



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 01:46 am GMT

PDB ID : 3TMK
Title : CRYSTAL STRUCTURE OF YEAST THYMIDYLATE KINASE COM-
PLEXED WITH THE BISUBSTRATE INHIBITOR TP5A AT 2.0 Å RESO-
LUTION: IMPLICATIONS FOR CATALYSIS AND AZT ACTIVATION
Authors : Lavie, A.; Schlichting, I.; Konrad, M.; Goody, R.S.; Brundiers, R.; Reinstein,
J.
Deposited on : 1998-01-26
Resolution : 2.00 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28683
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)	:	recalc28949

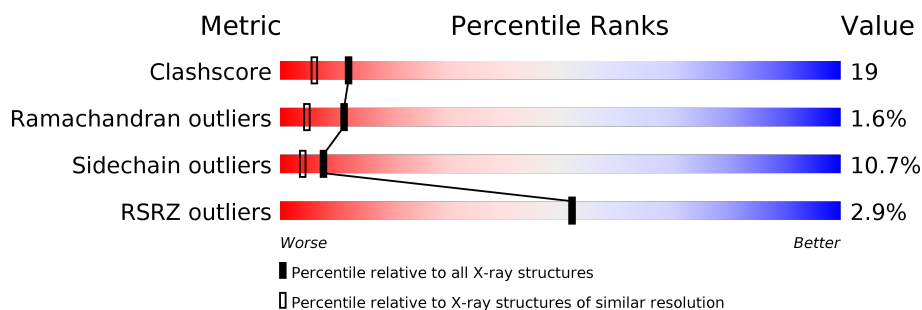
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	216	 6% 58% 34% 7%
1	B	216	 2% 72% 25% 1%
1	C	216	 2% 52% 32% 11% 5%
1	D	216	 1% 70% 25% 2%
1	E	216	 4% 61% 33% 5%
1	F	216	 2% 70% 25% 1%
1	G	216	 3% 61% 30% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	216	<div><div></div><div>3%</div><div>73%</div><div>24%</div><div>••</div></div>

2 Entry composition

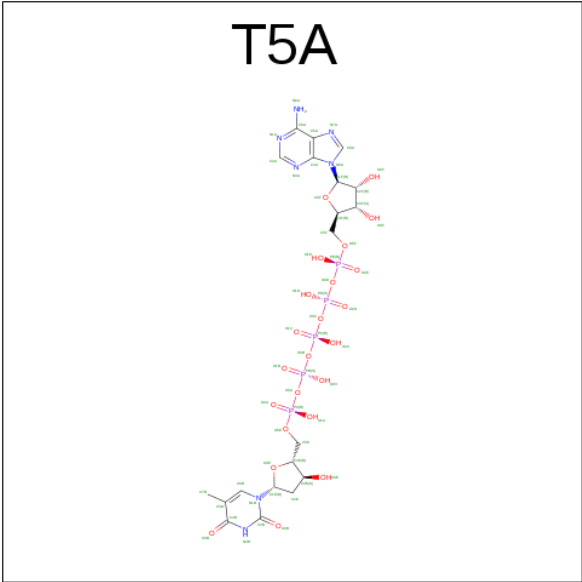
There are 3 unique types of molecules in this entry. The entry contains 15240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THYMIDYLATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1736	1107	289	332	8			
1	B	216	Total	C	N	O	S	0	0	0
			1733	1106	289	330	8			
1	C	205	Total	C	N	O	S	0	0	0
			1657	1060	275	314	8			
1	D	214	Total	C	N	O	S	0	0	0
			1707	1092	286	323	6			
1	E	215	Total	C	N	O	S	0	0	0
			1722	1096	288	331	7			
1	F	216	Total	C	N	O	S	0	0	0
			1729	1104	288	329	8			
1	G	215	Total	C	N	O	S	0	0	0
			1722	1096	288	331	7			
1	H	214	Total	C	N	O	S	0	0	0
			1706	1090	285	325	6			

- Molecule 2 is P1-(5'-ADENOSYL)P5-(5'-THYMIDYL)PENTAPHOSPHATE (three-letter code: T5A) (formula: C₂₀H₃₀N₇O₂₃P₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	B	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	C	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	D	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	E	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	F	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	G	1	Total	C	N	O	P	0	0
			55	20	7	23	5		
2	H	1	Total	C	N	O	P	0	0
			55	20	7	23	5		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	129	Total	O	0	0
			129	129		
3	B	161	Total	O	0	0
			161	161		
3	C	134	Total	O	0	0
			134	134		
3	D	144	Total	O	0	0
			144	144		

Continued on next page...

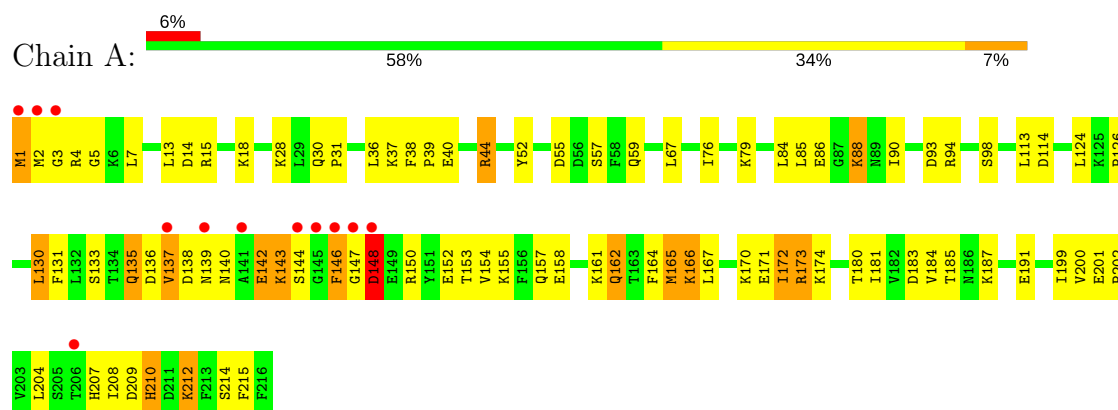
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	126	Total 126	O 126	0	0
3	F	147	Total 147	O 147	0	0
3	G	136	Total 136	O 136	0	0
3	H	111	Total 111	O 111	0	0

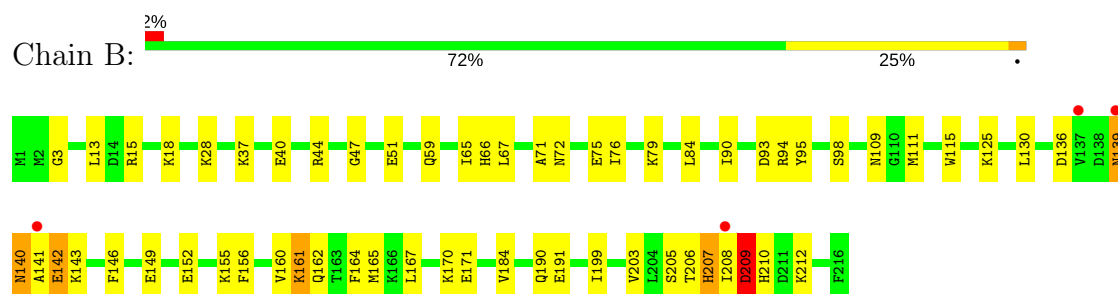
3 Residue-property plots [i](#)

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

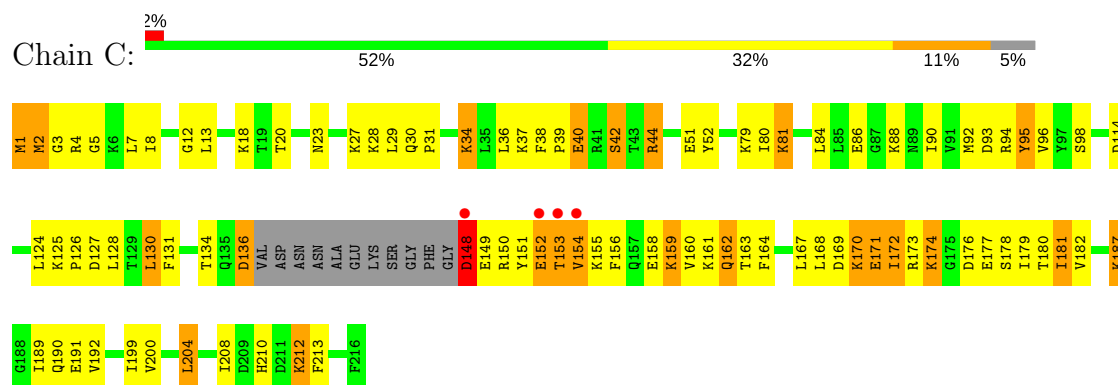
• Molecule 1: THYMIDYLATE KINASE



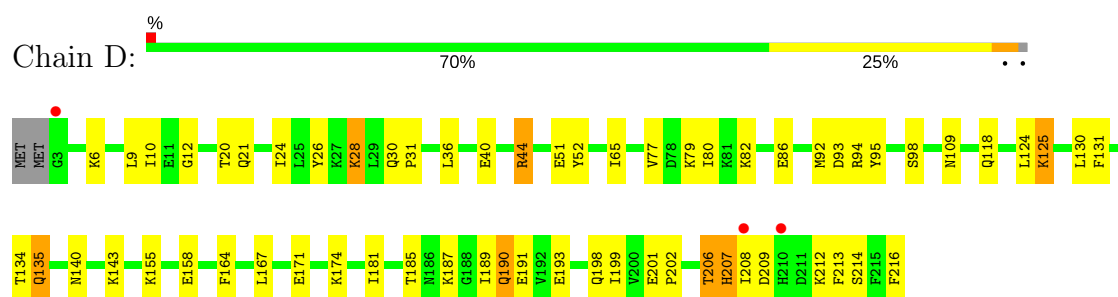
• Molecule 1: THYMIDYLATE KINASE



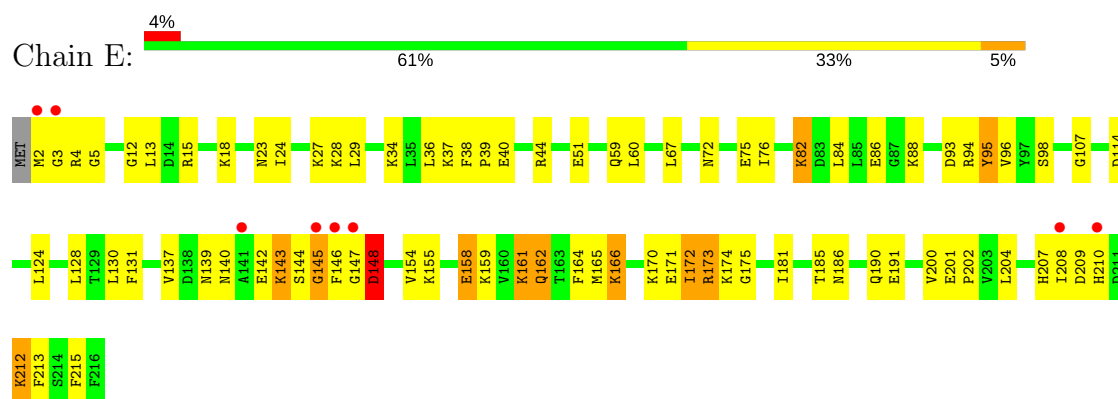
• Molecule 1: THYMIDYLATE KINASE



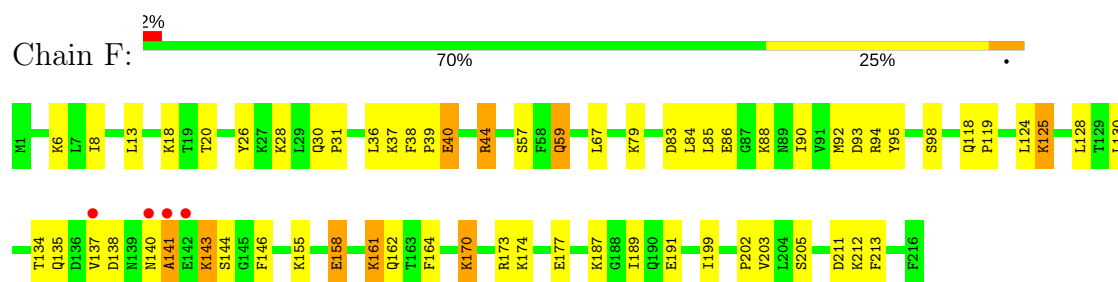
• Molecule 1: THYMIDYLATE KINASE



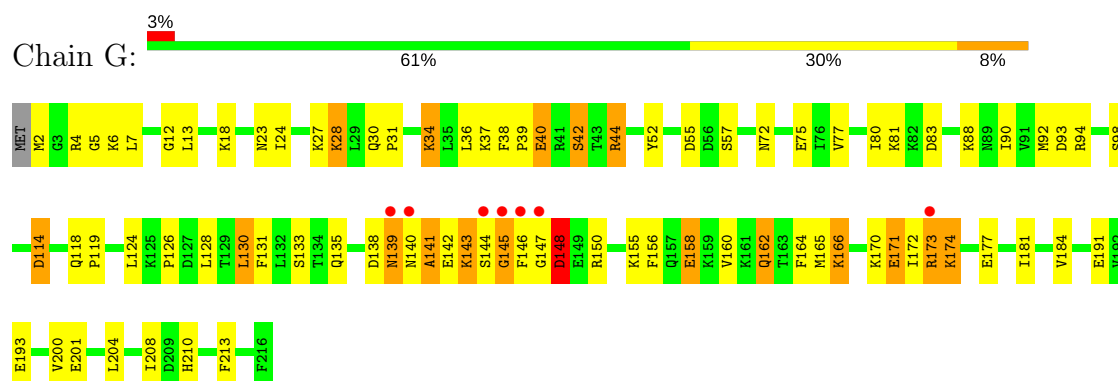
• Molecule 1: THYMIDYLATE KINASE



• Molecule 1: THYMIDYLATE KINASE

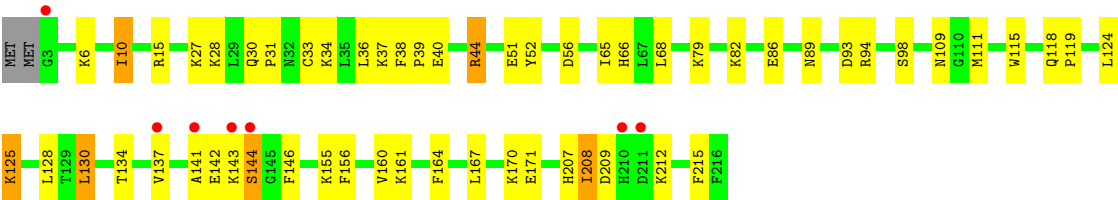


• Molecule 1: THYMIDYLATE KINASE



• Molecule 1: THYMIDYLATE KINASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.57Å 87.32Å 155.02Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	43.80 – 2.00 43.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.80-2.00) 82.0 (43.66-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.209 , 0.279 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	1.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 64.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	0.053 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15240	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.18 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1888e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: T5A

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	0.49	0/1765	0.68	0/2375
1	B	0.48	0/1762	0.67	0/2371
1	C	0.55	1/1684 (0.1%)	0.71	1/2265 (0.0%)
1	D	0.48	0/1736	0.65	0/2338
1	E	0.47	0/1750	0.65	0/2356
1	F	0.49	0/1758	0.67	0/2366
1	G	0.46	0/1750	0.67	0/2356
1	H	0.49	0/1735	0.67	0/2338
All	All	0.49	1/13940 (0.0%)	0.67	1/18765 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	148	ASP	C-N	9.34	1.55	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	ASP	C-N-CA	-5.75	107.32	121.70

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	1736	0	1757	98	1
1	B	1733	0	1755	42	0
1	C	1657	0	1687	113	0
1	D	1707	0	1724	53	0
1	E	1722	0	1738	79	0
1	F	1729	0	1749	44	1
1	G	1722	0	1738	78	0
1	H	1706	0	1715	43	0
2	A	55	0	25	1	0
2	B	55	0	25	1	0
2	C	55	0	25	3	0
2	D	55	0	25	0	0
2	E	55	0	25	1	0
2	F	55	0	25	0	0
2	G	55	0	25	0	0
2	H	55	0	25	1	0
3	A	129	0	0	12	0
3	B	161	0	0	13	0
3	C	134	0	0	10	0
3	D	144	0	0	13	0
3	E	126	0	0	14	0
3	F	147	0	0	14	0
3	G	136	0	0	17	0
3	H	111	0	0	8	0
All	All	15240	0	14063	535	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

The worst 5 of 535 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:162:GLN:H	1:C:162:GLN:NE2	1.33	1.24
1:C:162:GLN:N	1:C:162:GLN:HE21	1.44	1.12
1:A:2:MET:HG3	1:A:3:GLY:H	1.08	1.11
1:D:44:ARG:HG2	3:D:4143:HOH:O	1.51	1.10
1:H:44:ARG:HG3	1:H:44:ARG:HH11	1.15	1.09

All (1) 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:191:GLU:OE2	1:F:191:GLU:OE2[1_556]	2.11	0.09

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	214/216 (99%)	194 (91%)	16 (8%)	4 (2%)	9	4
1	B	214/216 (99%)	201 (94%)	10 (5%)	3 (1%)	13	6
1	C	201/216 (93%)	191 (95%)	8 (4%)	2 (1%)	18	10
1	D	212/216 (98%)	205 (97%)	6 (3%)	1 (0%)	32	26
1	E	213/216 (99%)	196 (92%)	11 (5%)	6 (3%)	6	2
1	F	214/216 (99%)	204 (95%)	8 (4%)	2 (1%)	20	12
1	G	213/216 (99%)	193 (91%)	14 (7%)	6 (3%)	6	2
1	H	212/216 (98%)	198 (93%)	11 (5%)	3 (1%)	13	6
All	All	1693/1728 (98%)	1582 (93%)	84 (5%)	27 (2%)	11	5

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	VAL
1	G	142	GLU
1	G	145	GLY
1	G	146	PHE
1	G	148	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	194/194 (100%)	171 (88%)	23 (12%)	6	3
1	B	193/194 (100%)	175 (91%)	18 (9%)	10	6
1	C	186/194 (96%)	158 (85%)	28 (15%)	3	1
1	D	188/194 (97%)	172 (92%)	16 (8%)	12	7
1	E	192/194 (99%)	169 (88%)	23 (12%)	6	3
1	F	192/194 (99%)	173 (90%)	19 (10%)	9	5
1	G	192/194 (99%)	171 (89%)	21 (11%)	7	4
1	H	188/194 (97%)	173 (92%)	15 (8%)	14	9
All	All	1525/1552 (98%)	1362 (89%)	163 (11%)	8	4

5 of 163 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	98	SER
1	E	98	SER
1	H	40	GLU
1	D	125	LYS
1	D	206	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	23	ASN
1	D	190	GLN
1	H	32	ASN
1	D	32	ASN
1	B	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

8 ligands 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	T5A	A	217	-	43,59,59	1.17	4 (9%)	43,93,93	3.01	5 (11%)
2	T5A	B	217	-	43,59,59	1.33	6 (13%)	43,93,93	2.83	7 (16%)
2	T5A	C	217	-	43,59,59	1.36	6 (13%)	43,93,93	3.23	8 (18%)
2	T5A	D	217	-	43,59,59	1.21	3 (6%)	43,93,93	2.44	8 (18%)
2	T5A	E	217	-	43,59,59	1.35	4 (9%)	43,93,93	3.22	11 (25%)
2	T5A	F	217	-	43,59,59	1.29	7 (16%)	43,93,93	2.66	8 (18%)
2	T5A	G	217	-	43,59,59	1.41	7 (16%)	43,93,93	3.19	6 (13%)
2	T5A	H	217	-	43,59,59	1.46	5 (11%)	43,93,93	3.06	14 (32%)

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	T5A	A	217	-	-	0/36/72/72	0/5/5/5
2	T5A	B	217	-	-	0/36/72/72	0/5/5/5
2	T5A	C	217	-	-	0/36/72/72	0/5/5/5
2	T5A	D	217	-	-	0/36/72/72	0/5/5/5
2	T5A	E	217	-	-	0/36/72/72	0/5/5/5
2	T5A	F	217	-	-	0/36/72/72	0/5/5/5
2	T5A	G	217	-	-	0/36/72/72	0/5/5/5
2	T5A	H	217	-	-	0/36/72/72	0/5/5/5

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	217	T5A	C2F-C1F	-3.37	1.48	1.53
2	E	217	T5A	C8A-N7A	-3.07	1.28	1.34
2	F	217	T5A	C6B-C5B	-2.83	1.32	1.40
2	B	217	T5A	C6B-C5B	-2.80	1.32	1.40
2	H	217	T5A	C6B-C5B	-2.80	1.32	1.40

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	217	T5A	C5B-C4B-N3B	-12.20	111.80	125.24
2	G	217	T5A	C5B-C4B-N3B	-11.98	112.04	125.24
2	E	217	T5A	C5B-C4B-N3B	-11.60	112.45	125.24
2	A	217	T5A	C5B-C4B-N3B	-11.03	113.08	125.24
2	H	217	T5A	C5B-C4B-N3B	-10.84	113.29	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	217	T5A	1	0
2	B	217	T5A	1	0
2	C	217	T5A	3	0
2	E	217	T5A	1	0
2	H	217	T5A	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 [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	216/216 (100%)	0.06	12 (5%) 25 25	8, 19, 42, 56	0
1	B	216/216 (100%)	-0.19	4 (1%) 67 66	8, 17, 42, 49	0
1	C	205/216 (94%)	-0.04	4 (1%) 65 65	8, 18, 38, 49	0
1	D	214/216 (99%)	-0.19	3 (1%) 75 75	8, 17, 36, 46	0
1	E	215/216 (99%)	0.04	8 (3%) 42 43	7, 20, 45, 49	0
1	F	216/216 (100%)	-0.19	4 (1%) 67 66	8, 17, 36, 49	0
1	G	215/216 (99%)	-0.06	7 (3%) 47 47	7, 19, 41, 47	0
1	H	214/216 (99%)	-0.10	7 (3%) 47 47	7, 17, 41, 50	0
All	All	1711/1728 (99%)	-0.08	49 (2%) 52 52	7, 18, 41, 56	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	ASP	7.7
1	A	2	MET	5.5
1	E	2	MET	5.3
1	G	146	PHE	4.8
1	A	1	MET	4.8

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 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
2	T5A	F	217	55/55	0.97	0.11	-0.06	3,18,28,29	0
2	T5A	B	217	55/55	0.98	0.10	-0.09	7,16,25,26	0
2	T5A	A	217	55/55	0.98	0.10	-0.42	7,15,26,28	0
2	T5A	C	217	55/55	0.98	0.10	-0.44	6,14,26,27	0
2	T5A	E	217	55/55	0.98	0.10	-0.47	4,15,27,28	0
2	T5A	H	217	55/55	0.98	0.09	-0.52	2,16,25,26	0
2	T5A	D	217	55/55	0.98	0.10	-0.65	2,13,24,26	0
2	T5A	G	217	55/55	0.98	0.10	-0.66	4,12,23,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.