



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:23 am GMT

PDB ID : 4P5A  
Title : Crystal structure of a UMP/dUMP methylase PolB from *Streptomyces cacaoi* bound with 5-Br UMP  
Authors : Li, Y.; Chen, W.; Li, J.; Xia, Z.; Deng, Z.; Zhou, J.  
Deposited on : 2014-03-15  
Resolution : 1.76 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](mailto: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.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

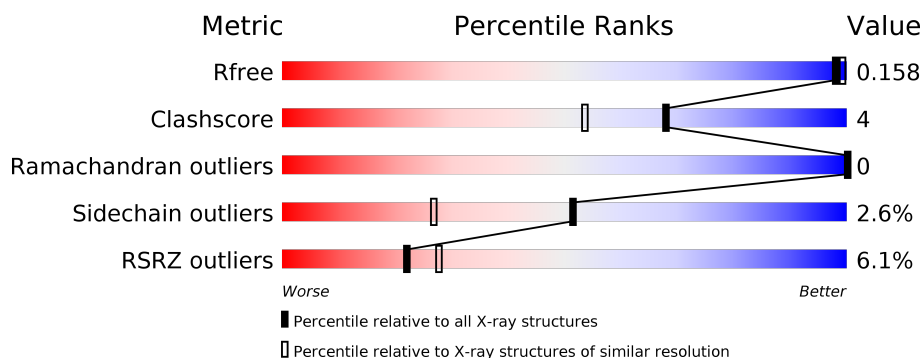
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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. 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	239	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	B	239	<div> <div>6%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	C	239	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 7%</div> </div> </div>
1	D	239	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>13%</div> <div>• 6%</div> </div> </div>

## 2 Entry composition [i](#)

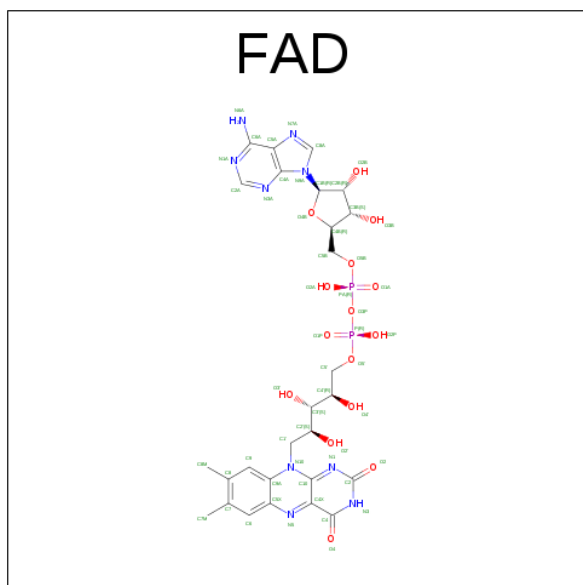
There are 4 unique types of molecules in this entry. The entry contains 8303 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ThyX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	1	0
			1816	1137	340	331	8			
1	B	227	Total	C	N	O	S	0	4	0
			1852	1160	347	337	8			
1	C	223	Total	C	N	O	S	0	2	0
			1798	1128	333	329	8			
1	D	225	Total	C	N	O	S	0	1	0
			1804	1129	335	332	8			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



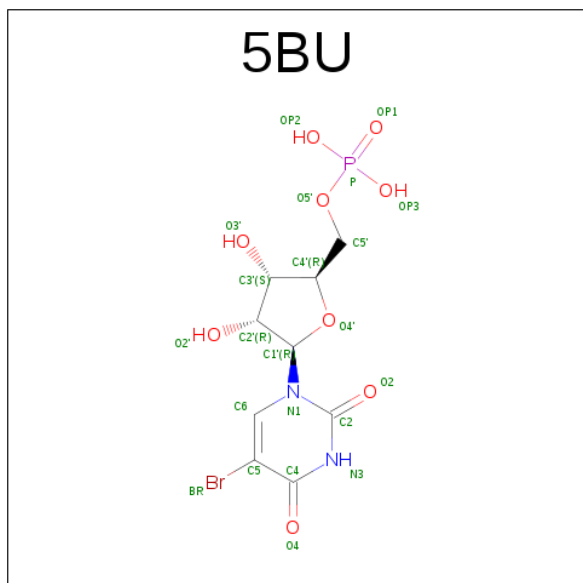
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 5-BROMO-URIDINE-5'-MONOPHOSPHATE (three-letter code: 5BU) (formula: C<sub>9</sub>H<sub>12</sub>BrN<sub>2</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 22	Br 1	C 9	N 2	O 9	P 1	0	0
3	B	1	Total 22	Br 1	C 9	N 2	O 9	P 1	0	0
3	C	1	Total 22	Br 1	C 9	N 2	O 9	P 1	0	0
3	D	1	Total 22	Br 1	C 9	N 2	O 9	P 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		
4	B	173	Total	O	0	0
			173	173		
4	C	185	Total	O	0	0
			185	185		

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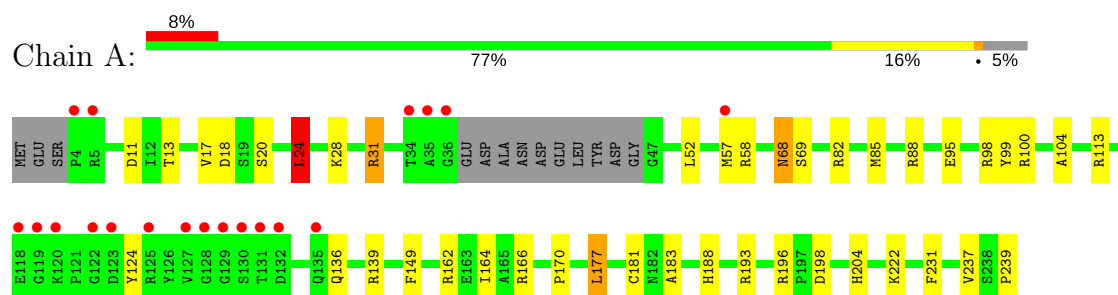
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	188	Total 188	O 188	0	0

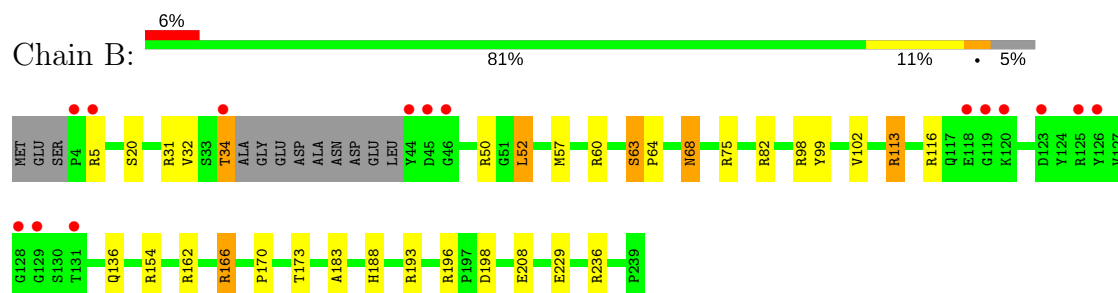
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

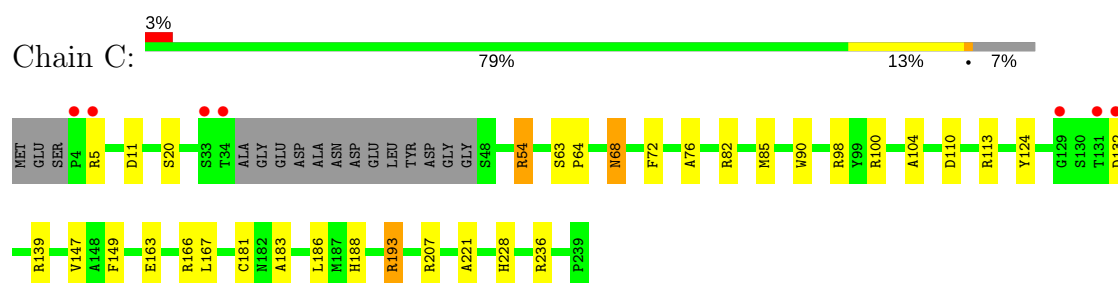
#### • Molecule 1: Thymidylate synthase ThyX



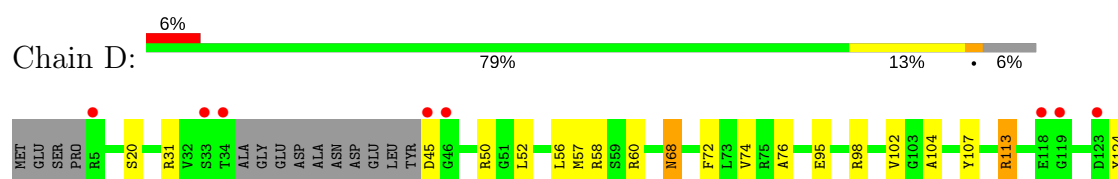
#### • Molecule 1: Thymidylate synthase ThyX



#### • Molecule 1: Thymidylate synthase ThyX



#### • Molecule 1: Thymidylate synthase ThyX





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.90Å 94.16Å 91.95Å 90.00° 98.30° 90.00°	Depositor
Resolution (Å)	50.00 – 1.76 36.46 – 1.76	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-1.76) 98.4 (36.46-1.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.154 , 0.193 0.157 , 0.158	Depositor DCC
$R_{free}$ test set	5176 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8303	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5BU, FAD

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	1.41	8/1856 (0.4%)	1.23	13/2511 (0.5%)
1	B	1.44	5/1900 (0.3%)	1.21	15/2570 (0.6%)
1	C	1.44	7/1844 (0.4%)	1.22	12/2495 (0.5%)
1	D	1.42	10/1846 (0.5%)	1.20	10/2497 (0.4%)
All	All	1.43	30/7446 (0.4%)	1.22	50/10073 (0.5%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	76	ALA	CA-CB	8.44	1.70	1.52
1	B	162	ARG	CB-CG	-7.57	1.32	1.52
1	D	107	TYR	CD1-CE1	7.54	1.50	1.39
1	B	63	SER	CB-OG	-7.43	1.32	1.42
1	C	163	GLU	CB-CG	7.37	1.66	1.52
1	D	76	ALA	CA-CB	7.07	1.67	1.52
1	C	181	CYS	CB-SG	-6.86	1.70	1.82
1	D	95	GLU	CD-OE2	6.71	1.33	1.25
1	A	95	GLU	CG-CD	6.30	1.61	1.51
1	A	17	VAL	CA-CB	6.19	1.67	1.54
1	B	198	ASP	CB-CG	6.07	1.64	1.51
1	B	208	GLU	CB-CG	5.81	1.63	1.52
1	C	147	VAL	CB-CG2	5.74	1.65	1.52
1	C	124	TYR	CD1-CE1	5.71	1.48	1.39
1	B	99	TYR	CD1-CE1	5.54	1.47	1.39
1	C	90	TRP	CZ3-CH2	5.42	1.48	1.40
1	D	147	VAL	CB-CG2	5.34	1.64	1.52
1	C	193	ARG	CZ-NH2	5.29	1.40	1.33
1	D	198	ASP	CB-CG	5.27	1.62	1.51
1	A	88	ARG	CG-CD	5.25	1.65	1.51
1	D	72	PHE	CE2-CZ	5.23	1.47	1.37
1	D	152	TYR	CD2-CE2	5.20	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	74	VAL	CB-CG1	5.18	1.63	1.52
1	D	214	GLU	CG-CD	5.17	1.59	1.51
1	A	181	CYS	CB-SG	-5.08	1.73	1.81
1	D	152	TYR	CD1-CE1	5.08	1.47	1.39
1	A	231	PHE	CD1-CE1	5.06	1.49	1.39
1	A	237	VAL	CB-CG1	5.06	1.63	1.52
1	A	69	SER	CA-CB	5.04	1.60	1.52
1	A	18	ASP	CB-CG	5.04	1.62	1.51

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	D	198	ASP	CB-CG-OD2	9.41	126.77	118.30
1	B	154	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	A	162	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	82	ARG	NE-CZ-NH2	8.57	124.59	120.30
1	B	196[A]	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	B	196[B]	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	58	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	52	LEU	CB-CG-CD2	7.59	123.91	111.00
1	C	11	ASP	CB-CG-OD1	7.44	124.99	118.30
1	A	196[A]	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	196[B]	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	82	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	B	162	ARG	CG-CD-NE	-7.21	96.66	111.80
1	B	196[A]	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	196[B]	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	D	196	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	50	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	C	186	LEU	CB-CG-CD2	-6.90	99.26	111.00
1	A	31	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	60	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	166	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	B	154	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	D	193	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	231	PHE	CB-CG-CD1	-6.24	116.44	120.80
1	D	198	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	C	207	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	C	100	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	C	236	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	C	110	ASP	CB-CG-OD1	5.84	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	57	MET	CA-CB-CG	5.76	123.10	113.30
1	B	236	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	50	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	D	60	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	54	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	24	LEU	CB-CG-CD2	5.49	120.33	111.00
1	D	154	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	88	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	D	139	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	C	85	MET	CA-CB-CG	-5.30	104.29	113.30
1	C	82	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	A	11	ASP	CB-CG-OD1	5.29	123.07	118.30
1	C	72	PHE	CB-CG-CD1	-5.29	117.10	120.80
1	B	57	MET	CA-CB-CG	5.29	122.29	113.30
1	D	227	THR	CA-CB-CG2	-5.21	105.10	112.40
1	A	85	MET	CA-CB-CG	-5.19	104.47	113.30
1	A	198	ASP	CB-CG-OD1	5.18	122.97	118.30
1	C	139	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	A	82	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	C	100	ARG	NE-CZ-NH1	5.05	122.82	120.30

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	1816	0	1792	19	0
1	B	1852	0	1824	16	0
1	C	1798	0	1778	18	0
1	D	1804	0	1775	16	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
3	A	22	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	10	2	0
3	C	22	0	10	2	0
3	D	22	0	10	2	0
4	A	187	0	0	4	0
4	B	173	0	0	6	0
4	C	185	0	0	6	0
4	D	188	0	0	5	0
All	All	8303	0	7333	65	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 4.

All (65) 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:198:ASP:HB3	4:D:413:HOH:O	1.50	1.10
1:B:68:ASN:HD21	1:B:183:ALA:H	1.19	0.90
1:C:193:ARG:HH12	3:D:301:5BU:H3	1.19	0.90
3:C:302:5BU:H3	1:D:193:ARG:HH12	1.17	0.89
1:A:193:ARG:HH12	3:B:301:5BU:H3	1.21	0.89
3:A:302:5BU:H3	1:B:193:ARG:HH12	1.20	0.88
1:A:68:ASN:HD21	1:A:183:ALA:H	1.19	0.86
1:C:54:ARG:HG3	1:C:54:ARG:HH21	1.38	0.86
1:C:68:ASN:HD21	1:C:183:ALA:H	1.23	0.85
1:D:68:ASN:HD21	1:D:183:ALA:H	1.22	0.84
1:C:54:ARG:CG	1:C:54:ARG:HH21	2.02	0.70
1:A:20:SER:HB2	1:D:20:SER:HB2	1.75	0.69
1:C:5:ARG:HD3	4:C:483:HOH:O	1.93	0.66
1:C:54:ARG:CG	1:C:54:ARG:NH2	2.58	0.64
1:C:54:ARG:HG3	1:C:54:ARG:NH2	2.13	0.63
1:A:68:ASN:HD21	1:A:183:ALA:N	1.96	0.62
1:D:113:ARG:HG2	4:D:561:HOH:O	2.02	0.60
1:A:136:GLN:NE2	1:A:139:ARG:HH21	1.99	0.59
1:B:68:ASN:HD21	1:B:183:ALA:N	1.96	0.59
1:A:99:TYR:HD2	1:A:100:ARG:HG3	1.68	0.59
1:B:20:SER:HB2	1:C:20:SER:HB2	1.84	0.59
1:C:68:ASN:HD21	1:C:183:ALA:N	1.98	0.57
1:D:68:ASN:HD21	1:D:183:ALA:N	2.00	0.57
1:B:188:HIS:HD2	4:B:559:HOH:O	1.88	0.56
1:D:31:ARG:NH2	4:D:401:HOH:O	2.20	0.56
1:D:104:ALA:HB2	1:D:149:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:NZ	4:A:570:HOH:O	2.40	0.53
1:A:104:ALA:HB2	1:A:149:PHE:CZ	2.44	0.53
1:C:104:ALA:HB2	1:C:149:PHE:CZ	2.44	0.53
1:C:188:HIS:HD2	4:C:548:HOH:O	1.91	0.53
1:A:24:LEU:HD22	1:A:28:LYS:HG3	1.90	0.52
1:D:124:TYR:HB2	1:D:204:HIS:HB3	1.91	0.52
1:A:98:ARG:HD3	3:A:302:5BU:BR	2.64	0.52
1:B:98:ARG:HD3	3:B:301:5BU:BR	2.65	0.52
1:B:75:ARG:NH2	4:B:539:HOH:O	2.42	0.52
1:C:188:HIS:HE1	4:C:544:HOH:O	1.95	0.50
1:D:58:ARG:HD2	4:D:497:HOH:O	2.12	0.49
1:A:188:HIS:HD2	4:A:422:HOH:O	1.97	0.48
1:C:54:ARG:NH2	4:C:401:HOH:O	1.98	0.47
1:D:52:LEU:HD21	1:D:56:LEU:HD11	1.95	0.47
1:D:52:LEU:C	1:D:52:LEU:HD23	2.35	0.47
1:C:63:SER:HB3	1:C:64:PRO:HD3	1.95	0.47
1:D:102:VAL:HG11	1:D:173:THR:HG21	1.97	0.47
1:A:57:MET:SD	1:A:239:PRO:HG3	2.56	0.46
1:D:98:ARG:HD3	3:D:301:5BU:BR	2.71	0.45
1:B:229:GLU:HG2	4:B:409:HOH:O	2.16	0.45
1:D:188:HIS:HD2	4:D:444:HOH:O	1.99	0.45
1:A:124:TYR:HB2	1:A:204:HIS:HB3	1.99	0.44
1:B:116:ARG:NH1	4:B:508:HOH:O	2.35	0.44
1:A:170:PRO:HA	1:B:170:PRO:HA	2.00	0.44
1:B:34:THR:HG23	4:B:513:HOH:O	2.18	0.43
1:C:98:ARG:HD3	3:C:302:5BU:BR	2.74	0.43
1:B:136:GLN:NE2	4:B:401:HOH:O	2.22	0.42
1:C:5:ARG:CD	4:C:483:HOH:O	2.60	0.42
1:A:31:ARG:CZ	1:A:52:LEU:HD22	2.50	0.42
1:C:188:HIS:CD2	4:C:548:HOH:O	2.69	0.42
1:A:177:LEU:HD22	1:A:177:LEU:O	2.19	0.42
1:B:63:SER:HB3	1:B:64:PRO:HD3	2.02	0.42
1:A:164:ILE:HD11	1:B:113:ARG:CZ	2.50	0.41
1:C:221:ALA:HB2	1:C:228:HIS:CD2	2.54	0.41
1:B:102:VAL:HG11	1:B:173:THR:HG21	2.03	0.41
1:A:13:THR:HG23	4:A:488:HOH:O	2.20	0.41
1:B:31:ARG:O	1:B:32:VAL:C	2.59	0.41
1:A:188:HIS:CD2	4:A:422:HOH:O	2.72	0.40
1:D:31:ARG:HH22	1:D:45:ASP:HB2	1.85	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	223/239 (93%)	221 (99%)	2 (1%)	0	100	100
1	B	227/239 (95%)	224 (99%)	3 (1%)	0	100	100
1	C	221/239 (92%)	218 (99%)	3 (1%)	0	100	100
1	D	222/239 (93%)	220 (99%)	2 (1%)	0	100	100
All	All	893/956 (93%)	883 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	191/201 (95%)	186 (97%)	5 (3%)	51	27
1	B	196/201 (98%)	190 (97%)	6 (3%)	45	20
1	C	192/201 (96%)	187 (97%)	5 (3%)	51	27
1	D	191/201 (95%)	187 (98%)	4 (2%)	59	35
All	All	770/804 (96%)	750 (97%)	20 (3%)	51	27

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	68	ASN

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Mol	Chain	Res	Type
1	A	113	ARG
1	A	166	ARG
1	A	177	LEU
1	B	5	ARG
1	B	34	THR
1	B	52	LEU
1	B	68	ASN
1	B	113	ARG
1	B	166	ARG
1	C	68	ASN
1	C	113	ARG
1	C	132	ASP
1	C	166	ARG
1	C	167	LEU
1	D	68	ASN
1	D	113	ARG
1	D	166	ARG
1	D	197	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	117	GLN
1	A	135	GLN
1	A	136	GLN
1	A	188	HIS
1	A	195	HIS
1	B	68	ASN
1	B	117	GLN
1	B	135	GLN
1	B	188	HIS
1	B	195	HIS
1	C	68	ASN
1	C	93	ASN
1	C	117	GLN
1	C	188	HIS
1	C	195	HIS
1	D	68	ASN
1	D	117	GLN
1	D	188	HIS
1	D	195	HIS

### 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 ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	FAD	A	301	-	51,58,58	2.17	10 (19%)	54,89,89	2.25	11 (20%)
3	5BU	A	302	-	18,23,23	1.73	4 (22%)	22,35,35	2.11	5 (22%)
3	5BU	B	301	-	18,23,23	1.83	5 (27%)	22,35,35	2.77	4 (18%)
2	FAD	B	302	-	51,58,58	2.04	12 (23%)	54,89,89	2.19	14 (25%)
2	FAD	C	301	-	51,58,58	2.16	9 (17%)	54,89,89	2.06	14 (25%)
3	5BU	C	302	-	18,23,23	1.46	2 (11%)	22,35,35	2.17	6 (27%)
3	5BU	D	301	-	18,23,23	1.67	6 (33%)	22,35,35	2.77	9 (40%)
2	FAD	D	302	-	51,58,58	2.16	13 (25%)	54,89,89	2.20	14 (25%)

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	FAD	A	301	-	-	0/28/50/50	0/6/6/6
3	5BU	A	302	-	-	0/6/26/26	0/2/2/2
3	5BU	B	301	-	-	0/6/26/26	0/2/2/2
2	FAD	B	302	-	-	0/28/50/50	0/6/6/6
2	FAD	C	301	-	-	0/28/50/50	0/6/6/6
3	5BU	C	302	-	-	0/6/26/26	0/2/2/2
3	5BU	D	301	-	-	0/6/26/26	0/2/2/2
2	FAD	D	302	-	-	0/28/50/50	0/6/6/6

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	FAD	C1'-N10	-4.87	1.43	1.48
2	D	302	FAD	C2-N1	-3.11	1.32	1.38
2	D	302	FAD	PA-O1A	-2.93	1.39	1.50
2	D	302	FAD	O5B-C5B	-2.56	1.34	1.44
3	A	302	5BU	O5'-C5'	-2.26	1.35	1.44
3	D	301	5BU	P-OP2	-2.22	1.45	1.54
2	B	302	FAD	PA-O2A	-2.21	1.44	1.55
3	B	301	5BU	P-OP3	-2.03	1.46	1.54
2	C	301	FAD	C2B-C3B	2.03	1.58	1.53
3	D	301	5BU	O2'-C2'	2.04	1.47	1.43
3	D	301	5BU	BR-C5	2.06	1.96	1.90
2	A	301	FAD	C2B-C1B	2.12	1.57	1.53
2	B	302	FAD	O2B-C2B	2.16	1.47	1.43
2	A	301	FAD	C2'-C3'	2.20	1.57	1.53
2	C	301	FAD	O2B-C2B	2.24	1.48	1.43
3	A	302	5BU	C4-C5	2.28	1.41	1.38
3	C	302	5BU	O2'-C2'	2.29	1.48	1.43
3	D	301	5BU	O4'-C4'	2.30	1.50	1.45
3	B	301	5BU	O4'-C1'	2.36	1.44	1.41
2	D	302	FAD	C4-N3	2.43	1.37	1.33
3	D	301	5BU	C5'-C4'	2.46	1.59	1.51
2	B	302	FAD	C2A-N3A	2.47	1.36	1.32
2	D	302	FAD	C8M-C8	2.51	1.56	1.51
2	D	302	FAD	C5B-C4B	2.51	1.59	1.51
2	B	302	FAD	C5'-C4'	2.53	1.55	1.51
2	C	301	FAD	C2A-N3A	2.53	1.36	1.32
2	D	302	FAD	C4X-N5	2.54	1.37	1.33
2	A	301	FAD	C4-N3	2.69	1.37	1.33
2	C	301	FAD	C4X-N5	2.75	1.37	1.33
2	B	302	FAD	C8M-C8	2.81	1.56	1.51
2	B	302	FAD	C9A-N10	2.89	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	FAD	C4'-C3'	2.98	1.59	1.53
2	A	301	FAD	C10-N1	3.02	1.37	1.33
3	B	301	5BU	O3'-C3'	3.05	1.50	1.43
3	B	301	5BU	O4'-C4'	3.22	1.52	1.45
2	D	302	FAD	C9A-N10	3.43	1.43	1.38
2	B	302	FAD	C4-N3	3.46	1.39	1.33
2	C	301	FAD	O4B-C1B	3.49	1.46	1.41
3	A	302	5BU	C5'-C4'	3.52	1.62	1.51
2	D	302	FAD	C2A-N3A	3.54	1.38	1.32
2	D	302	FAD	C5X-N5	3.56	1.40	1.35
2	D	302	FAD	C7M-C7	3.60	1.58	1.51
2	B	302	FAD	C10-N1	3.68	1.38	1.33
3	C	302	5BU	C5'-C4'	3.69	1.63	1.51
2	A	301	FAD	C2A-N3A	3.90	1.38	1.32
3	D	301	5BU	C4-N3	3.92	1.40	1.33
3	A	302	5BU	C4-N3	4.10	1.40	1.33
2	C	301	FAD	C9A-N10	4.17	1.44	1.38
3	B	301	5BU	C4-N3	4.27	1.40	1.33
2	B	302	FAD	C4'-C3'	4.55	1.62	1.53
2	A	301	FAD	C9A-N10	4.62	1.44	1.38
2	B	302	FAD	C5X-N5	5.06	1.43	1.35
2	B	302	FAD	O4B-C1B	5.32	1.48	1.41
2	B	302	FAD	C4X-N5	5.91	1.41	1.33
2	C	301	FAD	C5'-C4'	6.06	1.60	1.51
2	A	301	FAD	C4X-N5	6.06	1.42	1.33
2	C	301	FAD	C7M-C7	6.46	1.63	1.51
2	D	302	FAD	C10-N1	7.21	1.43	1.33
2	A	301	FAD	C5X-N5	7.34	1.46	1.35
2	D	302	FAD	O4B-C1B	7.46	1.51	1.41
2	C	301	FAD	C5X-N5	8.15	1.47	1.35

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	FAD	N3A-C2A-N1A	-8.58	121.39	128.86
2	B	302	FAD	N3A-C2A-N1A	-8.17	121.74	128.86
2	A	301	FAD	N3A-C2A-N1A	-8.02	121.87	128.86
3	D	301	5BU	C5-C4-N3	-7.71	114.41	123.64
3	B	301	5BU	C5-C4-N3	-7.18	115.05	123.64
2	D	302	FAD	N3A-C2A-N1A	-7.02	122.75	128.86
3	A	302	5BU	C5-C4-N3	-6.11	116.33	123.64
2	D	302	FAD	C4B-O4B-C1B	-5.43	103.99	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	5BU	C5-C4-N3	-5.08	117.56	123.64
2	C	301	FAD	C4B-O4B-C1B	-4.38	105.11	109.77
2	A	301	FAD	C4X-C4-N3	-3.64	118.30	123.48
2	D	302	FAD	C4A-C5A-N7A	-3.51	106.02	109.41
2	D	302	FAD	C4X-C4-N3	-3.42	118.61	123.48
2	B	302	FAD	C4A-C5A-N7A	-3.41	106.11	109.41
3	A	302	5BU	C5-C6-N1	-3.33	114.69	119.56
3	C	302	5BU	O4'-C1'-N1	-3.26	101.56	108.08
3	C	302	5BU	C5-C6-N1	-3.25	114.80	119.56
3	D	301	5BU	O5'-P-OP1	-3.09	97.81	106.47
2	B	302	FAD	C6-C5X-C9A	-3.09	114.99	119.00
2	D	302	FAD	O4B-C4B-C5B	-3.00	99.26	109.40
3	B	301	5BU	OP2-P-O5'	-2.88	99.07	106.73
2	D	302	FAD	O3B-C3B-C4B	-2.84	102.80	111.09
3	A	302	5BU	BR-C5-C4	-2.81	117.24	121.50
3	D	301	5BU	BR-C5-C4	-2.57	117.60	121.50
2	C	301	FAD	C8M-C8-C9	-2.56	113.93	120.34
2	B	302	FAD	C4X-C4-N3	-2.48	119.95	123.48
2	D	302	FAD	C7-C6-C5X	-2.40	117.36	121.08
2	B	302	FAD	C4-C4X-C10	-2.36	118.05	119.96
2	D	302	FAD	C7M-C7-C6	-2.35	114.45	120.34
2	B	302	FAD	O2'-C2'-C3'	-2.28	103.44	109.09
2	C	301	FAD	O5'-C5'-C4'	-2.27	103.31	109.36
2	B	302	FAD	C9-C8-C7	-2.25	115.93	119.95
2	A	301	FAD	C4X-N5-C5X	-2.20	114.44	116.76
2	C	301	FAD	C1B-N9A-C4A	-2.17	122.89	126.64
2	C	301	FAD	C6-C5X-C9A	-2.15	116.21	119.00
2	A	301	FAD	C4B-O4B-C1B	-2.14	107.49	109.77
2	C	301	FAD	C4X-C4-N3	-2.14	120.44	123.48
3	D	301	5BU	OP2-P-O5'	-2.09	101.16	106.73
3	D	301	5BU	O3'-C3'-C4'	-2.07	105.03	111.09
3	D	301	5BU	C2'-C3'-C4'	-2.03	98.66	102.62
2	D	302	FAD	C8M-C8-C9	-2.03	115.25	120.34
2	C	301	FAD	C2B-C3B-C4B	-2.02	98.68	102.62
2	C	301	FAD	C4A-C5A-N7A	-2.01	107.47	109.41
3	B	301	5BU	OP3-P-OP2	2.03	115.80	107.61
2	A	301	FAD	O3'-C3'-C2'	2.06	113.91	108.82
2	A	301	FAD	O4'-C4'-C5'	2.11	114.70	110.00
2	B	302	FAD	C4X-N5-C5X	2.13	119.02	116.76
2	B	302	FAD	C2A-N1A-C6A	2.20	122.62	118.77
3	C	302	5BU	OP3-P-OP2	2.26	116.72	107.61
2	A	301	FAD	C5A-C6A-N6A	2.27	125.09	120.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	FAD	O2'-C2'-C1'	2.38	115.30	109.79
2	D	302	FAD	C6-C7-C8	2.40	124.23	119.95
2	C	301	FAD	C2A-N1A-C6A	2.40	122.97	118.77
3	C	302	5BU	C4'-O4'-C1'	2.42	112.34	109.77
3	D	301	5BU	OP3-P-OP2	2.44	117.46	107.61
2	B	302	FAD	C1'-N10-C9A	2.57	120.70	118.35
2	C	301	FAD	C6-C5X-N5	2.61	122.03	118.97
2	D	302	FAD	C4X-C10-N10	2.76	122.44	120.52
3	D	301	5BU	OP2-P-OP1	2.92	121.91	110.50
2	C	301	FAD	C1'-N10-C9A	2.93	121.03	118.35
2	B	302	FAD	C4X-C10-N10	3.17	122.72	120.52
2	D	302	FAD	C8M-C8-C7	3.17	127.38	120.72
3	A	302	5BU	C4'-O4'-C1'	3.28	113.26	109.77
2	A	301	FAD	C4X-C10-N10	3.67	123.07	120.52
2	A	301	FAD	C1'-N10-C10	3.82	122.42	118.50
2	C	301	FAD	C4X-C10-N10	3.91	123.24	120.52
2	D	302	FAD	C1'-N10-C9A	4.11	122.11	118.35
2	B	302	FAD	C4-C4X-N5	4.23	123.31	118.68
2	B	302	FAD	C6-C5X-N5	4.23	123.93	118.97
3	A	302	5BU	C4-N3-C2	4.45	119.06	115.16
2	C	301	FAD	C4-N3-C2	5.33	119.82	115.16
3	C	302	5BU	C4-N3-C2	5.81	120.24	115.16
2	B	302	FAD	C4-N3-C2	6.76	121.07	115.16
3	D	301	5BU	C4-N3-C2	6.98	121.27	115.16
2	D	302	FAD	C4-N3-C2	7.38	121.61	115.16
3	B	301	5BU	C4-N3-C2	9.45	123.43	115.16
2	A	301	FAD	C4-N3-C2	9.70	123.64	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	5BU	2	0
3	B	301	5BU	2	0
3	C	302	5BU	2	0
3	D	301	5BU	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

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	226/239 (94%)	0.04	19 (8%) 12 15	7, 16, 43, 56	0
1	B	227/239 (94%)	-0.02	15 (6%) 19 25	7, 16, 41, 50	0
1	C	223/239 (93%)	-0.12	7 (3%) 49 57	6, 15, 34, 50	0
1	D	225/239 (94%)	-0.01	14 (6%) 21 27	8, 16, 39, 59	0
All	All	901/956 (94%)	-0.03	55 (6%) 22 28	6, 16, 40, 59	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	46	GLY	6.6
1	A	35	ALA	5.7
1	D	45	ASP	5.7
1	A	119	GLY	5.7
1	A	4	PRO	5.5
1	B	45	ASP	4.9
1	A	36	GLY	4.8
1	A	129	GLY	4.6
1	C	34	THR	4.5
1	D	34	THR	4.2
1	B	129	GLY	4.2
1	B	34	THR	4.0
1	A	125	ARG	4.0
1	A	131	THR	3.9
1	D	118	GLU	3.6
1	C	5	ARG	3.5
1	C	131	THR	3.5
1	D	131	THR	3.5
1	D	123	ASP	3.4
1	A	57	MET	3.3
1	D	5	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	4	PRO	3.2
1	B	118	GLU	3.1
1	A	120	LYS	3.0
1	C	132	ASP	3.0
1	A	132	ASP	2.9
1	B	44	TYR	2.9
1	B	46	GLY	2.9
1	D	119	GLY	2.9
1	B	5	ARG	2.8
1	A	128	GLY	2.8
1	B	131	THR	2.8
1	A	122	GLY	2.8
1	D	125	ARG	2.8
1	A	118	GLU	2.7
1	B	120	LYS	2.7
1	A	123	ASP	2.7
1	B	4	PRO	2.7
1	B	123	ASP	2.6
1	A	127	VAL	2.6
1	D	127	VAL	2.5
1	B	119	GLY	2.4
1	C	33	SER	2.4
1	B	128	GLY	2.4
1	D	128	GLY	2.3
1	C	129	GLY	2.3
1	A	34	THR	2.2
1	A	130	SER	2.2
1	B	125	ARG	2.2
1	B	126	TYR	2.2
1	D	129	GLY	2.1
1	D	126	TYR	2.1
1	A	135	GLN	2.1
1	A	5	ARG	2.1
1	D	33	SER	2.0

## 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 [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, 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	A	301	53/53	0.98	0.10	-0.04	6,11,15,17	0
2	FAD	C	301	53/53	0.98	0.09	-0.09	7,10,14,14	0
2	FAD	B	302	53/53	0.98	0.09	-0.15	7,11,16,20	0
2	FAD	D	302	53/53	0.99	0.08	-0.43	7,9,15,20	0
3	5BU	D	301	22/22	0.98	0.07	-0.66	7,12,15,17	0
3	5BU	B	301	22/22	0.99	0.07	-1.06	8,12,17,17	0
3	5BU	A	302	22/22	0.99	0.06	-1.11	9,11,16,17	0
3	5BU	C	302	22/22	0.99	0.06	-1.26	8,11,15,17	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.