



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 07:05 PM GMT

PDB ID : 4P5B  
Title : Crystal structure of a UMP/dUMP methylase PolB from *Streptomyces cacaoi* bound with 5-Br dUMP  
Authors : Li, Y.; Chen, W.; Li, J.; Xia, Z.; Deng, Z.; Zhou, J.  
Deposited on : 2014-03-15  
Resolution : 2.27 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

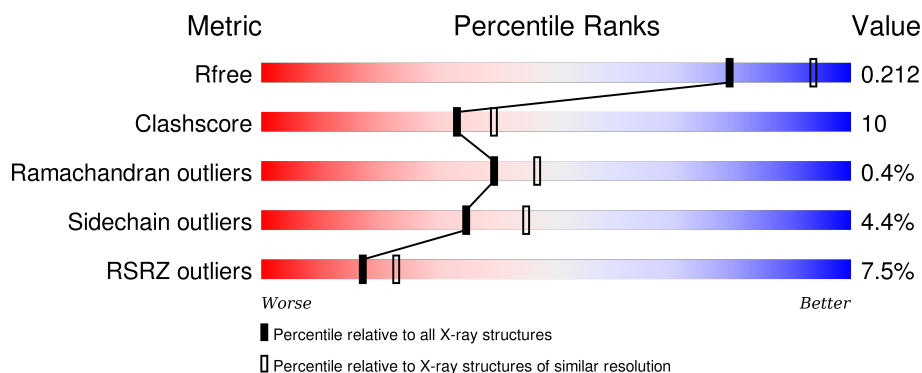
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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))
$R_{free}$	91344	5193 (2.30-2.26)
Clashscore	102246	5929 (2.30-2.26)
Ramachandran outliers	100387	5851 (2.30-2.26)
Sidechain outliers	100360	5850 (2.30-2.26)
RSRZ outliers	91569	5204 (2.30-2.26)

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>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	239	<div> <div>9%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>5% •</div> </div> </div>
1	C	239	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• • •</div> </div> </div>
1	D	239	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8125 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	229	Total	C	N	O	S	0	1	0
			1813	1132	336	337	8			
1	B	235	Total	C	N	O	S	0	1	0
			1874	1169	346	351	8			
1	C	234	Total	C	N	O	S	0	1	0
			1854	1157	339	350	8			
1	D	235	Total	C	N	O	S	0	1	0
			1881	1175	346	352	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 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

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- The chemical structure shows a 2'-methylthioadenine base (adenine) connected to a 2'-deoxyribose sugar, which is further connected to a phosphate group. The adenine base is a purine ring system with a methylthio group (-SCH<sub>3</sub>) at the 2-position. The sugar is a five-membered ring with a deoxy group at the 2' position and a phosphate group at the 5' position. The phosphate group is shown as a phosphorus atom (P) bonded to four oxygen atoms (O). The structure is labeled with atom names and numbers, including C1', C2', C3', C4', C5' for the sugar and N1, N3, C2, C4, C5, C6 for the base. The phosphate group is labeled with OP1, OP2, OP3, and OP4. The methylthio group is labeled with S1 and C5.

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $\text{O}_4\text{S}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

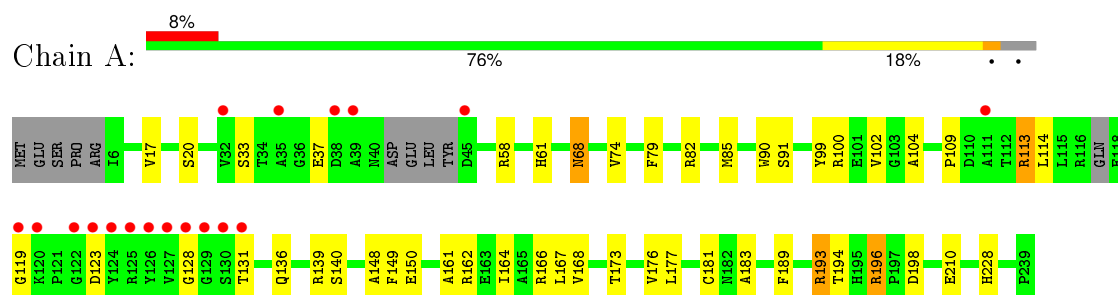
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	97	Total	O	0	0
			97	97		
5	C	93	Total	O	0	0
			93	93		
5	D	108	Total	O	0	0
			108	108		

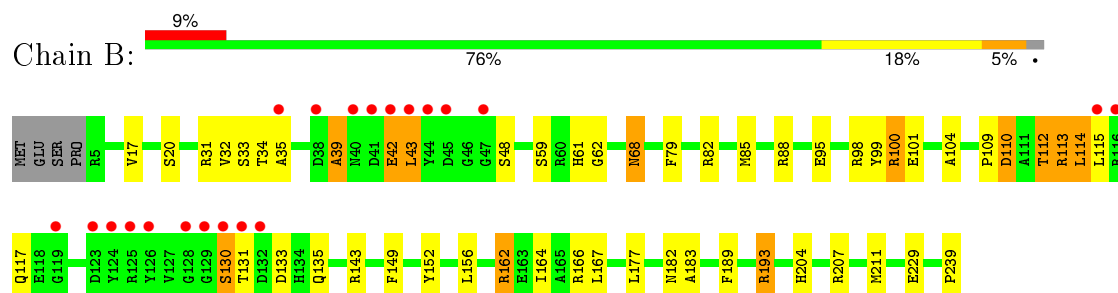
### 3 Residue-property plots [i](#)

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.

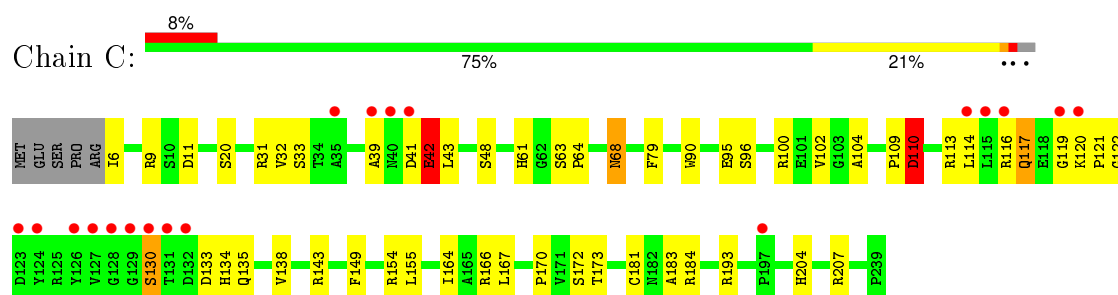
#### • Molecule 1: Thymidylate synthase ThyX



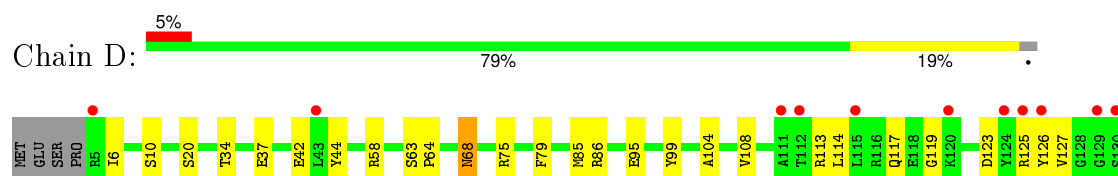
#### • Molecule 1: Thymidylate synthase ThyX



#### • Molecule 1: Thymidylate synthase ThyX



#### • Molecule 1: Thymidylate synthase ThyX





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	170.79Å 59.50Å 118.98Å 90.00° 120.31° 90.00°	Depositor
Resolution (Å)	50.00 – 2.27 34.24 – 2.27	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.27) 97.6 (34.24-2.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.164 , 0.216 0.163 , 0.212	Depositor DCC
$R_{free}$ test set	2332 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 46653 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BRU, SO4, 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	1.04	1/1851 (0.1%)	0.96	4/2505 (0.2%)
1	B	1.02	0/1915	0.91	2/2594 (0.1%)
1	C	1.05	0/1895	0.91	5/2569 (0.2%)
1	D	1.01	1/1923 (0.1%)	0.91	0/2605
All	All	1.03	2/7584 (0.0%)	0.92	11/10273 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	229	GLU	CG-CD	5.35	1.59	1.51
1	A	91	SER	CB-OG	5.00	1.48	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	A	193	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	A	196	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	C	207	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	C	154	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	C	110	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	193	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	119	GLY	N-CA-C	5.25	126.23	113.10
1	A	139	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	C	120	LYS	N-CA-C	5.22	125.10	111.00
1	B	162	ARG	NE-CZ-NH1	5.20	122.90	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	1813	0	1761	40	0
1	B	1874	0	1818	57	0
1	C	1854	0	1785	38	0
1	D	1881	0	1825	38	0
2	A	53	0	31	3	0
2	B	53	0	31	5	0
2	C	53	0	31	2	0
2	D	53	0	31	3	0
3	A	21	0	10	1	0
3	B	21	0	10	4	0
3	C	21	0	10	2	0
3	D	21	0	10	1	0
4	A	5	0	0	0	0
5	A	104	0	0	6	0
5	B	97	0	0	6	0
5	C	93	0	0	3	1
5	D	108	0	0	3	0
All	All	8125	0	7353	155	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (155) 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)
2:B:302:FAD:O1A	5:B:463:HOH:O	1.70	1.09
2:A:301:FAD:O1A	5:A:475:HOH:O	1.72	1.06
2:D:302:FAD:O1A	5:D:449:HOH:O	1.77	1.01
1:D:68:ASN:HD21	1:D:183:ALA:H	1.07	1.00
1:D:10:SER:HB3	1:D:108:VAL:O	1.61	0.99
1:A:193:ARG:HH12	3:B:301:BRU:HN3	1.15	0.93
1:A:119:GLY:HA2	5:A:477:HOH:O	1.66	0.93
1:B:68:ASN:HD21	1:B:183:ALA:H	1.08	0.93
1:A:68:ASN:HD21	1:A:183:ALA:H	1.11	0.90
3:A:302:BRU:HN3	1:B:193:ARG:HH12	1.17	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASN:HD21	1:C:183:ALA:H	1.19	0.90
1:C:193:ARG:HH12	3:D:301:BRU:HN3	1.22	0.84
3:C:302:BRU:HN3	1:D:193:ARG:HH12	1.26	0.82
1:A:119:GLY:CA	5:A:477:HOH:O	2.30	0.77
1:A:68:ASN:HD21	1:A:183:ALA:N	1.83	0.76
2:C:301:FAD:HM73	5:C:461:HOH:O	1.86	0.76
1:A:228:HIS:CD2	5:A:464:HOH:O	2.38	0.76
1:B:229:GLU:HG2	5:B:402:HOH:O	1.88	0.74
1:B:110:ASP:OD2	1:B:112:THR:HG23	1.88	0.73
1:A:79:PHE:CE1	1:B:167:LEU:HD22	2.24	0.72
1:B:68:ASN:HD21	1:B:183:ALA:N	1.86	0.72
1:D:58:ARG:HD3	5:D:499:HOH:O	1.90	0.71
1:B:115:LEU:HD23	1:B:130:SER:HA	1.73	0.70
1:C:68:ASN:HD21	1:C:183:ALA:N	1.88	0.70
1:A:161:ALA:H	1:B:117:GLN:HE21	1.40	0.69
1:D:68:ASN:HD21	1:D:183:ALA:N	1.87	0.68
1:B:114:LEU:HD13	1:B:117:GLN:OE1	1.94	0.68
1:C:114:LEU:O	1:C:117:GLN:HG3	1.96	0.66
1:C:63:SER:HB2	5:C:493:HOH:O	1.94	0.66
1:A:100:ARG:HD2	1:D:34:THR:O	1.96	0.66
1:B:20:SER:HB2	1:C:20:SER:HB2	1.79	0.64
1:A:104:ALA:HB2	1:A:149:PHE:CZ	2.32	0.64
1:B:59:SER:HB2	1:B:61[B]:HIS:CD2	2.33	0.63
1:B:33:SER:HA	1:C:95:GLU:HA	1.80	0.62
1:A:20:SER:HB2	1:D:20:SER:HB2	1.82	0.61
1:A:100:ARG:HD2	1:D:34:THR:C	2.22	0.60
1:B:99:TYR:CE2	3:B:301:BRU:BR	3.10	0.60
1:B:100:ARG:HA	1:B:162:ARG:HH11	1.68	0.59
5:A:482:HOH:O	1:D:37:GLU:HG3	2.02	0.58
1:B:42:GLU:HG2	1:B:43:LEU:H	1.69	0.58
1:B:62:GLY:HA2	1:B:239:PRO:HB2	1.85	0.58
1:B:68:ASN:ND2	1:B:183:ALA:H	1.92	0.57
1:A:196:ARG:NH1	5:A:458:HOH:O	2.36	0.57
1:A:161:ALA:HB2	1:B:117:GLN:HB3	1.87	0.57
1:D:119:GLY:HA3	1:D:126:TYR:HB3	1.87	0.56
1:B:104:ALA:HB2	1:B:149:PHE:CZ	2.40	0.56
1:A:161:ALA:H	1:B:117:GLN:NE2	2.03	0.56
1:B:131:THR:HG22	1:B:131:THR:O	2.06	0.56
1:C:104:ALA:HB2	1:C:149:PHE:CE2	2.41	0.56
1:C:114:LEU:HD13	1:C:134:HIS:HA	1.87	0.56
1:B:95:GLU:HA	1:C:33:SER:HA	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD12	1:B:133:ASP:CB	2.36	0.55
1:B:32:VAL:HA	1:B:39:ALA:HB2	1.87	0.55
1:C:167:LEU:HD22	1:D:79:PHE:CE1	2.42	0.55
1:C:143:ARG:HH21	1:D:154:ARG:HH11	1.52	0.54
2:B:302:FAD:HM73	5:D:508:HOH:O	2.06	0.54
1:A:99:TYR:O	1:A:162:ARG:NH1	2.38	0.54
1:C:164:ILE:O	1:C:167:LEU:HG	2.08	0.54
1:C:61[B]:HIS:O	1:C:64:PRO:HD2	2.09	0.53
1:C:122:GLY:HA2	1:C:204:HIS:CD2	2.43	0.53
1:A:164:ILE:O	1:A:167:LEU:HG	2.08	0.53
1:D:85:MET:CE	1:D:177:LEU:HD13	2.39	0.53
1:B:99:TYR:HE2	3:B:301:BRU:BR	2.47	0.52
1:B:85:MET:HE2	1:B:177:LEU:HD13	1.90	0.52
1:A:161:ALA:CB	1:B:117:GLN:HB3	2.39	0.52
2:A:301:FAD:H9	2:A:301:FAD:O4'	2.09	0.52
1:B:114:LEU:O	1:B:117:GLN:OE1	2.28	0.52
1:B:101:GLU:H	1:B:162:ARG:NH1	2.08	0.52
1:C:172:SER:HB3	1:D:167:LEU:HB3	1.92	0.51
1:A:167:LEU:HD22	1:B:79:PHE:CE1	2.46	0.51
1:B:59:SER:CB	1:B:61[B]:HIS:CD2	2.94	0.51
1:A:90:TRP:CD2	1:A:181:CYS:HB3	2.46	0.51
2:B:302:FAD:HM73	5:B:448:HOH:O	2.11	0.50
1:D:68:ASN:ND2	1:D:183:ALA:H	1.91	0.50
1:B:189:PHE:CE2	1:B:193:ARG:HG3	2.47	0.50
1:B:95:GLU:OE1	1:B:100:ARG:HD3	2.12	0.50
1:A:177:LEU:C	1:A:177:LEU:HD12	2.31	0.50
1:B:88:ARG:NE	2:B:302:FAD:O2A	2.34	0.50
1:B:164:ILE:O	1:B:167:LEU:HG	2.12	0.50
1:C:121:PRO:HD2	1:D:99:TYR:CE2	2.47	0.50
1:D:85:MET:HE3	1:D:177:LEU:HD13	1.94	0.50
1:C:130:SER:O	1:C:133:ASP:HB2	2.12	0.50
1:D:189:PHE:CE2	1:D:193:ARG:HG3	2.46	0.49
1:B:114:LEU:HD12	1:B:133:ASP:HB3	1.95	0.49
1:A:104:ALA:HB2	1:A:149:PHE:CE1	2.47	0.49
1:A:109:PRO:HB3	1:A:113:ARG:HG3	1.94	0.49
1:A:37:GLU:CB	1:D:75:ARG:HH12	2.25	0.49
1:B:182:ASN:ND2	2:D:302:FAD:N1A	2.59	0.49
3:C:302:BRU:HN3	1:D:193:ARG:NH1	2.04	0.48
1:B:95:GLU:OE1	1:B:100:ARG:NH2	2.44	0.48
1:B:34:THR:C	1:C:100:ARG:HD2	2.33	0.48
1:C:102:VAL:HG11	1:C:173:THR:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:FAD:N3A	5:B:452:HOH:O	2.35	0.48
1:D:10:SER:CB	1:D:108:VAL:O	2.49	0.48
1:C:42:GLU:HB3	1:C:43:LEU:H	1.53	0.48
1:B:115:LEU:CD2	1:B:130:SER:HA	2.44	0.47
1:B:182:ASN:HD21	2:D:302:FAD:C2A	2.28	0.47
1:C:61[B]:HIS:HD2	5:C:469:HOH:O	1.98	0.47
1:D:135:GLN:HG2	1:D:139:ARG:HD3	1.97	0.47
1:D:195:HIS:HD2	1:D:203:SER:O	1.98	0.46
1:C:110:ASP:C	1:C:110:ASP:OD1	2.53	0.46
1:A:189:PHE:CE2	1:A:193:ARG:HG3	2.50	0.46
1:B:114:LEU:HD12	1:B:133:ASP:HB2	1.98	0.45
1:A:90:TRP:CE3	1:A:181:CYS:HB3	2.52	0.45
1:D:123:ASP:OD1	1:D:125:ARG:HG2	2.15	0.45
1:C:116:ARG:O	1:C:117:GLN:O	2.33	0.45
1:C:31:ARG:CB	1:C:39:ALA:HB1	2.47	0.45
1:A:194:THR:HA	1:A:210:GLU:HG3	1.99	0.45
1:C:9:ARG:HB3	1:C:11:ASP:OD1	2.16	0.45
1:C:79:PHE:CE1	1:D:167:LEU:HD22	2.52	0.44
1:A:177:LEU:O	1:A:177:LEU:HD12	2.16	0.44
2:A:301:FAD:O3B	1:C:184:ARG:NH1	2.50	0.44
1:B:104:ALA:HB2	1:B:149:PHE:CE2	2.53	0.44
1:A:102:VAL:HG11	1:A:173:THR:HG21	1.99	0.44
1:B:59:SER:HB2	1:B:61[B]:HIS:HD2	1.79	0.44
1:B:204:HIS:ND1	5:B:469:HOH:O	2.37	0.44
1:D:114:LEU:CD1	1:D:134:HIS:HA	2.48	0.44
1:C:134:HIS:O	1:C:138:VAL:HG23	2.17	0.44
1:D:63:SER:OG	1:D:64:PRO:HD3	2.17	0.44
1:C:155:LEU:HD21	1:D:140:SER:CB	2.47	0.44
1:B:31:ARG:NH2	1:B:35:ALA:HB2	2.32	0.43
1:C:31:ARG:HB3	1:C:39:ALA:HB1	2.00	0.43
1:C:90:TRP:CD2	1:C:181:CYS:HB3	2.53	0.43
1:A:33:SER:HA	1:D:95:GLU:HA	2.00	0.43
1:B:207:ARG:HG3	1:B:211:MET:CE	2.49	0.43
1:D:136:GLN:O	1:D:140:SER:HB2	2.17	0.43
1:C:63:SER:N	1:C:64:PRO:CD	2.82	0.43
1:A:196:ARG:HD2	1:A:198:ASP:OD1	2.19	0.42
1:A:82:ARG:HD3	1:B:82:ARG:HD3	2.01	0.42
1:B:109:PRO:HB3	1:B:113:ARG:HD2	2.02	0.42
1:D:114:LEU:O	1:D:117:GLN:HG3	2.20	0.42
1:C:109:PRO:HG2	1:C:114:LEU:HD11	2.02	0.42
1:A:85:MET:HE2	1:A:177:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ASP:N	1:C:11:ASP:OD1	2.53	0.42
1:C:167:LEU:HB3	1:D:172:SER:HB3	2.02	0.42
1:D:86:ARG:HD2	1:D:86:ARG:HA	1.85	0.42
1:A:61[A]:HIS:HE1	2:C:301:FAD:O2'	2.03	0.41
1:D:42:GLU:HB2	1:D:44:TYR:CZ	2.56	0.41
1:B:62:GLY:CA	1:B:239:PRO:HB2	2.48	0.41
1:D:6:ILE:HA	1:D:104:ALA:HB1	2.03	0.41
1:A:148:ALA:HB1	1:A:168:VAL:O	2.21	0.41
1:A:79:PHE:CD1	1:B:167:LEU:HD22	2.56	0.41
1:B:114:LEU:HA	1:B:114:LEU:HD22	1.80	0.41
1:C:96:SER:O	1:C:100:ARG:HB2	2.20	0.41
1:D:164:ILE:O	1:D:167:LEU:HG	2.21	0.41
1:D:117:GLN:O	1:D:127:VAL:HA	2.21	0.41
1:A:74:VAL:O	1:A:176:VAL:HA	2.21	0.41
1:C:170:PRO:HA	1:D:170:PRO:HA	2.03	0.41
1:B:162:ARG:NH1	5:B:465:HOH:O	2.54	0.40
1:B:207:ARG:HG3	1:B:211:MET:HE3	2.02	0.40
1:A:114:LEU:HB3	1:A:128:GLY:O	2.21	0.40
1:A:150:GLU:OE1	1:B:143:ARG:NH1	2.46	0.40
1:B:152:TYR:CZ	1:B:156:LEU:HD11	2.57	0.40
1:B:98:ARG:HD3	3:B:301:BRU:BR	2.76	0.40
1:A:136:GLN:O	1:A:140:SER:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:401:HOH:O	5:C:409:HOH:O[2_556]	2.04	0.16

## 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	224/239 (94%)	220 (98%)	4 (2%)	0	100	100
1	B	234/239 (98%)	225 (96%)	7 (3%)	2 (1%)	21	22
1	C	233/239 (98%)	222 (95%)	9 (4%)	2 (1%)	21	22
1	D	234/239 (98%)	228 (97%)	6 (3%)	0	100	100
All	All	925/956 (97%)	895 (97%)	26 (3%)	4 (0%)	39	47

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	42	GLU
1	C	117	GLN
1	B	39	ALA
1	C	42	GLU

### 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	189/201 (94%)	182 (96%)	7 (4%)	41	54
1	B	196/201 (98%)	184 (94%)	12 (6%)	23	29
1	C	193/201 (96%)	182 (94%)	11 (6%)	25	32
1	D	197/201 (98%)	193 (98%)	4 (2%)	63	78
All	All	775/804 (96%)	741 (96%)	34 (4%)	35	45

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	58	ARG
1	A	68	ASN
1	A	113	ARG
1	A	123	ASP
1	A	131	THR
1	A	166	ARG

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Mol	Chain	Res	Type
1	B	17	VAL
1	B	43	LEU
1	B	48	SER
1	B	68	ASN
1	B	100	ARG
1	B	110	ASP
1	B	112	THR
1	B	113	ARG
1	B	114	LEU
1	B	130	SER
1	B	135	GLN
1	B	166	ARG
1	C	6	ILE
1	C	32	VAL
1	C	41	ASP
1	C	42	GLU
1	C	48	SER
1	C	68	ASN
1	C	110	ASP
1	C	113	ARG
1	C	130	SER
1	C	135	GLN
1	C	166	ARG
1	D	68	ASN
1	D	113	ARG
1	D	143	ARG
1	D	166	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	93	ASN
1	A	195	HIS
1	B	40	ASN
1	B	68	ASN
1	B	93	ASN
1	B	117	GLN
1	B	195	HIS
1	C	68	ASN
1	C	93	ASN
1	C	195	HIS

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Mol	Chain	Res	Type
1	C	204	HIS
1	D	68	ASN
1	D	93	ASN
1	D	195	HIS
1	D	204	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 ⓘ

9 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	-	52,58,58	1.77	12 (23%)	52,89,89	2.41	24 (46%)
3	BRU	A	302	-	17,22,22	1.69	3 (17%)	22,33,33	2.71	9 (40%)
4	SO4	A	303	-	4,4,4	0.27	0	6,6,6	0.54	0
3	BRU	B	301	-	17,22,22	1.33	2 (11%)	22,33,33	2.46	8 (36%)
2	FAD	B	302	-	52,58,58	1.79	10 (19%)	52,89,89	2.37	18 (34%)
2	FAD	C	301	-	52,58,58	2.03	12 (23%)	52,89,89	2.19	13 (25%)
3	BRU	C	302	-	17,22,22	1.56	2 (11%)	22,33,33	2.70	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BRU	D	301	-	17,22,22	1.73	5 (29%)	22,33,33	2.75	6 (27%)
2	FAD	D	302	-	52,58,58	2.09	11 (21%)	52,89,89	2.20	13 (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	-	-	0/30/50/50	0/6/6/6
3	BRU	A	302	-	-	0/6/22/22	0/2/2/2
4	SO4	A	303	-	-	0/0/0/0	0/0/0/0
3	BRU	B	301	-	-	0/6/22/22	0/2/2/2
2	FAD	B	302	-	-	0/30/50/50	0/6/6/6
2	FAD	C	301	-	-	0/30/50/50	0/6/6/6
3	BRU	C	302	-	-	0/6/22/22	0/2/2/2
3	BRU	D	301	-	-	0/6/22/22	0/2/2/2
2	FAD	D	302	-	-	0/30/50/50	0/6/6/6

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	BRU	P-OP3	-2.82	1.45	1.54
2	A	301	FAD	C1'-N10	-2.24	1.46	1.48
3	A	302	BRU	P-OP2	-2.13	1.47	1.54
3	D	301	BRU	O4'-C1'	-2.13	1.37	1.42
2	A	301	FAD	C6-C5X	-2.07	1.38	1.41
3	A	302	BRU	P-OP3	-2.06	1.47	1.54
2	A	301	FAD	C10-N1	2.02	1.39	1.35
2	C	301	FAD	PA-O2A	2.03	1.63	1.55
2	C	301	FAD	O5B-C5B	2.05	1.53	1.44
2	A	301	FAD	C8M-C8	2.09	1.55	1.51
2	B	302	FAD	C10-N10	2.17	1.41	1.39
2	C	301	FAD	C5'-C4'	2.28	1.55	1.51
2	A	301	FAD	C7M-C7	2.29	1.55	1.51
3	B	301	BRU	P-O5'	2.32	1.66	1.59
2	B	302	FAD	C8M-C8	2.39	1.55	1.51
2	A	301	FAD	C10-N10	2.43	1.42	1.39
3	D	301	BRU	C4-N3	2.45	1.37	1.33
2	D	302	FAD	PA-O2A	2.50	1.65	1.55
2	B	302	FAD	C7M-C7	2.52	1.56	1.51
2	D	302	FAD	C2-N3	2.53	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	BRU	C2'-C1'	2.56	1.59	1.52
2	C	301	FAD	C8M-C8	2.59	1.56	1.51
2	A	301	FAD	PA-O5B	2.78	1.71	1.59
2	B	302	FAD	C2-N1	2.81	1.44	1.38
2	D	302	FAD	O4B-C1B	2.84	1.45	1.41
2	D	302	FAD	C9A-N10	2.91	1.42	1.38
2	A	301	FAD	O3B-C3B	2.97	1.50	1.43
3	C	302	BRU	C4-N3	3.19	1.38	1.33
2	D	302	FAD	PA-O5B	3.23	1.72	1.59
2	B	302	FAD	C5X-N5	3.29	1.40	1.35
2	C	301	FAD	C10-N1	3.32	1.41	1.35
2	C	301	FAD	O4B-C1B	3.36	1.46	1.41
2	D	302	FAD	C2-N1	3.43	1.45	1.38
2	B	302	FAD	PA-O5B	3.49	1.74	1.59
2	C	301	FAD	PA-O1A	3.50	1.64	1.51
2	D	302	FAD	C10-N10	3.58	1.43	1.39
2	B	302	FAD	C4X-N5	3.60	1.38	1.33
3	B	301	BRU	O4'-C4'	3.64	1.53	1.45
2	B	302	FAD	C10-N1	3.69	1.41	1.35
2	A	301	FAD	O4B-C1B	3.77	1.46	1.41
2	C	301	FAD	PA-O5B	3.92	1.75	1.59
2	C	301	FAD	C9A-N10	4.02	1.44	1.38
3	D	301	BRU	P-O5'	4.05	1.71	1.59
2	A	301	FAD	C5X-N5	4.07	1.41	1.35
2	D	302	FAD	C5X-N5	4.07	1.41	1.35
3	C	302	BRU	P-O5'	4.29	1.72	1.59
2	B	302	FAD	C9A-N10	4.39	1.45	1.38
2	A	301	FAD	C4X-N5	4.63	1.40	1.33
3	A	302	BRU	P-O5'	4.73	1.73	1.59
2	A	301	FAD	C4-N3	5.19	1.42	1.33
2	D	302	FAD	C10-N1	5.21	1.44	1.35
2	C	301	FAD	C5X-N5	5.43	1.43	1.35
2	C	301	FAD	C4-N3	5.63	1.43	1.33
2	C	301	FAD	C4X-N5	6.01	1.42	1.33
2	B	302	FAD	C4-N3	6.09	1.44	1.33
2	D	302	FAD	C4X-N5	6.09	1.42	1.33
2	D	302	FAD	C4-N3	6.90	1.45	1.33

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	FAD	N3A-C2A-N1A	-8.24	122.39	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	FAD	N3A-C2A-N1A	-7.88	122.68	128.87
3	D	301	BRU	O5'-P-OP1	-6.29	91.27	107.08
3	A	302	BRU	C5-C4-N3	-6.13	117.46	124.00
2	B	302	FAD	O5B-PA-O1A	-6.12	84.15	109.21
2	D	302	FAD	O5B-PA-O1A	-6.09	84.27	109.21
2	C	301	FAD	N3A-C2A-N1A	-6.04	124.13	128.87
2	D	302	FAD	N3-C2-N1	-5.83	117.88	127.69
2	D	302	FAD	N3A-C2A-N1A	-5.77	124.34	128.87
3	D	301	BRU	OP2-P-O5'	-5.73	90.00	106.72
2	B	302	FAD	N3-C2-N1	-5.58	118.29	127.69
3	C	302	BRU	OP2-P-O5'	-5.56	90.49	106.72
3	D	301	BRU	C5-C4-N3	-5.36	118.28	124.00
3	B	301	BRU	C5-C4-N3	-5.33	118.31	124.00
2	C	301	FAD	O2A-PA-O5B	-5.11	83.86	108.24
3	C	302	BRU	OP3-P-O5'	-4.94	92.32	106.72
3	A	302	BRU	OP2-P-O5'	-4.86	92.55	106.72
2	C	301	FAD	N3-C2-N1	-4.60	119.95	127.69
2	A	301	FAD	O2A-PA-O5B	-4.44	87.07	108.24
3	C	302	BRU	O5'-P-OP1	-4.35	96.16	107.08
2	A	301	FAD	O4B-C4B-C5B	-4.26	94.03	109.29
2	D	302	FAD	O2A-PA-O5B	-4.25	87.96	108.24
2	C	301	FAD	C4B-O4B-C1B	-4.23	105.16	109.64
2	A	301	FAD	O5B-PA-O1A	-4.00	92.86	109.21
3	B	301	BRU	OP3-P-O5'	-3.83	95.55	106.72
3	C	302	BRU	C5-C4-N3	-3.82	119.92	124.00
2	A	301	FAD	C4B-O4B-C1B	-3.76	105.66	109.64
2	A	301	FAD	C4X-C4-N3	-3.72	118.67	123.52
3	A	302	BRU	OP3-P-O5'	-3.62	96.15	106.72
2	A	301	FAD	C1B-N9A-C4A	-3.59	122.79	126.81
2	C	301	FAD	O5B-PA-O1A	-3.36	95.47	109.21
2	B	302	FAD	O4B-C4B-C5B	-3.28	97.55	109.29
2	B	302	FAD	C1B-N9A-C4A	-3.22	123.21	126.81
2	B	302	FAD	O2A-PA-O5B	-3.22	92.90	108.24
2	A	301	FAD	N3-C2-N1	-3.20	122.30	127.69
3	A	302	BRU	O5'-P-OP1	-2.84	99.93	107.08
2	A	301	FAD	C5X-C9A-N10	-2.83	115.45	117.58
2	C	301	FAD	C4X-C4-N3	-2.82	119.83	123.52
3	B	301	BRU	OP2-P-O5'	-2.61	99.11	106.72
2	A	301	FAD	O4B-C1B-N9A	-2.52	103.34	108.11
3	B	301	BRU	BR-C5-C4	-2.48	117.30	121.48
3	A	302	BRU	O4'-C1'-N1	-2.38	103.56	107.71
2	C	301	FAD	O4B-C4B-C5B	-2.35	100.89	109.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	BRU	BR-C5-C4	-2.35	117.53	121.48
2	D	302	FAD	C4X-C4-N3	-2.24	120.59	123.52
2	A	301	FAD	C6-C5X-N5	-2.24	116.12	118.92
3	B	301	BRU	O5'-P-OP1	-2.24	101.46	107.08
2	C	301	FAD	C1B-N9A-C4A	-2.23	124.31	126.81
2	A	301	FAD	C7M-C7-C6	-2.16	114.23	120.33
2	B	302	FAD	C4X-C4-N3	-2.12	120.75	123.52
2	B	302	FAD	C5X-C9A-N10	-2.02	116.06	117.58
2	D	302	FAD	C4-C4X-N5	2.03	121.16	118.70
2	A	301	FAD	O3B-C3B-C4B	2.03	117.06	111.01
2	B	302	FAD	C2A-N1A-C6A	2.03	122.39	118.77
2	B	302	FAD	C7M-C7-C8	2.04	125.12	120.73
2	B	302	FAD	C2B-C1B-N9A	2.04	118.94	113.47
2	A	301	FAD	O5B-C5B-C4B	2.09	116.61	109.09
2	D	302	FAD	O2A-PA-O3P	2.10	114.27	105.27
3	A	302	BRU	OP3-P-OP1	2.10	117.49	110.63
2	D	302	FAD	N6A-C6A-N1A	2.17	122.15	118.52
3	B	301	BRU	OP3-P-OP1	2.19	117.77	110.63
2	D	302	FAD	C2B-C1B-N9A	2.27	119.54	113.47
2	D	302	FAD	C6-C5X-C9A	2.28	121.63	119.11
2	A	301	FAD	C2A-N1A-C6A	2.36	122.98	118.77
2	A	301	FAD	C4-C4X-C10	2.38	121.46	119.94
2	B	302	FAD	O5B-C5B-C4B	2.42	117.82	109.09
2	A	301	FAD	C7M-C7-C8	2.54	126.20	120.73
2	B	302	FAD	O3'-C3'-C2'	2.55	115.34	108.73
2	C	301	FAD	C4-C4X-N5	2.56	121.81	118.70
2	A	301	FAD	C1'-N10-C9A	2.57	121.81	118.83
2	A	301	FAD	O2A-PA-O3P	2.59	116.39	105.27
2	C	301	FAD	O2A-PA-O1A	2.61	126.12	112.56
2	A	301	FAD	C4X-N5-C5X	2.67	119.87	116.72
2	B	302	FAD	C6-C5X-C9A	2.67	122.06	119.11
2	A	301	FAD	O2A-PA-O1A	2.69	126.57	112.56
2	C	301	FAD	C4X-N5-C5X	2.72	119.93	116.72
3	D	301	BRU	OP2-P-OP1	2.85	119.92	110.63
2	B	302	FAD	O2A-PA-O3P	2.93	117.84	105.27
3	B	301	BRU	OP2-P-OP1	3.05	120.59	110.63
2	A	301	FAD	C4-C4X-N5	3.15	122.53	118.70
2	A	301	FAD	C4X-C10-N10	3.34	122.95	120.52
2	C	301	FAD	C1'-N10-C9A	3.37	122.74	118.83
2	D	302	FAD	C4X-N5-C5X	3.38	120.71	116.72
2	A	301	FAD	C4-N3-C2	3.50	118.08	115.16
3	D	301	BRU	C4-N3-C2	3.71	118.25	115.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	FAD	C4X-N5-C5X	3.73	121.11	116.72
2	D	302	FAD	C1'-N10-C9A	3.90	123.35	118.83
3	C	302	BRU	C4-N3-C2	3.95	118.45	115.16
2	B	302	FAD	C1'-N10-C9A	4.08	123.56	118.83
3	A	302	BRU	OP3-P-OP2	4.32	123.32	107.44
2	B	302	FAD	C4-N3-C2	4.65	119.04	115.16
3	D	301	BRU	OP3-P-OP2	5.37	127.14	107.44
3	A	302	BRU	C4-N3-C2	5.88	120.07	115.16
3	C	302	BRU	OP2-P-OP1	5.93	129.98	110.63
2	D	302	FAD	C4-N3-C2	5.96	120.13	115.16
2	C	301	FAD	C4-N3-C2	6.19	120.32	115.16
3	B	301	BRU	C4-N3-C2	6.86	120.88	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	FAD	3	0
3	A	302	BRU	1	0
3	B	301	BRU	4	0
2	B	302	FAD	5	0
2	C	301	FAD	2	0
3	C	302	BRU	2	0
3	D	301	BRU	1	0
2	D	302	FAD	3	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	229/239 (95%)	0.06	18 (7%) 15 21	12, 24, 74, 95	0
1	B	235/239 (98%)	-0.04	21 (8%) 12 16	13, 26, 67, 77	0
1	C	234/239 (97%)	-0.08	19 (8%) 15 20	13, 26, 72, 83	0
1	D	235/239 (98%)	-0.21	12 (5%) 32 39	15, 26, 62, 76	0
All	All	933/956 (97%)	-0.07	70 (7%) 17 23	12, 25, 69, 95	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	GLY	10.8
1	A	124	TYR	9.6
1	A	128	GLY	8.4
1	B	43	LEU	7.8
1	A	127	VAL	6.9
1	C	128	GLY	6.2
1	C	129	GLY	6.1
1	C	115	LEU	6.0
1	A	119	GLY	5.8
1	A	123	ASP	5.3
1	D	115	LEU	5.3
1	A	126	TYR	5.2
1	B	41	ASP	5.0
1	B	124	TYR	5.0
1	C	41	ASP	5.0
1	D	131	THR	4.9
1	B	44	TYR	4.9
1	C	124	TYR	4.7
1	A	130	SER	4.7
1	D	124	TYR	4.5
1	B	126	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	131	THR	4.2
1	B	123	ASP	4.2
1	B	130	SER	4.1
1	C	126	TYR	4.1
1	C	120	LYS	4.1
1	A	35	ALA	4.0
1	D	130	SER	4.0
1	B	115	LEU	4.0
1	D	129	GLY	3.8
1	B	35	ALA	3.6
1	A	125	ARG	3.4
1	A	120	LYS	3.4
1	A	45	ASP	3.3
1	B	132	ASP	3.3
1	D	5	ARG	3.3
1	B	128	GLY	3.2
1	A	39	ALA	3.2
1	A	122	GLY	3.0
1	B	131	THR	3.0
1	B	40	ASN	3.0
1	C	127	VAL	2.9
1	B	125	ARG	2.9
1	C	39	ALA	2.9
1	A	131	THR	2.8
1	C	116	ARG	2.8
1	C	119	GLY	2.7
1	C	114	LEU	2.7
1	C	123	ASP	2.7
1	C	197	PRO	2.6
1	B	38	ASP	2.6
1	B	45	ASP	2.6
1	B	42	GLU	2.6
1	D	112	THR	2.5
1	C	35	ALA	2.5
1	D	126	TYR	2.5
1	B	47	GLY	2.5
1	C	132	ASP	2.4
1	B	129	GLY	2.3
1	C	130	SER	2.3
1	B	116	ARG	2.2
1	D	125	ARG	2.2
1	A	32	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	120	LYS	2.1
1	A	111	ALA	2.1
1	C	40	ASN	2.1
1	D	43	LEU	2.1
1	D	111	ALA	2.1
1	A	38	ASP	2.1
1	B	119	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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(Å <sup>2</sup> )	Q<0.9
2	FAD	D	302	53/53	0.89	0.17	1.23	32,49,54,56	0
2	FAD	B	302	53/53	0.91	0.16	0.76	24,43,50,56	0
2	FAD	C	301	53/53	0.89	0.16	0.60	29,42,51,52	0
3	BRU	C	302	21/21	0.96	0.14	0.13	19,25,31,39	0
3	BRU	A	302	21/21	0.97	0.13	-0.10	13,18,23,30	0
4	SO4	A	303	5/5	0.97	0.10	-0.34	54,55,56,58	0
2	FAD	A	301	53/53	0.94	0.11	-0.45	17,34,40,43	0
3	BRU	B	301	21/21	0.96	0.11	-0.56	12,17,21,29	0
3	BRU	D	301	21/21	0.98	0.10	-0.81	16,22,25,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.