



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2017 – 12:54 AM EDT

PDB ID : 3N0B  
Title : TM0449 mutant crystals grown in loops/micromounts  
Authors : Mathews, I.I.  
Deposited on : unknown  
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](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.

---

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 : rb-20030345  
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) : rb-20030345

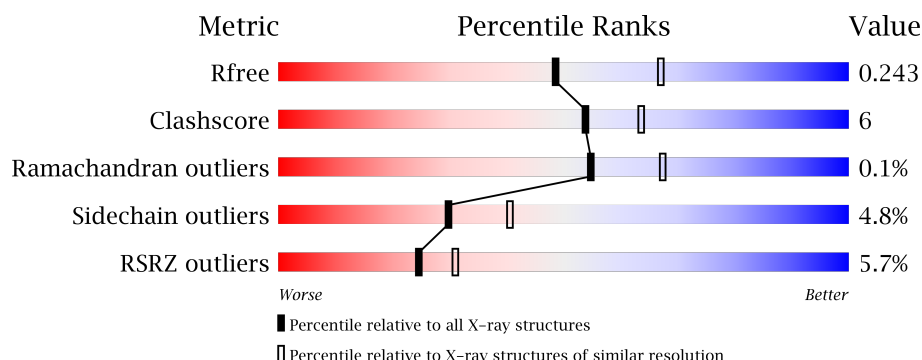
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (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  $\geq 3$ , 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	232	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>• 7%</div> </div> </div>
1	B	232	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div> </div>
1	C	232	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 7%</div> </div> </div>
1	D	232	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>14%</div> <div>• 9%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7464 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	216	Total	C	N	O	S	0	0	0
			1778	1153	307	312	6			
1	B	220	Total	C	N	O	S	0	0	0
			1821	1180	313	322	6			
1	C	216	Total	C	N	O	S	0	0	0
			1793	1162	308	318	5			
1	D	210	Total	C	N	O	S	0	0	0
			1741	1128	300	308	5			

There are 56 discrepancies between the modelled and reference sequences:

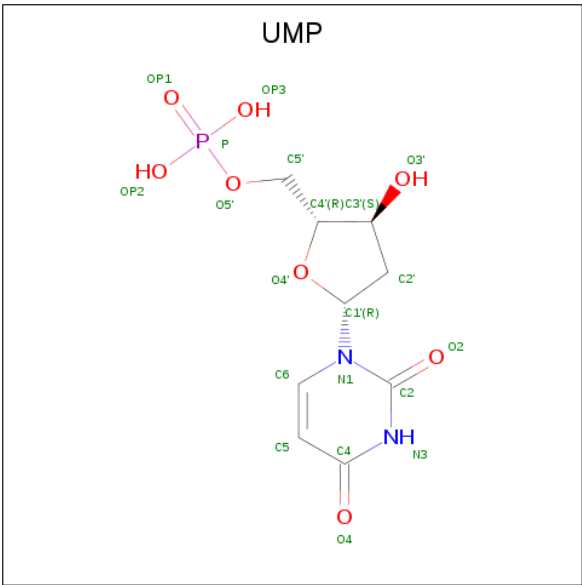
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q9WYT0
A	-10	GLY	-	EXPRESSION TAG	UNP Q9WYT0
A	-9	SER	-	EXPRESSION TAG	UNP Q9WYT0
A	-8	ASP	-	EXPRESSION TAG	UNP Q9WYT0
A	-7	LYS	-	EXPRESSION TAG	UNP Q9WYT0
A	-6	ILE	-	EXPRESSION TAG	UNP Q9WYT0
A	-5	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	-4	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	-3	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	-2	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	-1	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	0	HIS	-	EXPRESSION TAG	UNP Q9WYT0
A	158	ALA	PHE	ENGINEERED MUTATION	UNP Q9WYT0
A	160	ALA	TRP	ENGINEERED MUTATION	UNP Q9WYT0
B	-11	MET	-	EXPRESSION TAG	UNP Q9WYT0
B	-10	GLY	-	EXPRESSION TAG	UNP Q9WYT0
B	-9	SER	-	EXPRESSION TAG	UNP Q9WYT0
B	-8	ASP	-	EXPRESSION TAG	UNP Q9WYT0
B	-7	LYS	-	EXPRESSION TAG	UNP Q9WYT0
B	-6	ILE	-	EXPRESSION TAG	UNP Q9WYT0
B	-5	HIS	-	EXPRESSION TAG	UNP Q9WYT0

*Continued on next page...*

*Continued from previous page...*

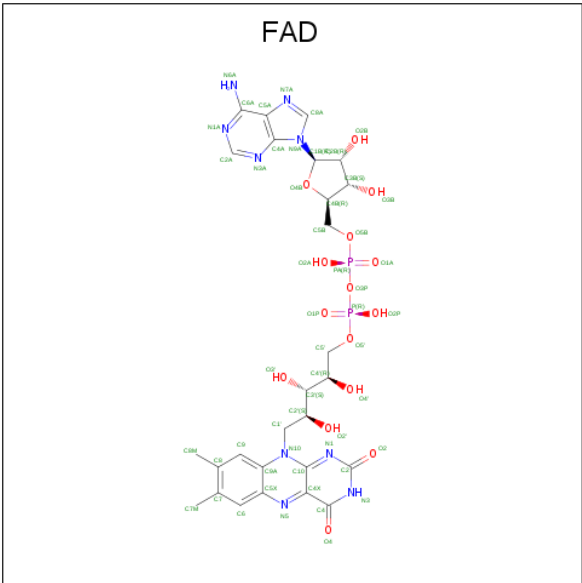
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	-3	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	-2	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	-1	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	0	HIS	-	EXPRESSION TAG	UNP Q9WYT0
B	158	ALA	PHE	ENGINEERED MUTATION	UNP Q9WYT0
B	160	ALA	TRP	ENGINEERED MUTATION	UNP Q9WYT0
C	-11	MET	-	EXPRESSION TAG	UNP Q9WYT0
C	-10	GLY	-	EXPRESSION TAG	UNP Q9WYT0
C	-9	SER	-	EXPRESSION TAG	UNP Q9WYT0
C	-8	ASP	-	EXPRESSION TAG	UNP Q9WYT0
C	-7	LYS	-	EXPRESSION TAG	UNP Q9WYT0
C	-6	ILE	-	EXPRESSION TAG	UNP Q9WYT0
C	-5	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	-4	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	-3	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	-2	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	-1	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	0	HIS	-	EXPRESSION TAG	UNP Q9WYT0
C	158	ALA	PHE	ENGINEERED MUTATION	UNP Q9WYT0
C	160	ALA	TRP	ENGINEERED MUTATION	UNP Q9WYT0
D	-11	MET	-	EXPRESSION TAG	UNP Q9WYT0
D	-10	GLY	-	EXPRESSION TAG	UNP Q9WYT0
D	-9	SER	-	EXPRESSION TAG	UNP Q9WYT0
D	-8	ASP	-	EXPRESSION TAG	UNP Q9WYT0
D	-7	LYS	-	EXPRESSION TAG	UNP Q9WYT0
D	-6	ILE	-	EXPRESSION TAG	UNP Q9WYT0
D	-5	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	-4	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	-3	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	-2	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	-1	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	0	HIS	-	EXPRESSION TAG	UNP Q9WYT0
D	158	ALA	PHE	ENGINEERED MUTATION	UNP Q9WYT0
D	160	ALA	TRP	ENGINEERED MUTATION	UNP Q9WYT0

- 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		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

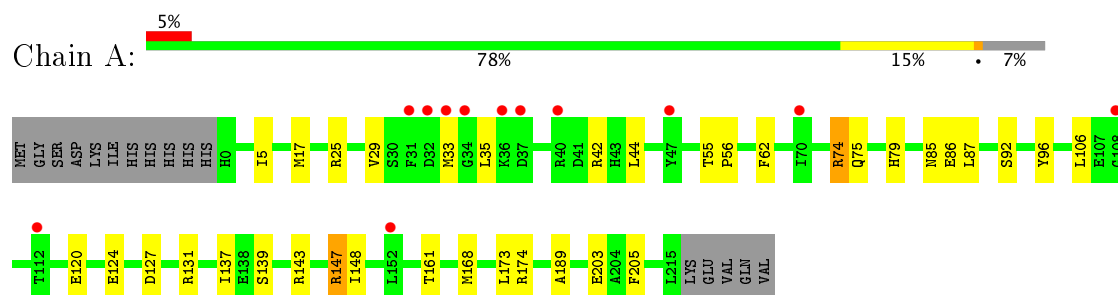
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	10	Total	O	0	0
			10	10		
4	C	9	Total	O	0	0
			9	9		
4	D	7	Total	O	0	0
			7	7		

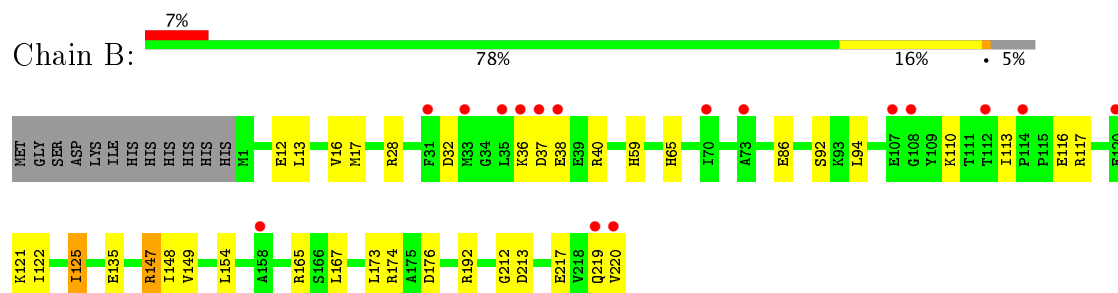
### 3 Residue-property plots [i](#)

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.

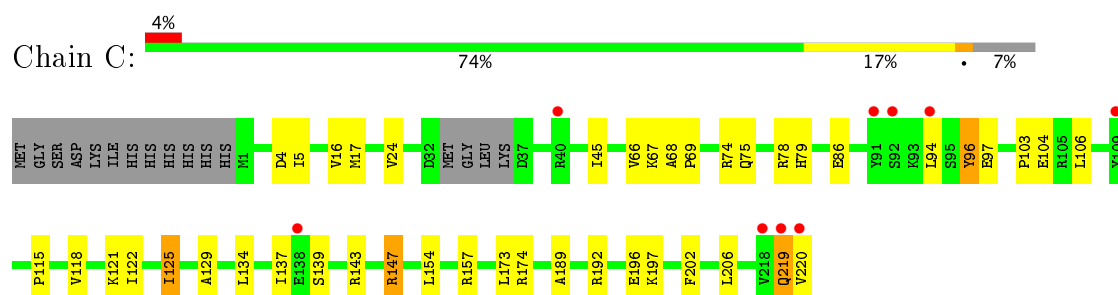
#### • Molecule 1: Thymidylate synthase thyX



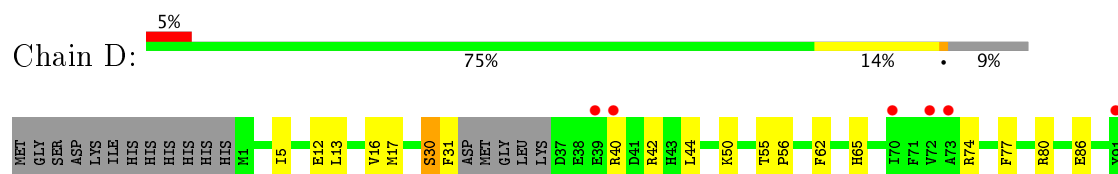
#### • Molecule 1: Thymidylate synthase thyX

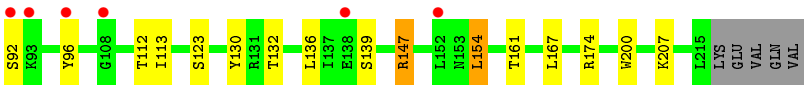


#### • Molecule 1: Thymidylate synthase thyX



#### • Molecule 1: Thymidylate synthase thyX







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.52Å 116.75Å 141.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.30) 99.8 (29.98-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.198 , 0.249 0.193 , 0.243	Depositor DCC
$R_{free}$ test set	2046 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7464	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: UMP, 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	0.83	0/1824	0.78	1/2465 (0.0%)
1	B	0.77	0/1867	0.79	1/2522 (0.0%)
1	C	0.81	0/1838	0.79	1/2483 (0.0%)
1	D	0.79	0/1785	0.78	1/2414 (0.0%)
All	All	0.80	0/7314	0.79	4/9884 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	B	213	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	134	LEU	CA-CB-CG	5.25	127.38	115.30
1	D	154	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	1778	0	1776	20	0
1	B	1821	0	1825	28	0
1	C	1793	0	1790	32	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1741	0	1737	18	0
2	A	20	0	11	1	0
2	B	20	0	11	3	0
2	C	20	0	11	3	0
2	D	20	0	11	2	0
3	A	53	0	31	0	0
3	B	53	0	31	2	0
3	C	53	0	31	1	0
3	D	53	0	31	2	0
4	A	13	0	0	0	0
4	B	10	0	0	0	0
4	C	9	0	0	0	0
4	D	7	0	0	0	0
All	All	7464	0	7296	89	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 6.

All (89) 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:C:17:MET:HB2	1:D:17:MET:HB2	1.39	1.02
2:A:303:UMP:HN3	1:D:174:ARG:HH12	1.08	1.00
1:B:174:ARG:HH12	2:C:313:UMP:HN3	1.15	0.92
2:B:308:UMP:HN3	1:C:174:ARG:HH12	1.17	0.86
1:B:122:ILE:O	1:B:125:ILE:HD12	1.76	0.86
1:A:5:ILE:HD11	1:A:189:ALA:HB2	1.63	0.78
1:A:17:MET:HB2	1:B:17:MET:HB2	1.67	0.76
1:C:137:ILE:HD12	1:C:143:ARG:HG2	1.67	0.74
1:C:106:LEU:HD11	1:C:118:VAL:HG11	1.70	0.73
1:B:122:ILE:HA	1:B:125:ILE:HD11	1.71	0.71
1:C:137:ILE:CD1	1:C:143:ARG:HG2	2.21	0.71
1:A:42:ARG:NH2	1:A:203:GLU:OE1	2.25	0.69
1:A:174:ARG:HH12	2:D:318:UMP:HN3	1.40	0.68
1:C:103:PRO:HB3	1:C:115:PRO:HB2	1.77	0.65
1:B:37:ASP:HB3	1:B:40:ARG:HB2	1.79	0.64
1:B:135:GLU:OE1	1:C:121:LYS:NZ	2.31	0.63
1:C:24:VAL:HG23	1:C:45:ILE:HD11	1.81	0.63
1:B:122:ILE:O	1:B:125:ILE:CD1	2.46	0.62
1:D:16:VAL:HG22	1:D:62:PHE:CD2	2.37	0.59
1:A:120:GLU:O	1:A:124:GLU:HG3	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:VAL:HB	1:C:125:ILE:HD13	1.85	0.59
1:D:12:GLU:HG3	1:D:65:HIS:HB3	1.84	0.58
1:B:117:ARG:NH2	1:B:121:LYS:HE3	2.19	0.57
1:B:94:LEU:HD13	1:B:154:LEU:HD21	1.86	0.56
1:D:42:ARG:HG2	1:D:200:TRP:CD2	2.41	0.56
1:B:117:ARG:HH21	1:B:121:LYS:HE3	1.69	0.56
1:A:127:ASP:OD2	1:A:131:ARG:NH1	2.39	0.55
1:B:125:ILE:HG21	1:C:129:ALA:HA	1.89	0.55
1:C:122:ILE:O	1:C:125:ILE:HD12	2.09	0.53
1:C:67:LYS:NZ	1:C:97:GLU:OE1	2.30	0.53
1:B:165:ARG:CZ	3:D:300:FAD:H2B	2.39	0.52
1:C:86:GLU:HB3	2:C:313:UMP:H4'	1.92	0.52
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.75	0.52
1:C:4:ASP:O	1:C:5:ILE:HD13	2.11	0.51
1:C:79:HIS:HE1	1:C:173:LEU:HD12	1.75	0.51
1:A:137:ILE:HD12	1:A:143:ARG:HG2	1.92	0.51
1:A:79:HIS:HE1	1:A:173:LEU:HD12	1.76	0.51
1:B:147:ARG:HD2	1:B:147:ARG:C	2.31	0.50
1:B:176:ASP:OD1	1:B:212:GLY:HA2	2.10	0.50
1:C:202:PHE:CE2	1:C:206:LEU:HD11	2.46	0.50
1:A:55:THR:OG1	1:A:56:PRO:HD3	2.11	0.50
1:B:86:GLU:HB3	2:B:308:UMP:H4'	1.94	0.50
1:A:85:ASN:ND2	1:B:59:HIS:NE2	2.58	0.50
1:A:74:ARG:HH22	1:D:86:GLU:CD	2.16	0.49
1:D:147:ARG:HD2	1:D:147:ARG:C	2.33	0.49
1:C:68:ALA:HB1	1:C:69:PRO:HD2	1.95	0.49
1:A:5:ILE:CD1	1:A:189:ALA:HB2	2.38	0.48
1:C:96:TYR:O	1:C:97:GLU:HG2	2.13	0.48
1:D:30:SER:O	1:D:31:PHE:CB	2.62	0.48
1:A:86:GLU:OE2	1:D:74:ARG:NH2	2.48	0.47
1:B:167:LEU:HD23	1:B:167:LEU:O	2.14	0.47
1:C:16:VAL:HG11	1:C:197:LYS:HD2	1.97	0.47
1:A:5:ILE:HD11	1:A:189:ALA:CB	2.39	0.46
1:B:174:ARG:NH1	2:C:313:UMP:HN3	1.98	0.46
1:B:37:ASP:OD1	1:B:38:GLU:N	2.49	0.46
1:C:192:ARG:CZ	1:C:220:VAL:CG2	2.94	0.46
1:B:167:LEU:HD23	1:B:167:LEU:C	2.37	0.45
1:C:219:GLN:HB2	1:C:219:GLN:HE21	1.57	0.45
1:C:74:ARG:O	1:C:78:ARG:HG2	2.17	0.45
1:B:13:LEU:HD21	1:B:16:VAL:HG23	1.99	0.45
1:C:106:LEU:CD1	1:C:118:VAL:HG11	2.42	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:LEU:HD11	1:D:16:VAL:HG23	1.98	0.45
1:D:62:PHE:O	1:D:161:THR:HA	2.17	0.44
1:C:67:LYS:HG3	1:C:157:ARG:HG2	1.99	0.44
1:D:77:PHE:N	1:D:77:PHE:CD1	2.86	0.43
1:D:55:THR:N	1:D:56:PRO:CD	2.82	0.43
1:A:168:MET:HB3	1:A:205:PHE:CE1	2.53	0.43
1:C:5:ILE:HD11	1:C:189:ALA:HB2	2.01	0.43
1:A:25:ARG:HG3	1:A:35:LEU:HD21	2.00	0.43
1:B:147:ARG:HD2	1:B:148:ILE:N	2.34	0.42
1:C:68:ALA:HB1	1:C:69:PRO:CD	2.48	0.42
1:B:192:ARG:HG3	1:B:220:VAL:CG1	2.50	0.42
2:B:308:UMP:C2	1:C:75:GLN:HG2	2.54	0.42
1:A:62:PHE:O	1:A:161:THR:HA	2.20	0.42
1:D:80:ARG:H	3:D:300:FAD:PA	2.43	0.42
1:C:143:ARG:O	1:C:147:ARG:HG3	2.19	0.42
1:B:173:LEU:HB3	3:B:310:FAD:HM81	2.02	0.42
1:A:139:SER:HB2	1:D:112:THR:HB	2.02	0.42
1:B:173:LEU:HB3	3:B:310:FAD:C8M	2.50	0.42
1:C:78:ARG:HH12	3:C:305:FAD:C2	2.33	0.41
1:A:75:GLN:HG2	2:D:318:UMP:C2	2.56	0.41
1:D:167:LEU:C	1:D:167:LEU:HD23	2.41	0.41
1:D:96:TYR:CD1	1:D:130:TYR:CD2	3.09	0.41
1:B:12:GLU:HB3	1:B:65:HIS:HB3	2.03	0.41
1:C:192:ARG:CZ	1:C:220:VAL:HG21	2.51	0.40
1:D:132:THR:O	1:D:136:LEU:HG	2.21	0.40
1:A:147:ARG:HD2	1:A:148:ILE:N	2.36	0.40
1:C:94:LEU:HD13	1:C:154:LEU:HD21	2.03	0.40
1:C:66:VAL:O	1:C:157:ARG:HA	2.22	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	214/232 (92%)	207 (97%)	7 (3%)	0	100	100
1	B	218/232 (94%)	209 (96%)	9 (4%)	0	100	100
1	C	212/232 (91%)	204 (96%)	7 (3%)	1 (0%)	32	39
1	D	206/232 (89%)	198 (96%)	8 (4%)	0	100	100
All	All	850/928 (92%)	818 (96%)	31 (4%)	1 (0%)	55	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	96	TYR

### 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	187/205 (91%)	179 (96%)	8 (4%)	33	45
1	B	193/205 (94%)	183 (95%)	10 (5%)	27	36
1	C	190/205 (93%)	184 (97%)	6 (3%)	44	60
1	D	184/205 (90%)	172 (94%)	12 (6%)	20	26
All	All	754/820 (92%)	718 (95%)	36 (5%)	30	40

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

Mol	Chain	Res	Type
1	A	29	VAL
1	A	33	MET
1	A	44	LEU
1	A	87	LEU
1	A	92	SER
1	A	96	TYR
1	A	106	LEU
1	A	147	ARG
1	B	32	ASP
1	B	36	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	92	SER
1	B	110	LYS
1	B	113	ILE
1	B	116	GLU
1	B	125	ILE
1	B	147	ARG
1	B	217	GLU
1	B	219	GLN
1	C	104	GLU
1	C	125	ILE
1	C	139	SER
1	C	147	ARG
1	C	196	GLU
1	C	219	GLN
1	D	5	ILE
1	D	30	SER
1	D	40	ARG
1	D	44	LEU
1	D	50	LYS
1	D	92	SER
1	D	113	ILE
1	D	123	SER
1	D	139	SER
1	D	147	ARG
1	D	154	LEU
1	D	207	LYS

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	85	ASN
1	A	169	ASN
1	A	185	GLN
1	B	219	GLN
1	C	219	GLN
1	D	75	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 ⓘ

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	UMP	A	303	-	17,21,21	0.83	1 (5%)	23,31,31	2.26	1 (4%)
3	FAD	A	315	-	51,58,58	3.67	14 (27%)	54,89,89	3.52	17 (31%)
2	UMP	B	308	-	17,21,21	0.88	1 (5%)	23,31,31	2.11	3 (13%)
3	FAD	B	310	-	51,58,58	3.31	14 (27%)	54,89,89	3.21	10 (18%)
3	FAD	C	305	-	51,58,58	3.30	15 (29%)	54,89,89	3.27	12 (22%)
2	UMP	C	313	-	17,21,21	0.80	0	23,31,31	2.35	4 (17%)
3	FAD	D	300	-	51,58,58	3.31	14 (27%)	54,89,89	3.42	13 (24%)
2	UMP	D	318	-	17,21,21	0.72	0	23,31,31	2.16	3 (13%)

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	303	-	-	0/6/22/22	0/2/2/2
3	FAD	A	315	-	-	0/28/50/50	0/6/6/6
2	UMP	B	308	-	-	0/6/22/22	0/2/2/2
3	FAD	B	310	-	-	0/28/50/50	0/6/6/6
3	FAD	C	305	-	-	0/28/50/50	0/6/6/6

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UMP	C	313	-	-	0/6/22/22	0/2/2/2
3	FAD	D	300	-	-	0/28/50/50	0/6/6/6
2	UMP	D	318	-	-	0/6/22/22	0/2/2/2

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	315	FAD	C9A-N10	-7.44	1.29	1.38
3	B	310	FAD	C9A-N10	-7.07	1.29	1.38
3	D	300	FAD	C9A-N10	-6.80	1.29	1.38
3	C	305	FAD	C9A-N10	-5.95	1.31	1.38
3	D	300	FAD	C2-N1	-5.64	1.27	1.38
3	A	315	FAD	C2-N1	-5.63	1.27	1.38
3	C	305	FAD	C2-N1	-5.06	1.28	1.38
3	B	310	FAD	C2-N1	-4.54	1.29	1.38
2	A	303	UMP	C2-N3	-2.20	1.33	1.38
2	B	308	UMP	C2-N3	-2.10	1.34	1.38
3	B	310	FAD	C2A-N3A	2.10	1.35	1.32
3	A	315	FAD	O4B-C1B	2.46	1.44	1.41
3	D	300	FAD	O4B-C1B	2.58	1.44	1.41
3	C	305	FAD	O4B-C1B	2.58	1.44	1.41
3	C	305	FAD	C2A-N3A	2.59	1.36	1.32
3	A	315	FAD	C9-C9A	2.69	1.46	1.40
3	B	310	FAD	C9-C9A	3.26	1.47	1.40
3	D	300	FAD	C5A-C4A	3.29	1.47	1.40
3	B	310	FAD	C5A-C4A	3.47	1.48	1.40
3	C	305	FAD	C9-C9A	3.75	1.48	1.40
3	D	300	FAD	C9-C9A	3.76	1.48	1.40
3	A	315	FAD	C5A-C4A	3.94	1.49	1.40
3	C	305	FAD	C5A-C4A	4.27	1.50	1.40
3	B	310	FAD	C8-C7	4.31	1.51	1.41
3	D	300	FAD	C9A-C5X	4.35	1.51	1.42
3	D	300	FAD	C8-C7	4.37	1.52	1.41
3	A	315	FAD	C8-C7	4.46	1.52	1.41
3	C	305	FAD	C8-C7	4.69	1.52	1.41
3	C	305	FAD	C9A-C5X	4.80	1.52	1.42
3	B	310	FAD	C9A-C5X	4.84	1.52	1.42
3	C	305	FAD	C4-C4X	5.28	1.51	1.41
3	A	315	FAD	C9A-C5X	5.30	1.53	1.42
3	D	300	FAD	C4-C4X	5.32	1.51	1.41
3	C	305	FAD	C6-C7	5.84	1.53	1.37
3	B	310	FAD	C4-C4X	5.86	1.52	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	310	FAD	C6-C7	6.03	1.53	1.37
3	D	300	FAD	C4X-C10	6.35	1.52	1.41
3	D	300	FAD	C6-C7	6.36	1.54	1.37
3	A	315	FAD	C6-C7	6.64	1.55	1.37
3	C	305	FAD	C5X-N5	6.82	1.45	1.35
3	A	315	FAD	C4-C4X	6.86	1.54	1.41
3	D	300	FAD	C5X-N5	6.91	1.45	1.35
3	B	310	FAD	C4X-C10	6.97	1.53	1.41
3	B	310	FAD	C5X-N5	7.04	1.46	1.35
3	C	305	FAD	C4X-C10	7.08	1.53	1.41
3	D	300	FAD	C4X-N5	7.31	1.43	1.33
3	C	305	FAD	C4X-N5	7.35	1.43	1.33
3	B	310	FAD	C6-C5X	7.97	1.53	1.41
3	A	315	FAD	C4X-C10	8.01	1.55	1.41
3	C	305	FAD	C6-C5X	8.07	1.53	1.41
3	D	300	FAD	C6-C5X	8.40	1.54	1.41
3	B	310	FAD	C4X-N5	8.49	1.45	1.33
3	A	315	FAD	C5X-N5	8.56	1.48	1.35
3	A	315	FAD	C6-C5X	8.74	1.54	1.41
3	B	310	FAD	C10-N1	9.75	1.46	1.33
3	A	315	FAD	C4X-N5	9.81	1.47	1.33
3	A	315	FAD	C10-N1	9.97	1.47	1.33
3	C	305	FAD	C10-N1	10.21	1.47	1.33
3	D	300	FAD	C10-N1	10.30	1.47	1.33

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	300	FAD	C1'-N10-C10	-10.19	108.05	118.50
3	C	305	FAD	C1'-N10-C10	-9.67	108.58	118.50
3	B	310	FAD	C1'-N10-C10	-9.35	108.92	118.50
3	A	315	FAD	C1'-N10-C10	-8.60	109.69	118.50
3	D	300	FAD	N3A-C2A-N1A	-7.88	121.99	128.86
3	B	310	FAD	N3A-C2A-N1A	-7.05	122.72	128.86
3	A	315	FAD	N3A-C2A-N1A	-6.85	122.90	128.86
3	C	305	FAD	N3A-C2A-N1A	-6.72	123.00	128.86
3	A	315	FAD	C4-C4X-C10	-5.38	115.61	119.96
3	D	300	FAD	C4X-C10-N10	-5.11	116.97	120.52
3	D	300	FAD	C7-C6-C5X	-5.07	113.24	121.08
3	D	300	FAD	C4X-C4-N3	-4.84	116.59	123.48
3	D	300	FAD	C4-C4X-C10	-4.71	116.16	119.96
3	B	310	FAD	C4-C4X-C10	-4.69	116.17	119.96

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	305	FAD	C4X-C4-N3	-4.54	117.01	123.48
3	B	310	FAD	C7-C6-C5X	-4.43	114.22	121.08
3	A	315	FAD	C10-C4X-N5	-4.32	115.63	120.59
3	B	310	FAD	C4X-C4-N3	-4.19	117.52	123.48
3	A	315	FAD	C4X-C4-N3	-4.16	117.56	123.48
3	C	305	FAD	C7-C6-C5X	-4.15	114.67	121.08
3	A	315	FAD	C7-C6-C5X	-3.82	115.17	121.08
3	C	305	FAD	C4-C4X-C10	-3.06	117.49	119.96
3	B	310	FAD	C4X-C10-N10	-3.00	118.44	120.52
3	A	315	FAD	C4A-C5A-N7A	-2.82	106.68	109.41
3	C	305	FAD	C4A-C5A-N7A	-2.65	106.84	109.41
3	C	305	FAD	C10-C4X-N5	-2.53	117.68	120.59
3	C	305	FAD	C6-C5X-N5	-2.43	116.12	118.97
2	C	313	UMP	C6-N1-C2	-2.18	117.75	121.28
3	D	300	FAD	C9A-C5X-N5	-2.17	119.00	122.24
3	A	315	FAD	C9A-C5X-N5	-2.17	119.01	122.24
3	A	315	FAD	O2B-C2B-C1B	-2.16	104.86	111.61
2	B	308	UMP	OP3-P-O5'	-2.15	101.01	106.73
3	D	300	FAD	C4A-C5A-N7A	-2.14	107.34	109.41
2	C	313	UMP	C5-C4-N3	-2.08	118.17	123.12
3	A	315	FAD	C4X-C10-N10	2.04	121.93	120.52
3	D	300	FAD	C4B-O4B-C1B	2.05	111.96	109.77
2	D	318	UMP	O4'-C1'-C2'	2.06	110.21	106.25
3	A	315	FAD	C2A-N1A-C6A	2.08	122.41	118.77
2	B	308	UMP	OP3-P-OP1	2.13	118.85	110.50
2	D	318	UMP	OP3-P-OP1	2.30	119.51	110.50
2	C	313	UMP	OP3-P-OP2	2.38	117.21	107.61
3	A	315	FAD	C4B-O4B-C1B	2.59	112.53	109.77
3	A	315	FAD	C9-C8-C7	2.92	125.16	119.95
3	C	305	FAD	C5X-C9A-N10	3.89	120.55	117.66
3	D	300	FAD	C5X-C9A-N10	3.94	120.58	117.66
3	B	310	FAD	C5X-C9A-N10	4.08	120.69	117.66
3	D	300	FAD	C4-C4X-N5	4.19	123.27	118.68
3	C	305	FAD	C4-C4X-N5	4.52	123.64	118.68
3	B	310	FAD	C4-C4X-N5	5.11	124.29	118.68
3	A	315	FAD	C5X-C9A-N10	6.69	122.62	117.66
3	A	315	FAD	C4-C4X-N5	8.23	127.70	118.68
2	B	308	UMP	C4-N3-C2	8.64	121.55	114.13
2	D	318	UMP	C4-N3-C2	8.96	121.83	114.13
2	A	303	UMP	C4-N3-C2	9.60	122.38	114.13
2	C	313	UMP	C4-N3-C2	9.93	122.66	114.13
3	B	310	FAD	C1'-N10-C9A	10.78	128.22	118.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	300	FAD	C1'-N10-C9A	11.00	128.43	118.35
3	A	315	FAD	C4-N3-C2	11.47	125.19	115.16
3	C	305	FAD	C4-N3-C2	11.57	125.28	115.16
3	B	310	FAD	C4-N3-C2	12.18	125.81	115.16
3	C	305	FAD	C1'-N10-C9A	12.44	129.75	118.35
3	A	315	FAD	C1'-N10-C9A	12.48	129.79	118.35
3	D	300	FAD	C4-N3-C2	12.49	126.09	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	303	UMP	1	0
2	B	308	UMP	3	0
3	B	310	FAD	2	0
3	C	305	FAD	1	0
2	C	313	UMP	3	0
3	D	300	FAD	2	0
2	D	318	UMP	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	216/232 (93%)	0.07	12 (5%) 25 32	25, 36, 66, 72	0
1	B	220/232 (94%)	0.25	16 (7%) 16 21	24, 38, 71, 77	0
1	C	216/232 (93%)	0.03	9 (4%) 37 44	24, 34, 61, 69	0
1	D	210/232 (90%)	0.16	12 (5%) 24 31	23, 36, 62, 72	0
All	All	862/928 (92%)	0.13	49 (5%) 24 31	23, 36, 66, 77	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	TYR	4.8
1	D	91	TYR	4.8
1	A	36	LYS	4.7
1	D	108	GLY	4.5
1	B	35	LEU	4.5
1	A	33	MET	4.4
1	B	220	VAL	4.2
1	B	33	MET	4.0
1	D	92	SER	3.9
1	A	108	GLY	3.8
1	A	34	GLY	3.7
1	B	112	THR	3.6
1	B	114	PRO	3.5
1	C	94	LEU	3.5
1	D	40	ARG	3.4
1	D	152	LEU	3.3
1	C	219	GLN	3.2
1	C	92	SER	3.1
1	B	31	PHE	3.0
1	C	138	GLU	3.0
1	C	220	VAL	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	32	ASP	2.9
1	A	31	PHE	2.9
1	B	219	GLN	2.9
1	D	73	ALA	2.9
1	B	107	GLU	2.9
1	C	109	TYR	2.9
1	D	93	LYS	2.8
1	A	40	ARG	2.8
1	A	37	ASP	2.7
1	A	112	THR	2.6
1	B	38	GLU	2.6
1	B	70	ILE	2.5
1	C	218	VAL	2.5
1	B	37	ASP	2.5
1	C	40	ARG	2.4
1	B	120	GLU	2.4
1	D	70	ILE	2.4
1	B	36	LYS	2.3
1	D	72	VAL	2.3
1	B	108	GLY	2.2
1	A	152	LEU	2.2
1	B	73	ALA	2.1
1	D	39	GLU	2.1
1	A	70	ILE	2.1
1	C	91	TYR	2.1
1	A	47	TYR	2.1
1	D	138	GLU	2.1
1	B	158	ALA	2.1

## 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
3	FAD	B	310	53/53	0.89	0.19	1.39	42,55,63,63	0
3	FAD	A	315	53/53	0.90	0.19	1.19	46,61,69,71	0
3	FAD	D	300	53/53	0.90	0.17	0.95	41,54,58,60	0
3	FAD	C	305	53/53	0.93	0.14	0.03	38,52,58,59	0
2	UMP	D	318	20/20	0.90	0.15	-0.21	49,53,56,56	0
2	UMP	B	308	20/20	0.96	0.14	-0.25	35,41,43,44	0
2	UMP	C	313	20/20	0.95	0.13	-0.64	38,42,48,49	0
2	UMP	A	303	20/20	0.97	0.12	-0.67	33,36,38,39	0

## 6.5 Other polymers

There are no such residues in this entry.