



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 04:11 AM EDT

PDB ID : 1Y97
Title : The human TREX2 3' exonuclease structure suggests a mechanism for efficient non-processive DNA catalysis
Authors : Perrino, F.W.; Harvey, S.; McMillin, S.; Hollis, T.
Deposited on : 2004-12-14
Resolution : 2.50 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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
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) : 2.37.1

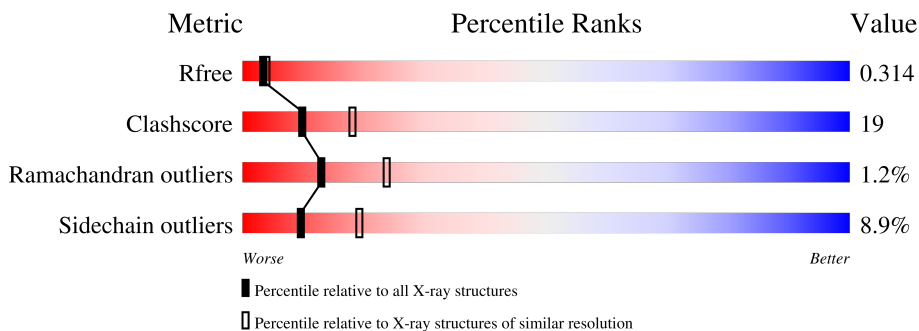
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	238	64% (green), 21% (yellow), 5% (orange), 10% (grey)
1	B	238	60% (green), 24% (yellow), . . (orange), 11% (grey)

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3340 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 Three prime repair exonuclease 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	214	1638	1044	288	297	6	3	0	0	0
1	B	211	1625	1036	282	299	6	2	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	CLONING ARTIFACT	UNP Q9BQ50
A	0	GLY	-	CLONING ARTIFACT	UNP Q9BQ50
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9BQ50
A	64	MSE	MET	MODIFIED RESIDUE	UNP Q9BQ50
A	225	MSE	MET	MODIFIED RESIDUE	UNP Q9BQ50
B	-1	ALA	-	CLONING ARTIFACT	UNP Q9BQ50
B	0	GLY	-	CLONING ARTIFACT	UNP Q9BQ50
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9BQ50
B	64	MSE	MET	MODIFIED RESIDUE	UNP Q9BQ50
B	225	MSE	MET	MODIFIED RESIDUE	UNP Q9BQ50

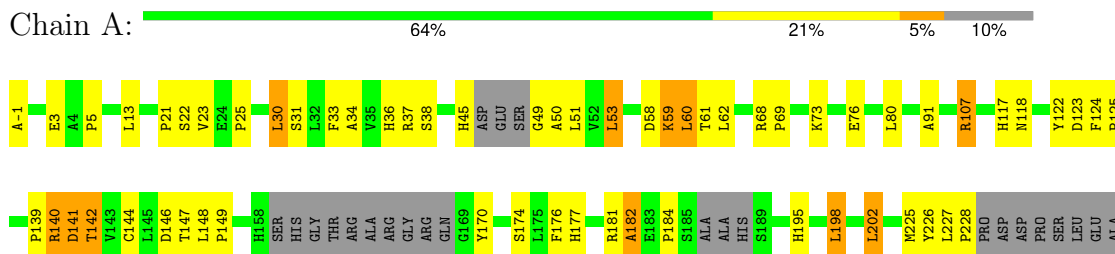
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total 45	O 45	0	0
2	B	32	Total 32	O 32	0	0

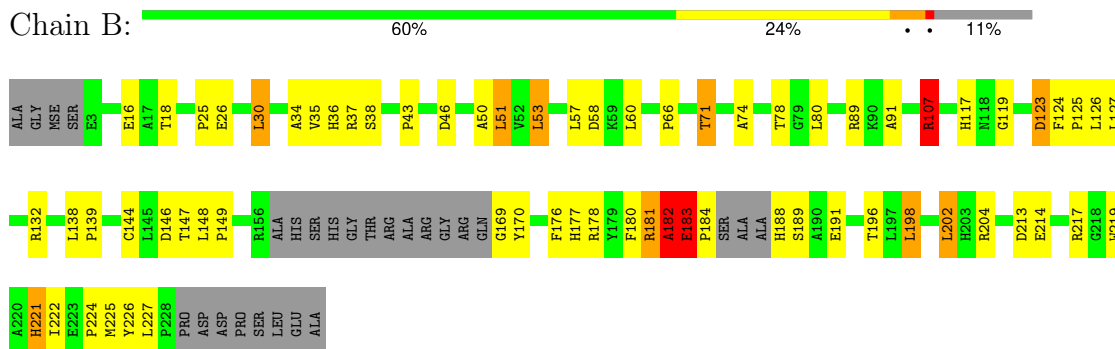
3 Residue-property plots

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. 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: Three prime repair exonuclease 2



- Molecule 1: Three prime repair exonuclease 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.50Å 77.20Å 101.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 43.41 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-2.50) 96.3 (43.41-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	53.90 (at 2.51Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.205 , 0.261 0.264 , 0.314	Depositor DCC
R_{free} test set	720 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtrriage
Anisotropy	0.763	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	3340	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.07% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.71	1/1672 (0.1%)	0.87	1/2264 (0.0%)
1	B	0.78	1/1661 (0.1%)	1.07	6/2254 (0.3%)
All	All	0.75	2/3333 (0.1%)	0.98	7/4518 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	182	ALA	C-N	-10.90	1.08	1.34
1	A	49	GLY	N-CA	5.03	1.53	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	182	ALA	O-C-N	-24.55	83.42	122.70
1	B	182	ALA	C-N-CA	6.92	139.01	121.70
1	B	182	ALA	CA-C-N	5.99	130.38	117.20
1	B	107	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	B	183	GLU	CA-C-N	-5.37	102.08	117.10
1	B	182	ALA	N-CA-C	5.23	125.11	111.00
1	A	37	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	182	ALA	Mainchain

5.2 Too-close contacts [i](#)

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	1638	0	1617	55	2
1	B	1625	0	1590	73	2
2	A	45	0	0	1	0
2	B	32	0	0	1	0
All	All	3340	0	3207	124	2

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 19.

All (124) 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:183:GLU:HB3	1:B:184:PRO:CD	1.34	1.40
1:B:183:GLU:CB	1:B:184:PRO:HD2	1.22	1.35
1:B:181:ARG:O	1:B:182:ALA:HB2	1.36	1.15
1:A:25:PRO:CD	1:A:225:MSE:HE1	1.84	1.08
1:A:25:PRO:HD2	1:A:225:MSE:HE1	1.14	1.07
1:B:181:ARG:O	1:B:182:ALA:CB	1.96	1.07
1:B:183:GLU:CG	1:B:184:PRO:HD2	1.84	1.06
1:B:183:GLU:CB	1:B:184:PRO:CD	2.06	1.05
1:A:25:PRO:HD2	1:A:225:MSE:CE	1.86	1.04
1:B:132:ARG:HH21	1:B:224:PRO:HD3	1.38	0.85
1:B:180:PHE:O	1:B:181:ARG:CB	2.26	0.82
1:B:183:GLU:CD	1:B:184:PRO:CD	2.47	0.82
1:B:124:PHE:HB3	1:B:222:ILE:HD13	1.63	0.80
1:B:126:LEU:HD13	1:B:225:MSE:CE	2.12	0.79
1:B:183:GLU:HB3	1:B:184:PRO:CG	2.14	0.77
1:B:183:GLU:CD	1:B:184:PRO:HD2	2.04	0.77
1:B:71:THR:HG22	1:B:74:ALA:H	1.50	0.76
1:B:183:GLU:CD	1:B:184:PRO:HD3	2.06	0.75
1:B:117:HIS:HD2	1:B:147:THR:OG1	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PRO:O	1:A:142:THR:HG23	1.87	0.73
1:A:139:PRO:O	1:A:142:THR:CG2	2.39	0.71
1:A:36:HIS:CD2	1:A:38:SER:H	2.08	0.71
1:A:25:PRO:CG	1:A:225:MSE:HE1	2.19	0.71
1:A:34:ALA:HB3	1:A:58:ASP:HB2	1.74	0.70
1:A:140:ARG:O	1:A:141:ASP:OD1	2.09	0.70
1:B:71:THR:HG22	1:B:74:ALA:CB	2.22	0.69
1:B:225:MSE:HE3	1:B:226:TYR:HE2	1.57	0.69
1:B:169:GLY:O	1:B:178:ARG:NH2	2.24	0.69
1:A:181:ARG:O	1:A:182:ALA:HB2	1.93	0.68
1:B:217:ARG:HD3	1:B:221:HIS:HE1	1.60	0.67
1:A:117:HIS:HD2	1:A:147:THR:OG1	1.78	0.67
1:B:25:PRO:HG2	1:B:225:MSE:HE1	1.78	0.66
1:B:71:THR:CG2	1:B:74:ALA:H	2.08	0.66
1:A:148:LEU:HB3	1:A:149:PRO:HD3	1.79	0.64
1:B:126:LEU:HD13	1:B:225:MSE:HE2	1.79	0.64
1:B:126:LEU:HD13	1:B:225:MSE:HE1	1.79	0.64
1:B:183:GLU:HB3	1:B:184:PRO:HD2	0.64	0.62
1:B:148:LEU:HB3	1:B:149:PRO:HD3	1.83	0.61
1:B:217:ARG:HD3	1:B:221:HIS:CE1	2.35	0.61
1:B:35:VAL:HG22	1:B:57:LEU:CD1	2.31	0.60
1:B:30:LEU:C	1:B:30:LEU:HD23	2.23	0.59
1:A:73:LYS:HD2	1:A:76:GLU:OE1	2.02	0.59
1:A:5:PRO:HG3	1:A:141:ASP:HB2	1.85	0.59
1:B:35:VAL:HG22	1:B:57:LEU:HD11	1.83	0.59
1:B:225:MSE:HE3	1:B:226:TYR:CE2	2.38	0.59
1:A:30:LEU:HD23	1:A:30:LEU:O	2.03	0.59
1:A:140:ARG:CG	1:A:140:ARG:HH11	2.17	0.57
1:B:36:HIS:HD2	1:B:38:SER:OG	1.87	0.57
1:B:46:ASP:HB3	1:B:50:ALA:H	1.69	0.57
1:B:183:GLU:O	1:B:184:PRO:O	2.22	0.57
1:B:18:THR:O	1:B:71:THR:HB	2.04	0.56
1:A:45:HIS:HA	1:A:50:ALA:O	2.06	0.56
1:B:107:ARG:HD3	2:B:525:HOH:O	2.06	0.56
1:A:36:HIS:HD2	1:A:38:SER:H	1.51	0.55
1:B:182:ALA:O	1:B:183:GLU:O	2.25	0.55
1:A:140:ARG:HH11	1:A:140:ARG:HG3	1.73	0.54
1:A:51:LEU:HD21	1:A:202:LEU:HB3	1.89	0.54
1:B:36:HIS:CD2	1:B:38:SER:H	2.26	0.54
1:A:59:LYS:NZ	1:B:191:GLU:OE1	2.30	0.54
1:A:176:PHE:HD2	1:A:182:ALA:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:HIS:CE1	1:A:184:PRO:HD3	2.43	0.53
1:A:122:TYR:O	1:A:125:PRO:HD2	2.08	0.52
1:B:26:GLU:HB2	1:B:66:PRO:HB3	1.91	0.52
1:B:37:ARG:NH2	1:B:213:ASP:OD2	2.41	0.52
1:B:183:GLU:OE1	1:B:184:PRO:CD	2.57	0.52
1:A:198:LEU:HD22	1:A:202:LEU:HD22	1.92	0.52
1:A:33:PHE:CE1	1:A:59:LYS:HD3	2.46	0.51
1:A:228:PRO:HD3	2:A:539:HOH:O	2.10	0.51
1:B:71:THR:HG22	1:B:74:ALA:HB3	1.92	0.51
1:B:132:ARG:NH2	1:B:224:PRO:HD3	2.17	0.51
1:B:138:LEU:HD12	1:B:219:TRP:CE2	2.46	0.50
1:A:181:ARG:O	1:A:182:ALA:CB	2.59	0.49
1:A:107:ARG:NH2	1:B:91:ALA:HB3	2.28	0.49
1:B:53:LEU:HG	1:B:198:LEU:HD12	1.93	0.49
1:A:36:HIS:CD2	1:A:38:SER:OG	2.65	0.48
1:B:217:ARG:CD	1:B:221:HIS:HE1	2.25	0.48
1:A:140:ARG:CG	1:A:140:ARG:NH1	2.75	0.48
1:A:21:PRO:HA	1:A:225:MSE:CE	2.43	0.48
1:A:59:LYS:HE2	1:B:191:GLU:OE2	2.12	0.48
1:B:198:LEU:HD22	1:B:202:LEU:HD22	1.96	0.48
1:B:30:LEU:HD23	1:B:30:LEU:O	2.14	0.48
1:A:36:HIS:HD2	1:A:38:SER:CB	2.27	0.47
1:B:71:THR:HG22	1:B:74:ALA:HB2	1.97	0.47
1:B:183:GLU:OE1	1:B:184:PRO:HD3	2.12	0.47
1:A:68:ARG:HB3	1:A:69:PRO:HD2	1.96	0.47
1:A:36:HIS:HD2	1:A:38:SER:OG	1.98	0.47
1:A:225:MSE:HE2	1:A:226:TYR:CE2	2.50	0.47
1:B:144:CYS:N	1:B:217:ARG:O	2.48	0.46
1:A:30:LEU:HD22	1:A:62:LEU:HB2	1.96	0.46
1:B:117:HIS:HE1	1:B:170:TYR:O	1.99	0.46
1:A:3:GLU:HA	1:A:3:GLU:OE1	2.16	0.46
1:A:23:VAL:HG12	1:A:23:VAL:O	2.15	0.45
1:A:225:MSE:HE2	1:A:226:TYR:CD2	2.51	0.45
1:B:71:THR:HG22	1:B:74:ALA:N	2.26	0.45
1:B:117:HIS:CD2	1:B:147:THR:OG1	2.61	0.45
1:B:43:PRO:HB3	1:B:51:LEU:HD21	1.98	0.45
1:B:181:ARG:O	1:B:182:ALA:HB3	2.07	0.45
1:A:91:ALA:HB3	1:B:107:ARG:NH2	2.32	0.45
1:A:124:PHE:HB2	1:A:125:PRO:HD3	1.99	0.44
1:B:138:LEU:O	1:B:139:PRO:C	2.55	0.44
1:B:46:ASP:HB2	1:B:50:ALA:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:HA	1:A:60:LEU:O	2.18	0.44
1:B:124:PHE:CE1	1:B:144:CYS:HB3	2.53	0.44
1:A:30:LEU:O	1:A:61:THR:HA	2.17	0.44
1:A:21:PRO:HA	1:A:225:MSE:HE3	2.01	0.43
1:A:177:HIS:ND1	1:A:182:ALA:C	2.72	0.43
1:B:202:LEU:HD13	1:B:202:LEU:HA	1.89	0.42
1:B:146:ASP:O	1:B:149:PRO:HD2	2.20	0.42
1:B:225:MSE:HG2	1:B:226:TYR:HD2	1.85	0.42
1:B:34:ALA:HB3	1:B:58:ASP:HB2	2.02	0.42
1:A:13:LEU:C	1:A:13:LEU:HD12	2.40	0.41
1:A:176:PHE:CD2	1:A:182:ALA:O	2.70	0.41
1:A:53:LEU:HD21	1:A:195:HIS:CD2	2.56	0.41
1:B:132:ARG:HH21	1:B:224:PRO:CD	2.22	0.41
1:A:117:HIS:HE1	1:A:170:TYR:O	2.03	0.41
1:A:124:PHE:CE1	1:A:144:CYS:HB3	2.55	0.41
1:A:117:HIS:CD2	1:A:147:THR:OG1	2.65	0.41
1:B:89:ARG:HG3	1:B:89:ARG:NH1	2.36	0.41
1:B:16:GLU:OE1	1:B:188:HIS:N	2.54	0.40
1:B:74:ALA:O	1:B:78:THR:HG23	2.22	0.40
1:B:119:GLY:O	1:B:125:PRO:HD2	2.21	0.40
1:A:117:HIS:O	1:A:118:ASN:HB3	2.22	0.40
1:A:146:ASP:CG	1:A:149:PRO:HD2	2.42	0.40
1:B:176:PHE:CE2	1:B:183:GLU:HA	2.57	0.40

All (2) 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)
1:A:22:SER:OG	1:B:214:GLU:OE2[2_764]	2.04	0.16
1:A:-1:ALA:N	1:B:123:ASP:OD1[2_664]	2.05	0.15

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	206/238 (87%)	197 (96%)	8 (4%)	1 (0%)	29	48
1	B	205/238 (86%)	196 (96%)	5 (2%)	4 (2%)	7	12
All	All	411/476 (86%)	393 (96%)	13 (3%)	5 (1%)	13	24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	181	ARG
1	B	182	ALA
1	A	182	ALA
1	B	189	SER
1	B	183	GLU

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	169/187 (90%)	155 (92%)	14 (8%)	11	22
1	B	169/187 (90%)	153 (90%)	16 (10%)	8	17
All	All	338/374 (90%)	308 (91%)	30 (9%)	9	19

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	53	LEU
1	A	59	LYS
1	A	60	LEU
1	A	80	LEU
1	A	107	ARG
1	A	123	ASP
1	A	140	ARG
1	A	141	ASP

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Mol	Chain	Res	Type
1	A	142	THR
1	A	174	SER
1	A	198	LEU
1	A	202	LEU
1	A	227	LEU
1	B	30	LEU
1	B	51	LEU
1	B	53	LEU
1	B	60	LEU
1	B	71	THR
1	B	80	LEU
1	B	107	ARG
1	B	123	ASP
1	B	127	LEU
1	B	177	HIS
1	B	196	THR
1	B	198	LEU
1	B	202	LEU
1	B	204	ARG
1	B	221	HIS
1	B	227	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	117	HIS
1	A	158	HIS
1	B	36	HIS
1	B	117	HIS
1	B	221	HIS

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	182:ALA	C	183:GLU	N	1.09

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.