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

wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2017 – 11:43 AM EDT

PDB ID : 5TXN

Title : STRUCTURE OF Q151M MUTANT HIV-1 REVERSE TRANSCRIPTASE (RT) TERNARY COMPLEX WITH A DOUBLE STRANDED DNA AND AN INCOMING DATP

Authors : Das, K.; Martinez, S.M.; Arnold, E.

Deposited on : unknown

Resolution : 2.55 Å(reported)

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

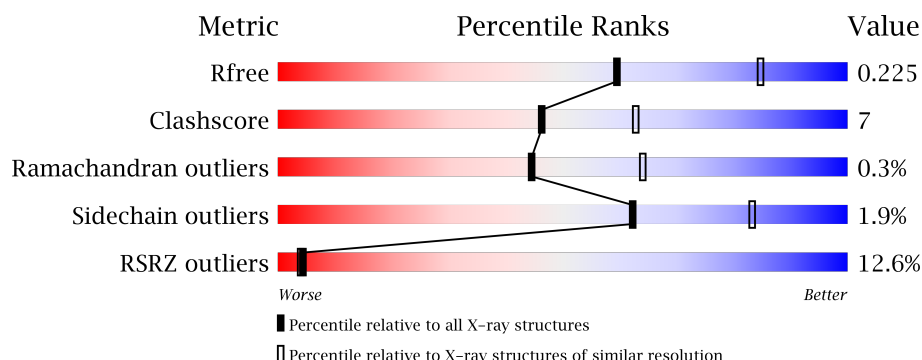|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029824

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 2.55 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		0.225
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		1.9%
RSRZ outliers		12.6%

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$_{free}$	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

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 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	A	556	15% 82% 17% •
1	C	556	15% 80% 20% •
2	B	428	7% 82% 14% • •
2	D	428	11% 82% 14% •
3	E	27	15% 37% 52% 11%

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Mol	Chain	Length	Quality of chain
3	T	27	22% · 59% · 26% · 11%
4	F	21	5% · 43% · 52% · 5%
4	P	21	10% · 38% · 52% · 5% 5%

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
5	MG	A	602	-	-	-	X
9	SO4	D	502	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 17923 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 HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4510	2920	750	831	9			
1	C	555	Total	C	N	O	S	0	0	0
			4510	2920	750	831	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	151	MET	GLN	engineered mutation	UNP P03366
A	258	CYS	GLN	engineered mutation	UNP P03366
A	280	SER	CYS	engineered mutation	UNP P03366
A	498	ASN	ASP	engineered mutation	UNP P03366
C	-1	MET	-	initiating methionine	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	151	MET	GLN	engineered mutation	UNP P03366
C	258	CYS	GLN	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366
C	498	ASN	ASP	engineered mutation	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			
2	D	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	engineered mutation	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*G)-3').

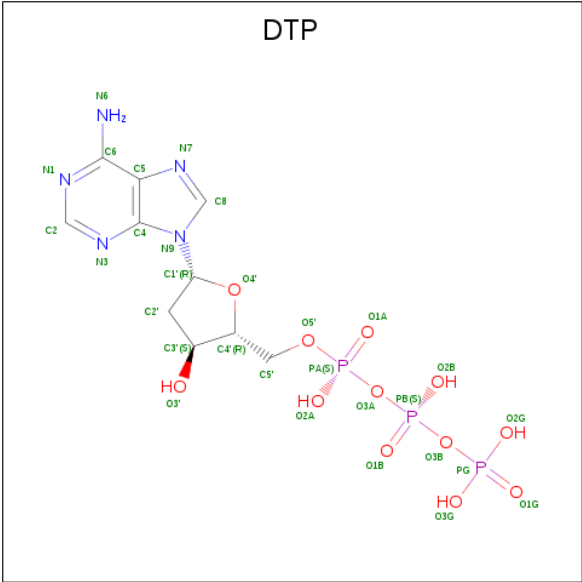| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	24	Total	C	N	O	P	0	0	0
			494	233	97	141	23			
3	E	24	Total	C	N	O	P	0	0	0
			494	233	97	141	23			

- Molecule 4 is a DNA chain called DNA (5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	P	20	Total	C	N	O	P	S	0	0	0
			407	195	72	120	19	1			
4	F	20	Total	C	N	O	P	S	0	0	0
			407	195	72	120	19	1			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 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
6	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
6	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 7 is SUCROSE (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).
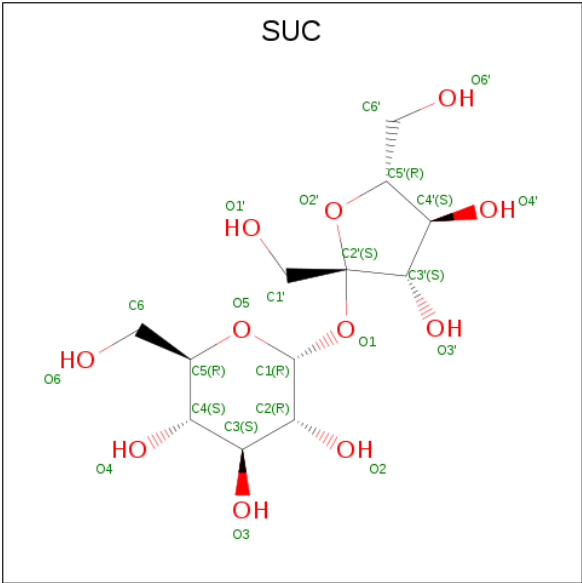
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			23	12	11		
7	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total C O 4 2 2		0	0
8	D	1	Total C O 4 2 2		0	0

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
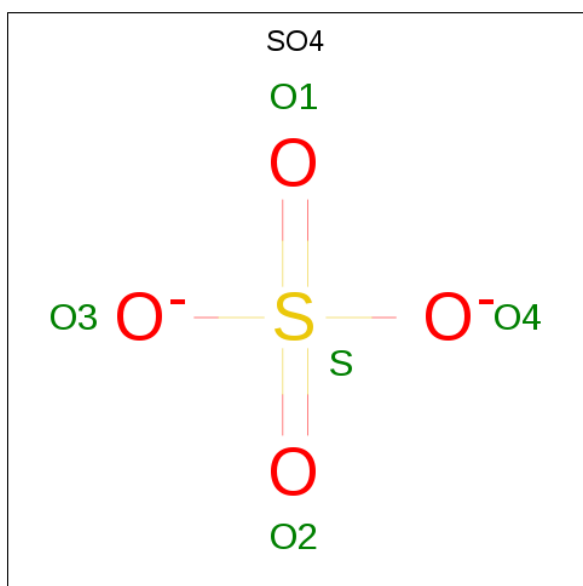
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total O S 5 4 1		0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	50	Total 50	O 50	0	0
10	B	42	Total 42	O 42	0	0
10	T	1	Total 1	O 1	0	0
10	P	1	Total 1	O 1	0	0
10	C	48	Total 48	O 48	0	0
10	D	33	Total 33	O 33	0	0
10	E	1	Total 1	O 1	0	0
10	F	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
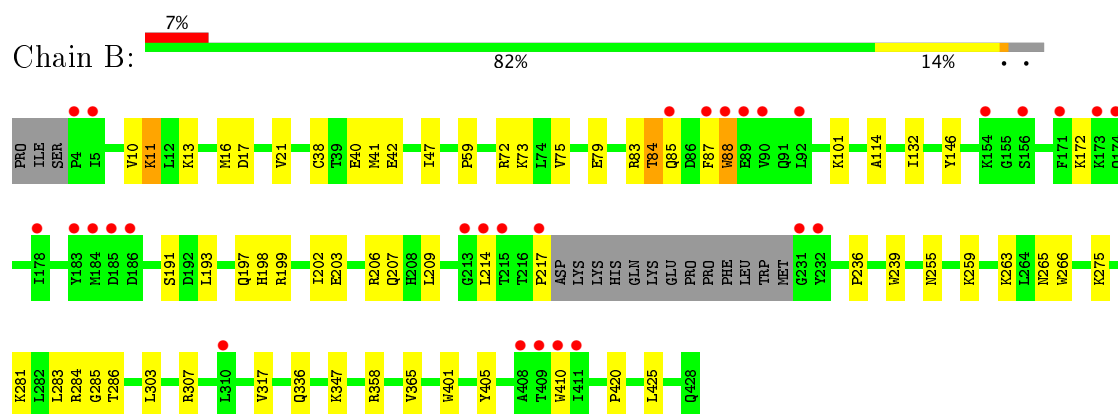
- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT
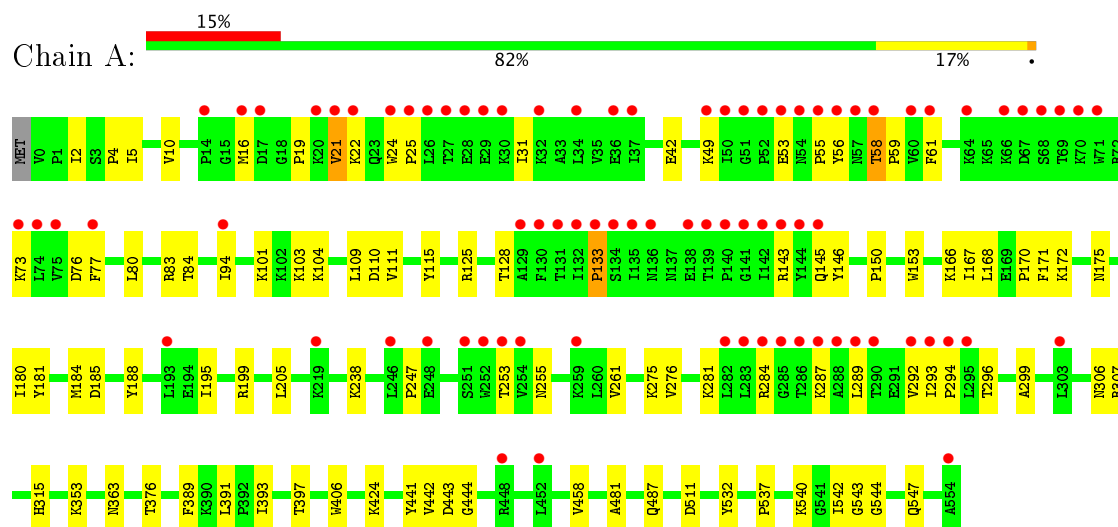
- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT
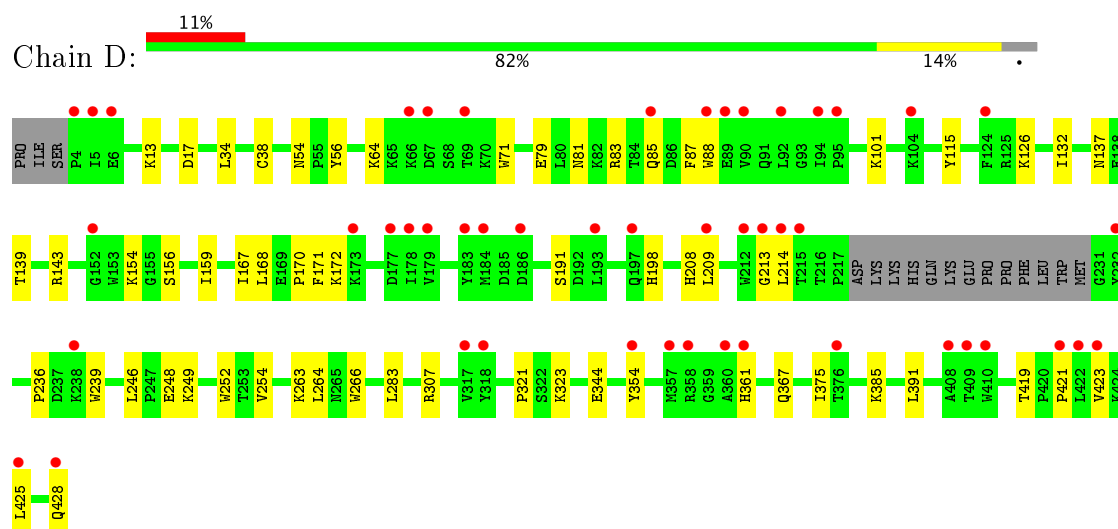
Chain B:

• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT

Chain D:

• Molecule 3: DNA (5'-D(*TP*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP
*AP*GP*GP*GP*AP*CP*TP*G)-3')

Chain T:

• Molecule 3: DNA (5'-D(*TP*GP*GP*TP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP
*AP*GP*GP*GP*AP*CP*TP*G)-3')

Chain E:

• Molecule 4: DNA (5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)
P*CP*GP*CP*CP*G)-3')

Chain P:
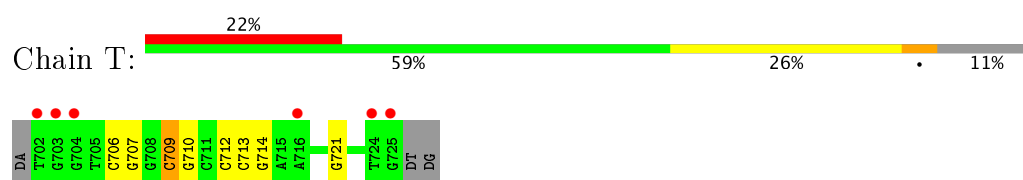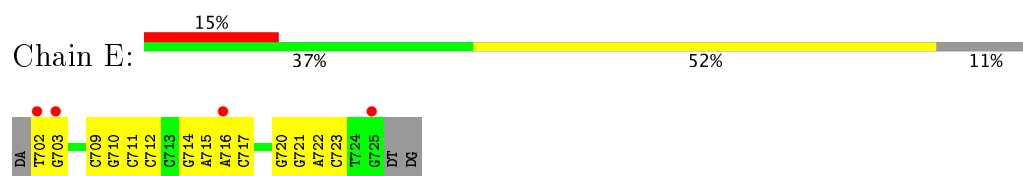
● Molecule 4: DNA (5'-D(*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*(MRG)P*CP*GP*CP*CP*G)-3')

4   Data and refinement statistics (i)

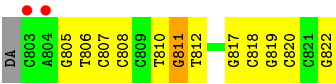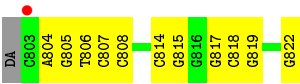| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.04Å 133.63Å 139.21Å 90.00° 97.88° 90.00°	Depositor
Resolution (Å)	33.38 – 2.55 36.37 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.2 (33.38-2.55) 97.4 (36.37-2.53)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.196 , 0.226 0.192 , 0.225	Depositor DCC
R_{free} test set	3042 reflections (2.92%)	DCC
Wilson B-factor (Å^2)	57.2	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.2	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17923	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MRG, SUC, EDO, SO4, 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	A	0.25	0/4628	0.45	1/6288 (0.0%)
1	C	0.27	1/4628 (0.0%)	0.43	1/6288 (0.0%)
2	B	0.27	1/3497 (0.0%)	0.45	1/4751 (0.0%)
2	D	0.28	2/3497 (0.1%)	0.44	1/4751 (0.0%)
3	E	0.52	0/555	0.85	0/856
3	T	0.51	0/555	0.87	1/856 (0.1%)
4	F	0.54	0/424	0.94	0/649
4	P	0.61	1/424 (0.2%)	1.03	2/649 (0.3%)
All	All	0.31	5/18208 (0.0%)	0.52	7/25088 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	172	LYS	CE-NZ	-6.31	1.33	1.49
2	D	172	LYS	CE-NZ	-6.27	1.33	1.49
1	C	172	LYS	CE-NZ	-6.27	1.33	1.49
2	D	391	LEU	C-N	5.66	1.45	1.34
4	P	811	DG	C4'-O4'	5.28	1.50	1.45

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	820	DC	O4'-C4'-C3'	-9.46	100.32	106.00
3	T	709	DC	O4'-C4'-C3'	-6.50	101.90	104.50
1	A	73	LYS	CB-CA-C	-5.77	98.86	110.40
2	B	172	LYS	CD-CE-NZ	5.37	124.04	111.70
2	D	172	LYS	CD-CE-NZ	5.36	124.03	111.70

There are no chirality outliers.

There are no planarity outliers.

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	4510	0	4571	67	0
1	C	4510	0	4571	61	0
2	B	3400	0	3433	46	0
2	D	3400	0	3433	41	0
3	E	494	0	269	9	0
3	T	494	0	269	9	0
4	F	407	0	229	13	0
4	P	407	0	229	11	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	A	30	0	12	2	0
6	C	30	0	12	0	0
7	B	23	0	22	0	0
7	D	23	0	22	0	0
8	B	4	0	6	0	0
8	D	4	0	6	3	0
9	D	5	0	0	0	0
10	A	50	0	0	2	0
10	B	42	0	0	2	0
10	C	48	0	0	2	0
10	D	33	0	0	4	0
10	E	1	0	0	0	0
10	F	2	0	0	0	0
10	P	1	0	0	1	0
10	T	1	0	0	0	0
All	All	17923	0	17084	245	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 7.

The worst 5 of 245 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)
4:P:817:MRG:H231	4:P:817:MRG:N3	1.90	0.87
1:A:167:ILE:O	1:A:170:PRO:HD2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.65	0.77
2:D:263:LYS:HE3	2:D:425:LEU:HA	1.69	0.75
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.24	0.71

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	553/556 (100%)	533 (96%)	17 (3%)	3 (0%)	32	52
1	C	553/556 (100%)	534 (97%)	17 (3%)	2 (0%)	38	57
2	B	408/428 (95%)	399 (98%)	9 (2%)	0	100	100
2	D	408/428 (95%)	394 (97%)	14 (3%)	0	100	100
All	All	1922/1968 (98%)	1860 (97%)	57 (3%)	5 (0%)	44	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	PRO
1	C	4	PRO
1	A	150	PRO
1	A	133	PRO
1	C	150	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	495/497 (100%)	489 (99%)	6 (1%)	75	90
1	C	495/497 (100%)	476 (96%)	19 (4%)	38	62
2	B	374/390 (96%)	367 (98%)	7 (2%)	62	83
2	D	374/390 (96%)	373 (100%)	1 (0%)	94	98
All	All	1738/1774 (98%)	1705 (98%)	33 (2%)	62	83

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	VAL
1	C	40	GLU
1	C	450	THR
1	C	23	GLN
1	C	28	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	GLN
1	A	182	GLN
1	C	367	GLN
1	C	498	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	#$|Z| > 2$
4	MRG	F	817	1,3,4	21,28,29	3.28	10 (47%)	24,39,42	2.02	8 (33%)
4	MRG	P	817	1,3,4	21,28,29	3.33	10 (47%)	24,39,42	2.12	9 (37%)

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
4	MRG	F	817	1,3,4	-	0/8/26/27	0/3/3/3
4	MRG	P	817	1,3,4	-	0/8/26/27	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	817	MRG	O5'-C5'	-4.21	1.38	1.44
4	F	817	MRG	O5'-C5'	-4.08	1.39	1.44
4	P	817	MRG	C2'-C3'	-3.27	1.44	1.52
4	F	817	MRG	C2'-C3'	-3.24	1.44	1.52
4	F	817	MRG	O4'-C4'	-2.62	1.39	1.45

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	817	MRG	N3-C2-N1	-4.54	119.37	126.23
4	F	817	MRG	N3-C2-N1	-4.25	119.80	126.23
4	F	817	MRG	C5-C6-N1	-2.48	119.95	123.48
4	P	817	MRG	C5-C6-N1	-2.38	120.09	123.48
4	F	817	MRG	C4-C5-N7	-2.33	107.16	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	817	MRG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	P	817	MRG	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	#$|Z| > 2$
6	DTP	A	603	5	26,32,32	1.45	6 (23%)	26,50,50	1.90	4 (15%)
7	SUC	B	501	-	24,24,24	0.30	0	36,36,36	0.67	0
8	EDO	B	502	-	3,3,3	0.36	0	2,2,2	0.46	0
6	DTP	C	601	5	26,32,32	1.45	6 (23%)	26,50,50	1.91	4 (15%)
7	SUC	D	501	-	24,24,24	0.27	0	36,36,36	0.84	1 (2%)
9	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.06	0
8	EDO	D	503	-	3,3,3	0.45	0	2,2,2	0.23	0

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
6	DTP	A	603	5	-	0/18/34/34	0/3/3/3
7	SUC	B	501	-	-	0/12/51/51	0/2/2/2
8	EDO	B	502	-	-	0/1/1/1	0/0/0/0
6	DTP	C	601	5	-	0/18/34/34	0/3/3/3
7	SUC	D	501	-	-	0/12/51/51	0/2/2/2
9	SO4	D	502	-	-	0/0/0/0	0/0/0/0
8	EDO	D	503	-	-	0/1/1/1	0/0/0/0

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	DTP	C5'-C4'	-3.08	1.41	1.51
6	C	601	DTP	C5'-C4'	-3.07	1.41	1.51
6	A	603	DTP	C2'-C3'	-2.60	1.46	1.52
6	C	601	DTP	C2'-C3'	-2.60	1.46	1.52
6	C	601	DTP	O5'-C5'	-2.46	1.35	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	601	DTP	N3-C2-N1	-8.06	121.83	128.86
6	A	603	DTP	N3-C2-N1	-7.97	121.92	128.86
6	C	601	DTP	C4-C5-N7	-2.29	107.20	109.41
6	A	603	DTP	C4-C5-N7	-2.17	107.32	109.41
7	D	501	SUC	C6-C5-C4	-2.16	107.94	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	603	DTP	2	0
8	D	503	EDO	3	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 (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	555/556 (99%)	0.73	83 (14%)	3	2	33, 84, 169, 230	0
1	C	555/556 (99%)	0.71	81 (14%)	3	2	36, 91, 160, 232	0
2	B	412/428 (96%)	0.42	29 (7%)	17	18	35, 70, 124, 162	0
2	D	412/428 (96%)	0.62	48 (11%)	5	5	37, 82, 142, 174	0
3	E	24/27 (88%)	1.01	4 (16%)	2	2	76, 116, 193, 231	0
3	T	24/27 (88%)	1.18	6 (25%)	1	0	76, 110, 203, 249	0
4	F	19/21 (90%)	0.55	1 (5%)	27	29	62, 99, 182, 186	0
4	P	19/21 (90%)	0.58	2 (10%)	7	7	69, 100, 158, 180	0
All	All	2020/2064 (97%)	0.65	254 (12%)	4	4	33, 81, 156, 249	0

The worst 5 of 254 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	214	LEU	14.6
3	T	702	DT	10.6
2	B	4	PRO	10.3
2	D	214	LEU	10.3
1	A	135	ILE	9.9

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th 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(Å²)	Q<0.9
4	MRG	F	817	26/27	0.85	0.16	-	105,119,149,157	0
4	MRG	P	817	26/27	0.90	0.14	-	90,114,145,155	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, 95th 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(Å²)	Q<0.9
9	SO4	D	502	5/5	0.71	0.31	4.07	160,162,164,165	0
5	MG	A	602	1/1	0.55	0.39	3.42	85,85,85,85	0
8	EDO	D	503	4/4	0.88	0.25	1.81	70,74,74,77	0
7	SUC	D	501	23/23	0.83	0.21	1.35	79,109,120,123	0
8	EDO	B	502	4/4	0.94	0.15	0.53	59,66,71,79	0
7	SUC	B	501	23/23	0.85	0.18	0.29	69,105,118,121	0
6	DTP	C	601	30/30	0.95	0.15	-0.61	76,97,131,138	0
6	DTP	A	603	30/30	0.92	0.13	-1.03	73,104,136,139	0
5	MG	C	602	1/1	0.90	0.07	-1.62	80,80,80,80	0
5	MG	A	601	1/1	0.84	0.04	-2.89	95,95,95,95	0
5	MG	C	603	1/1	0.92	0.25	-	96,96,96,96	0

6.5 Other polymers (i)

There are no such residues in this entry.