wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:17 AM GMT

PDB ID	:	3E0D
Title	:	Insights into the Replisome from the Crystral Structure of the Ternary Complex of the Eubacterial DNA Polymerase III alpha-subunit
Authors	:	Wing, R.A.; Bailey, S.; Steitz, T.A.
Deposited on	:	2008-07-31
Resolution	:	4.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

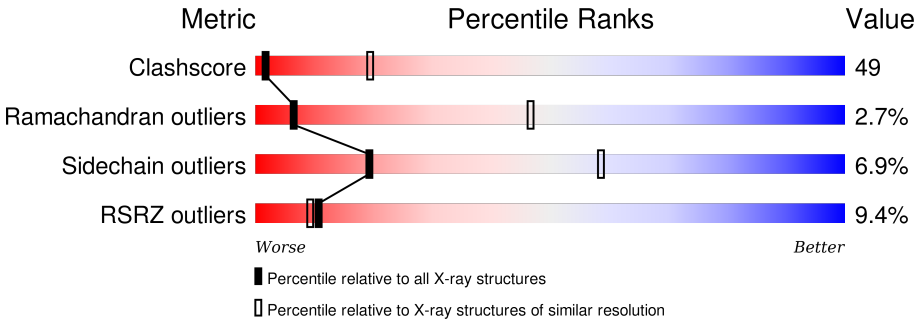
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 4.60 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))
Clashscore	102246	1004 (5.52-3.64)
Ramachandran outliers	100387	1131 (5.52-3.60)
Sidechain outliers	100360	1112 (5.50-3.60)
RSRZ outliers	91569	1092 (5.52-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	C	27	4% · 67% · 26%
1	E	27	70% · 26%
2	D	21	5% 62% 19% 5% 10%
2	F	21	86% 5% 10%
3	A	1220	10% 61% 28% · · 6%
3	B	1220	8% 61% 28% · · 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DOC	D	21	-	-	X	-
2	DOC	F	21	-	-	X	-
5	DTP	A	1222	-	-	X	-
5	DTP	B	1222	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19982 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 DNA chain called DNA substrate template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	20	Total	C	N	O	P	0	0	0
			407	195	69	124	19			
1	E	20	Total	C	N	O	P	0	0	0
			407	195	69	124	19			

- Molecule 2 is a DNA chain called DNA substrate primer strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	19	Total	C	N	O	P	0	0	0
			385	183	78	106	18			
2	F	19	Total	C	N	O	P	0	0	0
			385	183	78	106	18			

- Molecule 3 is a protein called DNA polymerase III subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1148	Total	C	N	O	S	0	0	0
			9168	5847	1605	1688	28			
3	B	1148	Total	C	N	O	S	0	0	0
			9168	5847	1605	1688	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	ASN	ASP	ENGINEERED	UNP Q9XDH5
A	212	ASN	ASP	ENGINEERED	UNP Q9XDH5
A	539	PHE	ILE	ENGINEERED	UNP Q9XDH5
A	540	GLU	GLN	ENGINEERED	UNP Q9XDH5
A	541	ALA	VAL	ENGINEERED	UNP Q9XDH5
A	542	GLU	VAL	ENGINEERED	UNP Q9XDH5
B	20	ASN	ASP	ENGINEERED	UNP Q9XDH5
B	212	ASN	ASP	ENGINEERED	UNP Q9XDH5

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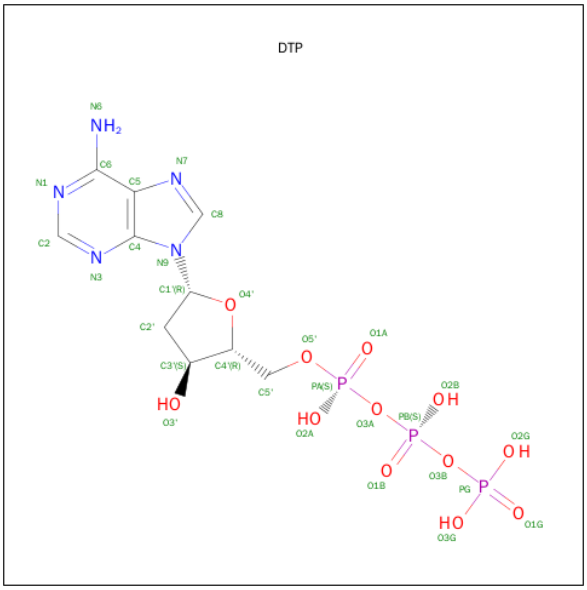
Chain	Residue	Modelled	Actual	Comment	Reference
B	539	PHE	ILE	ENGINEERED	UNP Q9XDH5
B	540	GLU	GLN	ENGINEERED	UNP Q9XDH5
B	541	ALA	VAL	ENGINEERED	UNP Q9XDH5
B	542	GLU	VAL	ENGINEERED	UNP Q9XDH5

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0
4	A	1	Total Ca 1 1	0	0

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



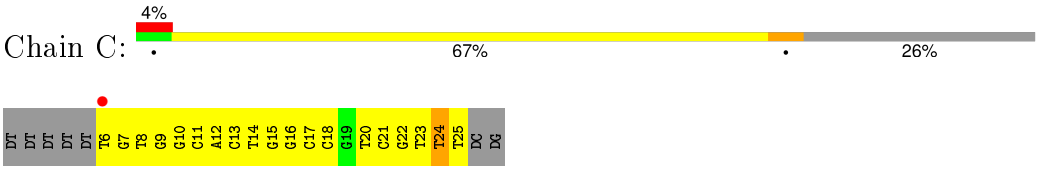
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 30 10 5 12 3	0	0
5	B	1	Total C N O P 30 10 5 12 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

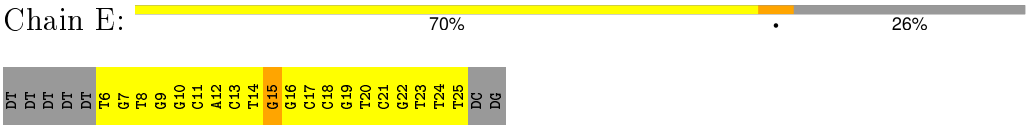
- Molecule 1: DNA substrate template strand

Chain C:



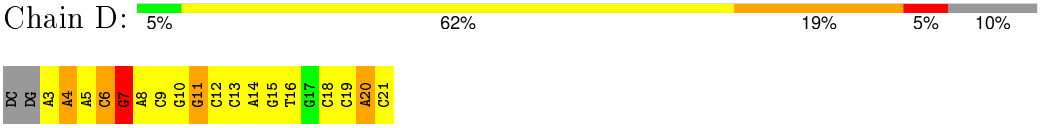
- Molecule 1: DNA substrate template strand

Chain E:



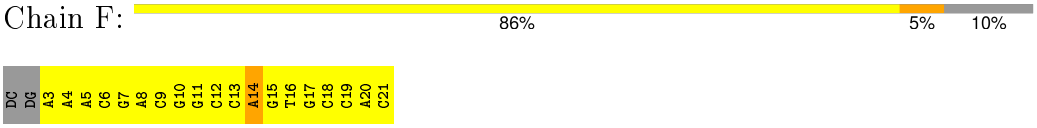
- Molecule 2: DNA substrate primer strand

Chain D:



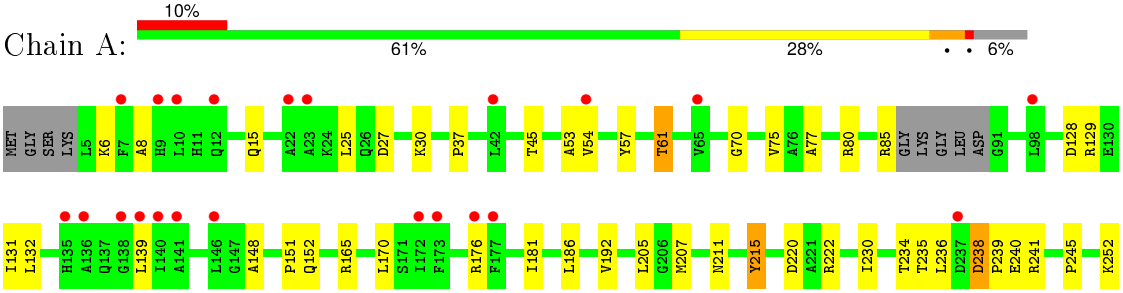
- Molecule 2: DNA substrate primer strand

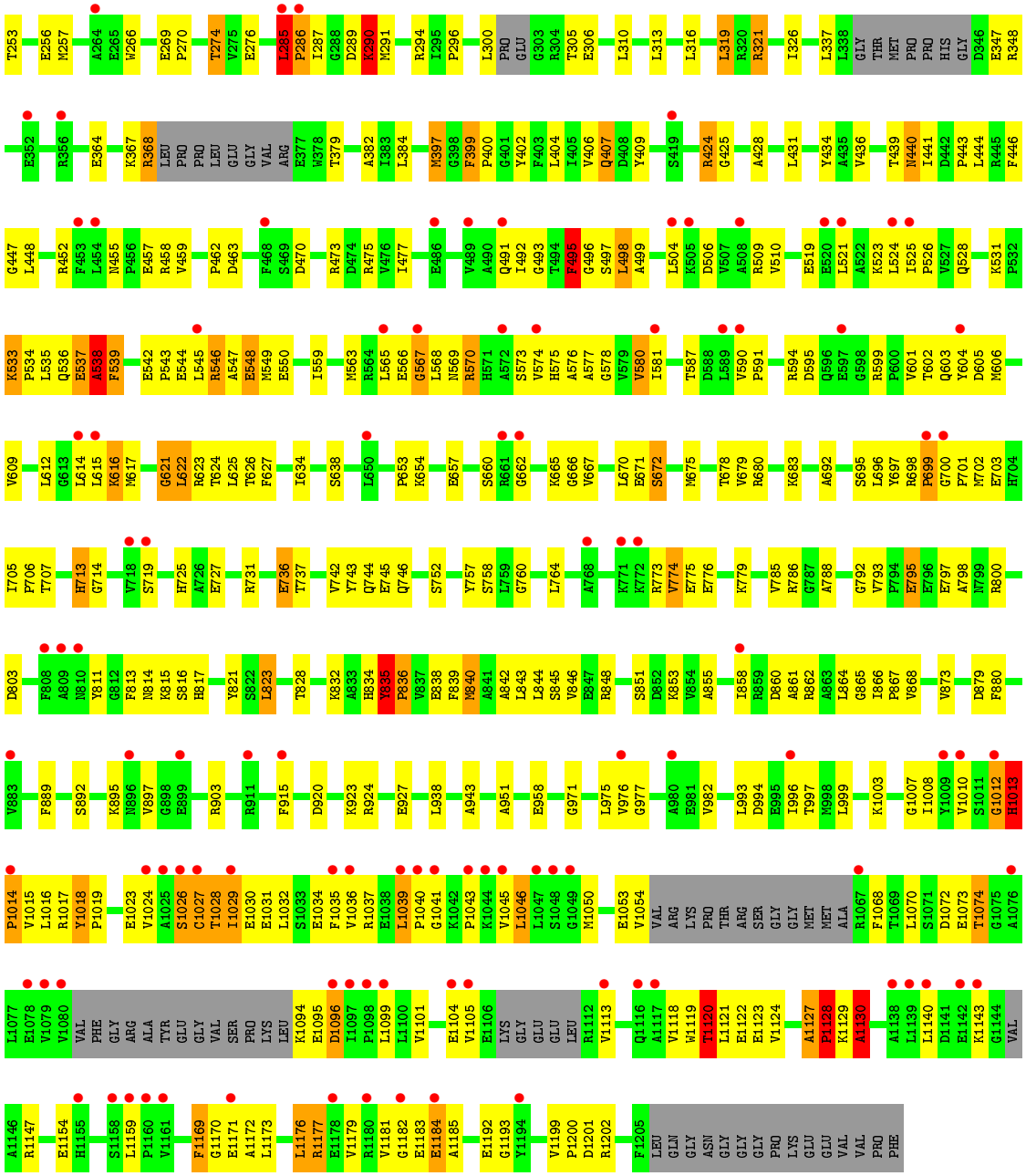
Chain F:



- Molecule 3: DNA polymerase III subunit alpha

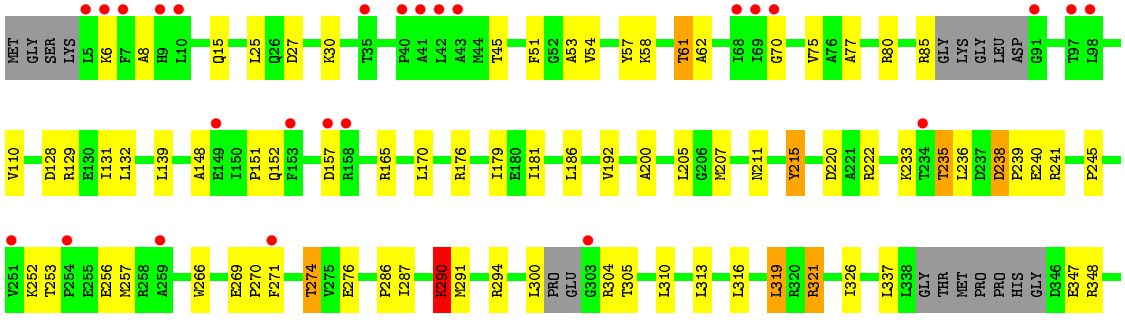
Chain A:

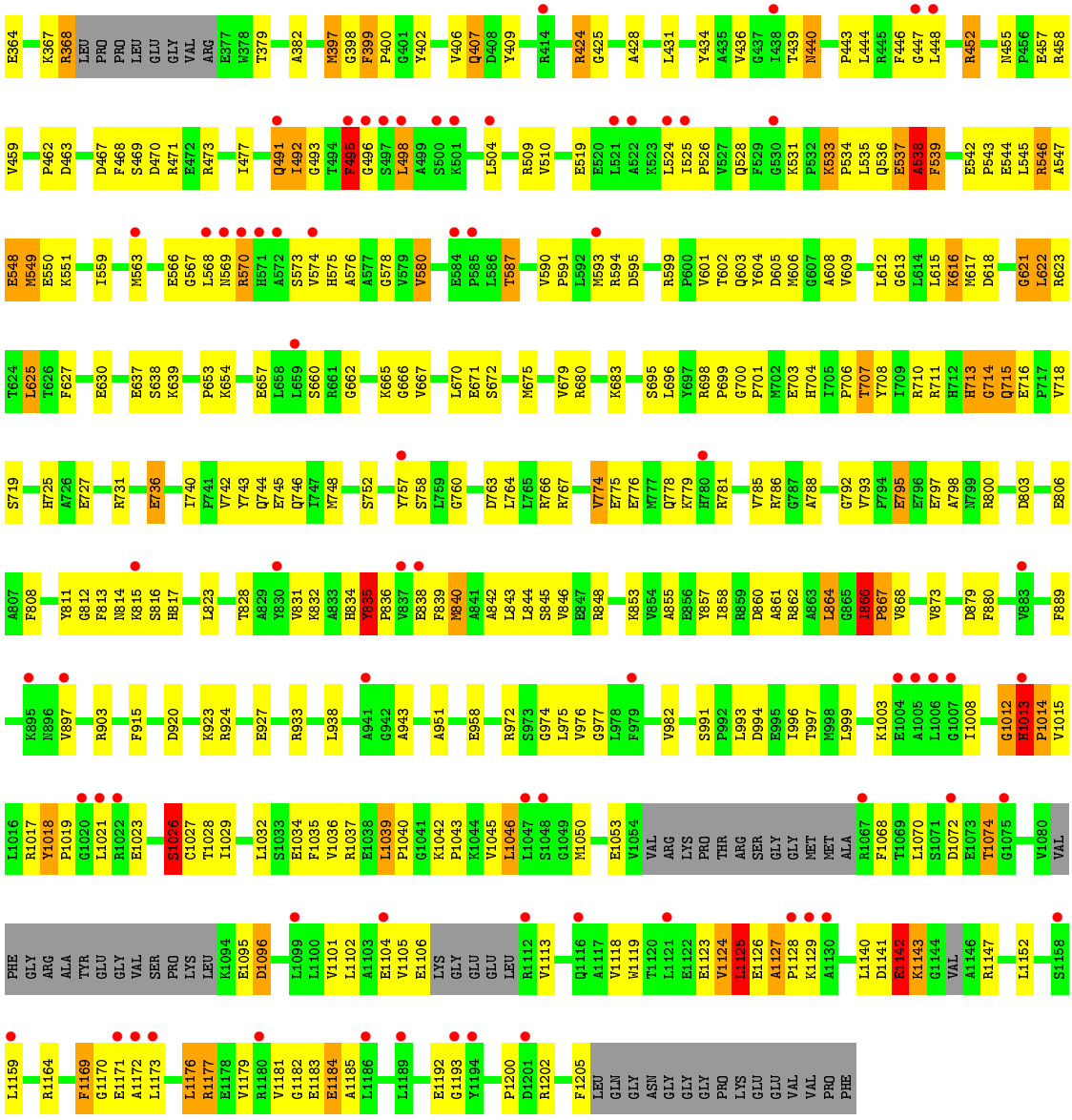




• Molecule 3: DNA polymerase III subunit alpha

Chain B:




E364 K367 R368 LEU PRO PRO LEU GLU GLY VAL ARG E377 W378 T379 A382 M397 G398 F399 P400 G401 Y402 V406 Q407 D408 Y409 R414 R424 G425 A428 L431 Y434 A435 V436 G437 I438 T439 N440 P443 L444 R445 F446 G447 L448 R452 N455 P456 E457 R458
V459 P462 D463 D467 F468 S469 D470 R471 E472 R473 I477 Q491 I492 G493 T494 P495 G496 S497 L498 A499 S500 K501 L504 R509 V510 E519 E520 L521 A522 K523 L524 I525 P526 V527 Q528 F529 G530 K531 P532 K533 P534 L535 Q536 E537 A538 F539 E542 P543 E544 L545 R546 A547
E548 M549 E550 K551 I559 M563 E566 G567 L568 N569 R570 H571 A572 S573 V574 H575 A576 A577 G578 V579 V580 E584 P585 L586 T587 V590 P591 L592 M593 R594 D595 R599 P600 V601 T602 Q603 Y604 D605 M606 G607 A608 V609 L612 G613 L614 L615 K616 M617 D618 G621 L622 R623
T624 L625 T626 F627 E630 E637 S638 K639 P653 K654 E657 L658 L659 S660 R661 G662 K665 G666 V667 L670 E671 S672 M675 V679 R680 K683 S695 L696 Y697 R698 P699 G700 P701 M702 E703 H704 I705 P706 T707 Y708 L709 R710 R711 H712 H713 G714 Q715 E716 P717 V718
S719 H725 A726 E727 R731 E736 I740 P741 V742 Y743 Q744 E745 Q746 I747 M748 S752 Y757 S758 L759 G760 D763 L764 L765 R766 R767 V774 E775 E776 M777 Q778 K779 H780 R781 V785 R786 G787 A788 G792 V793 P794 E795 E796 E797 A798 N799 R800 D803 E806
A807 F808 Y811 G812 F813 N814 K815 S816 H817 L823 T828 A829 Y830 V831 K832 A833 H834 Y835 P836 V837 E838 F839 M840 A841 A842 L843 L844 S845 V846 E847 R848 K853 V854 A855 E856 Y857 I858 R859 D860 A861 R862 A863 L864 G865 I866 P867 V868 V873 D879 F880 V883 F889
K895 N896 V897 R903 F915 D920 K923 R924 E927 R933 L938 A941 G942 A943 A961 E958 R972 S973 G974 L975 V976 G977 L978 F979 V982 S991 P992 L993 D994 E995 I996 T997 M998 L999 K1003 E1004 A1005 L1006 G1007 I1008 G1012 H1013 P1014 V1015
L1016 R1017 Y1018 P1019 G1020 L1021 R1022 E1023 S1026 C1027 T1028 I1029 L1032 S1033 E1034 F1035 V1036 R1037 E1038 L1039 P1040 G1041 K1042 P1043 K1044 V1045 L1046 L1047 S1048 G1049 M1050 E1053 V1054 VAL ARG LYS PRO THR ARG SER GLY GLY MET MET ALA R1067 F1068 T1069 L1070 S1071 D1072 E1073 T1074 G1075 V1080 VAL
PHE GLY ARG ALA TYR GLU GLY VAL SER PRO LYS LEU K1094 E1095 D1096 L1099 L1100 V1101 L1102 A1103 E1104 V1105 E1106 LYS GLY GLU GLU LEU R1112 V1113 Q1116 A1117 V1118 W1119 T1120 L1121 E1122 E1123 V1124 L1125 E1126 A1127 P1128 K1129 A1130 L1140 D1141 E1142 K1143 G1144 VAL A1146 R1147 L1152 S1158
L1159 R1164 F1169 G1170 E1171 A1172 L1173 L1176 R1177 E1178 V1179 R1180 V1181 G1182 E1183 E1184 A1185 L1186 L1189 E1192 G1193 Y1194 P1200 D1201 R1202 F1205 LEU GLN GLY ASN GLY GLY GLY PRO LYS GLU GLU VAL VAL PRO PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	149.55Å 149.55Å 163.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.60 49.85 – 4.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-4.60) 99.5 (49.85-4.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 4.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.287 , 0.271 0.303 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	215.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 198.0	EDS
Estimated twinning fraction	0.347 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 20097 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	19982	wwPDB-VP
Average B, all atoms (Å^2)	233.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, CA, DTP

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	C	2.18	1/454 (0.2%)	1.01	3/700 (0.4%)
1	E	0.74	1/454 (0.2%)	0.88	0/700
2	D	1.93	1/413 (0.2%)	1.24	6/635 (0.9%)
2	F	0.85	1/413 (0.2%)	0.95	0/635
3	A	0.68	13/9348 (0.1%)	1.00	21/12615 (0.2%)
3	B	0.79	14/9346 (0.1%)	0.84	20/12608 (0.2%)
All	All	0.84	31/20428 (0.2%)	0.94	50/27893 (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
2	D	0	3
3	A	3	8
3	B	4	11
All	All	7	22

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	DT	O3'-P	43.89	2.13	1.61
3	B	713	HIS	C-N	34.20	1.94	1.33
3	B	397	MET	C-N	29.55	1.86	1.33
2	D	3	DA	O3'-P	29.28	1.96	1.61
3	A	567	GLY	C-N	28.47	1.99	1.34

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	495	PHE	O-C-N	-47.05	43.21	123.20
3	A	699	PRO	CA-C-N	-41.86	32.49	116.20
3	A	699	PRO	C-N-CA	-39.91	38.49	122.30
3	A	1127	ALA	C-N-CD	-29.66	55.35	120.60
3	A	495	PHE	C-N-CA	-28.34	62.79	122.30

5 of 7 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	538	ALA	CA
3	A	1013	HIS	CA
3	A	1120	THR	CB
3	B	538	ALA	CA
3	B	866	ILE	CA

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	285	LEU	Mainchain
3	A	337	LEU	Mainchain
2	D	11	DG	Sidechain
2	D	20	DA	Sidechain
2	D	7	DG	Sidechain

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	C	407	0	230	199	0
1	E	407	0	229	139	0
2	D	385	0	212	143	1
2	F	385	0	212	79	0
3	A	9168	0	9186	856	33
3	B	9168	0	9182	793	35
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	30	0	12	24	0
5	B	30	0	11	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19982	0	19274	1892	36

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 49.

The worst 5 of 1892 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)
3:A:1013:HIS:CE1	3:A:1073:GLU:HB3	1.26	1.68
3:A:858:ILE:HD11	3:A:889:PHE:CZ	1.24	1.65
3:A:844:LEU:HB3	3:A:880:PHE:CE1	1.24	1.64
3:B:831:VAL:HG12	3:B:839:PHE:CD1	1.14	1.63
3:B:832:LYS:HB2	3:B:839:PHE:CE2	1.26	1.63

The worst 5 of 36 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)
3:A:1177:ARG:NH2	3:B:972:ARG:CA[3_655]	0.82	1.38
3:A:1154:GLU:O	3:B:157:ASP:OD2[1_655]	0.99	1.21
3:A:657:GLU:OE2	3:B:654:LYS:N[2_655]	1.00	1.20
3:A:1177:ARG:NH2	3:B:972:ARG:CB[3_655]	1.14	1.06
3:A:654:LYS:N	3:B:657:GLU:OE2[2_655]	1.22	0.98

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
3	A	1124/1220 (92%)	1006 (90%)	88 (8%)	30 (3%)	6 47
3	B	1120/1220 (92%)	1007 (90%)	82 (7%)	31 (3%)	6 46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2244/2440 (92%)	2013 (90%)	170 (8%)	61 (3%)	6 47

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	286	PRO
3	A	537	GLU
3	A	538	ALA
3	A	774	VAL
3	A	836	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
3	A	953/1008 (94%)	889 (93%)	64 (7%)	20 59
3	B	953/1008 (94%)	886 (93%)	67 (7%)	19 58
All	All	1906/2016 (94%)	1775 (93%)	131 (7%)	19 58

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	1104	GLU
3	B	222	ARG
3	B	1046	LEU
3	A	1169	PHE
3	B	75	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	9	HIS
3	B	440	ASN
3	B	1116	GLN

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Mol	Chain	Res	Type
3	B	15	GLN
3	B	455	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	DOC	D	21	1,2	11,19,20	0.87	1 (9%)	14,26,29	1.30	2 (14%)
2	DOC	F	21	1,2	11,19,20	0.91	1 (9%)	14,26,29	1.27	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DOC	D	21	1,2	-	0/3/18/19	0/2/2/2
2	DOC	F	21	1,2	-	0/3/18/19	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	21	DOC	C6-C5	-2.23	1.33	1.38
2	F	21	DOC	C6-C5	-2.16	1.33	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	21	DOC	C3'-C2'-C1'	2.46	105.45	102.71
2	D	21	DOC	C2-N3-C4	3.25	120.19	115.61
2	F	21	DOC	C2-N3-C4	3.27	120.23	115.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	21	DOC	25	0
2	F	21	DOC	16	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DTP	A	1222	4	24,32,32	1.25	2 (8%)	32,50,50	1.18	4 (12%)
5	DTP	B	1222	4	24,32,32	1.25	2 (8%)	32,50,50	1.18	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DTP	A	1222	4	-	0/18/34/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DTP	B	1222	4	-	0/18/34/34	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1222	DTP	O4'-C1'	-3.01	1.35	1.42
5	A	1222	DTP	O4'-C1'	-3.00	1.35	1.42
5	B	1222	DTP	PA-O2A	-2.88	1.42	1.54
5	A	1222	DTP	PA-O2A	-2.84	1.42	1.54

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1222	DTP	C2'-C1'-N9	-2.86	107.20	114.16
5	B	1222	DTP	C2'-C1'-N9	-2.83	107.28	114.16
5	A	1222	DTP	O3G-PG-O3B	-2.20	95.11	105.09
5	B	1222	DTP	O3G-PG-O3B	-2.19	95.17	105.09
5	B	1222	DTP	O2G-PG-O1G	2.21	117.70	110.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1222	DTP	24	0
5	B	1222	DTP	14	0

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	C	20/27 (74%)	-0.08	1 (5%) 32 26	228, 228, 228, 228	0
1	E	20/27 (74%)	-0.38	0 100 100	228, 228, 228, 228	0
2	D	18/21 (85%)	-0.26	0 100 100	66, 228, 228, 228	0
2	F	18/21 (85%)	-0.26	0 100 100	228, 228, 228, 228	0
3	A	1148/1220 (94%)	0.41	125 (10%) 7 7	201, 226, 296, 326	0
3	B	1148/1220 (94%)	0.39	97 (8%) 14 11	201, 226, 296, 326	0
All	All	2372/2536 (93%)	0.38	223 (9%) 11 9	66, 226, 296, 326	0

The worst 5 of 223 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	1026	SER	8.4
3	B	496	GLY	8.2
3	B	569	ASN	7.4
3	B	524	LEU	6.8
3	B	1129	LYS	6.6

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	DOC	D	21	18/19	0.78	0.19	-	227,227,227,227	0
2	DOC	F	21	18/19	0.67	0.26	-	227,227,227,227	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DTP	B	1222	30/30	0.80	0.28	0.38	242,242,242,242	0
5	DTP	A	1222	30/30	0.83	0.25	-0.73	242,242,242,242	0
4	CA	A	1221	1/1	0.97	0.26	-	47,47,47,47	0
4	CA	B	1221	1/1	0.96	0.24	-	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.