Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 10:44 AM EDT

PDB ID	:	6XGW
Title	:	ISCth4 transposase, pre-reaction complex, PRC
Authors	:	Kosek, D.; Dyda, F.
Deposited on	:	2020-06-18
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 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:

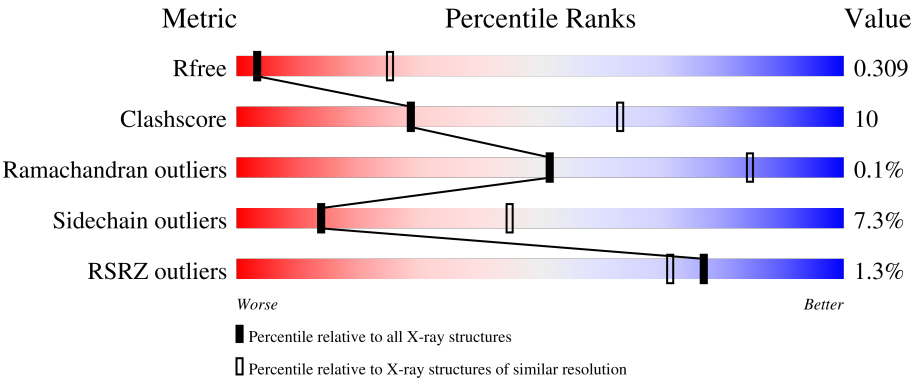
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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	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 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 <=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	71% 24%
1	B	410	2% 66% 18% 13%
2	D	32	41% 56%
3	E	32	50% 47%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7424 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	356	Total	C	N	O	S	0	0	0
			2888	1849	484	543	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 (32-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	31	Total	C	N	O	P	0	0	0
			628	303	117	178	30			

- Molecule 3 is a DNA chain called DNA (32-MER).

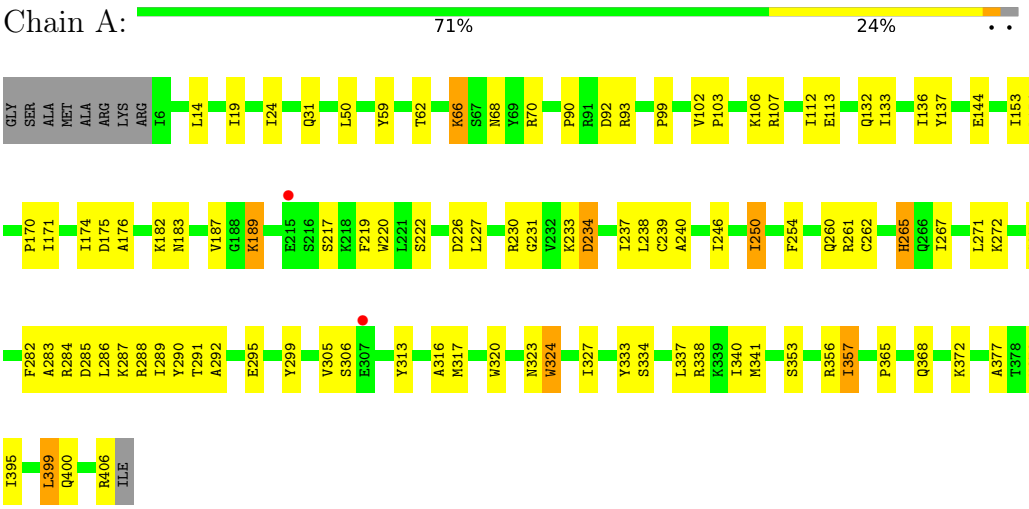
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	31	Total	C	N	O	P	0	0	0
			637	308	109	190	30			

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.

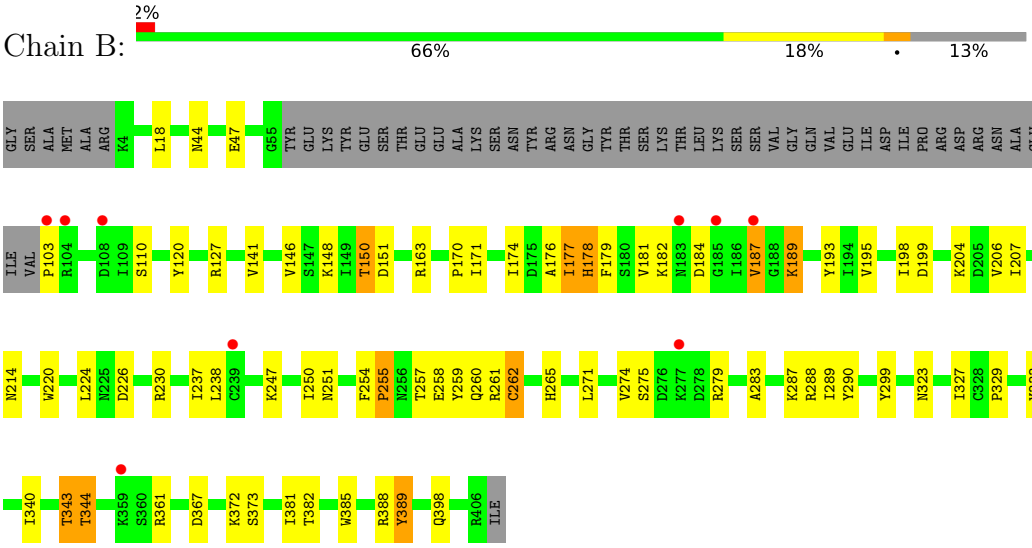
• Molecule 1: Mutator family transposase

Chain A:



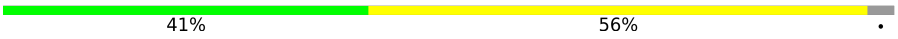
• Molecule 1: Mutator family transposase

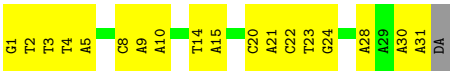
Chain B:



• Molecule 2: DNA (32-MER)

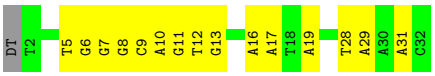
Chain D:





• Molecule 3: DNA (32-MER)

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.58Å 99.05Å 156.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.48 – 3.50 29.48 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.48-3.50) 99.4 (29.48-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 3.47Å)	Xtriage
Refinement program	BUSTER, PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.249 , 0.296 0.260 , 0.309	Depositor DCC
R_{free} test set	719 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å^2)	133.6	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 95.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7424	wwPDB-VP
Average B, all atoms (Å^2)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.24	0/3331	0.42	0/4489
1	B	0.24	0/2939	0.43	1/3960 (0.0%)
2	D	0.54	0/705	0.90	0/1084
3	E	0.53	0/713	0.99	0/1101
All	All	0.32	0/7688	0.57	1/10634 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	103	PRO	N-CA-CB	5.91	110.39	103.30

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	68	0
1	B	2888	0	2924	47	0
2	D	628	0	351	15	0
3	E	637	0	357	19	0
All	All	7424	0	6941	139	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 (139) 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:239:CYS:HB3	1:A:262:CYS:SG	2.16	0.86
1:B:381:ILE:O	1:B:385:TRP:HB2	1.79	0.83
2:D:8:DC:H2'	2:D:9:DA:C8	2.16	0.81
2:D:9:DA:H2'	2:D:10:DA:C8	2.22	0.75
1:B:340:ILE:HD12	1:B:389:TYR:HE2	1.58	0.69
1:B:261:ARG:NH2	1:B:329:PRO:O	2.27	0.68
2:D:23:DT:H2"	2:D:24:DG:H5"	1.76	0.66
2:D:20:DC:H2'	2:D:21:DA:C8	2.32	0.65
1:A:271:LEU:HD11	1:A:320:TRP:HE1	1.62	0.64
1:A:340:ILE:HD11	1:A:395:ILE:HD13	1.80	0.64
1:A:50:LEU:HD22	1:A:90:PRO:HB2	1.80	0.64
3:E:5:DT:H2'	3:E:6:DG:C8	2.33	0.64
1:B:382:THR:HA	1:B:385:TRP:HB3	1.80	0.63
3:E:10:DA:H2"	3:E:11:DG:H5"	1.81	0.62
1:A:19:ILE:HA	1:A:24:ILE:HD13	1.82	0.62
1:B:163:ARG:NH2	1:B:206:VAL:O	2.34	0.61
1:A:283:ALA:HA	1:A:286:LEU:HB3	1.83	0.60
1:B:120:TYR:CZ	1:B:361:ARG:HD2	2.37	0.58
1:A:272:LYS:HA	1:A:275:SER:HB2	1.84	0.58
1:A:262:CYS:HB3	1:A:265:HIS:HB2	1.85	0.58
1:B:170:PRO:HD2	1:B:199:ASP:HA	1.85	0.57
1:A:271:LEU:HD21	1:A:320:TRP:HE1	1.70	0.56
2:D:28:DA:N6	3:E:5:DT:H3	2.04	0.56
1:A:227:LEU:O	1:A:231:GLY:N	2.35	0.55
1:B:238:LEU:HD23	1:B:250:ILE:HD11	1.89	0.55
2:D:28:DA:H61	3:E:5:DT:H3	1.52	0.55
1:A:59:TYR:OH	2:D:3:DT:O2	2.25	0.55
1:B:151:ASP:OD1	1:B:372:LYS:NZ	2.29	0.55
2:D:1:DG:H2"	2:D:2:DT:H5"	1.88	0.55
1:A:187:VAL:HB	2:D:22:DC:H4'	1.88	0.54
1:A:267:ILE:HA	1:A:271:LEU:HD13	1.89	0.54
1:A:278:ASP:O	1:A:279:ARG:NH1	2.40	0.54
1:A:287:LYS:HA	1:A:290:TYR:CZ	2.42	0.54
1:A:175:ASP:OD1	1:A:176:ALA:N	2.41	0.54
1:A:271:LEU:HB3	1:A:282:PHE:HZ	1.74	0.53
3:E:11:DG:H2'	3:E:12:DT:C6	2.44	0.53
1:A:353:SER:O	1:A:356:ARG:HG2	2.08	0.53
1:A:306:SER:HA	1:A:317:MET:HG3	1.91	0.53
1:A:59:TYR:OH	3:E:31:DA:N3	2.42	0.53
1:A:357:ILE:HG21	1:A:377:ALA:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:HD11	1:A:133:ILE:HD12	1.91	0.52
1:B:336:GLU:O	1:B:340:ILE:HG12	2.09	0.51
1:B:171:ILE:HB	1:B:198:ILE:HG23	1.92	0.51
3:E:12:DT:H2'	3:E:13:DG:C8	2.45	0.51
1:A:154:LEU:HD11	1:A:372:LYS:HE2	1.92	0.51
1:A:226:ASP:OD1	1:A:230:ARG:NH1	2.43	0.51
1:A:271:LEU:HD11	1:A:320:TRP:NE1	2.25	0.51
1:A:333:TYR:HB3	1:A:337:LEU:HB3	1.93	0.51
1:B:198:ILE:HB	1:B:204:LYS:HD3	1.93	0.50
1:B:287:LYS:HA	1:B:290:TYR:CE2	2.47	0.50
1:A:323:ASN:O	1:A:327:ILE:HG13	2.11	0.50
1:A:292:ALA:O	1:A:338:ARG:NH1	2.44	0.50
2:D:22:DC:H2'	2:D:23:DT:C6	2.46	0.50
1:B:177:ILE:HG22	1:B:178:HIS:H	1.77	0.49
1:A:217:SER:O	1:A:220:TRP:HB2	2.11	0.49
1:B:247:LYS:O	1:B:251:ASN:ND2	2.38	0.49
1:A:286:LEU:HD12	1:A:289:ILE:HD12	1.93	0.49
3:E:12:DT:H4'	3:E:13:DG:OP1	2.13	0.49
1:B:181:VAL:HG11	1:B:187:VAL:HG12	1.94	0.49
1:A:234:ASP:N	1:A:234:ASP:OD1	2.45	0.48
3:E:6:DG:H2"	3:E:7:DG:H8	1.78	0.48
1:A:289:ILE:HD11	1:A:305:VAL:HG11	1.94	0.48
3:E:9:DC:H2"	3:E:10:DA:H8	1.79	0.47
1:A:19:ILE:HG23	1:A:24:ILE:HB	1.96	0.47
1:A:400:GLN:OE1	1:A:406:ARG:NH2	2.47	0.47
1:B:174:ILE:HG21	1:B:220:TRP:HZ3	1.80	0.47
1:B:262:CYS:SG	1:B:265:HIS:HB2	2.55	0.47
1:A:261:ARG:HB3	1:A:327:ILE:HG12	1.97	0.47
1:B:279:ARG:O	1:B:283:ALA:N	2.41	0.46
1:A:170:PRO:HB2	1:A:171:ILE:HD12	1.97	0.46
1:A:400:GLN:HB3	1:A:406:ARG:HH21	1.80	0.46
1:B:176:ALA:HB2	1:B:193:TYR:CE2	2.50	0.46
1:B:274:VAL:HG22	1:B:275:SER:H	1.81	0.46
1:B:174:ILE:HG12	1:B:195:VAL:HG13	1.96	0.46
1:B:207:ILE:O	1:B:230:ARG:NH1	2.49	0.46
1:A:219:PHE:O	1:A:222:SER:HB2	2.15	0.45
1:B:334:SER:OG	1:B:398:GLN:OE1	2.28	0.45
1:B:189:LYS:HD2	1:B:189:LYS:H	1.82	0.45
1:A:92:ASP:OD1	1:A:93:ARG:N	2.48	0.45
3:E:11:DG:C8	3:E:12:DT:H72	2.51	0.45
1:A:167:GLU:HB3	1:A:233:LYS:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ILE:HD13	1:A:240:ALA:HB2	1.97	0.45
1:A:288:ARG:HA	1:A:291:THR:HG22	1.98	0.45
1:A:31:GLN:HE22	1:B:110:SER:HB3	1.81	0.45
1:A:285:ASP:O	1:A:288:ARG:HB3	2.15	0.45
1:A:14:LEU:HD11	1:B:18:LEU:HA	1.99	0.45
1:A:133:ILE:O	1:A:137:TYR:HB2	2.15	0.45
1:A:313:TYR:CZ	1:A:316:ALA:HB2	2.51	0.45
1:B:333:TYR:HB3	1:B:337:LEU:HB2	1.99	0.45
1:B:170:PRO:HB2	1:B:171:ILE:HD12	1.99	0.44
1:B:181:VAL:HG21	1:B:187:VAL:HA	2.00	0.44
1:B:171:ILE:HG13	1:B:237:ILE:HD12	2.00	0.44
1:A:365:PRO:HG3	3:E:13:DG:N3	2.33	0.44
3:E:7:DG:H2"	3:E:8:DG:H8	1.82	0.44
1:B:44:ASN:HA	1:B:47:GLU:HG2	1.99	0.44
3:E:12:DT:H2'	3:E:13:DG:N7	2.33	0.44
1:A:295:GLU:HB2	1:A:324:TRP:HH2	1.83	0.44
1:B:146:VAL:O	1:B:150:THR:OG1	2.34	0.44
2:D:15:DA:C2	3:E:19:DA:C2	3.06	0.44
1:B:343:THR:O	1:B:344:THR:HG22	2.17	0.44
1:B:179:PHE:CZ	1:B:181:VAL:HA	2.53	0.43
1:B:271:LEU:O	1:B:274:VAL:HG12	2.18	0.43
1:A:132:GLN:O	1:A:136:ILE:HG12	2.19	0.43
1:B:323:ASN:O	1:B:327:ILE:HG13	2.19	0.43
1:B:171:ILE:HB	1:B:198:ILE:CG2	2.48	0.43
1:A:394:LEU:HD12	1:A:394:LEU:HA	1.82	0.43
1:B:288:ARG:HA	1:B:288:ARG:HD3	1.79	0.43
1:A:379:VAL:HA	1:A:382:THR:HG22	2.01	0.43
1:B:287:LYS:NZ	2:D:28:DA:OP2	2.52	0.43
3:E:28:DT:H2"	3:E:29:DA:C8	2.53	0.43
1:B:189:LYS:HE3	1:B:189:LYS:HB3	1.75	0.43
1:A:66:LYS:HE3	1:A:66:LYS:H	1.84	0.42
1:A:99:PRO:HB2	1:A:102:VAL:O	2.18	0.42
3:E:5:DT:H2'	3:E:6:DG:H8	1.84	0.42
3:E:5:DT:H2"	3:E:6:DG:O5'	2.19	0.42
1:A:136:ILE:HG13	1:A:137:TYR:CD1	2.54	0.42
1:A:189:LYS:HE3	1:A:189:LYS:HB3	1.86	0.42
1:A:237:ILE:HD11	1:A:260:GLN:HG2	2.01	0.42
1:B:210:TYR:OH	1:B:226:ASP:OD2	2.29	0.42
1:B:127:ARG:HD2	1:B:127:ARG:H	1.85	0.42
1:A:276:ASP:OD2	1:A:279:ARG:HB2	2.20	0.42
1:A:368:GLN:O	1:A:372:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:DT:H2"	2:D:15:DA:C8	2.55	0.42
1:A:103:PRO:HD2	1:A:106:LYS:HD3	2.00	0.42
1:B:213:GLU:H	1:B:213:GLU:HG2	1.39	0.42
2:D:30:DA:H2"	2:D:31:DA:N7	2.35	0.41
1:B:182:LYS:HD3	1:B:367:ASP:HA	2.01	0.41
1:A:220:TRP:CE3	1:A:246:ILE:HD11	2.55	0.41
1:B:251:ASN:HA	1:B:255:PRO:HB3	2.02	0.41
3:E:16:DA:H2"	3:E:17:DA:C8	2.55	0.41
1:A:136:ILE:HG13	1:A:137:TYR:HD1	1.85	0.41
1:A:167:GLU:O	1:A:233:LYS:HB2	2.19	0.41
1:A:267:ILE:HG12	1:A:286:LEU:HD21	2.02	0.41
1:A:66:LYS:H	1:A:66:LYS:CD	2.34	0.41
1:A:182:LYS:HB2	1:A:187:VAL:HG22	2.03	0.41
1:B:150:THR:HG22	1:B:372:LYS:HD3	2.02	0.40
2:D:4:DT:H2"	2:D:5:DA:C8	2.56	0.40
1:A:250:ILE:O	1:A:254:PHE:N	2.52	0.40
1:A:337:LEU:HD21	1:A:399:LEU:HD11	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 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%)	381 (96%)	18 (4%)	0	100 100
1	B	352/410 (86%)	336 (96%)	15 (4%)	1 (0%)	41 75
All	All	751/820 (92%)	717 (96%)	33 (4%)	1 (0%)	51 84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	PRO

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 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%)	336 (93%)	24 (7%)	16 48
1	B	315/366 (86%)	290 (92%)	25 (8%)	12 41
All	All	675/732 (92%)	626 (93%)	49 (7%)	14 45

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	THR
1	A	66	LYS
1	A	68	ASN
1	A	70	ARG
1	A	107	ARG
1	A	113	GLU
1	A	144	GLU
1	A	153	ILE
1	A	165	LEU
1	A	183	ASN
1	A	189	LYS
1	A	234	ASP
1	A	238	LEU
1	A	250	ILE
1	A	265	HIS
1	A	276	ASP
1	A	278	ASP
1	A	284	ARG
1	A	299	TYR
1	A	324	TRP
1	A	334	SER
1	A	341	MET
1	A	357	ILE
1	A	399	LEU
1	B	141	VAL
1	B	148	LYS
1	B	150	THR

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Mol	Chain	Res	Type
1	B	177	ILE
1	B	178	HIS
1	B	184	ASP
1	B	187	VAL
1	B	189	LYS
1	B	211	VAL
1	B	213	GLU
1	B	214	ASN
1	B	224	LEU
1	B	254	PHE
1	B	257	THR
1	B	258	GLU
1	B	259	TYR
1	B	260	GLN
1	B	262	CYS
1	B	289	ILE
1	B	299	TYR
1	B	343	THR
1	B	344	THR
1	B	373	SER
1	B	388	ARG
1	B	389	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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.

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, 95^{th} 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	401/410 (97%)	-0.27	2 (0%) 91 88	90, 146, 191, 233	0
1	B	356/410 (86%)	-0.20	9 (2%) 57 51	92, 158, 212, 242	0
2	D	31/32 (96%)	-0.40	0 100 100	115, 139, 251, 257	0
3	E	31/32 (96%)	-0.31	0 100 100	114, 135, 230, 236	0
All	All	819/884 (92%)	-0.24	11 (1%) 77 71	90, 151, 209, 257	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	PRO	3.6
1	B	187	VAL	3.4
1	B	108	ASP	3.1
1	B	104	ARG	2.9
1	B	277	LYS	2.7
1	B	359	LYS	2.4
1	A	307	GLU	2.2
1	B	183	ASN	2.2
1	A	215	GLU	2.2
1	B	185	GLY	2.1
1	B	239	CYS	2.1

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.