



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2017 – 06:06 AM EDT

PDB ID : 5X5D
Title : Human thymidylate synthase bound with dUMP
Authors : Chen, D.; Jansson, A.; Larsson, A.; Nordlund, P.
Deposited on : unknown
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 : 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

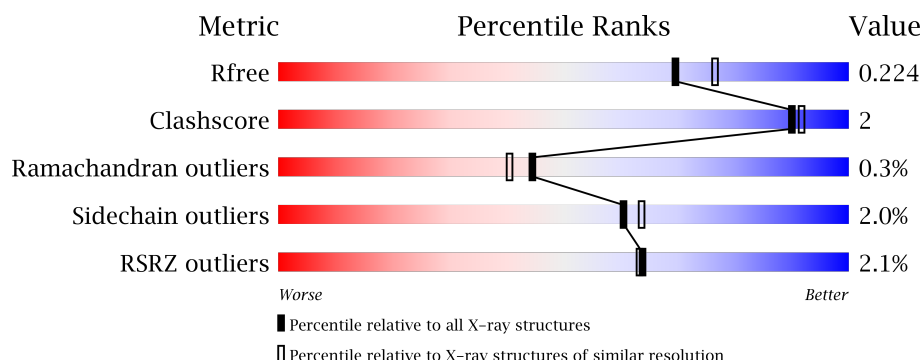
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	100719	6609 (2.00-2.00)
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	290	<div> <div></div> <div>93%</div> <div>5% ..</div> </div>
1	B	290	<div> <div></div> <div>92%</div> <div>6% ..</div> </div>
1	C	290	<div> <div>3%</div> <div>92%</div> <div>6% ..</div> </div>
1	D	290	<div> <div>3%</div> <div>91%</div> <div>7% ..</div> </div>
1	E	290	<div> <div>3%</div> <div>90%</div> <div>7% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	290	

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	UMP	E	401	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15521 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.

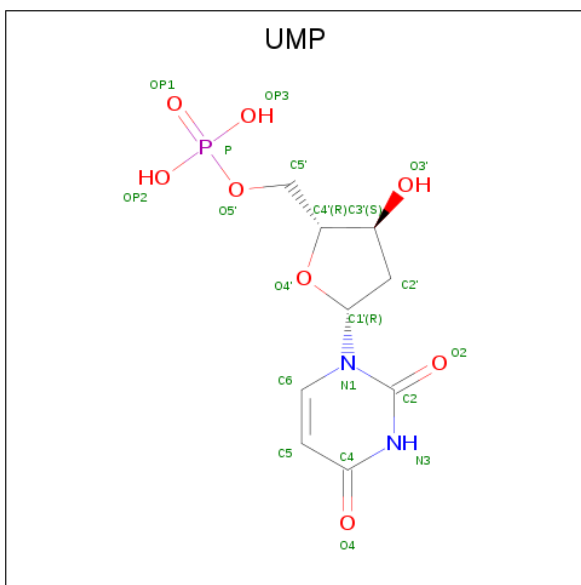
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	1	0
			2321	1483	405	421	12			
1	B	288	Total	C	N	O	S	0	0	0
			2324	1486	405	420	13			
1	C	286	Total	C	N	O	S	0	0	0
			2293	1466	401	414	12			
1	D	285	Total	C	N	O	S	0	1	0
			2305	1475	401	417	12			
1	E	281	Total	C	N	O	S	0	0	0
			2251	1442	390	408	11			
1	F	284	Total	C	N	O	S	0	0	0
			2283	1459	398	414	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP P04818
A	25	MET	-	expression tag	UNP P04818
B	24	SER	-	expression tag	UNP P04818
B	25	MET	-	expression tag	UNP P04818
C	24	SER	-	expression tag	UNP P04818
C	25	MET	-	expression tag	UNP P04818
D	24	SER	-	expression tag	UNP P04818
D	25	MET	-	expression tag	UNP P04818
E	24	SER	-	expression tag	UNP P04818
E	25	MET	-	expression tag	UNP P04818
F	24	SER	-	expression tag	UNP P04818
F	25	MET	-	expression tag	UNP P04818

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: C₉H₁₃N₂O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	F	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	309	Total	O	0	0
			309	309		
3	B	288	Total	O	0	0
			288	288		
3	C	242	Total	O	0	0
			242	242		
3	D	293	Total	O	0	0
			293	293		
3	E	280	Total	O	0	0
			280	280		
3	F	212	Total	O	0	0
			212	212		

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.

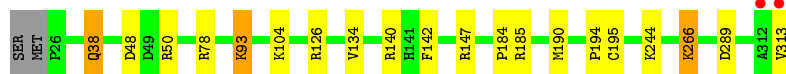
- Molecule 1: Thymidylate synthase

Chain A: 



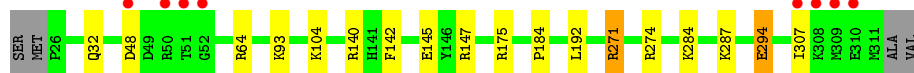
- Molecule 1: Thymidylate synthase

Chain B: 



- Molecule 1: Thymidylate synthase

Chain C: 




- Molecule 1: Thymidylate synthase

Chain D: 

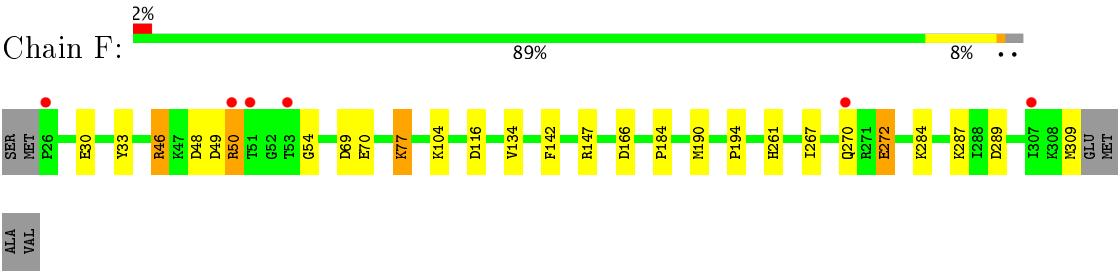


- Molecule 1: Thymidylate synthase

Chain E: 



- Molecule 1: Thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.74Å 109.74Å 317.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.57 – 2.00 22.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.1 (22.57-2.00) 88.2 (22.57-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.181 , 0.223 0.181 , 0.224	Depositor DCC
R_{free} test set	5800 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15521	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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 52.86 % 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 4.5801e-05. 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: UMP

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	0.99	0/2381	0.94	5/3223 (0.2%)
1	B	0.97	0/2384	0.95	7/3224 (0.2%)
1	C	0.93	1/2353 (0.0%)	0.91	9/3186 (0.3%)
1	D	1.04	2/2365 (0.1%)	0.92	5/3199 (0.2%)
1	E	1.00	1/2311 (0.0%)	0.96	9/3130 (0.3%)
1	F	0.94	2/2342 (0.1%)	0.93	5/3169 (0.2%)
All	All	0.98	6/14136 (0.0%)	0.94	40/19131 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	294	GLU	CD-OE1	-7.03	1.18	1.25
1	D	70	GLU	CD-OE1	-6.47	1.18	1.25
1	F	30	GLU	CD-OE1	-5.97	1.19	1.25
1	D	30	GLU	CD-OE1	-5.90	1.19	1.25
1	E	294	GLU	CD-OE2	5.31	1.31	1.25
1	F	33	TYR	CE1-CZ	5.25	1.45	1.38

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	70	GLU	CA-CB-CG	9.84	135.05	113.40
1	B	126	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	E	70	GLU	CA-CB-CG	9.12	133.47	113.40
1	E	70	GLU	OE1-CD-OE2	-8.39	113.23	123.30
1	A	126	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	C	48	ASP	CB-CG-OD1	7.79	125.31	118.30
1	D	140	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	F	116	ASP	CB-CG-OD1	7.48	125.03	118.30
1	C	140	ARG	NE-CZ-NH2	6.96	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	ARG	NE-CZ-NH2	6.93	123.77	120.30
1	B	266	LYS	CD-CE-NZ	-6.78	96.10	111.70
1	E	140	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	A	38	GLN	CA-CB-CG	6.52	127.74	113.40
1	E	185	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	C	147	ARG	CB-CG-CD	6.06	127.35	111.60
1	C	294	GLU	CA-CB-CG	6.02	126.65	113.40
1	A	140	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	E	294	GLU	CA-CB-CG	5.97	126.54	113.40
1	C	287	LYS	CD-CE-NZ	-5.94	98.05	111.70
1	D	78[A]	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	78[B]	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	38	GLN	CA-CB-CG	5.84	126.25	113.40
1	F	116	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	E	175	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	78	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	173	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	175	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	271	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	E	173	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	C	93	LYS	CB-CA-C	-5.23	99.94	110.40
1	B	93	LYS	CB-CA-C	-5.22	99.95	110.40
1	D	77	LYS	CA-CB-CG	5.21	124.87	113.40
1	E	93	LYS	CB-CA-C	-5.20	99.99	110.40
1	C	294	GLU	CG-CD-OE1	-5.20	107.91	118.30
1	E	289	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	271	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	116	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	B	185	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	F	50	ARG	CA-CB-CG	5.10	124.62	113.40
1	F	77	LYS	CA-CB-CG	5.03	124.47	113.40

There are no chirality outliers.

There are no planarity outliers.

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	2321	0	2278	13	0
1	B	2324	0	2297	9	0
1	C	2293	0	2246	8	0
1	D	2305	0	2266	11	0
1	E	2251	0	2199	7	0
1	F	2283	0	2243	17	0
2	A	20	0	11	0	0
2	B	20	0	10	1	0
2	C	20	0	11	0	0
2	D	20	0	11	0	0
2	E	20	0	9	0	0
2	F	20	0	10	1	0
3	A	309	0	0	5	0
3	B	288	0	0	5	0
3	C	242	0	0	4	0
3	D	293	0	0	4	1
3	E	280	0	0	4	1
3	F	212	0	0	5	0
All	All	15521	0	13591	57	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 2.

All (57) 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:D:46:ARG:NH2	3:D:501:HOH:O	2.08	0.87
1:F:272:GLU:HB3	3:F:524:HOH:O	1.79	0.80
1:A:147:ARG:NH1	3:A:501:HOH:O	2.16	0.77
1:F:50:ARG:HH11	1:F:50:ARG:HB3	1.52	0.73
1:F:166:ASP:OD1	3:F:501:HOH:O	2.13	0.67
1:F:50:ARG:NH1	1:F:50:ARG:HB3	2.09	0.67
1:F:69:ASP:HB3	3:F:657:HOH:O	1.95	0.66
1:F:261:HIS:CE1	1:F:309:MET:HB3	2.32	0.64
1:D:93:LYS:HE3	1:D:100:GLU:OE2	1.99	0.63
1:B:104:LYS:HE2	3:B:556:HOH:O	2.00	0.61
1:D:48:ASP:OD1	3:D:502:HOH:O	2.17	0.59
1:E:306:THR:HG22	3:E:514:HOH:O	2.01	0.59
1:B:266:LYS:HE2	3:B:707:HOH:O	2.03	0.58
1:F:267:ILE:O	1:F:270:GLN:HG2	2.04	0.58
1:A:166:ASP:OD1	3:A:502:HOH:O	2.16	0.57
1:F:50:ARG:NH1	2:F:401:UMP:OP3	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:HG11	3:C:506:HOH:O	2.07	0.55
1:F:147:ARG:NH1	3:F:504:HOH:O	2.39	0.54
1:B:147:ARG:NH1	3:B:506:HOH:O	2.41	0.54
1:F:261:HIS:ND1	1:F:309:MET:HB3	2.22	0.54
1:B:195:CYS:SG	2:B:401:UMP:C6	3.02	0.53
1:F:104:LYS:HE2	3:F:543:HOH:O	2.08	0.53
1:A:313:VAL:HG21	1:C:274:ARG:HH22	1.73	0.53
1:C:184:PRO:HD2	1:F:142:PHE:CE1	2.44	0.53
1:A:99:LYS:HE2	3:A:601:HOH:O	2.09	0.53
1:C:271:ARG:NH2	1:C:307:ILE:HD11	2.23	0.53
1:D:261:HIS:NE2	1:D:310:GLU:HB2	2.25	0.52
1:A:51:THR:CG2	1:A:313:VAL:HB	2.40	0.51
1:E:99:LYS:NZ	3:E:506:HOH:O	2.40	0.51
1:A:184:PRO:HD2	1:D:142:PHE:CE1	2.47	0.49
1:A:190:MET:SD	1:A:194:PRO:HD3	2.52	0.49
1:A:50:ARG:HG3	3:A:702:HOH:O	2.12	0.49
1:A:142:PHE:CE1	1:D:184:PRO:HD2	2.48	0.48
1:F:190:MET:SD	1:F:194:PRO:HD3	2.53	0.48
1:A:278:LYS:NZ	3:A:516:HOH:O	2.47	0.47
1:C:104:LYS:HE2	3:C:507:HOH:O	2.14	0.47
1:B:142:PHE:CE1	1:E:184:PRO:HD2	2.50	0.47
1:B:184:PRO:HD2	1:E:142:PHE:CE1	2.49	0.47
1:B:190:MET:SD	1:B:194:PRO:HD3	2.56	0.46
1:B:93:LYS:HE3	3:B:700:HOH:O	2.16	0.46
1:B:48:ASP:HB3	3:B:689:HOH:O	2.16	0.45
1:E:104:LYS:HE2	3:E:554:HOH:O	2.16	0.45
1:D:166:ASP:OD1	3:D:503:HOH:O	2.21	0.45
1:A:51:THR:HG22	1:A:313:VAL:HB	1.98	0.45
1:A:313:VAL:CG2	1:C:274:ARG:HH22	2.29	0.45
1:C:145:GLU:CB	3:C:693:HOH:O	2.65	0.45
1:C:142:PHE:CE1	1:F:184:PRO:HD2	2.52	0.44
1:E:306:THR:CG2	3:E:514:HOH:O	2.61	0.44
1:D:78[A]:ARG:NH1	3:D:507:HOH:O	2.44	0.42
1:C:32:GLN:NE2	1:C:64:ARG:O	2.43	0.42
1:E:196:HIS:HB3	1:E:212:LEU:HD11	2.02	0.41
1:F:147:ARG:HH11	1:F:147:ARG:HG3	1.85	0.41
1:D:261:HIS:NE2	1:D:310:GLU:CB	2.83	0.41
3:C:565:HOH:O	1:F:49:ASP:HA	2.20	0.41
1:F:46:ARG:NH1	1:F:54:GLY:HA3	2.35	0.40
1:D:50:ARG:CZ	1:D:50:ARG:HB3	2.52	0.40
1:D:190:MET:SD	1:D:194:PRO:HD3	2.62	0.40

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)
3:D:733:HOH:O	3:E:752:HOH:O[8_454]	2.03	0.17

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	287/290 (99%)	279 (97%)	7 (2%)	1 (0%)	44	40
1	B	286/290 (99%)	278 (97%)	7 (2%)	1 (0%)	44	40
1	C	284/290 (98%)	276 (97%)	8 (3%)	0	100	100
1	D	284/290 (98%)	276 (97%)	7 (2%)	1 (0%)	38	33
1	E	279/290 (96%)	272 (98%)	6 (2%)	1 (0%)	38	33
1	F	282/290 (97%)	274 (97%)	7 (2%)	1 (0%)	38	33
All	All	1702/1740 (98%)	1655 (97%)	42 (2%)	5 (0%)	44	40

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	VAL
1	B	134	VAL
1	E	134	VAL
1	F	134	VAL
1	D	134	VAL

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	249/253 (98%)	245 (98%)	4 (2%)	68	72
1	B	251/253 (99%)	246 (98%)	5 (2%)	60	64
1	C	245/253 (97%)	242 (99%)	3 (1%)	75	80
1	D	247/253 (98%)	243 (98%)	4 (2%)	68	72
1	E	240/253 (95%)	233 (97%)	7 (3%)	48	47
1	F	245/253 (97%)	238 (97%)	7 (3%)	48	47
All	All	1477/1518 (97%)	1447 (98%)	30 (2%)	60	64

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	115	ARG
1	A	126	ARG
1	A	313	VAL
1	B	38	GLN
1	B	50	ARG
1	B	244	LYS
1	B	289	ASP
1	B	313	VAL
1	C	192	LEU
1	C	284	LYS
1	C	294	GLU
1	D	53	THR
1	D	77	LYS
1	D	126	ARG
1	D	284	LYS
1	E	32	GLN
1	E	126	ARG
1	E	270	GLN
1	E	284	LYS
1	E	287	LYS
1	E	289	ASP
1	E	294	GLU
1	F	46	ARG
1	F	48	ASP
1	F	77	LYS
1	F	272	GLU

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Mol	Chain	Res	Type
1	F	284	LYS
1	F	287	LYS
1	F	289	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	UMP	A	401	-	17,21,21	2.95	6 (35%)	23,31,31	3.32	7 (30%)
2	UMP	B	401	-	17,21,21	2.73	6 (35%)	23,31,31	3.75	4 (17%)
2	UMP	C	401	-	17,21,21	3.06	8 (47%)	23,31,31	3.10	5 (21%)
2	UMP	D	401	-	17,21,21	3.08	6 (35%)	23,31,31	2.99	3 (13%)
2	UMP	E	401	-	17,21,21	2.94	13 (76%)	23,31,31	3.32	6 (26%)
2	UMP	F	401	-	17,21,21	3.06	5 (29%)	23,31,31	3.64	4 (17%)

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	UMP	A	401	-	-	0/6/22/22	0/2/2/2
2	UMP	B	401	-	-	0/6/22/22	0/2/2/2
2	UMP	C	401	-	-	0/6/22/22	0/2/2/2
2	UMP	D	401	-	-	0/6/22/22	0/2/2/2
2	UMP	E	401	-	-	0/6/22/22	0/2/2/2
2	UMP	F	401	-	-	0/6/22/22	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	UMP	C2'-C3'	-4.16	1.41	1.52
2	E	401	UMP	O3'-C3'	-3.07	1.36	1.43
2	E	401	UMP	O4-C4	-2.80	1.17	1.24
2	E	401	UMP	P-OP3	-2.78	1.43	1.54
2	F	401	UMP	C2'-C3'	-2.65	1.45	1.52
2	C	401	UMP	C2'-C3'	-2.60	1.46	1.52
2	D	401	UMP	C2'-C3'	-2.59	1.46	1.52
2	E	401	UMP	P-OP2	-2.57	1.44	1.54
2	B	401	UMP	C2'-C3'	-2.47	1.46	1.52
2	E	401	UMP	C3'-C4'	-2.46	1.46	1.53
2	E	401	UMP	P-O5'	-2.46	1.52	1.60
2	C	401	UMP	C3'-C4'	-2.41	1.46	1.53
2	E	401	UMP	O5'-C5'	-2.33	1.35	1.44
2	D	401	UMP	O5'-C5'	-2.32	1.35	1.44
2	A	401	UMP	P-O5'	-2.28	1.52	1.60
2	E	401	UMP	O4'-C4'	-2.28	1.39	1.45
2	B	401	UMP	O5'-C5'	-2.26	1.35	1.44
2	C	401	UMP	P-O5'	-2.10	1.53	1.60
2	C	401	UMP	O5'-C5'	-2.05	1.36	1.44
2	A	401	UMP	O5'-C5'	-2.02	1.36	1.44
2	C	401	UMP	C2-N3	3.26	1.44	1.38
2	E	401	UMP	C2-N3	3.33	1.44	1.38
2	A	401	UMP	C6-C5	3.52	1.45	1.38
2	E	401	UMP	C6-C5	3.83	1.46	1.38
2	E	401	UMP	C4-N3	4.07	1.40	1.33
2	B	401	UMP	C4-N3	4.10	1.40	1.33
2	B	401	UMP	C6-C5	4.17	1.47	1.38
2	A	401	UMP	C2-N3	4.27	1.46	1.38
2	C	401	UMP	C6-C5	4.37	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	UMP	C4-N3	4.46	1.41	1.33
2	F	401	UMP	C4-N3	4.80	1.41	1.33
2	A	401	UMP	C4-N3	4.93	1.42	1.33
2	F	401	UMP	C2-N3	4.94	1.48	1.38
2	D	401	UMP	C2-N3	4.94	1.48	1.38
2	B	401	UMP	C2-N3	4.96	1.48	1.38
2	F	401	UMP	C6-C5	5.02	1.48	1.38
2	E	401	UMP	C6-N1	5.02	1.42	1.35
2	D	401	UMP	C6-C5	5.05	1.49	1.38
2	C	401	UMP	C4-N3	5.61	1.43	1.33
2	B	401	UMP	C6-N1	6.88	1.45	1.35
2	F	401	UMP	C6-N1	8.08	1.46	1.35
2	A	401	UMP	C6-N1	8.20	1.46	1.35
2	C	401	UMP	C6-N1	8.38	1.47	1.35
2	D	401	UMP	C6-N1	8.62	1.47	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	UMP	O3'-C3'-C2'	-3.34	98.68	110.83
2	C	401	UMP	O3'-C3'-C2'	-2.99	99.94	110.83
2	E	401	UMP	C5-C4-N3	-2.21	117.85	123.12
2	F	401	UMP	O4'-C1'-C2'	2.03	110.14	106.25
2	D	401	UMP	P-O5'-C5'	2.09	124.04	118.30
2	C	401	UMP	O5'-P-OP1	2.10	112.36	106.47
2	A	401	UMP	O4'-C1'-N1	2.16	111.42	107.78
2	F	401	UMP	P-O5'-C5'	2.16	124.25	118.30
2	A	401	UMP	OP3-P-O5'	2.29	112.82	106.73
2	E	401	UMP	P-O5'-C5'	2.44	125.02	118.30
2	B	401	UMP	O4'-C1'-N1	2.49	111.98	107.78
2	A	401	UMP	C6-N1-C2	2.88	125.95	121.28
2	E	401	UMP	O4'-C1'-N1	3.00	112.83	107.78
2	E	401	UMP	O5'-C5'-C4'	3.06	119.84	109.00
2	C	401	UMP	O4'-C1'-N1	3.08	112.97	107.78
2	A	401	UMP	P-O5'-C5'	3.25	127.26	118.30
2	B	401	UMP	O5'-P-OP1	4.02	117.76	106.47
2	A	401	UMP	C2'-C1'-N1	5.47	127.14	114.23
2	C	401	UMP	C2'-C1'-N1	6.19	128.85	114.23
2	B	401	UMP	C2'-C1'-N1	6.91	130.56	114.23
2	D	401	UMP	C2'-C1'-N1	7.07	130.94	114.23
2	E	401	UMP	C2'-C1'-N1	7.14	131.10	114.23
2	F	401	UMP	C2'-C1'-N1	7.40	131.71	114.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	UMP	C4-N3-C2	11.82	124.28	114.13
2	C	401	UMP	C4-N3-C2	12.14	124.56	114.13
2	E	401	UMP	C4-N3-C2	12.84	125.16	114.13
2	A	401	UMP	C4-N3-C2	13.28	125.54	114.13
2	F	401	UMP	C4-N3-C2	14.76	126.81	114.13
2	B	401	UMP	C4-N3-C2	15.25	127.23	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	UMP	1	0
2	F	401	UMP	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	288/290 (99%)	-0.45	3 (1%) 82 82	12, 21, 39, 77	0
1	B	288/290 (99%)	-0.41	2 (0%) 87 87	15, 23, 39, 60	0
1	C	286/290 (98%)	-0.21	8 (2%) 53 53	15, 26, 46, 100	0
1	D	285/290 (98%)	-0.35	9 (3%) 48 48	13, 22, 43, 81	0
1	E	281/290 (96%)	-0.30	8 (2%) 53 53	15, 23, 45, 86	0
1	F	284/290 (97%)	-0.16	6 (2%) 64 63	16, 26, 52, 75	0
All	All	1712/1740 (98%)	-0.31	36 (2%) 64 63	12, 23, 44, 100	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	51	THR	9.1
1	F	51	THR	8.5
1	E	51	THR	8.2
1	E	52	GLY	7.2
1	A	312	ALA	5.5
1	E	48	ASP	5.3
1	D	52	GLY	5.3
1	C	307	ILE	5.0
1	A	313	VAL	4.9
1	D	51	THR	4.8
1	E	53	THR	4.5
1	E	28	HIS	4.0
1	F	307	ILE	3.7
1	C	310	GLU	3.7
1	E	49	ASP	3.6
1	D	53	THR	3.4
1	E	50	ARG	3.1
1	C	309	MET	3.0
1	D	307	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	52	GLY	2.8
1	F	26	PRO	2.8
1	C	50	ARG	2.8
1	D	308	LYS	2.8
1	A	311	MET	2.6
1	C	308	LYS	2.5
1	C	48	ASP	2.4
1	D	50	ARG	2.3
1	F	270	GLN	2.3
1	F	50	ARG	2.2
1	B	312	ALA	2.2
1	D	28	HIS	2.1
1	D	310	GLU	2.1
1	D	27	PRO	2.1
1	B	313	VAL	2.1
1	F	53	THR	2.0
1	E	26	PRO	2.0

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	UMP	E	401	20/20	0.97	0.14	3.11	22,28,32,32	0
2	UMP	A	401	20/20	0.98	0.09	0.70	17,24,29,31	0
2	UMP	C	401	20/20	0.98	0.12	0.18	23,30,33,34	0
2	UMP	F	401	20/20	0.97	0.10	-0.03	23,31,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	UMP	D	401	20/20	0.98	0.09	-0.16	21,26,29,30	0
2	UMP	B	401	20/20	0.98	0.08	-0.19	20,27,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.