:29:DA:H2''	4:D:30:DA:C8	2.52	0.44
1:A:88:ASP:HA	1:A:89:ARG:NH2	2.32	0.44
1:B:148:LYS:O	1:B:152:VAL:HG22	2.18	0.44
1:B:305:CYS:HB3	1:B:437:LEU:HD21	2.00	0.44
1:B:520:ASN:ND2	1:B:556:GLU:O	2.46	0.44
2:C:13:DT:H2''	2:C:14:DA:C8	2.52	0.44
1:B:494:ALA:HB2	1:B:549:LEU:HD21	1.98	0.44
1:A:100:SER:HA	1:B:550:ASP:O	2.18	0.43
2:C:15:DT:H3	4:D:41:DA:H61	1.65	0.43
1:A:502:GLU:HG2	1:A:519:TYR:CD1	2.53	0.43
1:A:134:VAL:HG11	1:A:145:LEU:HD22	2.01	0.43
1:A:297:THR:HB	1:A:467:VAL:HG23	2.00	0.43
1:B:262:ALA:O	1:B:263:MET:HB2	2.18	0.43
1:B:134:VAL:HG11	1:B:145:LEU:HD22	2.01	0.43
1:B:297:THR:HB	1:B:467:VAL:HG23	2.00	0.43
1:B:502:GLU:HG2	1:B:519:TYR:CD1	2.54	0.43
3:E:8:DC:H2''	3:E:9:DA:C8	2.53	0.43
1:A:362:ASP:OD1	1:A:364:LYS:HB2	2.18	0.43
1:A:93:TRP:CD1	1:B:481:THR:HG21	2.53	0.43
1:A:425:ASN:HB3	1:A:429:ARG:NE	2.34	0.43
1:A:472:TYR:O	1:A:475:THR:HG22	2.17	0.43
4:D:10:DC:H2''	4:D:11:DG:C8	2.54	0.43
1:A:305:CYS:HB3	1:A:437:LEU:HD21	2.01	0.43
1:B:202:LYS:HG3	1:B:203:CYS:N	2.34	0.42
2:C:64:DT:H2''	2:C:65:DT:C6	2.54	0.42
4:D:8:DA:H2''	4:D:9:DG:C8	2.54	0.42
4:D:26:DC:H2''	4:D:27:DG:H5''	2.01	0.42
1:B:212:ARG:HH11	1:B:212:ARG:CG	2.30	0.42
1:A:228:ILE:HA	1:A:231:LEU:HG	2.02	0.42
1:B:598:LEU:O	1:B:602:GLU:HG2	2.18	0.42
2:C:32:DG:H2''	2:C:33:DT:C6	2.54	0.42
1:A:479:LYS:HD3	1:A:479:LYS:HA	1.90	0.42
1:A:182:GLU:O	1:A:186:GLN:HG3	2.20	0.42
2:C:31:DC:H2''	2:C:32:DG:C8	2.54	0.42
1:A:274:ASN:O	1:A:274:ASN:ND2	2.41	0.42
1:A:531:VAL:HG21	1:A:546:CYS:HB3	2.02	0.42
1:A:93:TRP:CD1	1:B:481:THR:HG1	2.38	0.41
1:A:294:ASP:HB2	1:A:301:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PRO:CB	1:A:352:ASN:HB3	2.49	0.41
1:B:276:PHE:CE2	1:B:415:THR:HG21	2.55	0.41
1:A:296:LYS:NZ	1:A:471:GLU:OE1	2.53	0.41
1:B:232:ASP:HB3	1:B:235:MET:HG2	2.02	0.41
1:B:296:LYS:NZ	1:B:471:GLU:OE1	2.53	0.41
1:A:191:ASP:HB3	1:A:203:CYS:SG	2.60	0.41
4:D:30:DA:H2''	4:D:31:DG:C8	2.56	0.41
1:A:204:TYR:O	1:A:208:GLU:HG3	2.20	0.41
1:B:290:TRP:CD2	1:B:314:ILE:HG12	2.56	0.41
1:B:583:SER:HA	1:B:586:LYS:HD2	2.02	0.41
1:B:143:SER:HB3	4:D:48:DC:C5	2.55	0.41
1:B:294:ASP:HB2	1:B:301:LEU:HD11	2.01	0.41
2:C:46:DG:H2''	2:C:47:DC:C6	2.56	0.41
1:B:157:LYS:N	1:B:158:PRO:HD2	2.36	0.41
1:A:290:TRP:CD2	1:A:314:ILE:HG12	2.56	0.40
1:B:205:GLU:O	1:B:208:GLU:HB2	2.21	0.40
1:A:157:LYS:N	1:A:158:PRO:HD2	2.36	0.40
1:B:298:ARG:HD3	1:B:298:ARG:HA	1.87	0.40
1:A:106:LEU:O	1:A:110:TRP:HD1	2.04	0.40
1:B:290:TRP:CG	1:B:314:ILE:HG12	2.57	0.40
2:C:42:DC:H2''	2:C:43:DG:C8	2.57	0.40
2:C:49:DT:H3	4:D:7:DA:N6	2.17	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 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	
1	A	431/529 (82%)	414 (96%)	15 (4%)	2 (0%)	24	56
1	B	466/529 (88%)	450 (97%)	14 (3%)	2 (0%)	30	60
All	All	897/1058 (85%)	864 (96%)	29 (3%)	4 (0%)	30	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	352	ASN
1	B	355	ARG
1	A	231	LEU
1	B	231	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	
1	A	370/430 (86%)	354 (96%)	16 (4%)	26	50
1	B	387/430 (90%)	372 (96%)	15 (4%)	28	53
All	All	757/860 (88%)	726 (96%)	31 (4%)	27	52

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ARG
1	A	141	SER
1	A	159	ASP
1	A	165	VAL
1	A	212	ARG
1	A	217	SER
1	A	226	ARG
1	A	239	CYS
1	A	274	ASN
1	A	310	ASN
1	A	432	ASP
1	A	440	LEU
1	A	525	LEU
1	A	528	VAL
1	A	531	VAL
1	A	592	GLN
1	B	89	ARG
1	B	141	SER
1	B	159	ASP

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Mol	Chain	Res	Type
1	B	165	VAL
1	B	178	SER
1	B	191	ASP
1	B	212	ARG
1	B	217	SER
1	B	226	ARG
1	B	310	ASN
1	B	378	SER
1	B	432	ASP
1	B	440	LEU
1	B	525	LEU
1	B	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	274	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/529 (83%)	1.11	86 (19%)  	134, 303, 577, 797	0
1	B	476/529 (89%)	0.88	76 (15%)  	130, 264, 400, 526	0
2	C	68/68 (100%)	1.07	11 (16%)  	200, 257, 409, 476	0
3	E	13/13 (100%)	0.73	0  	290, 364, 508, 517	0
4	D	49/49 (100%)	1.06	7 (14%)  	201, 256, 336, 350	0
All	All	1049/1188 (88%)	1.00	180 (17%)  	130, 277, 475, 797	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	GLN	10.3
1	B	397	VAL	8.8
1	A	286	ARG	7.4
1	A	408	PRO	6.5
1	B	146	ARG	6.2
1	A	205	GLU	6.1
1	A	226	ARG	6.0
1	A	147	ASP	5.8
1	A	285	ILE	5.8
1	A	265	TRP	5.7
1	A	309	GLU	5.5
1	A	191	ASP	5.5
1	B	296	LYS	5.1
1	B	370	MET	5.1
1	B	535	PHE	5.1
1	A	146	ARG	4.7
1	B	165	VAL	4.5
1	A	187	PHE	4.5
1	A	451	THR	4.5
1	A	336	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	369	LEU	4.3
1	A	333	ILE	4.2
1	A	335	ILE	4.2
1	B	396	GLY	4.2
1	A	360	GLU	4.2
1	B	318	PHE	4.2
1	B	153	GLN	4.2
1	B	537	PRO	4.1
1	B	291	PHE	4.0
1	A	269	ASP	4.0
1	B	111	LEU	4.0
1	A	400	LEU	3.9
1	B	437	LEU	3.9
1	B	161	ALA	3.9
1	A	209	LEU	3.8
1	B	292	TRP	3.8
1	A	554	ILE	3.8
1	A	206	ARG	3.7
1	A	238	ALA	3.7
1	A	361	ASP	3.7
1	B	200	PHE	3.7
1	B	148	LYS	3.6
1	A	234	ALA	3.6
1	B	272	LEU	3.6
1	B	226	ARG	3.6
1	A	292	TRP	3.6
1	A	236	VAL	3.6
1	A	270	GLY	3.6
1	A	111	LEU	3.5
1	A	446	MET	3.5
4	D	46	DT	3.5
1	B	95	LYS	3.4
1	A	192	TYR	3.4
1	A	96	TRP	3.4
1	A	419	PRO	3.4
2	C	54	DT	3.3
1	A	359	LYS	3.3
1	B	219	PRO	3.3
1	B	354	TYR	3.3
1	A	559	CYS	3.2
1	A	417	PRO	3.2
1	B	533	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	204	TYR	3.2
1	B	602	GLU	3.2
1	B	457	MET	3.2
1	B	490	LEU	3.2
1	A	300	ILE	3.2
1	B	331	PHE	3.2
1	B	523	LEU	3.2
1	A	291	PHE	3.2
4	D	34	DT	3.1
1	A	266	ILE	3.1
4	D	35	DT	3.1
1	A	315	ARG	3.1
1	A	424	ASP	3.1
1	B	96	TRP	3.0
1	A	165	VAL	3.0
1	B	128	LYS	3.0
2	C	21	DA	3.0
1	B	590	LYS	3.0
1	B	503	PHE	3.0
4	D	9	DG	2.9
2	C	53	DC	2.9
1	B	603	LEU	2.9
1	A	235	MET	2.9
1	A	244	HIS	2.9
1	A	450	ARG	2.9
1	A	143	SER	2.9
1	B	140	VAL	2.9
1	A	228	ILE	2.8
1	A	199	ALA	2.8
1	B	489	LEU	2.8
1	B	505	LEU	2.8
1	B	367	PHE	2.8
1	B	131	PHE	2.8
1	B	204	TYR	2.7
1	A	402	GLU	2.7
1	B	222	ALA	2.7
1	B	540	LEU	2.7
1	B	300	ILE	2.7
1	A	145	LEU	2.7
2	C	69	DG	2.7
1	A	583	SER	2.7
1	B	115	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	142	ALA	2.7
1	A	421	ALA	2.7
1	B	162	ALA	2.7
1	B	546	CYS	2.7
1	A	376	TRP	2.6
1	A	358	VAL	2.6
1	B	158	PRO	2.6
1	A	190	ALA	2.6
1	A	492	ALA	2.6
2	C	57	DT	2.6
1	B	487	MET	2.6
1	A	131	PHE	2.6
1	B	228	ILE	2.6
1	B	385	TRP	2.5
2	C	56	DA	2.5
1	B	605	PRO	2.5
1	B	150	TYR	2.5
1	B	236	VAL	2.5
1	B	223	THR	2.5
2	C	55	DG	2.5
1	A	95	LYS	2.5
1	B	322	VAL	2.5
1	A	153	GLN	2.4
1	B	552	ARG	2.4
1	A	144	THR	2.4
1	A	347	THR	2.4
1	A	454	GLU	2.4
1	A	488	LEU	2.4
1	A	202	LYS	2.4
1	A	247	MET	2.4
1	A	515	LYS	2.4
1	A	423	PRO	2.3
1	A	267	ASN	2.3
1	B	221	ARG	2.3
1	B	368	LEU	2.3
1	B	486	ARG	2.3
2	C	3	DT	2.3
4	D	42	DT	2.3
1	B	594	GLN	2.2
1	B	189	ILE	2.2
1	B	266	ILE	2.2
1	B	314	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	151	GLN	2.2
1	B	263	MET	2.2
1	A	298	ARG	2.2
2	C	52	DT	2.2
1	A	594	GLN	2.2
1	A	188	LEU	2.2
1	A	560	LEU	2.2
1	B	241	GLU	2.2
1	B	515	LYS	2.2
1	A	374	MET	2.2
1	B	201	ARG	2.2
1	A	271	TYR	2.2
1	A	107	ALA	2.1
1	A	276	PHE	2.1
1	B	100	SER	2.1
1	A	372	ALA	2.1
1	A	90	GLU	2.1
1	A	194	ARG	2.1
1	A	91	ALA	2.1
1	B	285	ILE	2.1
2	C	67	DA	2.1
1	A	357	LYS	2.1
1	B	500	LYS	2.1
1	A	200	PHE	2.1
2	C	58	DG	2.1
4	D	47	DG	2.1
1	B	185	TRP	2.1
1	B	305	CYS	2.1
1	B	155	PHE	2.1
1	B	544	VAL	2.1
1	A	415	THR	2.1
1	A	207	LEU	2.1
4	D	45	DA	2.0
1	B	160	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.