Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:39 AM GMT

PDB ID	:	2BBQ
Title	:	STRUCTURAL BASIS FOR RECOGNITION OF POLYGLUTAMYL FOLATES BY THYMIDYLATE SYNTHASE
Authors	:	Kamb, A.; Finer-Moore, J.; Stroud, R.M.
Deposited on	:	1992-09-16
Resolution	:	2.30 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 (i)) were used in the production of this report:

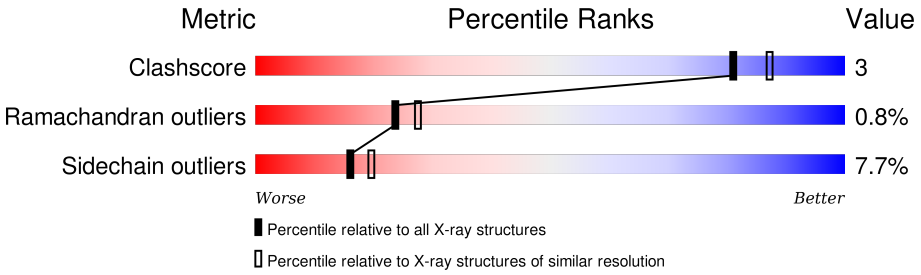
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	81% 16% •
1	B	264	77% 20% • •

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	B	530	X	-	-	-
3	PFG	A	531	X	-	-	-
3	PFG	B	532	X	-	-	-

2 Entry composition

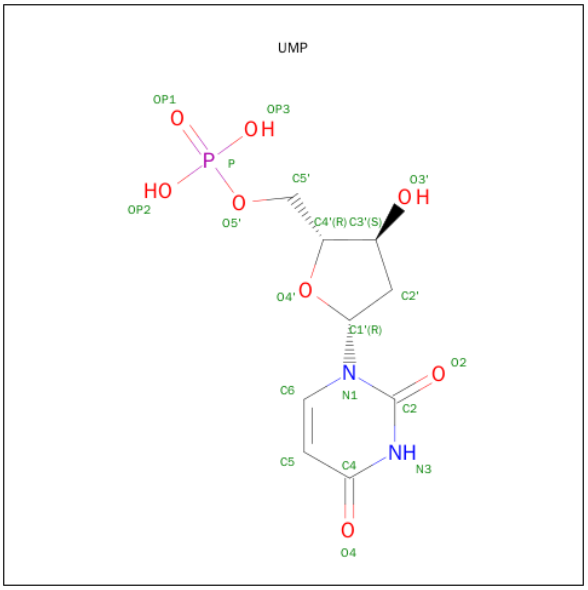
There are 4 unique types of molecules in this entry. The entry contains 4540 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

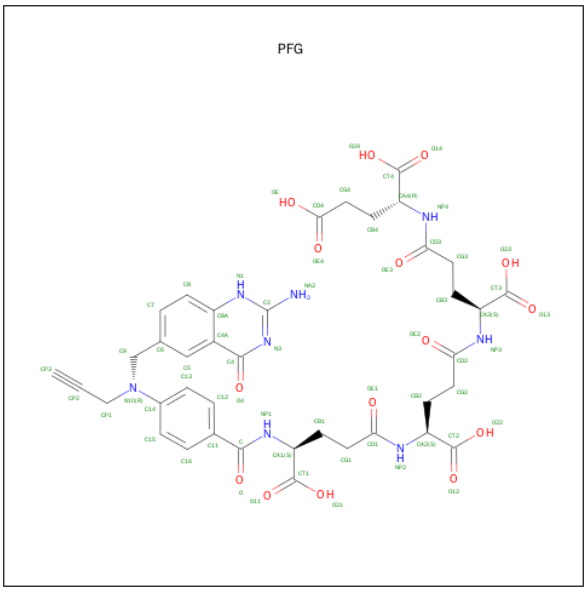
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2150	1374	371	393	12			
1	B	264	Total	C	N	O	S	0	0	0
			2150	1374	371	393	12			

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



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		

- Molecule 3 is 10-PARPARGYL-5,8-DIDEAZAFOLATE-4-GLUTAMIC ACID (three-letter code: PFG) (formula: $C_{39}H_{44}N_8O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 53 34 8 11	0	0
3	B	1	Total C N O 43 29 6 8	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	67	Total O 67 67	0	0
4	B	37	Total O 37 37	0	0

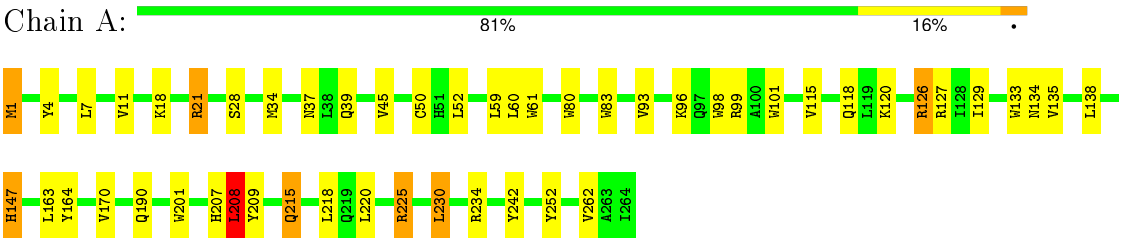
3 Residue-property plots (i)

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.

Note EDS was not executed.

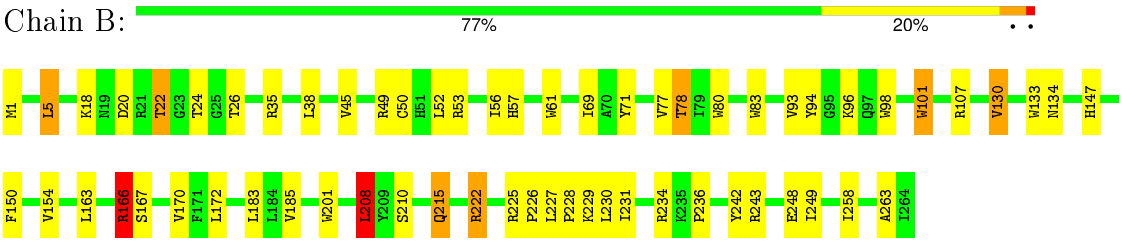
- Molecule 1: THYMIDYLATE SYNTHASE

Chain A:



- Molecule 1: THYMIDYLATE SYNTHASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	127.10Å 127.10Å 67.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4540	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.86	0/2210	1.66	42/3000 (1.4%)
1	B	0.87	0/2210	1.72	47/3000 (1.6%)
All	All	0.87	0/4420	1.69	89/6000 (1.5%)

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	B	0	1

There are no bond length outliers.

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	ARG	NE-CZ-NH1	20.85	130.72	120.30
1	B	166	ARG	NE-CZ-NH2	-12.84	113.88	120.30
1	A	126	ARG	NE-CZ-NH1	12.45	126.53	120.30
1	A	126	ARG	NE-CZ-NH2	-12.14	114.23	120.30
1	A	21	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	B	80	TRP	CD1-CG-CD2	9.54	113.93	106.30
1	A	80	TRP	CD1-CG-CD2	9.45	113.86	106.30
1	A	98	TRP	CD1-CG-CD2	9.17	113.64	106.30
1	A	234	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	A	234	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	A	61	TRP	CD1-CG-CD2	8.74	113.30	106.30
1	B	133	TRP	CD1-CG-CD2	8.53	113.12	106.30
1	B	80	TRP	CE2-CD2-CG	-8.20	100.74	107.30
1	B	83	TRP	CD1-CG-CD2	8.06	112.75	106.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	TRP	CD1-CG-CD2	7.93	112.64	106.30
1	A	80	TRP	CE2-CD2-CG	-7.89	100.99	107.30
1	A	98	TRP	CE2-CD2-CG	-7.75	101.10	107.30
1	B	243	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	B	94	TYR	CB-CG-CD2	-7.49	116.50	121.00
1	A	61	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	B	201	TRP	CD1-CG-CD2	7.15	112.02	106.30
1	A	208	LEU	CA-CB-CG	7.00	131.41	115.30
1	A	83	TRP	CE2-CD2-CG	-6.97	101.72	107.30
1	A	98	TRP	CG-CD1-NE1	-6.89	103.21	110.10
1	A	201	TRP	CE2-CD2-CG	-6.84	101.82	107.30
1	A	80	TRP	CG-CD1-NE1	-6.83	103.27	110.10
1	A	225	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	B	222	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	B	133	TRP	CE2-CD2-CG	-6.69	101.95	107.30
1	A	101	TRP	CE2-CD2-CG	-6.68	101.95	107.30
1	B	147	HIS	CA-CB-CG	6.63	124.88	113.60
1	A	83	TRP	CD1-CG-CD2	6.62	111.60	106.30
1	A	101	TRP	CD1-CG-CD2	6.62	111.59	106.30
1	B	166	ARG	CG-CD-NE	-6.61	97.92	111.80
1	B	80	TRP	CG-CD2-CE3	6.48	139.74	133.90
1	B	83	TRP	CE2-CD2-CG	-6.46	102.13	107.30
1	B	201	TRP	CE2-CD2-CG	-6.46	102.13	107.30
1	A	242	TYR	CB-CG-CD2	-6.44	117.13	121.00
1	B	166	ARG	CB-CG-CD	6.43	128.31	111.60
1	B	61	TRP	CD1-CG-CD2	6.42	111.44	106.30
1	A	99	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	185	VAL	CG1-CB-CG2	-6.39	100.68	110.90
1	A	133	TRP	CD1-CG-CD2	6.38	111.41	106.30
1	B	5	LEU	CA-CB-CG	6.38	129.97	115.30
1	B	133	TRP	CG-CD1-NE1	-6.32	103.78	110.10
1	A	133	TRP	CE2-CD2-CG	-6.28	102.27	107.30
1	B	222	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	242	TYR	CB-CG-CD2	-6.21	117.28	121.00
1	A	225	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	99	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	B	77	VAL	CA-C-N	-6.09	103.81	117.20
1	B	166	ARG	CD-NE-CZ	6.08	132.12	123.60
1	B	61	TRP	CE2-CD2-CG	-6.07	102.44	107.30
1	B	80	TRP	CG-CD1-NE1	-6.04	104.06	110.10
1	B	101	TRP	CE2-CD2-CG	-5.97	102.52	107.30
1	B	98	TRP	CE2-CD2-CG	-5.96	102.53	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	252	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	B	107	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	1	MET	CG-SD-CE	-5.82	90.89	100.20
1	A	61	TRP	CG-CD1-NE1	-5.82	104.28	110.10
1	B	172	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	B	80	TRP	CB-CG-CD1	-5.76	119.51	127.00
1	B	98	TRP	CD1-CG-CD2	5.74	110.89	106.30
1	A	34	MET	CA-CB-CG	5.73	123.05	113.30
1	A	101	TRP	CG-CD2-CE3	5.69	139.02	133.90
1	A	98	TRP	CG-CD2-CE3	5.68	139.01	133.90
1	B	49	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	230	LEU	CA-CB-CG	5.64	128.27	115.30
1	B	201	TRP	CG-CD1-NE1	-5.60	104.50	110.10
1	B	208	LEU	CA-CB-CG	5.54	128.05	115.30
1	A	201	TRP	CG-CD1-NE1	-5.46	104.64	110.10
1	A	209	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	B	101	TRP	CD1-CG-CD2	5.38	110.61	106.30
1	A	220	LEU	CA-CB-CG	5.33	127.57	115.30
1	B	130	VAL	CG1-CB-CG2	5.32	119.41	110.90
1	B	98	TRP	CG-CD2-CE3	5.29	138.66	133.90
1	A	147	HIS	CA-CB-CG	5.27	122.56	113.60
1	A	61	TRP	CG-CD2-CE3	5.24	138.62	133.90
1	A	164	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	B	35	ARG	CA-CB-CG	5.21	124.87	113.40
1	B	225	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	4	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	B	78	THR	N-CA-CB	-5.20	100.42	110.30
1	B	210	SER	CA-CB-OG	-5.12	97.37	111.20
1	B	53	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	230	LEU	CA-CB-CG	5.08	127.00	115.30
1	B	83	TRP	CG-CD1-NE1	-5.08	105.02	110.10
1	A	127	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	22	THR	N-CA-CB	-5.04	100.73	110.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	166	ARG	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	2150	0	2081	14	0
1	B	2150	0	2081	18	0
2	A	20	0	9	0	0
2	B	20	0	9	0	0
3	A	53	0	33	2	0
3	B	43	0	27	0	0
4	A	67	0	0	1	0
4	B	37	0	0	1	0
All	All	4540	0	4240	29	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 3.

All (29) 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:B:22:THR:HG21	1:B:263:ALA:HB1	1.49	0.92
1:B:231:ILE:HB	1:B:248:GLU:HB2	1.78	0.66
1:A:215:GLN:NE2	1:A:215:GLN:H	1.95	0.65
1:A:28:SER:HB3	1:A:207:HIS:HB3	1.83	0.61
1:B:20:ASP:OD2	1:B:22:THR:HB	2.02	0.59
1:A:215:GLN:HE21	1:A:215:GLN:H	1.52	0.55
1:B:215:GLN:HE21	1:B:215:GLN:H	1.54	0.55
3:A:531:PFG:H15	3:A:531:PFG:CP2	2.37	0.55
1:B:22:THR:CG2	1:B:263:ALA:HB1	2.30	0.54
1:A:18:LYS:HE3	1:B:154:VAL:O	2.08	0.53
1:B:57:HIS:HD2	1:B:71:TYR:OH	1.92	0.52
1:B:170:VAL:HB	1:B:208:LEU:HD13	1.91	0.52
1:A:129:ILE:HD11	1:B:166:ARG:HG3	1.91	0.52
1:A:115:VAL:HA	1:A:118:GLN:HE21	1.77	0.49
1:B:1:MET:N	4:B:568:HOH:O	2.45	0.49
1:A:1:MET:N	4:A:547:HOH:O	2.34	0.47
1:B:234:ARG:O	1:B:236:PRO:HD3	2.14	0.47
1:A:45:VAL:HG22	1:A:50:CYS:SG	2.55	0.46
1:B:22:THR:HG22	1:B:24:THR:H	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:HIS:HB2	1:A:163:LEU:HD11	1.99	0.44
1:B:52:LEU:HD12	1:B:249:ILE:HG21	2.00	0.44
1:B:130:VAL:HG22	1:B:150:PHE:CE1	2.53	0.44
1:A:126:ARG:HD3	1:B:167:SER:OG	2.19	0.43
1:B:45:VAL:HG22	1:B:50:CYS:SG	2.60	0.42
1:A:170:VAL:HB	1:A:208:LEU:HD13	2.00	0.41
1:A:126:ARG:HD3	1:B:167:SER:HG	1.85	0.41
1:A:135:VAL:HB	1:B:101:TRP:CE2	2.55	0.41
1:A:218:LEU:HA	1:A:218:LEU:HD12	1.90	0.40
3:A:531:PFG:C15	3:A:531:PFG:CP2	2.96	0.40

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	262/264 (99%)	252 (96%)	9 (3%)	1 (0%)	39	48
1	B	262/264 (99%)	250 (95%)	9 (3%)	3 (1%)	17	18
All	All	524/528 (99%)	502 (96%)	18 (3%)	4 (1%)	24	27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	VAL
1	B	258	ILE
1	B	93	VAL
1	B	228	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	233/233 (100%)	215 (92%)	18 (8%)	16	20
1	B	233/233 (100%)	215 (92%)	18 (8%)	16	20
All	All	466/466 (100%)	430 (92%)	36 (8%)	16	20

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	11	VAL
1	A	21	ARG
1	A	37	ASN
1	A	39	GLN
1	A	52	LEU
1	A	59	LEU
1	A	60	LEU
1	A	96	LYS
1	A	120	LYS
1	A	134	ASN
1	A	138	LEU
1	A	190	GLN
1	A	208	LEU
1	A	215	GLN
1	A	225	ARG
1	A	230	LEU
1	A	262	VAL
1	B	5	LEU
1	B	18	LYS
1	B	26	THR
1	B	38	LEU
1	B	56	ILE
1	B	69	ILE
1	B	78	THR
1	B	96	LYS
1	B	134	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	163	LEU
1	B	166	ARG
1	B	183	LEU
1	B	208	LEU
1	B	215	GLN
1	B	222	ARG
1	B	226	PRO
1	B	227	LEU
1	B	229	LYS

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	19	ASN
1	A	32	HIS
1	A	33	GLN
1	A	37	ASN
1	A	97	GLN
1	A	108	HIS
1	A	118	GLN
1	A	134	ASN
1	A	151	GLN
1	A	162	GLN
1	A	186	HIS
1	A	190	GLN
1	A	215	GLN
1	B	51	HIS
1	B	57	HIS
1	B	118	GLN
1	B	134	ASN
1	B	151	GLN
1	B	215	GLN

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)

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	UMP	A	529	1	16,21,21	2.51	4 (25%)	23,31,31	4.19	8 (34%)
3	PFG	A	531	-	46,55,64	1.31	2 (4%)	48,75,87	1.70	11 (22%)
2	UMP	B	530	1	16,21,21	2.70	4 (25%)	23,31,31	3.84	6 (26%)
3	PFG	B	532	-	39,45,64	1.27	2 (5%)	40,61,87	1.69	9 (22%)

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	529	1	-	0/6/22/22	0/2/2/2
3	PFG	A	531	-	1/1/11/18	0/41/54/67	0/3/3/3
2	UMP	B	530	1	1/1/4/4	0/6/22/22	0/2/2/2
3	PFG	B	532	-	1/1/7/18	0/30/40/67	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	530	UMP	P-OP3	-2.45	1.45	1.54
2	A	529	UMP	P-OP3	-2.34	1.46	1.54
3	B	532	PFG	C11-C	-2.13	1.45	1.50
2	A	529	UMP	C4-N3	2.13	1.37	1.33
3	A	531	PFG	CA2-NP2	2.28	1.49	1.46
2	A	529	UMP	C6-C5	4.17	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	530	UMP	C4-N3	4.53	1.41	1.33
2	B	530	UMP	C6-C5	5.07	1.49	1.38
3	B	532	PFG	O4-C4	5.22	1.37	1.24
3	A	531	PFG	O4-C4	5.33	1.37	1.24
2	B	530	UMP	C6-N1	7.60	1.46	1.35
2	A	529	UMP	C6-N1	7.89	1.46	1.35

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	531	PFG	N1-C2-N3	-4.95	119.90	127.44
2	A	529	UMP	C6-N1-C2	-4.28	114.35	121.28
2	B	530	UMP	C6-C5-C4	-4.18	109.46	117.28
2	A	529	UMP	C6-C5-C4	-4.18	109.46	117.28
3	B	532	PFG	N1-C2-N3	-4.14	121.13	127.44
2	A	529	UMP	C5-C6-N1	-3.84	111.17	120.58
2	B	530	UMP	C5-C6-N1	-3.74	111.42	120.58
3	B	532	PFG	CG1-CD1-NP2	-3.63	109.91	115.83
2	B	530	UMP	C5-C4-N3	-3.21	114.88	123.12
2	A	529	UMP	C5-C4-N3	-3.16	115.02	123.12
3	A	531	PFG	CG1-CD1-NP2	-3.11	110.76	115.83
3	B	532	PFG	CP1-N10-C9	-2.61	110.86	117.28
3	B	532	PFG	OE1-CD1-NP2	-2.55	118.69	123.01
3	A	531	PFG	C4-C4A-C8A	-2.17	116.42	118.54
3	A	531	PFG	CG3-CD3-NP4	-2.03	110.15	116.53
3	B	532	PFG	NA2-C2-N1	2.09	121.81	117.80
3	A	531	PFG	CG3-CB3-CA3	2.15	117.36	112.98
3	B	532	PFG	C9-N10-C14	2.32	125.11	120.93
3	A	531	PFG	C5-C4A-C8A	2.35	120.94	118.14
2	A	529	UMP	OP3-P-O5'	2.36	113.35	106.56
3	B	532	PFG	C5-C4A-C8A	2.41	121.02	118.14
3	A	531	PFG	NA2-C2-N1	2.50	122.59	117.80
3	B	532	PFG	CP1-N10-C14	2.64	123.86	119.05
3	A	531	PFG	C9-N10-C14	2.96	126.25	120.93
3	A	531	PFG	C6-C9-N10	2.99	119.48	114.51
2	A	529	UMP	C2'-C1'-N1	3.05	121.58	114.16
3	A	531	PFG	CG2-CB2-CA2	3.13	119.34	112.98
3	B	532	PFG	C4-N3-C2	3.55	120.87	115.94
3	A	531	PFG	C4-N3-C2	4.11	121.64	115.94
2	B	530	UMP	C2'-C1'-N1	4.39	124.83	114.16
2	B	530	UMP	O4'-C1'-N1	10.12	125.25	107.72
2	A	529	UMP	C4-N3-C2	12.03	126.06	114.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	530	UMP	C4-N3-C2	12.57	126.59	114.14
2	A	529	UMP	O4'-C1'-N1	13.12	130.44	107.72

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	530	UMP	C1'
3	A	531	PFG	N10
3	B	532	PFG	N10

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	531	PFG	2	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.