



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 07:44 PM GMT

PDB ID : 4PQU
Title : Crystal structure of HIV-1 Reverse Transcriptase in complex with RNA/DNA and dATP
Authors : Das, K.; Bandwar, R.P.; Arnold, E.
Deposited on : 2014-03-04
Resolution : 2.51 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

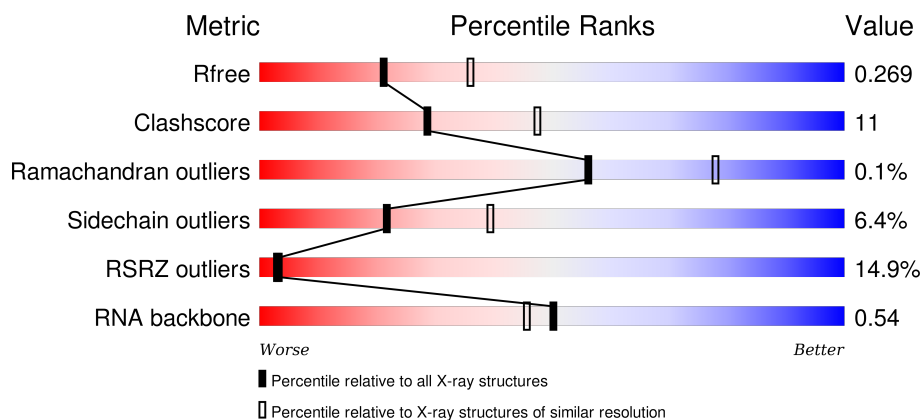
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

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 $\leq 5\%$. 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	<div> <div>9%</div> <div>71%</div> <div>24%</div> <div>• •</div> </div>
1	C	556	<div> <div>29%</div> <div>66%</div> <div>29%</div> <div>• •</div> </div>
2	B	428	<div> <div>4%</div> <div>72%</div> <div>22%</div> <div>• •</div> </div>
2	D	428	<div> <div>12%</div> <div>71%</div> <div>22%</div> <div>• •</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	E	27	
3	T	27	
4	F	21	
4	P	21	

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
8	SO4	A	607	-	-	-	X
8	SO4	C	604	-	-	-	X
9	GOL	B	502	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17849 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	545	Total	C	N	O	S	0	0	0
			4432	2872	736	816	8			
1	C	545	Total	C	N	O	S	0	0	0
			4432	2872	736	816	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P03366
A	0	VAL	-	EXPRESSION TAG	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	-	EXPRESSION TAG	UNP P03366
C	0	VAL	-	EXPRESSION TAG	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	413	Total	C	N	O	S	0	0	0
			3406	2215	564	621	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

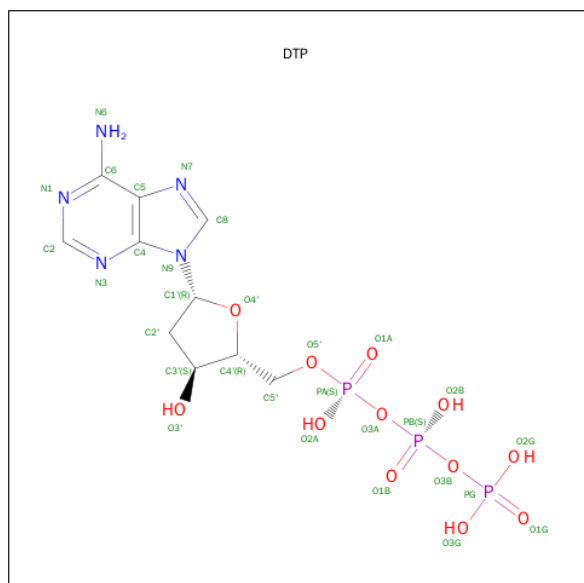
- Molecule 3 is a RNA chain called 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	21	Total	C	N	O	P	0	0	0
			452	202	88	142	20			
3	E	21	Total	C	N	O	P	0	0	0
			452	202	88	142	20			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	18	Total	C	N	O	P	0	0	0
			363	173	64	109	17			
4	F	18	Total	C	N	O	P	0	0	0
			363	173	64	109	17			

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃).

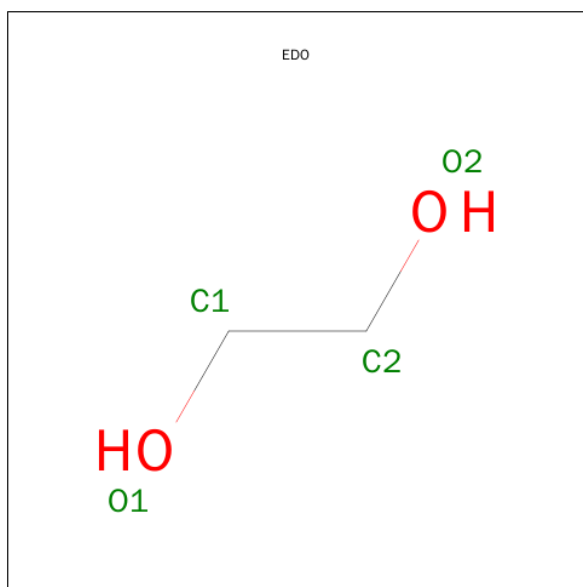


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
5	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

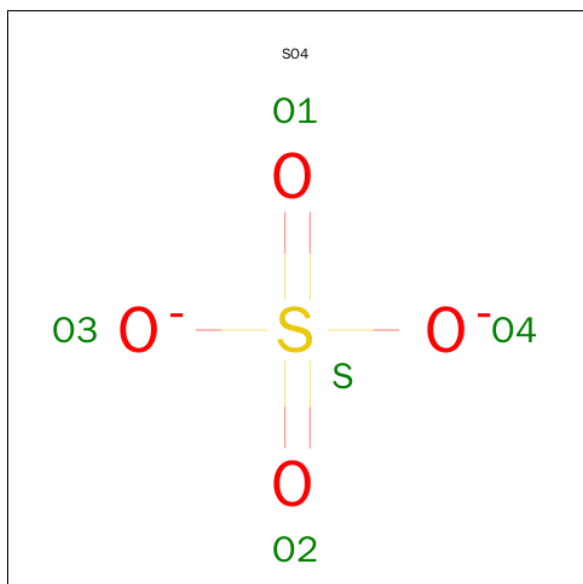
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		
6	C	2	Total	Mg	0	0
			2	2		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



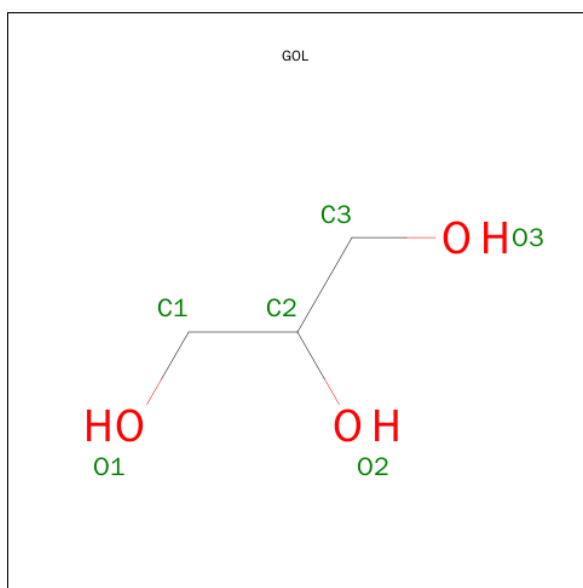
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	B	1	Total O S 5 4 1	0	0
8	C	1	Total O S 5 4 1	0	0
8	D	1	Total O S 5 4 1	0	0
8	D	1	Total O S 5 4 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 6 3 3	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	131	Total O 131 131	0	0

Continued on next page...

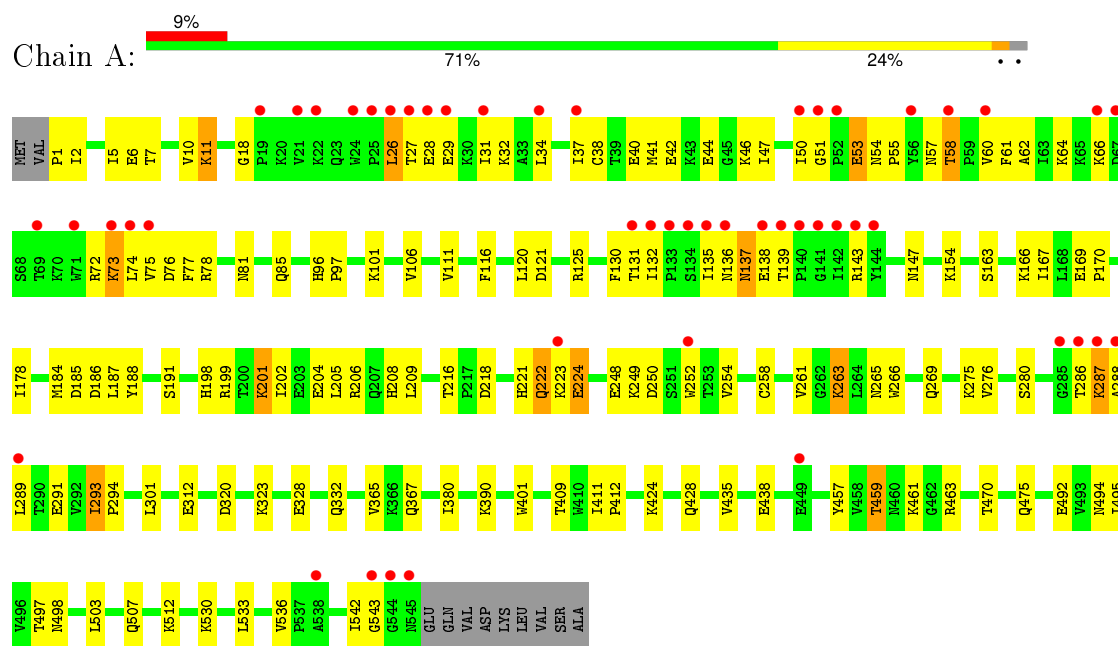
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	139	Total 139	O 139	0	0
10	C	80	Total 80	O 80	0	0
10	D	76	Total 76	O 76	0	0
10	T	3	Total 3	O 3	0	0
10	P	4	Total 4	O 4	0	0
10	E	1	Total 1	O 1	0	0
10	F	1	Total 1	O 1	0	0

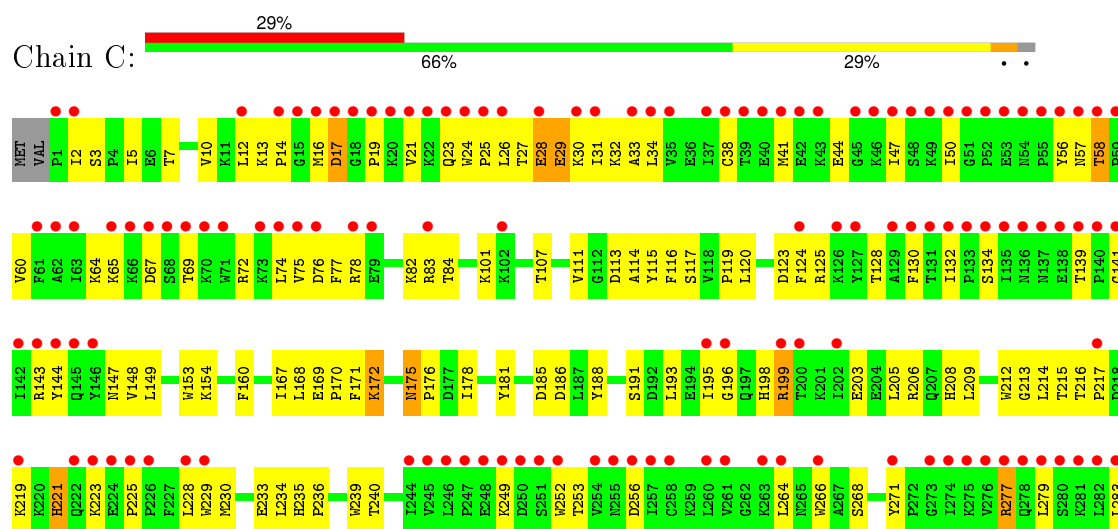
3 Residue-property plots

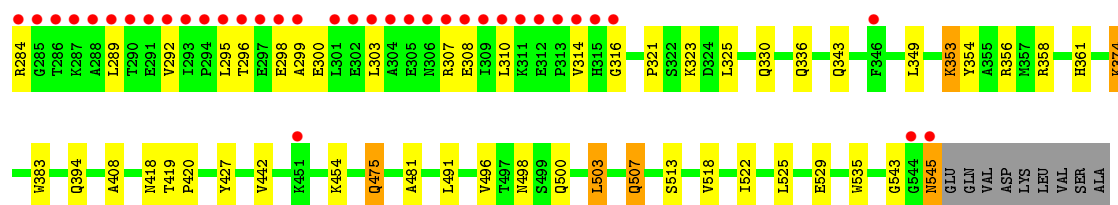
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: HIV-1 Reverse Transcriptase, p66 subunit

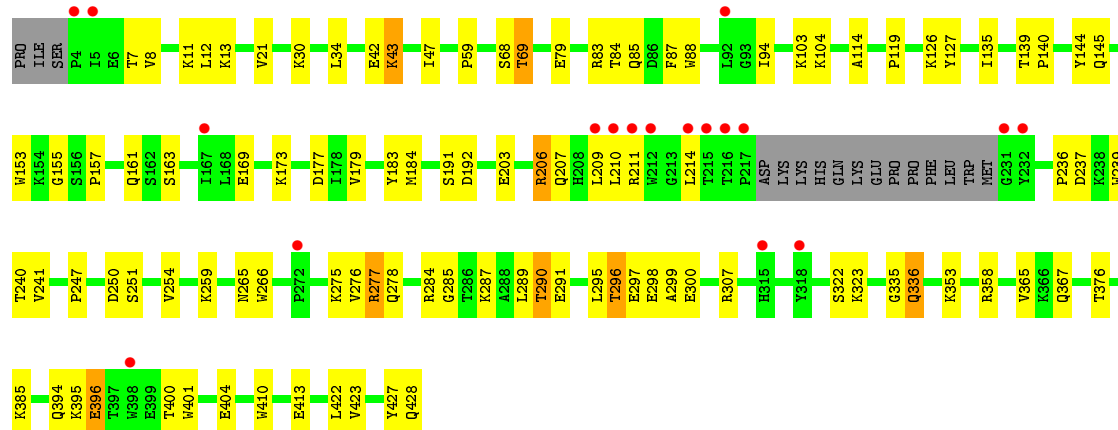


- Molecule 1: HIV-1 Reverse Transcriptase, p66 subunit

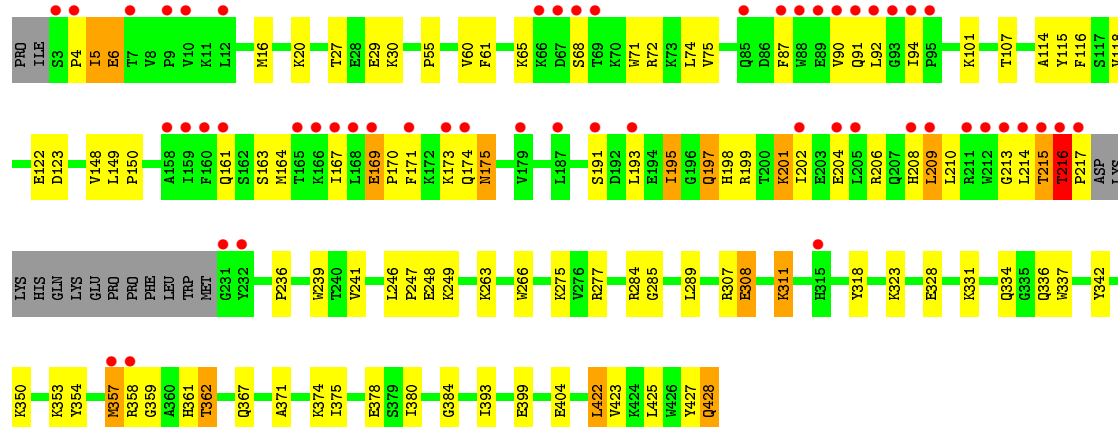




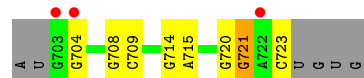
• Molecule 2: HIV-1 Reverse Transcriptase, p51 subunit



• Molecule 2: HIV-1 Reverse Transcriptase, p51 subunit

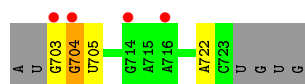


• Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*A
P*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'



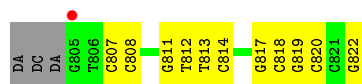
- Molecule 3: 5'-R(*AP*UP*GP*GP*UP*CP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*UP*GP*UP*G)-3'

Chain E: 



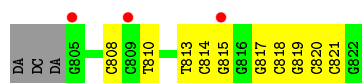
- Molecule 4: 5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3'

Chain P: 



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

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.44Å 128.29Å 130.68Å 90.00° 101.76° 90.00°	Depositor
Resolution (Å)	40.47 – 2.51 50.11 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.1 (40.47-2.51) 98.1 (50.11-2.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.202 , 0.266 0.214 , 0.269	Depositor DCC
R_{free} test set	2923 reflections (3.11%)	DCC
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 96937 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17849	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, DTP, EDO, SO4

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	0.56	1/4550 (0.0%)	0.64	1/6183 (0.0%)
1	C	0.48	1/4550 (0.0%)	0.61	2/6183 (0.0%)
2	B	0.56	0/3497	0.64	0/4751
2	D	0.53	0/3503	0.65	3/4760 (0.1%)
3	E	0.50	0/506	0.98	0/789
3	T	0.63	0/506	1.03	0/789
4	F	0.88	0/405	1.00	0/623
4	P	1.00	0/405	1.05	0/623
All	All	0.56	2/17922 (0.0%)	0.69	6/24701 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	312	GLU	CB-CG	5.29	1.62	1.52
1	C	176	PRO	N-CD	5.15	1.55	1.47

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	GLU	C-N-CD	5.80	140.58	128.40
1	A	169	GLU	C-N-CD	5.78	140.53	128.40
1	C	175	ASN	C-N-CD	5.68	140.32	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	213	GLY	N-CA-C	5.55	126.97	113.10
2	D	215	THR	N-CA-C	5.41	125.60	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	ASP	Peptide

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	4432	0	4488	97	0
1	C	4432	0	4488	133	0
2	B	3400	0	3433	69	0
2	D	3406	0	3437	81	0
3	E	452	0	232	2	0
3	T	452	0	232	4	0
4	F	363	0	202	14	0
4	P	363	0	202	12	0
5	A	30	0	12	1	0
5	C	30	0	12	2	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
7	A	4	0	6	1	0
8	A	15	0	0	2	0
8	B	10	0	0	1	0
8	C	5	0	0	0	0
8	D	10	0	0	1	0
9	B	6	0	8	2	0
10	A	131	0	0	5	0
10	B	139	0	0	7	0
10	C	80	0	0	0	0
10	D	76	0	0	3	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	P	4	0	0	1	0
10	T	3	0	0	0	0
All	All	17849	0	16752	389	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 11.

The worst 5 of 389 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:C:32:LYS:HD3	1:C:33:ALA:N	1.75	1.01
1:C:168:LEU:HB3	1:C:172:LYS:HE2	1.45	0.96
1:A:459:THR:HG22	1:A:461:LYS:H	1.33	0.94
1:C:175:ASN:HB3	1:C:178:ILE:HD13	1.49	0.92
2:D:191:SER:HG	2:D:198:HIS:HD1	1.22	0.87

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	543/556 (98%)	505 (93%)	37 (7%)	1 (0%)	52	75
1	C	543/556 (98%)	489 (90%)	54 (10%)	0	100	100
2	B	408/428 (95%)	386 (95%)	22 (5%)	0	100	100
2	D	409/428 (96%)	379 (93%)	29 (7%)	1 (0%)	52	75
All	All	1903/1968 (97%)	1759 (92%)	142 (8%)	2 (0%)	56	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	362	THR
1	A	18	GLY

5.3.2 Protein sidechains ⓘ

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	486/497 (98%)	455 (94%)	31 (6%)	22	39
1	C	486/497 (98%)	460 (95%)	26 (5%)	28	50
2	B	374/390 (96%)	353 (94%)	21 (6%)	26	47
2	D	375/390 (96%)	343 (92%)	32 (8%)	13	25
All	All	1721/1774 (97%)	1611 (94%)	110 (6%)	22	39

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	396	GLU
1	C	172	LYS
2	D	308	GLU
2	B	428	GLN
1	C	27	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	269	GLN
1	C	306	ASN
2	D	91	GLN
1	C	147	ASN
1	C	208	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	E	20/27 (74%)	2 (10%)	0
3	T	20/27 (74%)	3 (15%)	0
All	All	40/54 (74%)	5 (12%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	704	G
3	T	721	G
3	T	723	C
3	E	704	G
3	E	722	A

There are no RNA pucker outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	601	6	24,32,32	1.87	7 (29%)	32,50,50	2.38	4 (12%)
7	EDO	A	604	-	3,3,3	0.83	0	2,2,2	0.29	0
8	SO4	A	605	-	4,4,4	0.24	0	6,6,6	0.92	1 (16%)
8	SO4	A	606	-	4,4,4	0.17	0	6,6,6	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	SO4	A	607	-	4,4,4	0.24	0	6,6,6	0.30	0
8	SO4	B	501	-	4,4,4	0.22	0	6,6,6	0.78	0
9	GOL	B	502	-	5,5,5	0.57	0	5,5,5	0.66	0
8	SO4	B	503	-	4,4,4	0.24	0	6,6,6	0.37	0
5	DTP	C	601	6	24,32,32	1.82	6 (25%)	32,50,50	2.69	7 (21%)
8	SO4	C	604	-	4,4,4	0.19	0	6,6,6	0.40	0
8	SO4	D	501	-	4,4,4	0.15	0	6,6,6	0.24	0
8	SO4	D	502	-	4,4,4	0.15	0	6,6,6	0.69	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
5	DTP	A	601	6	-	0/18/34/34	0/3/3/3
7	EDO	A	604	-	-	0/1/1/1	0/0/0/0
8	SO4	A	605	-	-	0/0/0/0	0/0/0/0
8	SO4	A	606	-	-	0/0/0/0	0/0/0/0
8	SO4	A	607	-	-	0/0/0/0	0/0/0/0
8	SO4	B	501	-	-	0/0/0/0	0/0/0/0
9	GOL	B	502	-	-	0/4/4/4	0/0/0/0
8	SO4	B	503	-	-	0/0/0/0	0/0/0/0
5	DTP	C	601	6	-	0/18/34/34	0/3/3/3
8	SO4	C	604	-	-	0/0/0/0	0/0/0/0
8	SO4	D	501	-	-	0/0/0/0	0/0/0/0
8	SO4	D	502	-	-	0/0/0/0	0/0/0/0

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	DTP	C5'-C4'	-3.85	1.39	1.51
5	C	601	DTP	C5'-C4'	-3.65	1.39	1.51
5	C	601	DTP	O3'-C3'	-2.62	1.37	1.43
5	A	601	DTP	O3'-C3'	-2.47	1.37	1.43
5	A	601	DTP	C3'-C4'	-2.23	1.46	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	DTP	N3-C2-N1	-11.84	119.83	128.89
5	A	601	DTP	N3-C2-N1	-11.17	120.34	128.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	DTP	C1'-N9-C4	-4.15	120.13	127.16
5	A	601	DTP	PB-O3B-PG	-3.38	121.32	132.67
5	C	601	DTP	C4-C5-N7	-2.74	106.96	109.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	DTP	1	0
7	A	604	EDO	1	0
8	A	605	SO4	1	0
8	A	607	SO4	1	0
9	B	502	GOL	2	0
8	B	503	SO4	1	0
5	C	601	DTP	2	0
8	D	501	SO4	1	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, 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	545/556 (98%)	0.62	50 (9%) 11 12	14, 40, 95, 132	0
1	C	545/556 (98%)	1.62	164 (30%) 1 0	19, 64, 140, 157	0
2	B	412/428 (96%)	0.49	18 (4%) 38 43	15, 36, 71, 84	0
2	D	413/428 (96%)	0.80	53 (12%) 5 5	18, 45, 88, 119	0
3	E	21/27 (77%)	1.60	4 (19%) 2 1	56, 92, 122, 154	0
3	T	21/27 (77%)	0.91	3 (14%) 4 3	35, 83, 95, 128	0
4	F	18/21 (85%)	1.16	3 (16%) 2 2	59, 89, 122, 124	0
4	P	18/21 (85%)	0.79	1 (5%) 28 31	34, 81, 107, 109	0
All	All	1993/2064 (96%)	0.92	296 (14%) 3 3	14, 45, 121, 157	0

The worst 5 of 296 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	PRO	11.9
1	C	247	PRO	11.2
2	D	214	LEU	10.8
1	C	252	TRP	10.2
1	C	135	ILE	10.1

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 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(Å ²)	Q<0.9
8	SO4	A	607	5/5	0.90	0.29	7.60	45,46,60,70	0
9	GOL	B	502	6/6	0.77	0.29	5.55	36,36,43,47	0
8	SO4	C	604	5/5	0.92	0.21	2.91	51,63,69,83	0
8	SO4	D	502	5/5	0.89	0.27	1.99	58,67,72,86	0
7	EDO	A	604	4/4	0.97	0.25	1.31	21,22,23,24	0
8	SO4	A	605	5/5	0.97	0.18	0.99	37,39,51,57	0
8	SO4	A	606	5/5	0.93	0.14	-0.95	53,58,66,77	0
5	DTP	C	601	30/30	0.89	0.17	-0.99	63,71,85,88	0
5	DTP	A	601	30/30	0.95	0.14	-1.05	33,43,53,55	0
6	MG	C	602	1/1	0.95	0.13	-1.32	59,59,59,59	0
8	SO4	B	503	5/5	0.96	0.14	-2.08	54,54,65,77	0
6	MG	A	602	1/1	0.94	0.12	-2.10	30,30,30,30	0
8	SO4	B	501	5/5	0.96	0.14	-7.67	32,37,46,54	0
6	MG	C	603	1/1	0.50	0.14	-	63,63,63,63	0
8	SO4	D	501	5/5	0.96	0.09	-	49,57,63,68	0
6	MG	A	603	1/1	0.95	0.12	-	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.