wwPDB X-ray Structure Validation Summary Report (i)

Feb 17, 2024 – 11:02 AM EST

PDB ID	:	3S4Z
Title	:	Structure of a Y DNA-FANCI complex
Authors	:	Pavletich, N.P.
Deposited on	:	2011-05-20
Resolution	:	7.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

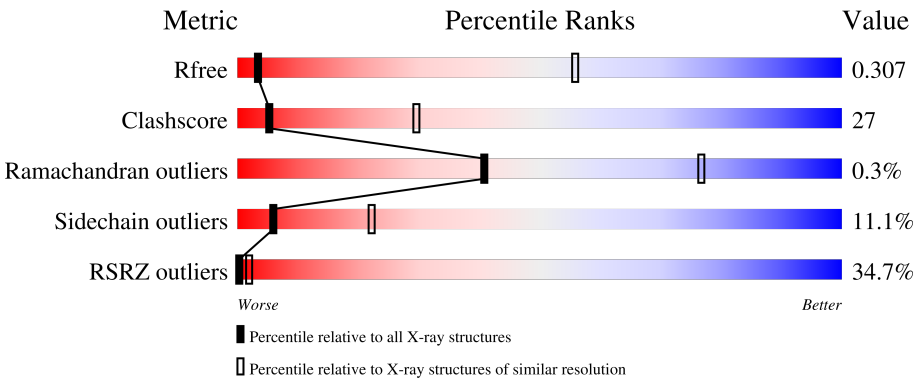
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 7.80 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))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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 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	1308	22%; 44%, 37%, 6%, 14%
1	B	1308	35%; 44%, 37%, 5%, 14%
1	C	1308	33%; 43%, 38%, 5%, 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 26814 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 dna repair 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1131	8938	5748	1485	1652	53	0	0	0
1	B	1131	8938	5748	1485	1652	53	0	0	0
1	C	1131	8938	5748	1485	1652	53	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

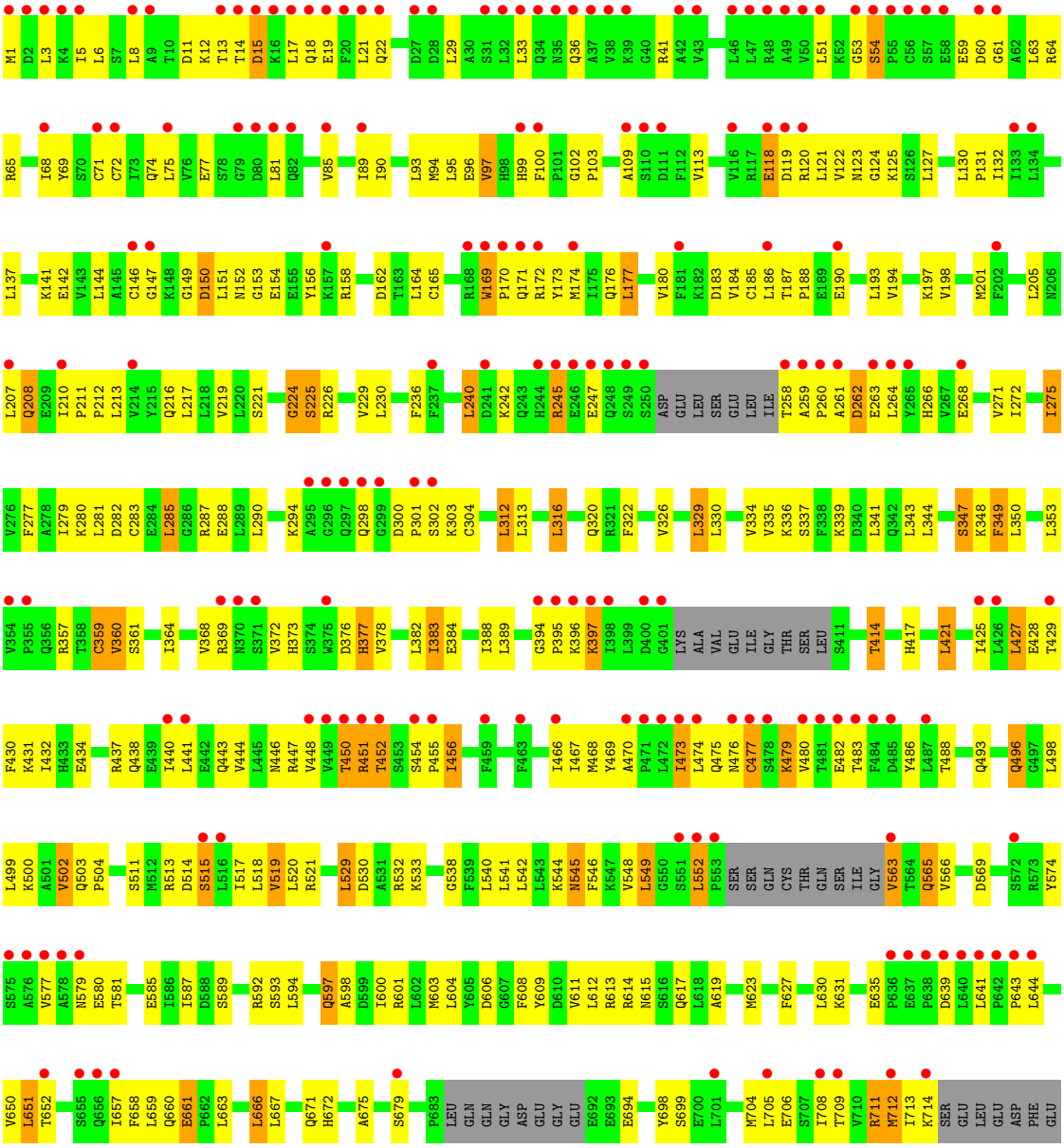
Chain	Residue	Modelled	Actual	Comment	Reference
A	1303	HIS	-	expression tag	UNP Q8K368
A	1304	HIS	-	expression tag	UNP Q8K368
A	1305	HIS	-	expression tag	UNP Q8K368
A	1306	HIS	-	expression tag	UNP Q8K368
A	1307	HIS	-	expression tag	UNP Q8K368
A	1308	HIS	-	expression tag	UNP Q8K368
B	1303	HIS	-	expression tag	UNP Q8K368
B	1304	HIS	-	expression tag	UNP Q8K368
B	1305	HIS	-	expression tag	UNP Q8K368
B	1306	HIS	-	expression tag	UNP Q8K368
B	1307	HIS	-	expression tag	UNP Q8K368
B	1308	HIS	-	expression tag	UNP Q8K368
C	1303	HIS	-	expression tag	UNP Q8K368
C	1304	HIS	-	expression tag	UNP Q8K368
C	1305	HIS	-	expression tag	UNP Q8K368
C	1306	HIS	-	expression tag	UNP Q8K368
C	1307	HIS	-	expression tag	UNP Q8K368
C	1308	HIS	-	expression tag	UNP Q8K368

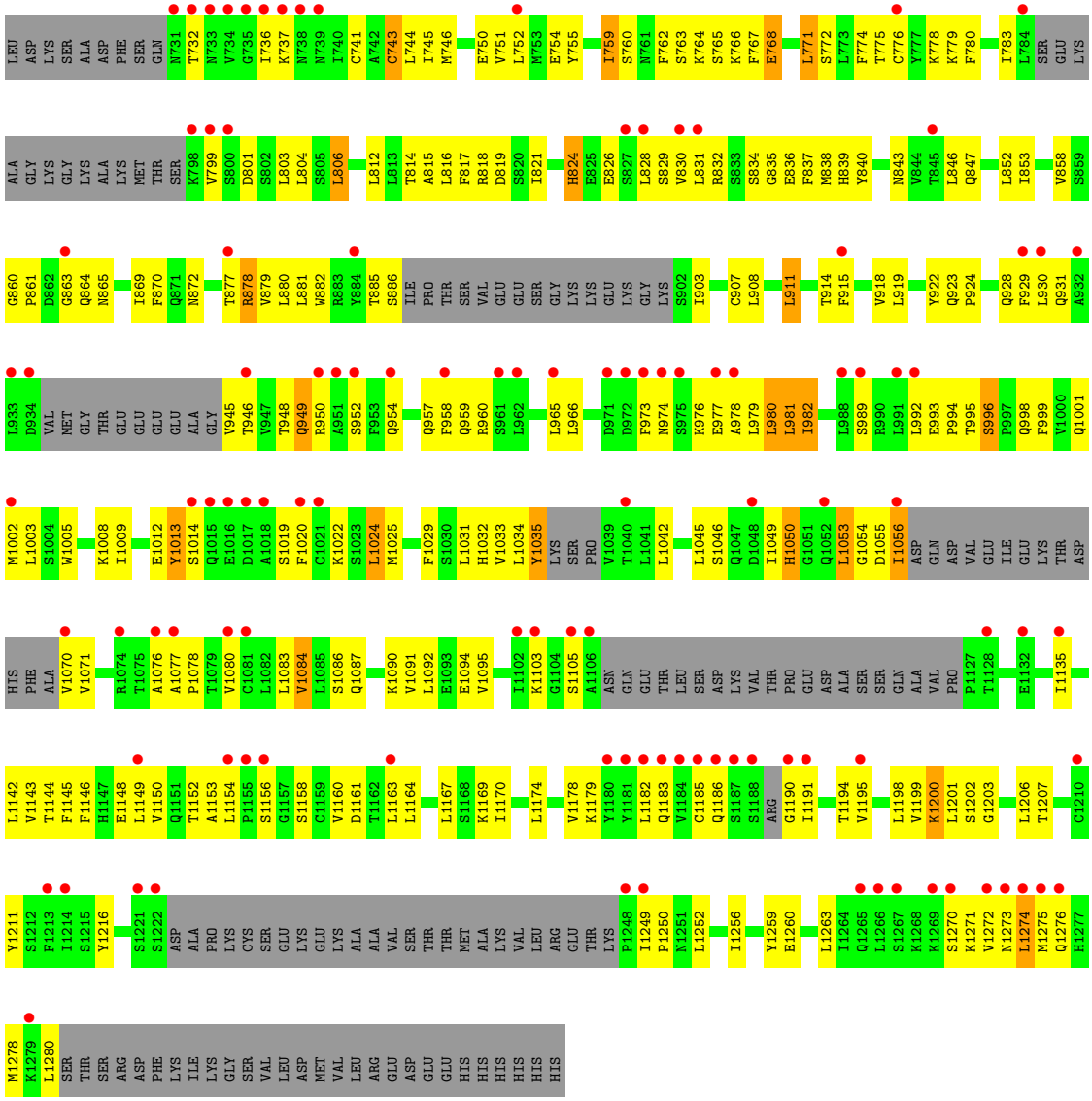
3 Residue-property plots (i)

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: dna repair 1

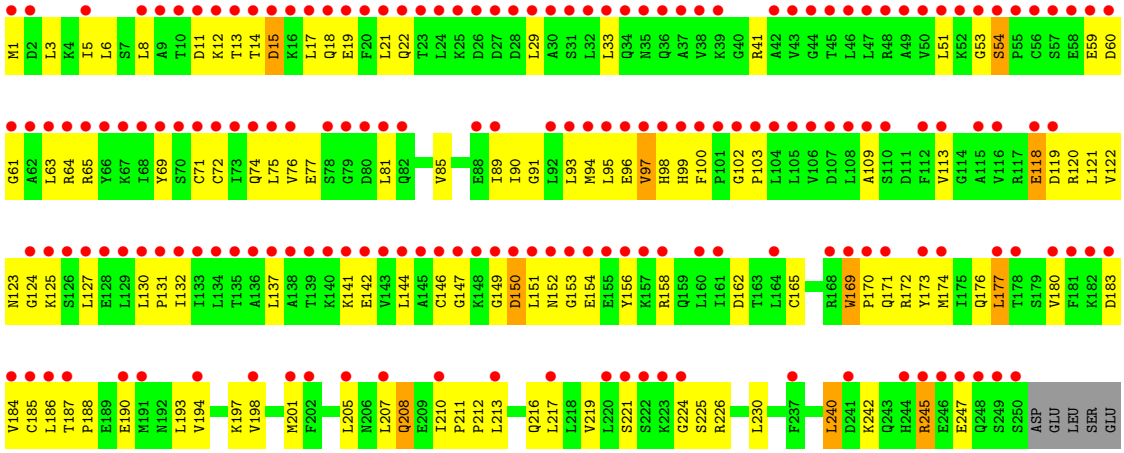
Chain A: 22% 44% 37% 6% 14%

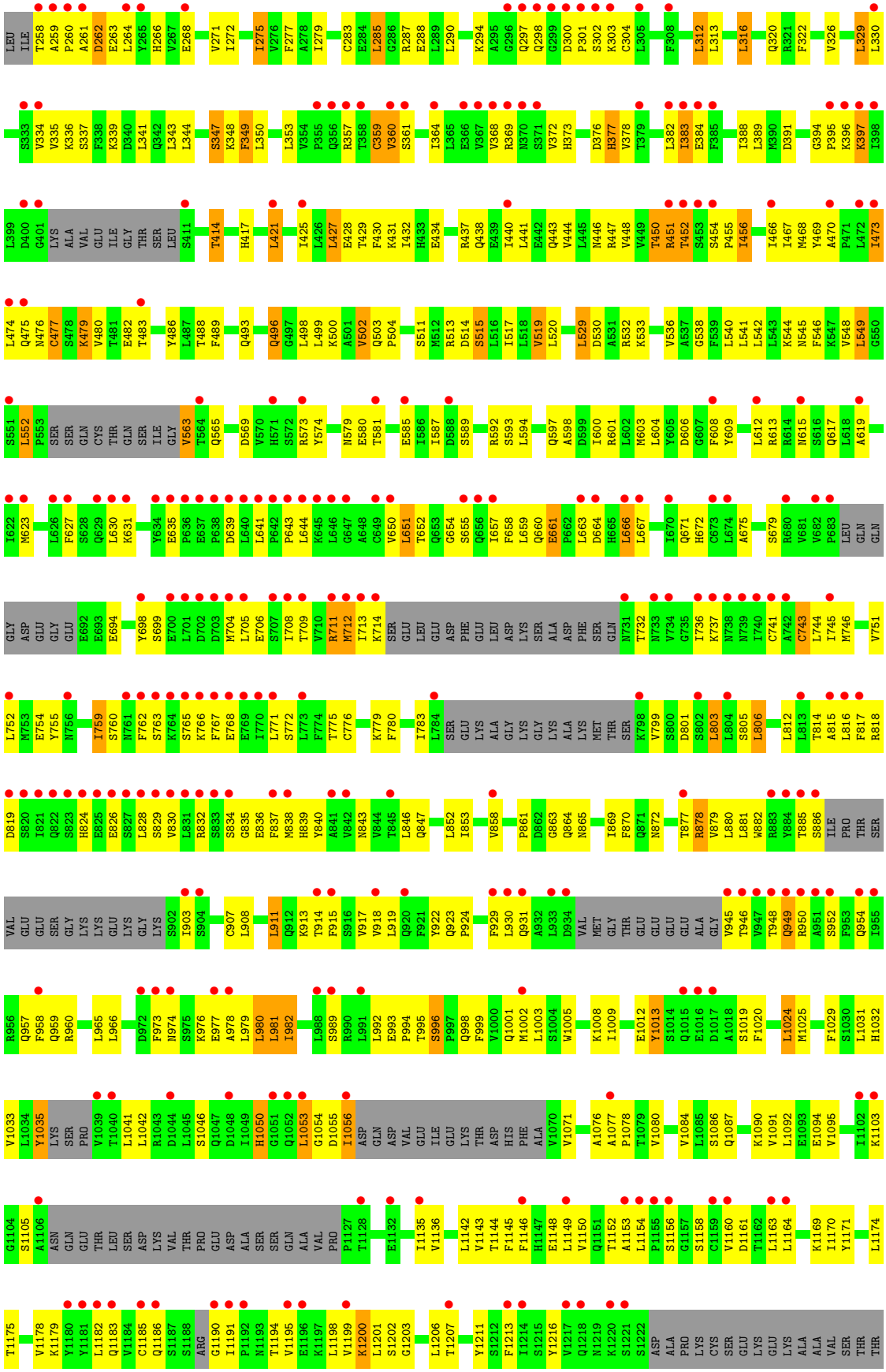


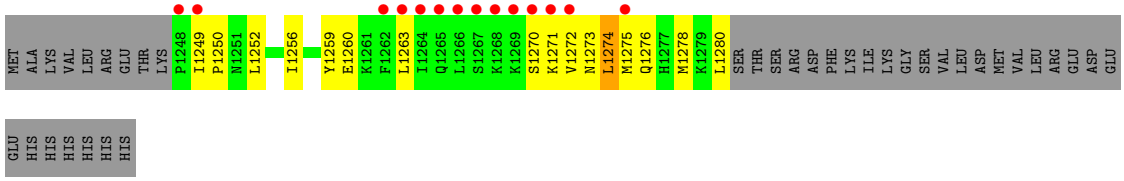


- Molecule 1: dna repair 1

Chain B:

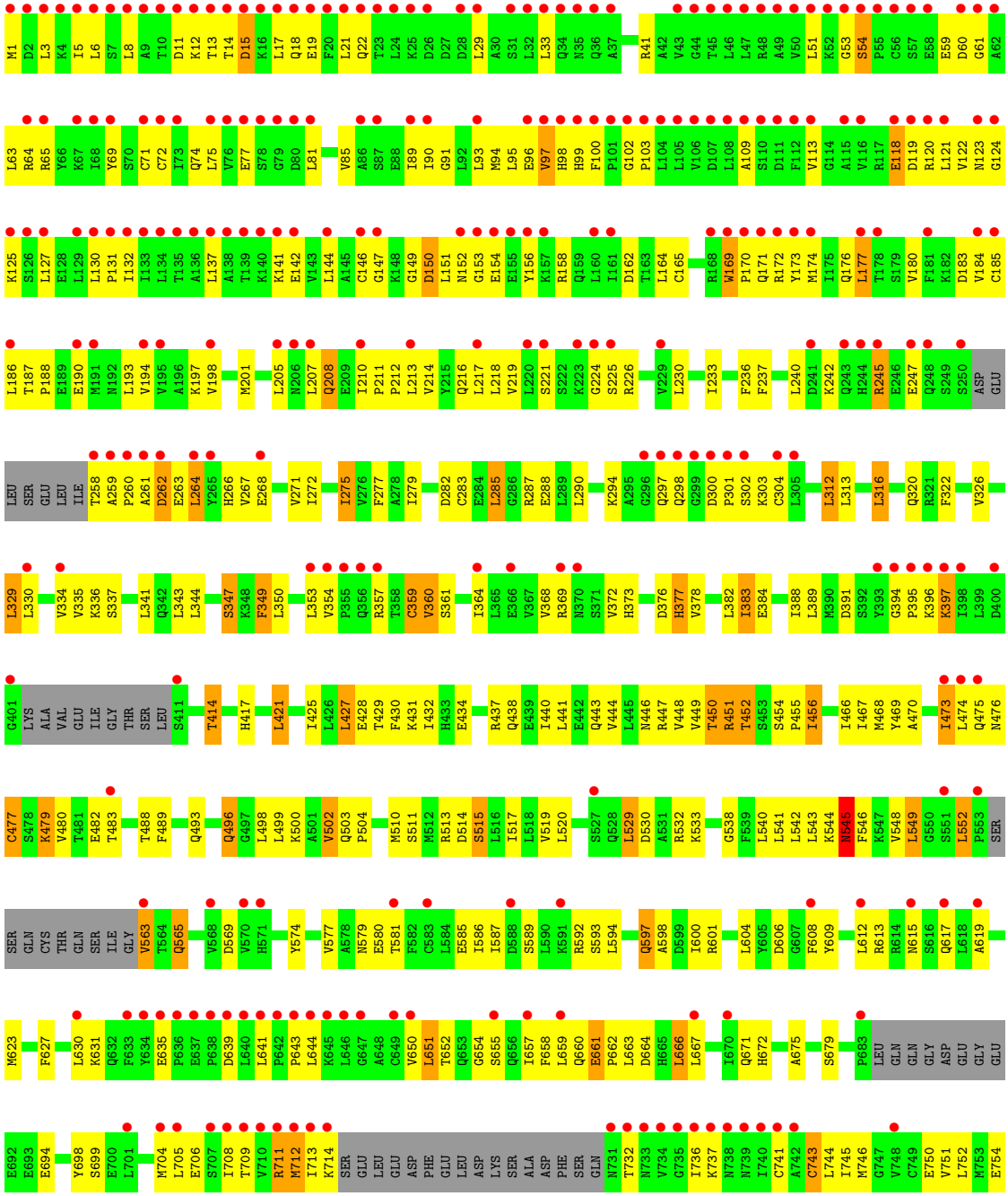


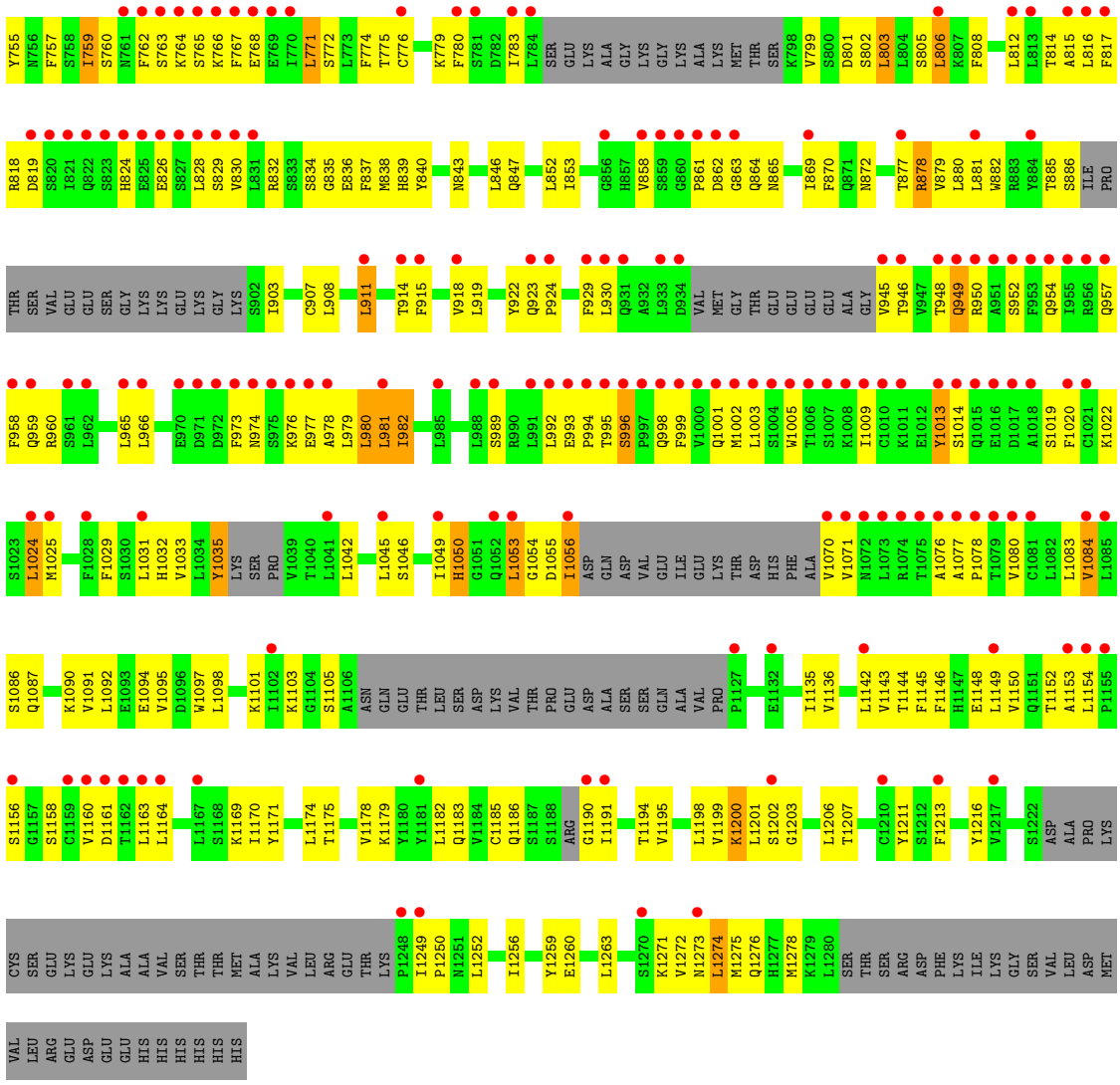

LEU ILE T258 A259 P260 A261 D262 E263 L264 Y265 H266 V267 E268 V271 I272 I275 V276 F277 A278 I279 C283 E284 L285 G286 R287 E288 L289 L290 K294 A295 G296 Q297 Q298 G299 D300 P301 S302 K303 C304 L305 F308 L312 L313 L316 Q320 R321 F322 V326 L329 L330
S333 V334 V335 K336 S337 F338 K339 D340 L341 Q342 L343 L344 S347 K348 F349 L350 L353 V354 P355 Q356 R357 T358 C359 V360 S361 I364 L365 E366 V367 V368 R369 M370 S371 V372 H373 D376 H377 V378 T379 L382 I383 E384 F385 I388 L389 M390 D391 G394 P395 K396 K397 I398
L399 D400 G401 LYS ALA VAL GLU ILE GLY THR SER LEU S411 T414 H417 L421 I425 L426 L427 E428 T429 F430 K431 I432 H433 E434 R437 Q438 E439 I440 L441 E442 Q443 V444 L445 N446 R447 V448 V449 T450 R451 T452 S453 S454 P455 I456 I466 I467 M468 Y469 A470 P471 L472 I473
L474 Q475 N476 C477 S478 K479 V480 T481 E482 T483 Y486 L487 T488 F489 Q493 Q496 G497 L498 L499 K500 A501 V502 Q503 P504 S511 M512 R513 D514 S515 L516 I517 L518 V519 L520 L529 D530 A531 R532 K533 V536 A537 G538 F539 L540 L541 L542 L543 K544 N545 F546 K547 V548 L549 G550
S551 L552 P553 SER SER GLN CYS THR GLN SER ILE GLY V563 T564 Q565 D569 V570 H571 S572 R573 Y574 N579 E580 T581 E585 I586 I587 D588 S589 R592 S593 L594 Q597 A598 D599 I600 R601 L602 M603 L604 Y605 D606 G607 F608 Y609 L612 R613 R614 N615 S616 Q617 L618 A619
I622 M623 L626 F627 S628 Q629 L630 K631 Y634 E635 P636 E637 P638 D639 L640 L641 P642 P643 L644 K645 L646 G647 A648 G649 V650 L651 T652 Q653 G654 S655 Q656 I657 F658 L659 Q660 E661 P662 L663 D664 H665 L666 L667 I670 Q671 H672 G673 L674 A675 S679 R680 V681 V682 P683 LEU GLN GLN
GLY ASP GLU GLY GLU E692 E693 E694 Y698 S699 E700 L701 D702 D703 M704 L705 E706 S707 I708 T709 V710 R711 M712 I713 K714 SER GLU LEU GLU ASP PHE GLU LEU ASP LYS SER ALA ASP PHE SER GLN N731 T732 N733 V734 G735 I736 K737 N738 N739 I740 C741 A742 C743 L744 I745 N746 V751
L752 M753 E754 Y755 N756 I759 S760 N761 F762 S763 K764 S765 K766 F767 E768 E769 I770 L771 S772 L773 F774 T775 C776 K779 F780 I783 L784 SER GLU GLU LYS ALA GLY LYS LYS ALA ALA LYS MET THR SER K798 V799 S800 D801 S802 L803 L804 S805 L806 L812 L813 T814 A815 L816 F817 R818
D819 S820 I821 Q822 S823 H824 E825 E826 S827 L828 S829 V830 L831 R832 S833 S834 G835 E836 F837 M838 H839 Y840 A841 V842 N843 V844 T845 L846 Q847 L852 I853 V858 P861 D862 G863 Q864 N865 I869 F870 Q871 N872 T877 R878 V879 L880 L881 W882 R883 Y884 T885 S886 ILE PRO THR SER
VAL GLU GLU SER GLY LYS LYS GLU LYS GLY LYS S902 I903 S904 C907 L908 L911 Q912 K913 T914 F915 S916 V917 V918 L919 Q920 F921 Y922 Q923 P924 F929 L930 Q931 A932 L933 D934 VAL MET GLY THR GLU GLU GLU GLU ALA GLY V945 T946 V947 T948 Q949 R950 A951 S952 F953 Q954 I955
R956 Q957 F958 Q959 R960 L965 L966 D972 F973 N974 S975 K976 E977 A978 L979 L980 L981 I982 L988 S989 R990 L991 L992 E993 P994 T995 S996 F997 Q998 F999 V1000 Q1001 M1002 L1003 S1004 W1005 K1008 I1009 E1012 Y1013 S1014 Q1015 E1016 D1017 A1018 S1019 F1020 L1024 M1025 F1029 S1030 L1031 H1032
V1033 L1034 Y1035 LYS SER PRO V1039 T1040 L1041 L1042 R1043 D1044 L1045 S1046 Q1047 D1048 I1049 H1050 G1051 Q1052 L1053 G1054 D1055 I1056 ASP GLN ASP VAL GLU ILE GLU LYS THR ASP HIS PHE ALA V1070 V1071 A1076 A1077 P1078 T1079 V1080 V1084 L1085 S1086 Q1087 K1090 V1091 L1092 E1093 E1094 V1095 I1102 K1103
G1104 S1105 A1106 ASN GLN GLU THR LEU SER ASP LYS VAL THR PRO GLU ASP ALA SER SER GLN ALA VAL PRO P1127 T1128 E1132 I1135 V1136 L1142 V1143 T1144 F1145 F1146 H1147 E1148 L1149 V1150 Q1151 T1152 A1153 L1154 P1155 S1156 G1157 S1158 C1159 V1160 D1161 T1162 L1163 L1164 K1169 I1170 Y1171 L1174
T1175 V1178 K1179 Y1180 Y1181 L1182 Q1183 V1184 C1185 Q1186 S1187 S1188 ARG G1190 I1191 P1192 N1193 T1194 V1195 E1196 K1197 L1198 V1199 K1200 L1201 S1202 G1203 L1206 T1207 Y1211 S1212 F1213 I1214 S1215 Y1216 V1217 Q1218 N1219 K1220 S1221 S1222 ASP ALA PRO LYS CYS SER GLU LYS GLU LYS ALA ALA VAL SER THR THR



• Molecule 1: dna repair 1

Chain C:




Y755 N756 F757 S758 I759 S760 N761 F762 S763 K764 S765 K766 F767 E768 E769 I770 L771 S772 L773 F774 T775 C776 K779 F780 S781 D782 I783 L784 SER GLU LYS ALA GLY LYS GLY LYS ALA LYS MET THR SER K798 V799 S800 D801 S802 L803 L804 S805 L806 K807 F808 L812 L813 T814 A815 L816 F817
R818 D819 S820 I821 Q822 S823 H824 E825 E826 S827 L828 S829 V830 L831 R832 S833 S834 G835 E836 F837 M838 H839 Y840 N843 L846 Q847 L852 I853 G856 H857 V858 S859 G860 P861 D862 G863 Q864 N865 I869 F870 Q871 N872 T877 R878 V879 L880 L881 W882 R883 Y884 T885 S886 ILE PRO
THR SER VAL GLU GLU SER GLY LYS LYS GLU LYS GLY LYS S902 I903 C907 L908 L911 T914 F915 V918 L919 Y922 Q923 P924 F929 L930 Q931 A932 L933 D934 VAL MET GLY THR GLU GLU GLU GLU ALA GLY V945 T946 V947 T948 Q949 R950 A951 S952 F953 Q954 I955 R956 Q957
F958 Q959 R960 S961 L962 L965 L966 E970 D971 D972 F973 N974 S975 K976 E977 A978 L979 L980 L981 I982 L985 L988 S989 R990 L991 L992 E993 P994 T995 S996 P997 Q998 F999 V1000 Q1001 M1002 L1003 S1004 W1005 T1006 S1007 K1008 I1009 C1010 K1011 E1012 Y1013 S1014 Q1015 E1016 D1017 A1018 S1019 F1020 C1021 K1022
S1023 L1024 M1025 F1028 F1029 S1030 L1031 H1032 V1033 L1034 Y1035 LYS SER PRO V1039 T1040 L1041 L1042 L1045 S1046 I1049 H1050 G1051 Q1052 L1053 G1054 D1055 I1056 ASP GLN ASP VAL GLU ILE GLU LYS THR ASP HIS PHE ALA V1070 V1071 N1072 L1073 R1074 T1075 A1076 A1077 P1078 T1079 V1080 C1081 L1082 L1083 V1084 L1085
S1086 Q1087 K1090 V1091 L1092 E1093 E1094 V1095 D1096 W1097 L1098 K1101 I1102 K1103 G1104 S1105 A1106 ASN GLN GLU THR LEU SER ASP LYS VAL THR PRO GLU ASP ALA SER SER GLN ALA VAL PRO P1127 E1132 I1135 V1136 L1142 V1143 T1144 F1145 F1146 H1147 E1148 L1149 V1150 Q1151 T1152 A1153 L1154 P1155
S1156 G1157 S1158 C1159 V1160 D1161 T1162 L1163 L1164 L1167 S1168 K1169 I1170 Y1171 L1174 T1175 V1178 K1179 Y1180 Y1181 L1182 Q1183 V1184 C1185 Q1186 S1187 S1188 ARG G1190 I1191 T1194 V1195 L1198 V1199 K1200 L1201 S1202 G1203 L1206 T1207 C1210 Y1211 S1212 F1213 Y1216 V1217 S1222 ASP ALA PRO LYS
CYS SER GLU LYS GLU LYS ALA ALA VAL SER THR THR MET ALA LYS VAL LEU ARG GLU THR LYS P1248 I1249 P1250 N1251 L1252 I1256 Y1259 E1260 L1263 S1270 K1271 V1272 N1273 L1274 M1275 Q1276 H1277 M1278 K1279 L1280 SER THR SER ARG ASP PHE LYS ILE LYS GLY SER VAL LEU ASP MET
VAL LEU ARG GLU ASP GLU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	235.20Å 307.90Å 375.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 7.80 50.02 – 7.80	Depositor EDS
% Data completeness (in resolution range)	85.3 (33.00-7.80) 85.2 (50.02-7.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.35 (at 7.37Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.310 , 0.324 0.303 , 0.307	Depositor DCC
R_{free} test set	604 reflections (4.10%)	wwPDB-VP
Wilson B-factor (Å^2)	473.6	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 619.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	26814	wwPDB-VP
Average B, all atoms (Å^2)	413.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.76% 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 (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	0.42	4/9075 (0.0%)	0.62	6/12252 (0.0%)
1	B	0.26	2/9073 (0.0%)	0.46	0/12246
1	C	0.27	3/9074 (0.0%)	0.48	3/12249 (0.0%)
All	All	0.33	9/27222 (0.0%)	0.52	9/36747 (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	A	0	1
1	B	0	1
1	C	0	2
All	All	0	4

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	GLY	C-N	25.03	1.91	1.34
1	A	545	ASN	C-N	18.55	1.76	1.34
1	B	320	GLN	CD-NE2	-6.82	1.15	1.32
1	A	320	GLN	CD-NE2	-6.82	1.15	1.32
1	C	320	GLN	CD-NE2	-6.80	1.15	1.32

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	224	GLY	O-C-N	-34.14	68.08	122.70
1	A	224	GLY	CA-C-N	21.55	164.61	117.20
1	A	224	GLY	C-N-CA	15.07	159.37	121.70
1	C	545	ASN	C-N-CA	-11.18	93.76	121.70
1	A	545	ASN	O-C-N	10.27	139.13	122.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1053	LEU	Peptide
1	B	1053	LEU	Peptide
1	C	1053	LEU	Peptide
1	C	545	ASN	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	8938	0	9247	507	13
1	B	8938	0	9247	452	0
1	C	8938	0	9248	527	0
All	All	26814	0	27742	1452	13

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 27.

The worst 5 of 1452 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:208:GLN:HE22	1:A:263:GLU:CG	1.18	1.57
1:C:210:ILE:CD1	1:C:236:PHE:CE2	1.90	1.52
1:C:207:LEU:HD22	1:C:237:PHE:CE2	1.48	1.46
1:A:545:ASN:C	1:A:546:PHE:N	1.76	1.37
1:A:208:GLN:NE2	1:A:263:GLU:HG2	1.38	1.34

The worst 5 of 13 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:281:LEU:CD1	1:A:486:TYR:CZ[7_455]	0.71	1.49
1:A:281:LEU:CD1	1:A:486:TYR:CE2[7_455]	0.84	1.36
1:A:280:LYS:NZ	1:A:446:ASN:OD1[7_455]	1.39	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:LYS:NZ	1:A:446:ASN:CG[7_455]	1.47	0.73
1:A:281:LEU:CD1	1:A:486:TYR:CE1[7_455]	1.61	0.59

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	1103/1308 (84%)	1019 (92%)	80 (7%)	4 (0%)	34 72
1	B	1099/1308 (84%)	1016 (92%)	80 (7%)	3 (0%)	41 77
1	C	1101/1308 (84%)	1019 (93%)	79 (7%)	3 (0%)	41 77
All	All	3303/3924 (84%)	3054 (92%)	239 (7%)	10 (0%)	41 77

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	150	ASP
1	A	225	SER
1	B	122	VAL
1	B	150	ASP

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	1029/1188 (87%)	914 (89%)	115 (11%)	6 22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1029/1188 (87%)	914 (89%)	115 (11%)	6	22
1	C	1029/1188 (87%)	915 (89%)	114 (11%)	6	22
All	All	3087/3564 (87%)	2743 (89%)	344 (11%)	6	22

5 of 344 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	19	GLU
1	C	529	LEU
1	C	119	ASP
1	C	349	PHE
1	C	661	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	377	HIS
1	C	672	HIS
1	B	377	HIS
1	B	597	GLN
1	B	672	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	2
1	A	2
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	224:GLY	C	225:SER	N	4.08
1	B	224:GLY	C	225:SER	N	2.63
1	B	545:ASN	C	546:PHE	N	2.09
1	A	224:GLY	C	225:SER	N	1.91
1	A	545:ASN	C	546:PHE	N	1.76

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	1131/1308 (86%)	1.37	289 (25%)	0	2	267, 382, 546, 649	0
1	B	1131/1308 (86%)	2.17	453 (40%)	0	1	285, 384, 602, 757	0
1	C	1131/1308 (86%)	2.05	437 (38%)	0	1	302, 421, 620, 719	0
All	All	3393/3924 (86%)	1.87	1179 (34%)	0	2	267, 397, 598, 757	0

The worst 5 of 1179 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	GLY	19.1
1	C	105	LEU	13.8
1	B	49	ALA	13.7
1	B	99	HIS	13.3
1	B	52	LYS	13.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.