



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:03 PM GMT

PDB ID : 1TLS  
Title : THYMIDYLATE SYNTHASE TERNARY COMPLEX WITH FDUMP AND  
METHYLENETETRAHYDROFOLATE  
Authors : Hyatt, D.C.; Maley, F.; Montfort, W.R.  
Deposited on : 1996-12-03  
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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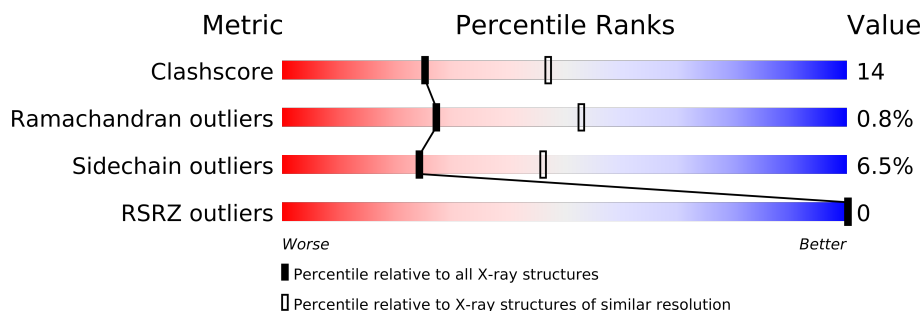
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance



The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	264	
1	B	264	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	C2F	B	266	-	X

## 2 Entry composition i

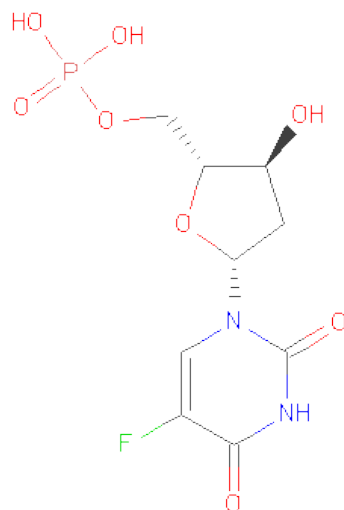
There are 4 unique types of molecules in this entry. The entry contains 4608 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

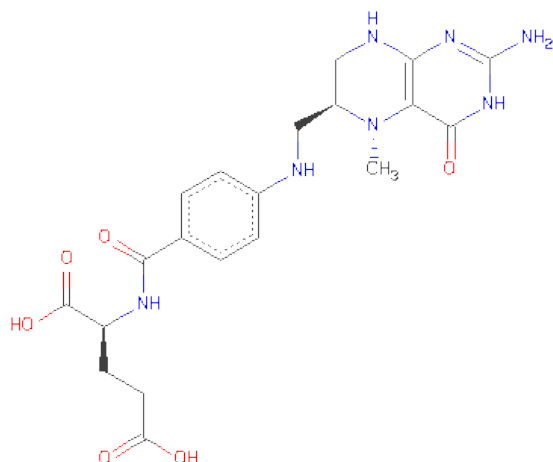
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2153	1375	371	395	12			
1	B	264	Total	C	N	O	S	0	0	0
			2153	1375	371	395	12			

- Molecule 2 is 5-FLUORO-2'-DEOXYURIDINE-5'-MONOPHOSPHATE (three-letter code: UFP) (formula: C<sub>9</sub>H<sub>12</sub>FN<sub>2</sub>O<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0
			21	9	1	2	8	1	
2	B	1	Total	C	F	N	O	P	0
			21	9	1	2	8	1	

- Molecule 3 is 5-METHYL-5,6,7,8-TETRAHYDROFOLICACID (three-letter code: C2F) (formula: C<sub>20</sub>H<sub>25</sub>N<sub>7</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	20	7	6		
3	B	1	Total	C	N	O	0	0
			33	20	7	6		

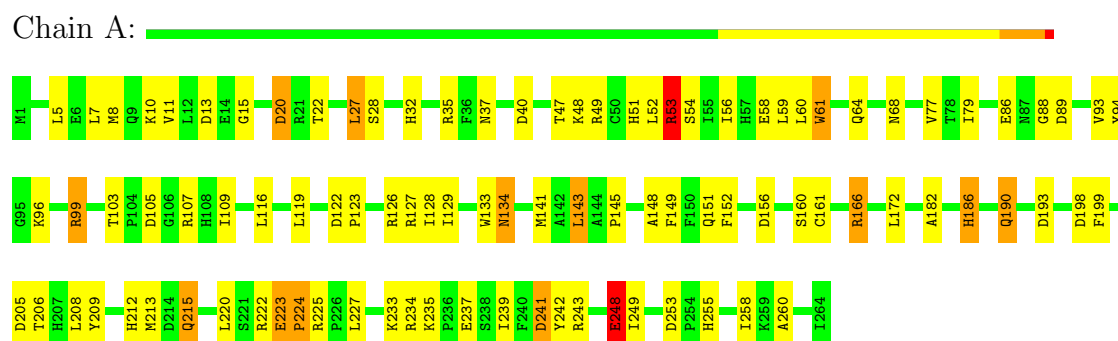
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		
4	B	84	Total	O	0	0
			84	84		

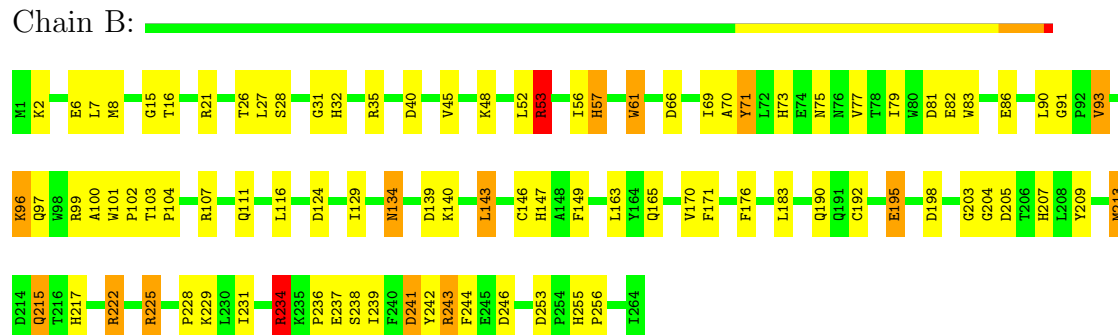
### 3 Residue-property plots

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: THYMIDYLATE SYNTHASE



#### • Molecule 1: THYMIDYLATE SYNTHASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.78Å 126.78Å 67.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	14.80 – 2.60 14.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (14.80-2.60) 89.5 (14.85-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.76 (at 2.61Å)	Xtriage
Refinement program	GPRLSA	Depositor
R, $R_{free}$	0.180 , (Not available) 0.161 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 19.5	EDS
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 19140 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: UFP, C2F, CXM

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	0.97	0/2202	1.87	47/2990 (1.6%)
1	B	0.96	0/2202	1.74	35/2990 (1.2%)
All	All	0.97	0/4404	1.80	82/5980 (1.4%)

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	2

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ARG	NE-CZ-NH2	-18.01	111.29	120.30
1	A	198	ASP	CB-CG-OD1	14.30	131.17	118.30
1	A	35	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	A	243	ARG	NE-CZ-NH1	12.69	126.64	120.30
1	A	53	ARG	NE-CZ-NH1	11.57	126.09	120.30
1	B	99	ARG	NE-CZ-NH2	10.43	125.51	120.30
1	B	35	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	A	99	ARG	NE-CZ-NH2	10.12	125.36	120.30
1	A	166	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	35	ARG	NE-CZ-NH1	9.73	125.16	120.30
1	A	198	ASP	CB-CG-OD2	-9.40	109.84	118.30
1	B	225	ARG	NE-CZ-NH2	-8.89	115.85	120.30
1	A	166	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	B	124	ASP	CB-CG-OD2	-8.32	110.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	B	21	ARG	NE-CZ-NH2	7.75	124.17	120.30
1	B	53	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	59	LEU	CB-CG-CD2	-7.51	98.24	111.00
1	B	243	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	40	ASP	CB-CG-OD2	7.40	124.96	118.30
1	B	99	ARG	NE-CZ-NH1	-7.33	116.63	120.30
1	A	99	ARG	NH1-CZ-NH2	-7.31	111.36	119.40
1	B	139	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	107	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	241	ASP	CB-CG-OD2	6.84	124.46	118.30
1	B	198	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	61	TRP	CA-CB-CG	6.66	126.35	113.70
1	A	13	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	161	CYS	O-C-N	6.65	133.35	122.70
1	B	222	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	40	ASP	CB-CG-OD1	-6.53	112.42	118.30
1	B	234	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	A	20	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	253	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	193	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	B	107	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	148	ALA	N-CA-CB	-6.37	101.18	110.10
1	A	205	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	195	GLU	N-CA-CB	-6.29	99.28	110.60
1	B	71	TYR	CB-CG-CD1	6.28	124.77	121.00
1	B	205	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	71	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	237	GLU	CG-CD-OE1	6.14	130.58	118.30
1	A	53	ARG	CD-NE-CZ	6.12	132.17	123.60
1	B	243	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	75	ASN	CB-CA-C	6.08	122.56	110.40
1	B	48	LYS	N-CA-CB	6.07	121.52	110.60
1	A	103	THR	CA-CB-CG2	6.05	120.86	112.40
1	A	53	ARG	NH1-CZ-NH2	-6.04	112.76	119.40
1	A	105	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	126	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	99	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	160	SER	N-CA-CB	5.87	119.31	110.50
1	A	22	THR	CA-CB-CG2	5.69	120.37	112.40
1	B	6	GLU	CG-CD-OE2	-5.66	106.98	118.30
1	A	199	PHE	N-CA-CB	5.65	120.77	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	LEU	CA-CB-CG	5.64	128.26	115.30
1	B	86	GLU	CA-CB-CG	5.62	125.76	113.40
1	B	35	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	227	LEU	N-CA-CB	-5.48	99.44	110.40
1	B	45	VAL	CA-CB-CG2	-5.45	102.72	110.90
1	A	94	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	B	16	THR	N-CA-CB	5.44	120.64	110.30
1	B	143	LEU	N-CA-CB	-5.35	99.70	110.40
1	A	156	ASP	CB-CG-OD1	-5.33	113.51	118.30
1	A	61	TRP	CA-CB-CG	5.31	123.79	113.70
1	A	224	PRO	O-C-N	5.30	131.18	122.70
1	A	241	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	139	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	172	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	234	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	94	TYR	CB-CG-CD1	5.15	124.09	121.00
1	A	186	HIS	CA-CB-CG	5.15	122.36	113.60
1	B	246	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	A	48	LYS	CA-C-O	-5.14	109.31	120.10
1	B	195	GLU	CB-CA-C	-5.12	100.16	110.40
1	A	198	ASP	N-CA-CB	-5.10	101.43	110.60
1	A	86	GLU	CG-CD-OE2	5.09	128.49	118.30
1	B	190	GLN	CB-CG-CD	5.07	124.79	111.60
1	B	244	PHE	CB-CA-C	5.06	120.52	110.40
1	B	57	HIS	CA-CB-CG	-5.04	105.03	113.60
1	A	248	GLU	CG-CD-OE1	-5.02	108.26	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	49	ARG	Sidechain
1	A	99	ARG	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2153	0	2079	66	0
1	B	2153	0	2079	52	0
2	A	21	0	9	1	0
2	B	21	0	9	1	0
3	A	33	0	21	5	0
3	B	33	0	21	0	0
4	A	110	0	0	3	0
4	B	84	0	0	1	0
All	All	4608	0	4218	117	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (117) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:52:LEU:CD1	1:A:249:ILE:HD13	1.54	1.33
1:A:52:LEU:HD11	1:A:249:ILE:CD1	1.84	1.08
1:B:129:ILE:HG21	1:B:149:PHE:CZ	2.02	0.95
1:A:52:LEU:CD1	1:A:249:ILE:CD1	2.42	0.94
1:A:215:GLN:HE21	1:A:215:GLN:H	1.19	0.90
1:B:215:GLN:HE21	1:B:215:GLN:N	1.69	0.90
1:B:215:GLN:NE2	1:B:215:GLN:H	1.68	0.90
1:A:52:LEU:HD11	1:A:249:ILE:HD13	0.87	0.84
1:B:215:GLN:HE21	1:B:215:GLN:H	0.85	0.82
1:B:96:LYS:NZ	1:B:102:PRO:HG3	1.96	0.80
1:B:27:LEU:HD12	1:B:213:MET:HE1	1.68	0.76
1:A:215:GLN:NE2	1:A:215:GLN:H	1.85	0.75
1:A:222:ARG:NH1	1:A:258:ILE:HD11	2.06	0.71
1:A:53:ARG:HH11	1:A:53:ARG:HB2	1.56	0.71
1:B:56:ILE:HG12	1:B:183:LEU:HD21	1.73	0.71
1:A:129:ILE:HG21	1:A:149:PHE:CE2	2.26	0.70
1:A:5:LEU:HD23	1:A:8:MET:HE2	1.76	0.67
1:B:129:ILE:CG2	1:B:149:PHE:CZ	2.75	0.67
1:B:134:ASN:C	1:B:134:ASN:HD22	1.98	0.67
1:B:96:LYS:HZ3	1:B:102:PRO:HG3	1.61	0.66
1:A:52:LEU:HD13	1:A:249:ILE:HD13	1.71	0.66
1:A:233:LYS:NZ	1:A:248:GLU:HG3	2.12	0.64
1:A:52:LEU:HD21	1:A:249:ILE:HD11	1.81	0.63
1:A:10:LYS:HE2	1:A:32:HIS:CD2	2.34	0.63
1:A:190:GLN:NE2	1:A:242:TYR:OH	2.33	0.61
1:A:10:LYS:HE2	1:A:32:HIS:HD2	1.65	0.60
1:A:129:ILE:CG2	1:A:149:PHE:CE2	2.84	0.59
1:A:52:LEU:CD2	1:A:249:ILE:CD1	2.80	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:238:SER:O	1:B:241:ASP:HB2	2.02	0.59
1:A:233:LYS:HZ2	1:A:248:GLU:HG3	1.69	0.58
1:A:151:GLN:HE22	1:B:204:GLY:HA3	1.69	0.57
1:B:57:HIS:HD2	1:B:71:TYR:OH	1.86	0.57
1:A:52:LEU:HD21	1:A:249:ILE:CD1	2.34	0.57
1:A:52:LEU:HD13	1:A:249:ILE:CD1	2.30	0.57
1:B:96:LYS:HZ1	1:B:102:PRO:HG3	1.69	0.56
1:A:7:LEU:HD11	1:A:206:THR:HG21	1.87	0.56
1:B:26:THR:HG22	1:B:209:TYR:CD1	2.41	0.55
1:A:53:ARG:HB2	1:A:53:ARG:NH1	2.19	0.55
1:A:129:ILE:HG13	1:A:151:GLN:HG3	1.88	0.55
1:A:215:GLN:N	1:A:215:GLN:HE21	1.98	0.55
1:B:27:LEU:HD12	1:B:213:MET:CE	2.36	0.54
1:B:69:ILE:HD12	1:B:73:HIS:CE1	2.42	0.54
1:B:171:PHE:CZ	1:B:215:GLN:HB3	2.43	0.54
1:B:27:LEU:CD1	1:B:213:MET:HE1	2.38	0.54
1:B:82:GLU:HG2	1:B:83:TRP:CZ3	2.43	0.54
1:A:47:THR:HA	1:A:255:HIS:CD2	2.44	0.53
1:B:147:HIS:HB2	1:B:163:LEU:HD11	1.91	0.53
1:B:53:ARG:NH1	1:B:53:ARG:HG3	2.23	0.52
1:B:222:ARG:HB3	1:B:255:HIS:CE1	2.45	0.52
1:A:5:LEU:HD23	1:A:8:MET:CE	2.38	0.52
1:A:134:ASN:C	1:A:134:ASN:HD22	2.14	0.51
1:A:47:THR:HA	1:A:255:HIS:HD2	1.75	0.51
1:B:242:TYR:O	1:B:243:ARG:HG2	2.11	0.51
1:B:61:TRP:CD1	1:B:66:ASP:HB3	2.46	0.51
1:A:143:LEU:CD2	3:A:266:C2F:H72	2.41	0.50
1:A:11:VAL:HG12	1:A:27:LEU:HD13	1.93	0.50
1:A:68:ASN:ND2	1:A:89:ASP:OD1	2.34	0.49
1:A:8:MET:HE3	1:A:220:LEU:HG	1.94	0.48
1:A:5:LEU:HD11	1:A:47:THR:HG21	1.94	0.48
1:A:53:ARG:CB	1:A:53:ARG:HH11	2.23	0.48
1:B:116:LEU:HD23	1:B:192:CYS:SG	2.53	0.48
1:A:56:ILE:O	1:A:60:LEU:HG	2.13	0.48
1:A:235:LYS:NZ	4:A:455:HOH:O	2.34	0.48
1:A:129:ILE:HG21	1:A:149:PHE:CZ	2.48	0.48
1:B:73:HIS:NE2	1:B:81:ASP:OD1	2.35	0.48
1:B:236:PRO:HG2	1:B:242:TYR:CE1	2.50	0.47
1:A:143:LEU:CD2	3:A:266:C2F:C7	2.92	0.47
1:B:129:ILE:HD13	1:B:149:PHE:CZ	2.49	0.47
1:B:165:GLN:O	1:B:203:GLY:HA2	2.15	0.47
1:A:11:VAL:HG12	1:A:27:LEU:CD1	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:234:ARG:O	1:B:236:PRO:HD3	2.14	0.46
1:A:127:ARG:HH22	1:B:143:LEU:HD12	1.81	0.46
1:A:133:TRP:CZ3	1:A:166:ARG:HD3	2.50	0.46
1:A:11:VAL:O	1:A:15:GLY:N	2.48	0.46
1:B:239:ILE:HA	1:B:242:TYR:HE1	1.81	0.45
1:A:143:LEU:HD21	3:A:266:C2F:N8	2.31	0.45
1:A:119:LEU:HD23	1:A:128:ILE:HD13	1.98	0.45
1:B:100:ALA:O	1:B:102:PRO:HD3	2.16	0.45
1:B:70:ALA:O	1:B:73:HIS:HB2	2.16	0.45
1:A:64:GLN:HG2	4:A:404:HOH:O	2.15	0.45
1:A:77:VAL:HG13	1:A:79:ILE:HG12	1.98	0.45
1:B:7:LEU:HD13	1:B:32:HIS:ND1	2.32	0.45
1:B:103:THR:HB	1:B:104:PRO:HD2	1.98	0.45
1:B:27:LEU:CD1	1:B:213:MET:CE	2.95	0.44
1:A:128:ILE:CG2	1:A:152:PHE:HB2	2.48	0.44
1:A:51:HIS:CE1	1:A:54:SER:HG	2.36	0.44
1:B:91:GLY:O	1:B:93:VAL:N	2.46	0.43
1:B:101:TRP:CH2	1:B:134:ASN:HA	2.53	0.43
1:B:134:ASN:ND2	1:B:134:ASN:C	2.69	0.43
1:A:53:ARG:HH11	1:A:53:ARG:CG	2.31	0.43
1:B:15:GLY:HA2	1:B:28:SER:O	2.19	0.43
1:A:223:GLU:HA	1:A:224:PRO:HD3	1.86	0.42
1:A:64:GLN:CG	4:A:404:HOH:O	2.67	0.42
1:B:231:ILE:HA	4:B:463:HOH:O	2.20	0.42
1:A:58:GLU:O	1:A:61:TRP:HB3	2.19	0.42
1:A:166:ARG:NH2	2:A:265:UFP:O3P	2.41	0.42
1:A:11:VAL:CG1	1:A:208:LEU:HD12	2.50	0.42
1:A:129:ILE:HD13	1:A:149:PHE:HZ	1.85	0.42
1:A:20:ASP:OD2	1:A:209:TYR:HE1	2.02	0.42
1:A:239:ILE:O	1:A:242:TYR:HD1	2.03	0.42
1:A:141:MET:SD	1:A:145:PRO:HD3	2.60	0.42
1:B:213:MET:O	1:B:217:HIS:CD2	2.73	0.41
1:A:68:ASN:HA	1:A:88:GLY:O	2.19	0.41
1:B:146:CYS:HB2	2:B:265:UFP:C4	2.50	0.41
1:A:143:LEU:HD23	3:A:266:C2F:H72	2.02	0.41
1:A:182:ALA:O	1:A:186:HIS:HD2	2.04	0.41
1:A:212:HIS:CD2	1:A:260:ALA:HB1	2.55	0.41
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.76	0.41
1:B:77:VAL:CG1	1:B:79:ILE:HG12	2.51	0.41
1:B:69:ILE:HG23	1:B:90:LEU:HD11	2.02	0.41
3:A:266:C2F:H92	3:A:266:C2F:H16	1.82	0.41
1:B:255:HIS:HB3	1:B:256:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:165:GLN:O	1:B:204:GLY:N	2.49	0.40
1:B:97:GLN:O	1:B:111:GLN:NE2	2.46	0.40
1:B:170:VAL:HG23	1:B:207:HIS:O	2.21	0.40
1:B:70:ALA:O	1:B:73:HIS:N	2.54	0.40
1:A:122:ASP:N	1:A:123:PRO:CD	2.85	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	262/264 (99%)	249 (95%)	12 (5%)	1 (0%)	43	72
1	B	262/264 (99%)	248 (95%)	11 (4%)	3 (1%)	21	42
All	All	524/528 (99%)	497 (95%)	23 (4%)	4 (1%)	27	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	VAL
1	B	228	PRO
1	B	31	GLY
1	B	93	VAL

### 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	232/232 (100%)	218 (94%)	14 (6%)	27	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	232/232 (100%)	216 (93%)	16 (7%)	22	42
All	All	464/464 (100%)	434 (94%)	30 (6%)	24	46

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

Mol	Chain	Res	Type
1	A	27	LEU
1	A	28	SER
1	A	37	ASN
1	A	53	ARG
1	A	96	LYS
1	A	109	ILE
1	A	134	ASN
1	A	190	GLN
1	A	213	MET
1	A	215	GLN
1	A	223	GLU
1	A	225	ARG
1	A	241	ASP
1	A	248	GLU
1	B	2	LYS
1	B	8	MET
1	B	52	LEU
1	B	53	ARG
1	B	96	LYS
1	B	134	ASN
1	B	140	LYS
1	B	176	PHE
1	B	195	GLU
1	B	213	MET
1	B	215	GLN
1	B	225	ARG
1	B	229	LYS
1	B	234	ARG
1	B	237	GLU
1	B	253	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS

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Mol	Chain	Res	Type
1	A	37	ASN
1	A	97	GLN
1	A	117	ASN
1	A	118	GLN
1	A	134	ASN
1	A	151	GLN
1	A	190	GLN
1	A	215	GLN
1	A	217	HIS
1	B	32	HIS
1	B	57	HIS
1	B	117	ASN
1	B	118	GLN
1	B	121	ASN
1	B	134	ASN
1	B	151	GLN
1	B	215	GLN
1	B	217	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z  > 2$
1	CXM	A	1	1	10,10,11	6.30	3 (30%)	8,11,13	1.15	0
1	CXM	B	1	1	10,10,11	5.89	3 (30%)	8,11,13	2.59	4 (50%)

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
1	CXM	A	1	1	-	0/8/10/12	0/0/0/0
1	CXM	B	1	1	-	0/8/10/12	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	CXM	O-C	19.52	1.24	1.11
1	B	1	CXM	O-C	18.27	1.24	1.11
1	A	1	CXM	CA-C	2.50	1.52	1.48
1	B	1	CXM	CA-C	2.29	1.52	1.48
1	A	1	CXM	CN-N	-2.11	1.30	1.33
1	B	1	CXM	ON1-CN	2.08	1.25	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	CXM	ON2-CN-N	4.73	122.22	116.33
1	B	1	CXM	ON1-CN-N	-3.81	118.11	124.90
1	B	1	CXM	CB-CA-N	3.46	115.26	110.48
1	B	1	CXM	ON2-CN-ON1	-2.12	119.52	122.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

4 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	UFP	A	265	1,3	22,22,22	5.46	7 (31%)	28,33,33	2.42	8 (28%)
3	C2F	A	266	2	35,35,35	2.65	15 (42%)	47,49,49	1.96	14 (29%)
2	UFP	B	265	1,3	22,22,22	5.38	6 (27%)	28,33,33	2.45	7 (25%)
3	C2F	B	266	2,4	35,35,35	2.40	13 (37%)	47,49,49	2.62	11 (23%)

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	UFP	A	265	1,3	-	0/7/22/22	0/2/2/2
3	C2F	A	266	2	-	0/22/35/35	0/1/3/3
2	UFP	B	265	1,3	-	0/7/22/22	0/2/2/2
3	C2F	B	266	2,4	-	0/22/35/35	0/1/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	265	UFP	C4-C5	19.89	1.63	1.38
2	B	265	UFP	C4-C5	19.43	1.63	1.38
2	B	265	UFP	C6-C5	12.76	1.62	1.38
2	A	265	UFP	C6-C5	11.37	1.59	1.38
2	B	265	UFP	C6-N1	7.38	1.52	1.34
2	A	265	UFP	F5-C5	-7.11	1.27	1.36
2	A	265	UFP	C6-N1	7.03	1.51	1.34
3	A	266	C2F	C2-NA2	6.01	1.41	1.32
3	A	266	C2F	C4-C4A	5.98	1.52	1.41
3	B	266	C2F	C4-C4A	5.84	1.52	1.41
3	A	266	C2F	C2-N1	5.77	1.40	1.33
3	B	266	C2F	C2-N1	5.05	1.39	1.33
3	B	266	C2F	C9-N10	5.00	1.56	1.45
3	A	266	C2F	C8A-N8	4.63	1.44	1.34
3	B	266	C2F	C6-N5	-4.13	1.42	1.47
3	B	266	C2F	C8A-N1	4.08	1.42	1.34
3	A	266	C2F	C6-N5	-3.96	1.43	1.47
3	A	266	C2F	C8A-N1	3.71	1.42	1.34
3	B	266	C2F	C2-NA2	3.49	1.37	1.32
2	B	265	UFP	F5-C5	-3.48	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	266	C2F	C-N	3.45	1.41	1.34
3	A	266	C2F	C9-N10	3.31	1.52	1.45
3	B	266	C2F	C7-C6	-3.25	1.48	1.52
2	B	265	UFP	O4'-C4'	3.20	1.52	1.45
3	B	266	C2F	C4-N3	3.06	1.42	1.37
3	B	266	C2F	CG-CD	3.04	1.58	1.50
3	B	266	C2F	C-N	2.94	1.40	1.34
3	A	266	C2F	C4-N3	2.91	1.42	1.37
3	A	266	C2F	C2-N3	2.80	1.41	1.36
2	A	265	UFP	C4-N3	2.72	1.41	1.37
3	A	266	C2F	C14-C15	2.71	1.43	1.39
2	A	265	UFP	P-O2P	-2.59	1.45	1.54
3	B	266	C2F	C15-N10	2.54	1.45	1.38
2	B	265	UFP	O3'-C3'	-2.54	1.37	1.43
2	A	265	UFP	C2-N1	2.43	1.41	1.38
3	A	266	C2F	C12-C	2.40	1.55	1.50
3	B	266	C2F	C2-N3	2.30	1.40	1.36
3	A	266	C2F	CA-CT	2.18	1.58	1.52
3	B	266	C2F	C16-C15	2.07	1.42	1.39
3	A	266	C2F	CB-CA	2.02	1.58	1.53
3	A	266	C2F	CG-CD	2.01	1.55	1.50

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	266	C2F	C4-C4A-C8A	10.67	123.25	114.43
3	B	266	C2F	CG-CB-CA	9.77	132.15	112.99
2	B	265	UFP	C5-C6-N1	-7.77	113.86	122.75
2	A	265	UFP	C5-C6-N1	-7.16	114.57	122.75
3	A	266	C2F	C4-C4A-C8A	6.35	119.68	114.43
2	B	265	UFP	C6-C5-C4	-5.72	104.45	117.33
2	A	265	UFP	C6-C5-C4	-5.08	105.89	117.33
2	B	265	UFP	N3-C2-N1	4.74	119.93	115.97
2	A	265	UFP	N3-C2-N1	4.69	119.89	115.97
3	A	266	C2F	CA-N-C	-4.33	112.12	121.80
2	A	265	UFP	O4'-C1'-N1	3.97	115.14	107.68
3	A	266	C2F	O2-CT-O1	3.56	132.12	124.07
3	B	266	C2F	C9-C6-N5	3.52	115.61	111.75
2	B	265	UFP	C6-N1-C2	-3.36	121.45	122.41
3	B	266	C2F	N8-C8A-N1	3.15	120.44	115.82
3	B	266	C2F	C6-C9-N10	-3.13	103.67	111.57
3	B	266	C2F	O2-CT-O1	3.13	131.14	124.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	266	C2F	CB-CG-CD	-3.12	105.30	112.88
3	A	266	C2F	OE1-CD-CG	-3.12	112.30	123.03
3	A	266	C2F	C7-C6-N5	3.09	111.59	108.42
3	A	266	C2F	CB-CA-N	-2.98	105.16	110.83
3	B	266	C2F	C8A-C4A-N5	-2.98	115.37	120.22
2	A	265	UFP	O3P-P-O1P	-2.89	101.00	110.44
3	A	266	C2F	NA2-C2-N3	2.74	120.88	117.86
2	B	265	UFP	O3P-P-O2P	2.73	118.24	107.61
3	B	266	C2F	C7-C6-N5	2.71	111.20	108.42
2	A	265	UFP	P-O5'-C5'	2.67	125.91	118.19
3	A	266	C2F	C6-C9-N10	-2.64	104.89	111.57
2	B	265	UFP	O4'-C1'-C2'	2.51	111.20	106.25
2	A	265	UFP	C2'-C3'-C4'	-2.50	97.13	102.73
3	B	266	C2F	C2-N1-C8A	2.42	121.05	117.61
3	B	266	C2F	C4A-C8A-N8	2.38	122.42	119.39
3	A	266	C2F	N8-C8A-N1	2.37	119.30	115.82
3	A	266	C2F	CT-CA-N	-2.34	104.50	110.53
3	A	266	C2F	C8A-C4A-N5	-2.27	116.52	120.22
3	B	266	C2F	CT-CA-N	-2.22	104.80	110.53
2	A	265	UFP	F5-C5-C6	-2.12	116.34	119.38
3	A	266	C2F	C9-C6-C7	2.11	116.01	112.89
3	A	266	C2F	CG-CB-CA	2.11	117.12	112.99
2	B	265	UFP	C6-N1-C1'	-2.07	114.20	119.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	264/264 (100%)	-0.97	0 100 100	2, 13, 28, 45	0
1	B	264/264 (100%)	-0.82	0 100 100	3, 18, 39, 54	0
All	All	528/528 (100%)	-0.90	0 100 100	2, 15, 35, 54	0

There are no RSRZ outliers to report.

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	CXM	B	1	11/12	0.10	-0.40	17,20,26,26	0
1	CXM	A	1	11/12	0.09	-0.61	13,17,20,20	0

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C2F	B	266	33/33	0.18	2.07	20,33,50,53	0
2	UFP	B	265	21/21	0.12	1.83	13,17,19,20	0
2	UFP	A	265	21/21	0.12	1.54	8,13,16,18	0
3	C2F	A	266	33/33	0.15	1.40	15,26,46,47	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.