Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:57 PM GMT

PDB ID	:	1VZA
Title	:	THYMIDYLATE SYNTHASE E60D MUTANT BINARY COMPLEX WITH 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (DUMP)
Authors	:	Birdsall, D.L.; Finer-Moore, J.; Stroud, R.M.
Deposited on	:	1996-09-18
Resolution	:	2.50 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 (i) symbol.

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

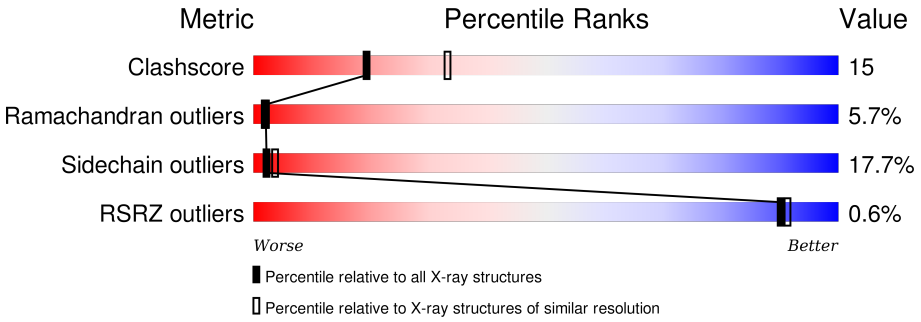
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	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)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	% 45% 39% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3246 atoms, of which 608 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.

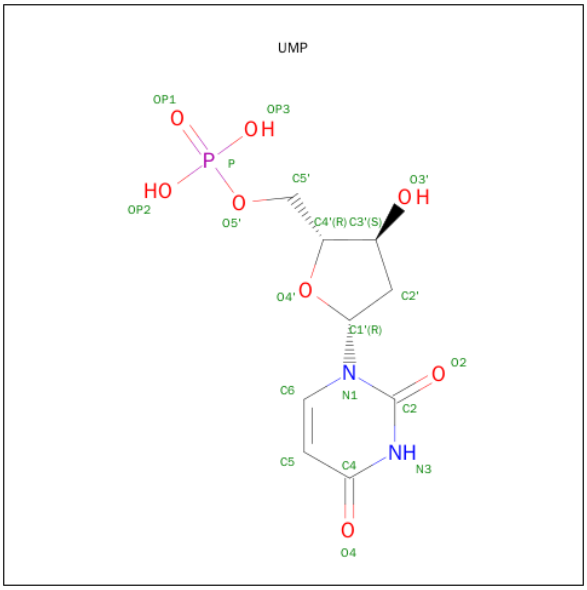
- Molecule 1 is a protein called THYMIDYLATE SYNTHASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	316	3138	1676	549	438	467	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLU	ENGINEERED	UNP P00469
A	111	ALA	ASP	CONFLICT	UNP P00469

- Molecule 2 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



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

- Molecule 3 is water.

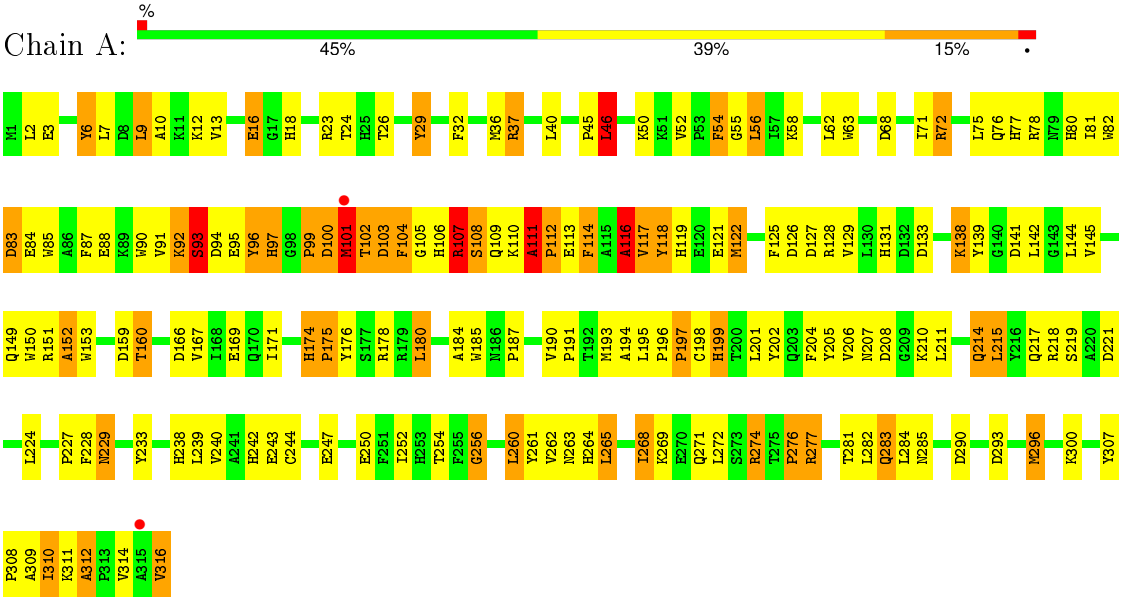
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	H	O		
3	A	29	87	58	29	0	0

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 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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	79.10Å 79.10Å 230.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.50 51.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.50) 61.3 (51.11-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.20Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.210 , (Not available) 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 98.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 13861 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3246	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.24	4/2673 (0.1%)	2.12	103/3633 (2.8%)

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	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	TRP	CG-CD2	-6.28	1.32	1.43
1	A	185	TRP	CG-CD2	-6.04	1.33	1.43
1	A	219	SER	CA-CB	-5.64	1.44	1.52
1	A	84	GLU	CG-CD	5.59	1.60	1.51

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	ARG	NE-CZ-NH1	13.82	127.21	120.30
1	A	128	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	A	151	ARG	NE-CZ-NH2	-10.79	114.90	120.30
1	A	96	TYR	CB-CG-CD2	-10.53	114.68	121.00
1	A	90	TRP	CD1-CG-CD2	9.63	114.00	106.30
1	A	153	TRP	CD1-CG-CD2	9.52	113.92	106.30
1	A	178	ARG	NE-CZ-NH2	-9.39	115.61	120.30
1	A	202	TYR	CB-CG-CD1	-9.23	115.46	121.00
1	A	82	TRP	CD1-CG-CD2	9.21	113.67	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	63	TRP	CD1-CG-CD2	8.76	113.30	106.30
1	A	185	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	A	169	GLU	CA-CB-CG	-8.36	95.01	113.40
1	A	150	TRP	CD1-CG-CD2	8.32	112.96	106.30
1	A	122	MET	CG-SD-CE	-8.17	87.13	100.20
1	A	37	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	A	233	TYR	CB-CG-CD2	-8.03	116.18	121.00
1	A	78	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	77	HIS	CA-CB-CG	-7.88	100.20	113.60
1	A	106	HIS	CA-CB-CG	-7.74	100.44	113.60
1	A	85	TRP	CD1-CG-CD2	7.70	112.46	106.30
1	A	185	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	A	90	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	A	153	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	A	284	LEU	N-CA-C	-7.45	90.89	111.00
1	A	166	ASP	CB-CG-OD2	7.38	124.95	118.30
1	A	63	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	A	97	HIS	CA-C-N	-7.30	101.60	116.20
1	A	99	PRO	N-CA-C	7.29	131.06	112.10
1	A	82	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	A	36	MET	CG-SD-CE	7.26	111.81	100.20
1	A	201	LEU	CA-CB-CG	7.25	131.97	115.30
1	A	284	LEU	CA-CB-CG	7.25	131.97	115.30
1	A	221	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	6	TYR	CB-CG-CD2	-7.23	116.66	121.00
1	A	159	ASP	N-CA-CB	-7.11	97.81	110.60
1	A	37	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	72	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	150	TRP	CE2-CD2-CG	-6.92	101.77	107.30
1	A	85	TRP	CE2-CD2-CG	-6.88	101.79	107.30
1	A	107	ARG	N-CA-C	-6.86	92.48	111.00
1	A	23	ARG	CA-CB-CG	6.85	128.47	113.40
1	A	205	TYR	CB-CG-CD1	-6.84	116.90	121.00
1	A	141	ASP	N-CA-C	-6.81	92.60	111.00
1	A	128	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	29	TYR	N-CA-C	-6.63	93.11	111.00
1	A	101	MET	CG-SD-CE	-6.62	89.61	100.20
1	A	78	ARG	CB-CG-CD	6.61	128.78	111.60
1	A	90	TRP	O-C-N	6.42	132.97	122.70
1	A	176	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	A	90	TRP	CG-CD1-NE1	-6.31	103.79	110.10
1	A	2	LEU	N-CA-CB	-6.15	98.10	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	126	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	195	LEU	N-CA-C	-6.05	94.66	111.00
1	A	214	GLN	CA-CB-CG	-6.05	100.09	113.40
1	A	96	TYR	CB-CG-CD1	6.03	124.62	121.00
1	A	180	LEU	CA-CB-CG	6.02	129.15	115.30
1	A	233	TYR	CA-CB-CG	-5.99	102.01	113.40
1	A	274	ARG	CA-CB-CG	-5.98	100.24	113.40
1	A	46	LEU	N-CA-C	-5.87	95.15	111.00
1	A	254	THR	CA-CB-CG2	5.84	120.57	112.40
1	A	205	TYR	CA-C-N	5.81	129.99	117.20
1	A	90	TRP	CB-CG-CD1	-5.77	119.49	127.00
1	A	97	HIS	CA-CB-CG	-5.71	103.90	113.60
1	A	108	SER	N-CA-C	-5.65	95.75	111.00
1	A	167	VAL	CA-CB-CG2	-5.64	102.44	110.90
1	A	99	PRO	N-CA-CB	-5.60	96.44	102.60
1	A	85	TRP	CG-CD2-CE3	5.55	138.90	133.90
1	A	116	ALA	CA-C-N	5.55	129.41	117.20
1	A	262	VAL	CG1-CB-CG2	-5.47	102.15	110.90
1	A	150	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	A	244	CYS	CA-C-N	5.45	127.10	116.20
1	A	221	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	A	274	ARG	CB-CG-CD	5.41	125.67	111.60
1	A	178	ARG	CA-CB-CG	-5.36	101.61	113.40
1	A	68	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	A	10	ALA	CB-CA-C	-5.33	102.10	110.10
1	A	272	LEU	CA-CB-CG	-5.32	103.06	115.30
1	A	174	HIS	N-CA-CB	5.32	120.17	110.60
1	A	82	TRP	CG-CD1-NE1	-5.32	104.78	110.10
1	A	310	ILE	CG1-CB-CG2	-5.32	99.70	111.40
1	A	85	TRP	CB-CA-C	-5.29	99.83	110.40
1	A	290	ASP	CA-CB-CG	-5.28	101.78	113.40
1	A	85	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	A	118	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	A	309	ALA	N-CA-CB	-5.26	102.74	110.10
1	A	72	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	152	ALA	CA-C-N	-5.21	105.73	117.20
1	A	160	THR	N-CA-CB	-5.20	100.43	110.30
1	A	199	HIS	N-CA-C	-5.17	97.04	111.00
1	A	174	HIS	CB-CA-C	-5.16	100.09	110.40
1	A	174	HIS	CA-CB-CG	5.14	122.34	113.60
1	A	178	ARG	CB-CG-CD	5.14	124.95	111.60
1	A	228	PHE	N-CA-CB	-5.14	101.35	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	152	ALA	CA-C-O	5.12	130.84	120.10
1	A	102	THR	O-C-N	5.10	130.85	122.70
1	A	166	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	A	316	VAL	CA-CB-CG2	5.09	118.54	110.90
1	A	54	PHE	CA-C-N	5.08	126.36	116.20
1	A	93	SER	O-C-N	5.08	130.82	122.70
1	A	68	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	9	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	90	TRP	CG-CD2-CE3	5.03	138.43	133.90
1	A	314	VAL	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	THR	Mainchain
1	A	111	ALA	Peptide
1	A	312	ALA	Peptide
1	A	6	TYR	Sidechain

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	2589	549	2497	77	0
2	A	20	1	11	0	0
3	A	29	58	0	0	0
All	All	2638	608	2508	77	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 15.

All (77) 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:A:101:MET:SD	1:A:118:TYR:HA	2.18	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:HIS:HB3	1:A:215:LEU:HD21	1.72	0.72
1:A:55:GLY:HA2	1:A:58:LYS:NZ	2.04	0.72
1:A:24:THR:HG21	1:A:316:VAL:HB	1.73	0.70
1:A:274:ARG:HG2	1:A:307:TYR:CE2	2.26	0.70
1:A:72:ARG:HG2	1:A:76:GLN:NE2	2.06	0.70
1:A:210:LYS:HA	1:A:247:GLU:O	1.92	0.70
1:A:87:PHE:HD2	1:A:122:MET:SD	2.18	0.67
1:A:274:ARG:NH2	1:A:310:ILE:HD11	2.09	0.67
1:A:260:LEU:HD21	1:A:268:ILE:HG13	1.75	0.66
1:A:87:PHE:CE2	1:A:122:MET:HA	2.31	0.65
1:A:55:GLY:HA2	1:A:58:LYS:HZ3	1.62	0.65
1:A:93:SER:HB3	1:A:139:TYR:OH	1.96	0.64
1:A:92:LYS:HE2	1:A:93:SER:HA	1.79	0.64
1:A:117:VAL:HG23	1:A:118:TYR:H	1.62	0.64
1:A:101:MET:HG3	1:A:121:GLU:HG2	1.80	0.63
1:A:114:PHE:O	1:A:118:TYR:HB3	1.98	0.63
1:A:12:LYS:O	1:A:16:GLU:HG2	1.99	0.61
1:A:87:PHE:HE2	1:A:122:MET:HA	1.66	0.60
1:A:37:ARG:HD3	1:A:250:GLU:OE1	2.03	0.59
1:A:190:VAL:HG23	1:A:191:PRO:HD3	1.83	0.59
1:A:13:VAL:HB	1:A:260:LEU:HD12	1.85	0.59
1:A:92:LYS:HE2	1:A:93:SER:CA	2.32	0.58
1:A:122:MET:O	1:A:125:PHE:HB3	2.04	0.57
1:A:101:MET:SD	1:A:118:TYR:CA	2.92	0.57
1:A:71:ILE:HD11	1:A:142:LEU:HD11	1.87	0.57
1:A:71:ILE:O	1:A:75:LEU:HG	2.05	0.56
1:A:204:PHE:CD2	1:A:211:LEU:HD21	2.40	0.56
1:A:138:LYS:NZ	1:A:139:TYR:CE2	2.74	0.56
1:A:271:GLN:O	1:A:274:ARG:HB2	2.06	0.56
1:A:100:ASP:HB3	1:A:114:PHE:CZ	2.41	0.55
1:A:40:LEU:HB3	1:A:238:HIS:HE1	1.73	0.53
1:A:87:PHE:HE2	1:A:122:MET:CA	2.21	0.53
1:A:87:PHE:CD2	1:A:122:MET:SD	3.01	0.52
1:A:116:ALA:O	1:A:118:TYR:N	2.42	0.52
1:A:125:PHE:O	1:A:129:VAL:HG23	2.10	0.52
1:A:214:GLN:HG3	1:A:252:ILE:HB	1.91	0.52
1:A:229:ASN:HD22	1:A:229:ASN:N	2.08	0.52
1:A:311:LYS:HD3	1:A:312:ALA:C	2.30	0.52
1:A:24:THR:HG21	1:A:316:VAL:CB	2.39	0.52
1:A:32:PHE:HA	1:A:256:GLY:O	2.11	0.51
1:A:46:LEU:HD11	1:A:54:PHE:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HB2	1:A:112:PRO:HD3	1.93	0.49
1:A:110:LYS:O	1:A:111:ALA:HB3	2.13	0.49
1:A:72:ARG:HG2	1:A:76:GLN:HE22	1.78	0.48
1:A:131:HIS:O	1:A:133:ASP:N	2.47	0.48
1:A:204:PHE:HB3	1:A:211:LEU:HD11	1.95	0.47
1:A:265:LEU:O	1:A:269:LYS:HG3	2.15	0.47
1:A:224:LEU:HD12	1:A:264:HIS:CE1	2.50	0.46
1:A:88:GLU:O	1:A:91:VAL:HG12	2.15	0.46
1:A:87:PHE:CE1	1:A:91:VAL:HB	2.49	0.46
1:A:198:CYS:HA	1:A:218:ARG:HH11	1.81	0.45
1:A:91:VAL:HG23	1:A:96:TYR:CE1	2.51	0.45
1:A:56:LEU:HD23	1:A:81:ILE:HD11	1.99	0.45
1:A:93:SER:O	1:A:95:GLU:N	2.50	0.45
1:A:54:PHE:HZ	1:A:282:LEU:HD11	1.83	0.44
1:A:62:LEU:HD12	1:A:296:MET:HG3	1.99	0.44
1:A:190:VAL:HG12	1:A:196:PRO:HB3	2.00	0.44
1:A:100:ASP:HB3	1:A:114:PHE:HZ	1.80	0.44
1:A:229:ASN:N	1:A:229:ASN:ND2	2.66	0.43
1:A:198:CYS:O	1:A:217:GLN:HA	2.18	0.43
1:A:107:ARG:NH1	1:A:114:PHE:CZ	2.86	0.43
1:A:184:ALA:O	1:A:197:PRO:HG3	2.18	0.43
1:A:207:ASN:OD1	1:A:208:ASP:N	2.52	0.43
1:A:95:GLU:O	1:A:97:HIS:N	2.52	0.42
1:A:91:VAL:O	1:A:91:VAL:HG22	2.19	0.42
1:A:277:ARG:NH1	1:A:307:TYR:CE1	2.87	0.42
1:A:87:PHE:CD2	1:A:122:MET:HA	2.54	0.42
1:A:54:PHE:O	1:A:58:LYS:HG3	2.21	0.41
1:A:80:HIS:HB3	1:A:83:ASP:HB2	2.02	0.41
1:A:171:ILE:O	1:A:175:PRO:HB3	2.20	0.41
1:A:72:ARG:HG2	1:A:76:GLN:HE21	1.81	0.41
1:A:204:PHE:CZ	1:A:240:VAL:HG21	2.55	0.41
1:A:283:GLN:NE2	1:A:300:LYS:NZ	2.69	0.41
1:A:83:ASP:OD2	1:A:122:MET:SD	2.79	0.41
1:A:261:TYR:HB2	1:A:264:HIS:ND1	2.35	0.41
1:A:103:ASP:O	1:A:104:PHE:C	2.59	0.41

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	314/316 (99%)	253 (81%)	43 (14%)	18 (6%)	2 2

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASP
1	A	99	PRO
1	A	101	MET
1	A	105	GLY
1	A	108	SER
1	A	111	ALA
1	A	117	VAL
1	A	296	MET
1	A	308	PRO
1	A	103	ASP
1	A	112	PRO
1	A	116	ALA
1	A	104	PHE
1	A	152	ALA
1	A	194	ALA
1	A	242	HIS
1	A	256	GLY
1	A	276	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	277/277 (100%)	228 (82%)	49 (18%)	2 4

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	7	LEU
1	A	9	LEU
1	A	16	GLU
1	A	18	HIS
1	A	26	THR
1	A	29	TYR
1	A	45	PRO
1	A	46	LEU
1	A	50	LYS
1	A	52	VAL
1	A	56	LEU
1	A	83	ASP
1	A	92	LYS
1	A	93	SER
1	A	100	ASP
1	A	107	ARG
1	A	109	GLN
1	A	113	GLU
1	A	114	PHE
1	A	119	HIS
1	A	127	ASP
1	A	138	LYS
1	A	144	LEU
1	A	145	VAL
1	A	149	GLN
1	A	160	THR
1	A	174	HIS
1	A	175	PRO
1	A	180	LEU
1	A	187	PRO
1	A	193	MET
1	A	197	PRO
1	A	206	VAL
1	A	215	LEU
1	A	227	PRO
1	A	229	ASN
1	A	239	LEU

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Mol	Chain	Res	Type
1	A	243	GLU
1	A	260	LEU
1	A	263	ASN
1	A	265	LEU
1	A	268	ILE
1	A	276	PRO
1	A	277	ARG
1	A	281	THR
1	A	283	GLN
1	A	285	ASN
1	A	293	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	76	GLN
1	A	214	GLN
1	A	238	HIS
1	A	271	GLN
1	A	283	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

1 ligand is 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	317	-	16,21,21	1.33	3 (18%)	20,31,31	1.82	4 (20%)

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	317	-	-	0/6/22/22	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	317	UMP	P-OP3	-2.09	1.47	1.54
2	A	317	UMP	C6-C5	2.30	1.43	1.38
2	A	317	UMP	C4-N3	2.72	1.40	1.36

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	317	UMP	OP2-P-O5'	-2.63	99.00	106.56
2	A	317	UMP	O4'-C1'-C2'	-2.34	101.60	106.27
2	A	317	UMP	O5'-P-OP1	2.09	112.45	107.14
2	A	317	UMP	O4'-C1'-N1	6.13	118.34	107.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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	316/316 (100%)	-0.78	2 (0%)	90	91	10, 22, 37, 44	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	MET	2.9
1	A	315	ALA	2.2

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

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^{th} 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	A	317	20/20	0.97	0.08	-1.24	15,28,32,33	0

6.5 Other polymers (i)

There are no such residues in this entry.