W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2020 – 12:08 PM EDT

PDB ID	:	6XG8
Title	:	ISCth4 transposase, pre-cleaved complex, PCC
Authors	:	Kosek, D.; Dyda, F.
Deposited on	:	2020-06-17
Resolution	:	3.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 3.50 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	Percentile Ranks	Value
Rfree		0.275
Clashscore		10
Ramachandran outliers		0.1%
Sidechain outliers		5.8%
RSRZ outliers		1.0%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
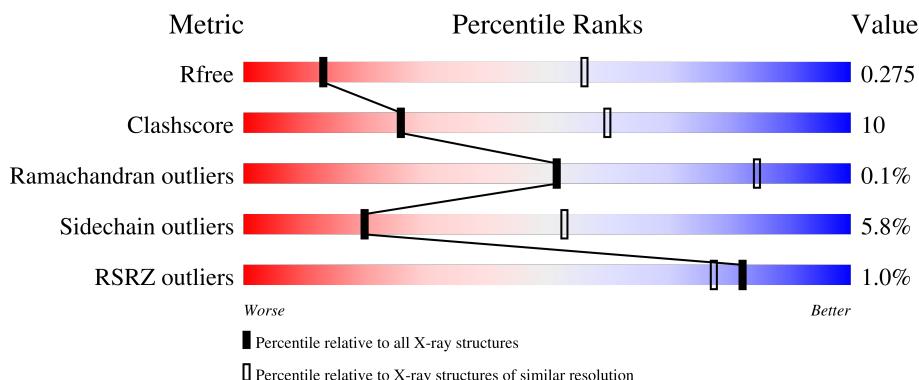
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 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% 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	410	72% 23% · ·
1	B	410	% 63% 21% · 14%
2	D	26	35% 65%
3	E	26	50% 50%
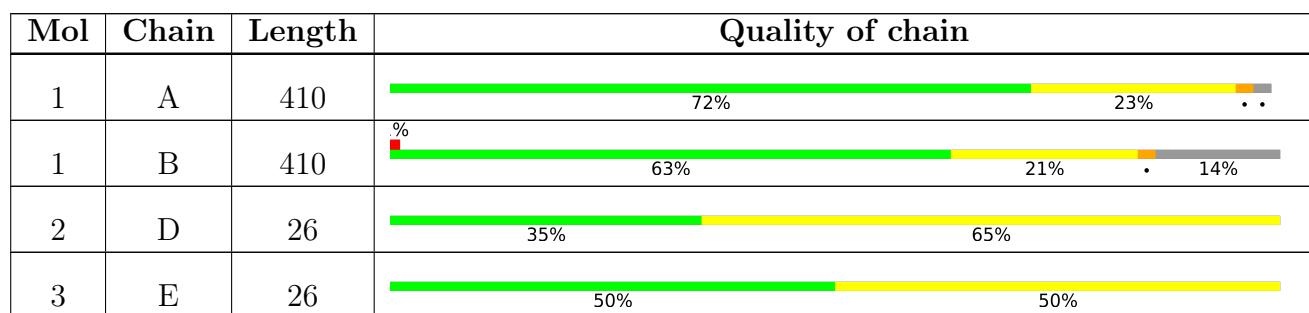
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 7187 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 Mutator family transposase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	0	0
			3271	2087	550	622	12			
1	B	351	Total	C	N	O	S	0	0	0
			2856	1828	479	537	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A3DBR0
A	-1	SER	-	expression tag	UNP A3DBR0
A	0	ALA	-	expression tag	UNP A3DBR0
B	-2	GLY	-	expression tag	UNP A3DBR0
B	-1	SER	-	expression tag	UNP A3DBR0
B	0	ALA	-	expression tag	UNP A3DBR0

- Molecule 2 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	26	Total	C	N	O	P	0	0	0
			525	254	94	152	25			

- Molecule 3 is a DNA chain called DNA (26-MER).

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	26	Total	C	N	O	P	0	0	0
			535	258	96	156	25			

3 Residue-property plots ⓘ

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: Mutator family transposase

Chain A:

• Molecule 1: Mutator family transposase

Chain B:

• Molecule 2: DNA (26-MER)

Chain D:

G1 T2 T3 T4 A5 C6 A9 A10 A15 T16 T17 T18 A19 C20 A21 C22 T23 G24 C25 C26
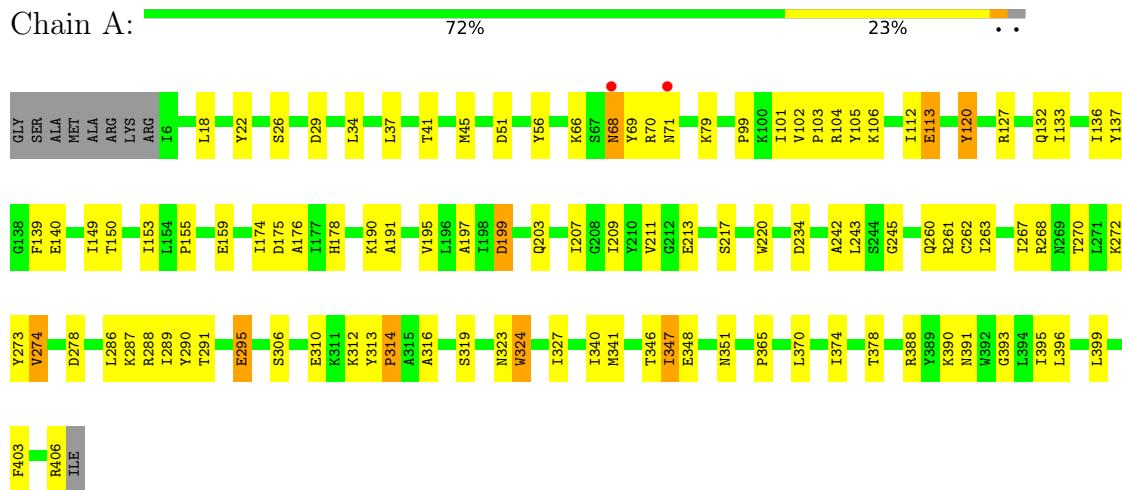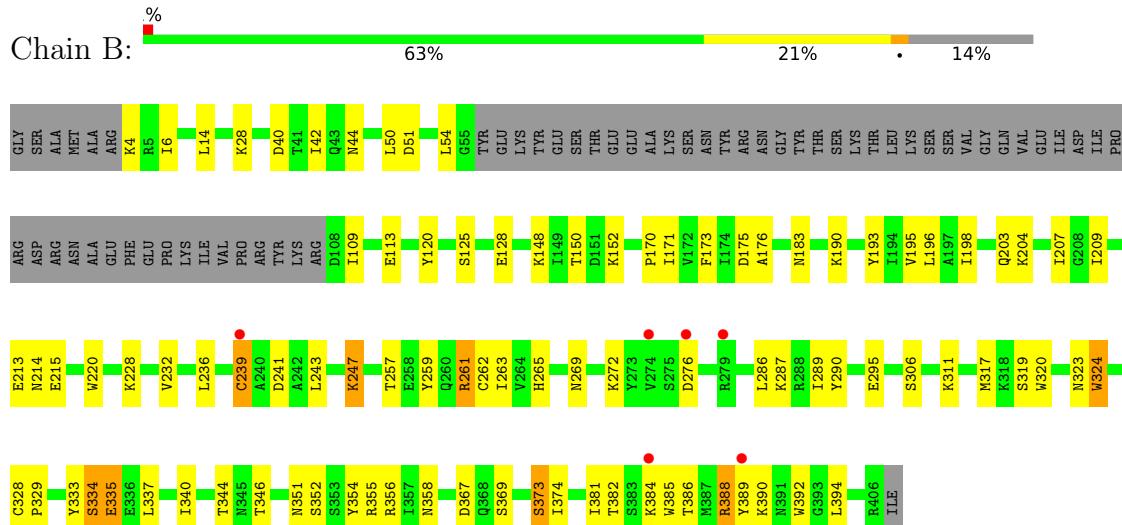
• Molecule 3: DNA (26-MER)

Chain E:

50%   50%

G1 G2 C3 A4 G5 T6 G7 A13 T18 G19 T20 G21 T22 A23 C26

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.68Å 109.50Å 157.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.61 – 3.50	Depositor
	29.61 – 3.50	EDS
% Data completeness	99.7 (29.61-3.50)	Depositor
(in resolution range)	99.8 (29.61-3.50)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 3.47Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.221 , 0.267	Depositor
	0.230 , 0.275	DCC
R_{free} test set	604 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	147.3	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 110.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7187	wwPDB-VP
Average B, all atoms (Å^2)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.26	0/3331	0.46	0/4489
1	B	0.26	0/2906	0.45	0/3914
2	D	0.61	0/588	0.95	0/904
3	E	0.60	0/600	1.01	0/926
All	All	0.34	0/7425	0.58	0/10233

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 ⓘ

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	3271	0	3309	65	0
1	B	2856	0	2907	60	0
2	D	525	0	296	13	0
3	E	535	0	298	18	0
All	All	7187	0	6810	147	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 (147) 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:317:MET:HA	1:B:320:TRP:HD1	1.53	0.74
3:E:4:DA:H2"	3:E:5:DG:H5"	1.69	0.74
1:B:354:TYR:O	1:B:358:ASN:ND2	2.22	0.72
1:B:351:ASN:OD1	1:B:355:ARG:NH2	2.26	0.69
2:D:20:DC:H2"	2:D:21:DA:C8	2.28	0.68
1:B:295:GLU:HG2	1:B:324:TRP:HH2	1.57	0.68
1:A:199:ASP:OD1	1:A:199:ASP:N	2.26	0.68
1:A:120:TYR:HD2	1:A:150:THR:HG21	1.60	0.67
1:B:382:THR:HA	1:B:385:TRP:HE3	1.61	0.65
2:D:9:DA:H2'	2:D:10:DA:C8	2.31	0.65
1:A:346:THR:HG23	1:A:347:ILE:HD12	1.81	0.62
3:E:6:DT:H2'	3:E:7:DG:C8	2.34	0.62
1:B:388:ARG:H	1:B:388:ARG:HD3	1.64	0.62
2:D:23:DT:H2'	2:D:24:DG:C8	2.35	0.62
1:A:203:GLN:HA	1:A:388:ARG:HD2	1.82	0.62
1:A:175:ASP:OD2	1:A:351:ASN:ND2	2.25	0.60
1:B:382:THR:HG22	1:B:385:TRP:HZ3	1.67	0.59
3:E:2:DG:H2'	3:E:3:DC:C6	2.36	0.59
1:B:247:LYS:H	1:B:247:LYS:HD3	1.66	0.59
1:B:213:GLU:O	1:B:214:ASN:ND2	2.35	0.59
1:B:190:LYS:HE3	1:B:213:GLU:HG2	1.84	0.58
1:A:103:PRO:HD2	1:A:106:LYS:HD3	1.86	0.58
1:B:382:THR:HG22	1:B:385:TRP:CZ3	2.39	0.58
1:A:274:VAL:HB	1:A:314:PRO:HG2	1.85	0.58
1:A:79:LYS:HD2	1:A:139:PHE:HB2	1.85	0.57
1:B:204:LYS:HD2	1:B:346:THR:HG21	1.87	0.57
1:A:393:GLY:HA2	1:A:396:LEU:HB3	1.87	0.57
1:B:295:GLU:HG2	1:B:324:TRP:CH2	2.38	0.57
1:B:286:LEU:O	1:B:289:ILE:HG22	2.04	0.57
1:A:69:TYR:HD2	2:D:3:DT:H2'	1.70	0.56
3:E:20:DT:H2"	3:E:21:DG:C8	2.41	0.56
1:B:317:MET:HA	1:B:320:TRP:CD1	2.39	0.55
1:A:263:ILE:O	1:A:267:ILE:HG12	2.07	0.55
1:B:287:LYS:HD2	3:E:1:DG:H4'	1.88	0.54
1:A:403:PHE:HB3	1:A:406:ARG:HG3	1.89	0.54
1:A:120:TYR:CD2	1:A:150:THR:HG21	2.42	0.54
1:A:340:ILE:HD11	1:A:395:ILE:HD13	1.89	0.54
3:E:5:DG:H2'	3:E:6:DT:C6	2.41	0.54
1:A:365:PRO:HB3	3:E:7:DG:H21	1.74	0.53
2:D:17:DT:H2'	2:D:18:DT:H72	1.91	0.53
1:A:313:TYR:HD2	1:A:316:ALA:H	1.56	0.53
1:B:109:ILE:HD12	1:B:152:LYS:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:THR:HB	1:A:316:ALA:HB1	1.90	0.52
1:B:170:PRO:HB2	1:B:171:ILE:HD12	1.91	0.52
1:B:228:LYS:HA	1:B:232:VAL:HG12	1.90	0.52
1:A:287:LYS:HA	1:A:290:TYR:CZ	2.44	0.52
3:E:3:DC:H2"	3:E:4:DA:C8	2.44	0.52
1:A:209:ILE:HD11	1:A:378:THR:HG21	1.91	0.52
1:B:170:PRO:HA	1:B:236:LEU:HB2	1.91	0.52
1:B:259:TYR:O	1:B:261:ARG:NH2	2.43	0.52
1:A:395:ILE:HG22	1:A:399:LEU:HD23	1.93	0.51
1:B:334:SER:OG	1:B:335:GLU:N	2.43	0.51
1:A:26:SER:OG	1:A:29:ASP:OD1	2.29	0.51
1:B:306:SER:HA	1:B:317:MET:HG3	1.92	0.51
1:A:391:ASN:O	1:A:395:ILE:HG13	2.11	0.51
1:A:56:TYR:O	1:A:70:ARG:NH2	2.44	0.51
1:B:287:LYS:HA	1:B:290:TYR:CZ	2.46	0.51
2:D:22:DC:H2'	2:D:23:DT:C6	2.45	0.51
1:A:71:ASN:OD1	2:D:6:DC:N4	2.43	0.51
1:A:323:ASN:O	1:A:327:ILE:HG13	2.11	0.51
3:E:18:DT:H2"	3:E:19:DG:C8	2.46	0.51
1:B:40:ASP:O	1:B:44:ASN:ND2	2.38	0.50
1:A:234:ASP:OD1	1:A:406:ARG:NH2	2.36	0.50
1:A:175:ASP:OD1	1:A:176:ALA:N	2.45	0.50
1:A:112:ILE:HD11	1:A:133:ILE:HD12	1.93	0.50
1:B:50:LEU:HB3	1:B:148:LYS:HE2	1.93	0.50
1:A:34:LEU:HD11	1:B:42:ILE:HD11	1.94	0.49
2:D:15:DA:C2	3:E:13:DA:C2	3.00	0.49
1:A:174:ILE:HD12	1:A:195:VAL:HG22	1.94	0.49
1:B:173:PHE:HE1	1:B:263:ILE:HD11	1.77	0.49
1:B:209:ILE:HD13	1:B:374:ILE:HG22	1.95	0.49
1:B:195:VAL:O	1:B:207:ILE:N	2.45	0.48
3:E:18:DT:H2"	3:E:19:DG:H8	1.79	0.48
1:A:66:LYS:HG3	1:A:68:ASN:H	1.78	0.48
1:B:257:THR:HB	1:B:259:TYR:CE1	2.49	0.48
1:B:356:ARG:NH1	3:E:5:DG:OP1	2.47	0.48
1:A:197:ALA:HB3	1:A:207:ILE:HG13	1.95	0.48
1:B:120:TYR:CD2	1:B:150:THR:HG21	2.50	0.47
1:B:170:PRO:HD2	1:B:198:ILE:O	2.14	0.47
1:A:242:ALA:HB2	1:A:261:ARG:NH1	2.29	0.47
1:A:268:ARG:HD3	1:A:348:GLU:OE1	2.15	0.47
1:B:220:TRP:HZ2	1:B:243:LEU:HD13	1.79	0.47
1:B:381:ILE:O	1:B:385:TRP:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:DG:H2"	2:D:25:DC:C6	2.49	0.47
1:B:183:ASN:HD21	1:B:367:ASP:CG	2.18	0.47
1:B:269:ASN:HA	1:B:272:LYS:HG3	1.96	0.47
1:A:178:HIS:CD2	1:A:191:ALA:HB2	2.50	0.47
1:B:175:ASP:O	1:B:193:TYR:HA	2.15	0.47
2:D:4:DT:H2"	2:D:5:DA:H8	1.80	0.46
1:A:310:GLU:HA	1:A:313:TYR:CD1	2.50	0.46
1:A:242:ALA:HB2	1:A:261:ARG:CZ	2.45	0.46
2:D:1:DG:H2"	2:D:2:DT:H5"	1.98	0.46
1:A:113:GLU:HG3	1:A:149:ILE:HG23	1.97	0.46
1:A:18:LEU:HD23	1:B:14:LEU:HD21	1.97	0.45
1:B:295:GLU:HG3	1:B:328:CYS:SG	2.56	0.45
1:A:41:THR:O	1:A:45:MET:HG3	2.17	0.45
1:A:396:LEU:HA	1:A:399:LEU:HG	1.99	0.45
1:A:220:TRP:CZ2	1:A:243:LEU:HD13	2.52	0.45
1:B:317:MET:O	1:B:320:TRP:HB2	2.17	0.45
1:B:352:SER:HA	1:B:355:ARG:HE	1.82	0.45
3:E:2:DG:H2"	3:E:3:DC:O5'	2.16	0.44
1:A:101:ILE:HG22	1:A:102:VAL:HG23	1.99	0.44
1:A:203:GLN:OE1	1:A:203:GLN:N	2.41	0.44
1:B:125:SER:HB2	1:B:128:GLU:HG3	1.99	0.44
1:B:319:SER:O	1:B:323:ASN:ND2	2.38	0.44
1:B:328:CYS:HB3	1:B:329:PRO:HD3	2.00	0.44
1:B:287:LYS:HA	1:B:290:TYR:CE2	2.53	0.44
1:A:370:LEU:O	1:A:374:ILE:HG12	2.18	0.43
1:B:276:ASP:OD1	1:B:276:ASP:N	2.51	0.43
1:A:234:ASP:OD2	1:A:406:ARG:NE	2.51	0.43
1:A:190:LYS:HA	1:A:190:LYS:HD3	1.82	0.43
1:B:369:SER:O	1:B:373:SER:OG	2.37	0.43
3:E:6:DT:H4'	3:E:7:DG:OP1	2.18	0.43
1:B:355:ARG:HA	1:B:358:ASN:HB2	2.00	0.43
1:A:288:ARG:HA	1:A:291:THR:HG22	2.01	0.42
1:B:175:ASP:OD1	1:B:176:ALA:N	2.52	0.42
2:D:17:DT:H2'	2:D:18:DT:C7	2.49	0.42
1:A:211:VAL:HG12	1:A:213:GLU:HG2	2.00	0.42
1:A:217:SER:OG	1:A:245:GLY:O	2.36	0.42
1:A:286:LEU:HD12	1:A:289:ILE:HD12	2.00	0.42
1:B:109:ILE:HG22	1:B:113:GLU:HB2	2.00	0.42
1:A:99:PRO:HB2	1:A:102:VAL:O	2.19	0.42
1:A:306:SER:O	1:A:310:GLU:N	2.52	0.42
1:A:319:SER:O	1:A:323:ASN:ND2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:CE2	1:A:37:LEU:HD23	2.55	0.42
1:B:333:TYR:HB3	1:B:337:LEU:HB3	2.01	0.42
1:A:153:ILE:H	1:A:153:ILE:HG13	1.63	0.42
1:A:316:ALA:O	1:A:319:SER:OG	2.29	0.42
1:A:51:ASP:OD1	1:A:70:ARG:NH2	2.45	0.42
1:B:239:CYS:HA	1:B:261:ARG:HA	2.01	0.41
1:B:183:ASN:ND2	1:B:367:ASP:OD1	2.49	0.41
1:A:155:PRO:O	1:A:159:GLU:HG2	2.19	0.41
3:E:5:DG:H3'	3:E:6:DT:H71	2.01	0.41
1:A:295:GLU:HB2	1:A:324:TRP:HH2	1.85	0.41
1:A:104:ARG:O	1:A:105:TYR:HB2	2.20	0.41
1:A:268:ARG:HB3	1:A:272:LYS:HE2	2.02	0.41
1:B:196:LEU:HD11	1:B:385:TRP:HH2	1.86	0.41
1:B:337:LEU:O	1:B:340:ILE:HG22	2.20	0.41
2:D:5:DA:C2	3:E:23:DA:C2	3.08	0.41
1:B:4:LYS:HG3	1:B:6:ILE:HG12	2.02	0.41
1:A:133:ILE:O	1:A:137:TYR:HB2	2.21	0.41
3:E:19:DG:H2"	3:E:20:DT:O4'	2.21	0.40
1:B:384:LYS:HB3	1:B:384:LYS:HE3	1.95	0.40
3:E:2:DG:H2"	3:E:3:DC:C5'	2.51	0.40
1:A:132:GLN:O	1:A:136:ILE:HG12	2.22	0.40
1:B:220:TRP:CZ2	1:B:243:LEU:HD13	2.56	0.40
1:A:312:LYS:HE2	1:A:312:LYS:HB3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	399/410 (97%)	388 (97%)	10 (2%)	1 (0%)	41	75
1	B	347/410 (85%)	337 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	746/820 (91%)	725 (97%)	20 (3%)	1 (0%)	51	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	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 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	360/366 (98%)	344 (96%)	16 (4%)	28	62
1	B	314/366 (86%)	291 (93%)	23 (7%)	14	45
All	All	674/732 (92%)	635 (94%)	39 (6%)	20	53

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	113	GLU
1	A	120	TYR
1	A	127	ARG
1	A	140	GLU
1	A	199	ASP
1	A	260	GLN
1	A	262	CYS
1	A	273	TYR
1	A	274	VAL
1	A	278	ASP
1	A	295	GLU
1	A	324	TRP
1	A	341	MET
1	A	347	ILE
1	A	390	LYS
1	B	28	LYS

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Mol	Chain	Res	Type
1	B	51	ASP
1	B	54	LEU
1	B	203	GLN
1	B	215	GLU
1	B	239	CYS
1	B	241	ASP
1	B	247	LYS
1	B	261	ARG
1	B	262	CYS
1	B	265	HIS
1	B	311	LYS
1	B	324	TRP
1	B	334	SER
1	B	335	GLU
1	B	344	THR
1	B	373	SER
1	B	386	THR
1	B	388	ARG
1	B	389	TYR
1	B	390	LYS
1	B	392	TRP
1	B	394	LEU

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

Mol	Chain	Res	Type
1	A	94	ASN
1	B	203	GLN

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 monosaccharides 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(Å²)	Q<0.9
1	A	401/410 (97%)	-0.36	2 (0%)	91	88	106, 157, 201, 240	0
1	B	351/410 (85%)	-0.30	6 (1%)	70	64	102, 173, 237, 267	0
2	D	26/26 (100%)	-0.63	0	100	100	137, 163, 196, 227	0
3	E	26/26 (100%)	-0.52	0	100	100	129, 157, 215, 231	0
All	All	804/872 (92%)	-0.35	8 (0%)	82	77	102, 162, 226, 267	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	276	ASP	2.8
1	B	384	LYS	2.7
1	B	279	ARG	2.4
1	B	389	TYR	2.4
1	B	239	CYS	2.2
1	A	71	ASN	2.2
1	B	274	VAL	2.1
1	A	68	ASN	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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.