



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:06 AM GMT

PDB ID : 2FMN  
Title : Ala177Val mutant of E. coli Methylenetetrahydrofolate Reductase complex with LY309887  
Authors : Pejchal, R.; Campbell, E.; Guenther, B.D.; Lennon, B.W.; Matthews, R.G.; Ludwig, M.L.  
Deposited on : 2006-01-09  
Resolution : 2.05 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 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

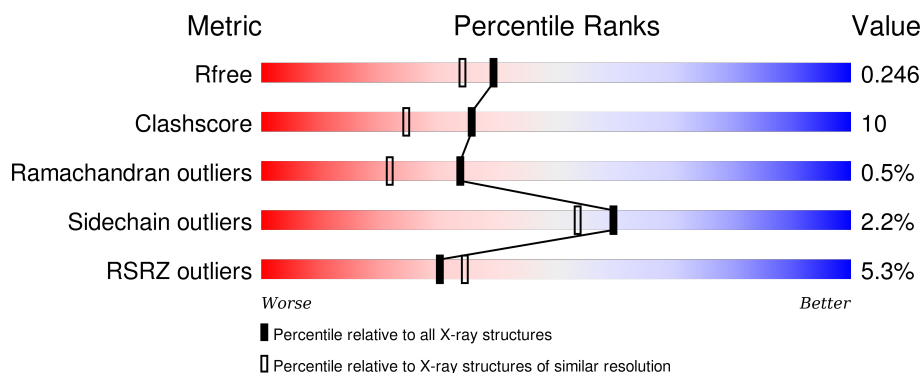
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	304	<div> <div>11%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>• 5%</div> </div> </div>
1	B	304	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>16%</div> <div>• 6%</div> </div> </div>
1	C	304	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7066 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 5,10-methylenetetrahydrofolate reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	288	Total	C	N	O	S	0	0	0
			2216	1401	388	416	11			
1	B	287	Total	C	N	O	S	0	0	0
			2230	1413	392	414	11			
1	C	271	Total	C	N	O	S	0	0	0
			2087	1327	362	387	11			

There are 27 discrepancies between the modelled and reference sequences:

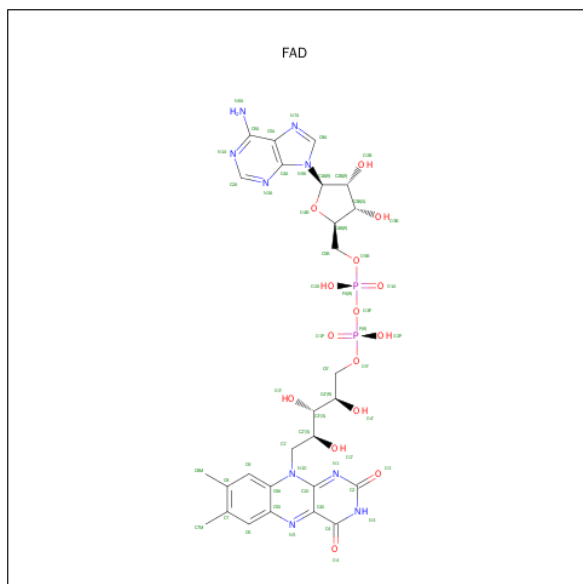
Chain	Residue	Modelled	Actual	Comment	Reference
A	177	VAL	ALA	ENGINEERED	UNP P0AEZ1
A	297	LEU	-	CLONING ARTIFACT	UNP P0AEZ1
A	298	GLU	-	CLONING ARTIFACT	UNP P0AEZ1
A	299	HIS	-	EXPRESSION TAG	UNP P0AEZ1
A	300	HIS	-	EXPRESSION TAG	UNP P0AEZ1
A	301	HIS	-	EXPRESSION TAG	UNP P0AEZ1
A	302	HIS	-	EXPRESSION TAG	UNP P0AEZ1
A	303	HIS	-	EXPRESSION TAG	UNP P0AEZ1
A	304	HIS	-	EXPRESSION TAG	UNP P0AEZ1
B	177	VAL	ALA	ENGINEERED	UNP P0AEZ1
B	297	LEU	-	CLONING ARTIFACT	UNP P0AEZ1
B	298	GLU	-	CLONING ARTIFACT	UNP P0AEZ1
B	299	HIS	-	EXPRESSION TAG	UNP P0AEZ1
B	300	HIS	-	EXPRESSION TAG	UNP P0AEZ1
B	301	HIS	-	EXPRESSION TAG	UNP P0AEZ1
B	302	HIS	-	EXPRESSION TAG	UNP P0AEZ1
B	303	HIS	-	EXPRESSION TAG	UNP P0AEZ1
B	304	HIS	-	EXPRESSION TAG	UNP P0AEZ1
C	177	VAL	ALA	ENGINEERED	UNP P0AEZ1
C	297	LEU	-	CLONING ARTIFACT	UNP P0AEZ1
C	298	GLU	-	CLONING ARTIFACT	UNP P0AEZ1
C	299	HIS	-	EXPRESSION TAG	UNP P0AEZ1
C	300	HIS	-	EXPRESSION TAG	UNP P0AEZ1

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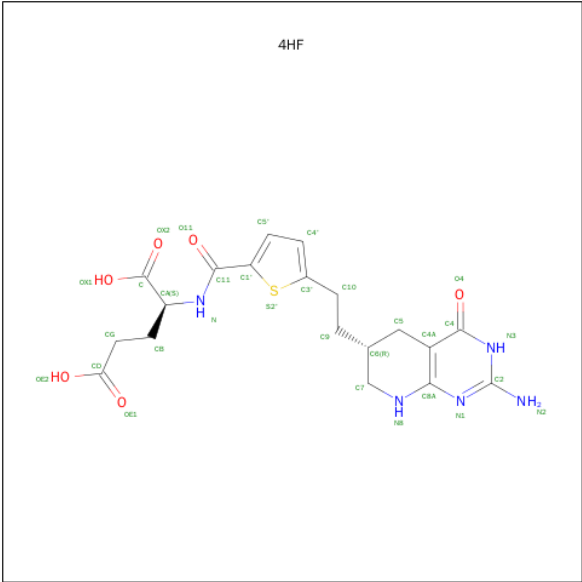
Chain	Residue	Modelled	Actual	Comment	Reference
C	301	HIS	-	EXPRESSION TAG	UNP P0AEZ1
C	302	HIS	-	EXPRESSION TAG	UNP P0AEZ1
C	303	HIS	-	EXPRESSION TAG	UNP P0AEZ1
C	304	HIS	-	EXPRESSION TAG	UNP P0AEZ1

- 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		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is N-[(5-{2-[(6R)-2-AMINO-4-OXO-3,4,5,6,7,8-HEXAHYDROPYRIDO[2,3-D]PYRIMIDIN-6-YL]ETHYL}-2-THIENYL)CARBONYL]-L-GLUTAMIC ACID (three-letter code: 4HF) (formula:  $C_{19}H_{23}N_5O_6S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			31	19	5	6	1		
3	B	1	Total	C	N	O	S	0	0
			31	19	5	6	1		
3	C	1	Total	C	N	O	S	0	0
			31	19	5	6	1		

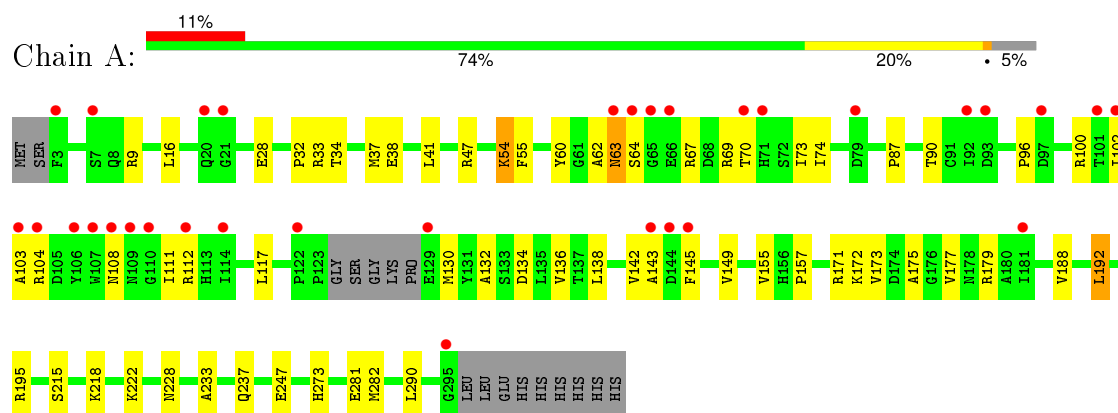
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	124	Total	O	0	0
			124	124		
4	C	95	Total	O	0	0
			95	95		

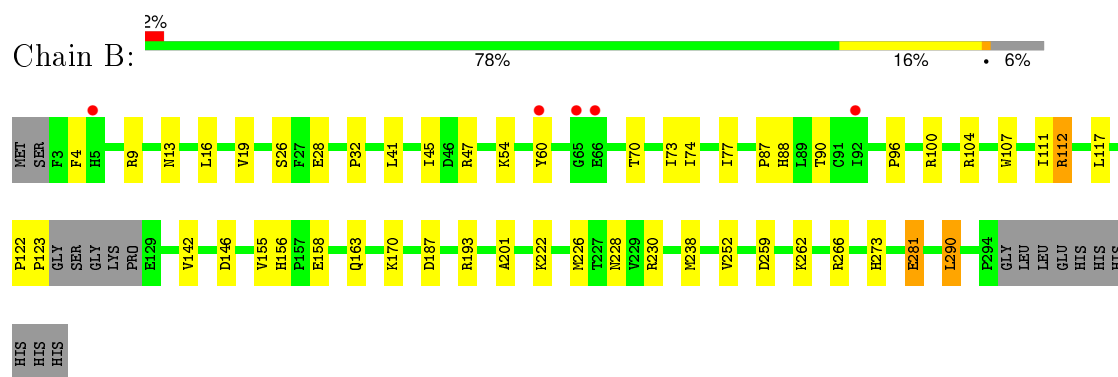
### 3 Residue-property plots

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.

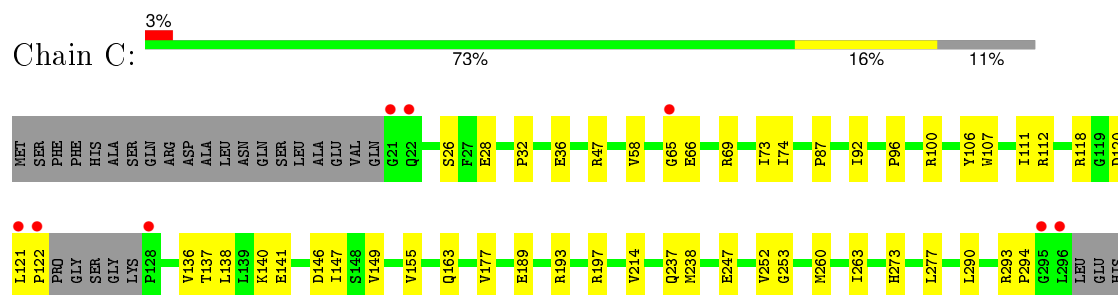
- Molecule 1: 5,10-methylenetetrahydrofolate reductase



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SIH  
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.56Å 128.64Å 96.74Å 90.00° 120.87° 90.00°	Depositor
Resolution (Å)	35.78 – 2.05 35.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.3 (35.78-2.05) 91.8 (35.78-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.217 , 0.250 0.213 , 0.246	Depositor DCC
$R_{free}$ test set	3160 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.4	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.4	EDS
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 69153 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: 4HF, 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	0.31	0/2260	0.54	0/3068
1	B	0.36	0/2276	0.59	1/3088 (0.0%)
1	C	0.34	0/2131	0.59	1/2893 (0.0%)
All	All	0.34	0/6667	0.57	2/9049 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	ASP	N-CA-C	-5.52	96.09	111.00
1	B	146	ASP	N-CA-C	-5.30	96.67	111.00

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	2216	0	2139	54	0
1	B	2230	0	2173	34	0
1	C	2087	0	2026	46	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	21	0	0
3	B	31	0	21	0	0
3	C	31	0	21	1	0
4	A	62	0	0	2	0
4	B	124	0	0	2	0
4	C	95	0	0	2	0
All	All	7066	0	6494	129	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 10.

All (129) 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:163:GLN:HE22	1:C:197:ARG:HH22	1.20	0.86
1:C:189:GLU:HB3	1:C:193:ARG:NH2	1.90	0.84
1:A:96:PRO:O	1:A:100:ARG:HG3	1.89	0.72
1:B:16:LEU:HD11	1:B:290:LEU:HD12	1.74	0.70
1:C:92:ILE:HG12	1:C:118:ARG:O	1.91	0.70
1:C:112:ARG:HG3	1:C:112:ARG:HH11	1.58	0.68
1:B:60:TYR:HB2	1:B:88:HIS:O	1.93	0.67
1:B:16:LEU:O	1:B:19:VAL:HG12	1.97	0.65
1:C:238:MET:HG3	1:C:252:VAL:HG11	1.78	0.64
1:B:13:ASN:HD21	1:B:262:LYS:NZ	1.96	0.64
1:A:9:ARG:HG3	1:C:263:ILE:HD11	1.80	0.64
1:B:9:ARG:C	1:B:9:ARG:HD2	2.18	0.63
1:A:149:VAL:HB	1:A:172:LYS:HD3	1.78	0.63
1:C:28:GLU:OE1	1:C:273:HIS:HE1	1.83	0.62
1:B:28:GLU:HB2	1:B:273:HIS:CE1	2.36	0.60
1:B:238:MET:HG3	1:B:252:VAL:HG11	1.82	0.60
1:A:63:ASN:HD22	1:A:64:SER:N	2.00	0.59
1:A:102:ILE:HD12	1:A:103:ALA:N	2.19	0.58
1:C:193:ARG:HG3	1:C:193:ARG:HH21	1.69	0.58
1:C:28:GLU:HB2	1:C:273:HIS:CE1	2.38	0.58
1:A:32:PRO:HD3	1:A:41:LEU:HD22	1.86	0.57
1:A:173:VAL:HA	1:A:177:VAL:HG22	1.86	0.57
1:C:96:PRO:O	1:C:100:ARG:HG3	2.04	0.57
1:A:74:ILE:HG13	1:A:87:PRO:HB3	1.87	0.57
1:A:149:VAL:CB	1:A:172:LYS:HD3	2.34	0.57
1:B:222:LYS:O	1:B:226:MET:HG3	2.05	0.57
1:A:9:ARG:CG	1:C:263:ILE:HD11	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:THR:O	1:C:141:GLU:HG3	2.04	0.57
1:B:96:PRO:O	1:B:100:ARG:HG3	2.05	0.56
1:A:34:THR:HG23	1:A:37:MET:HE3	1.88	0.56
1:B:32:PRO:HD3	1:B:41:LEU:HD22	1.88	0.56
1:A:33:ARG:HB2	1:A:37:MET:HE3	1.88	0.56
1:B:107:TRP:O	1:B:112:ARG:NH1	2.38	0.56
1:C:32:PRO:HG2	4:C:746:HOH:O	2.04	0.56
1:B:32:PRO:HD2	1:B:73:ILE:HD11	1.89	0.55
1:B:156:HIS:CE1	1:B:158:GLU:HB2	2.42	0.55
1:A:281:GLU:OE2	1:C:247:GLU:HG2	2.07	0.55
1:A:54:LYS:HD2	1:A:55:PHE:HD1	1.71	0.55
1:B:28:GLU:OE1	1:B:273:HIS:HE1	1.90	0.54
1:C:107:TRP:CZ3	1:C:112:ARG:HG2	2.43	0.54
1:A:34:THR:HG23	1:A:37:MET:CE	2.39	0.53
1:A:111:ILE:HD12	1:A:111:ILE:N	2.23	0.53
1:C:163:GLN:NE2	1:C:197:ARG:HH22	1.99	0.53
1:C:118:ARG:NH2	4:C:556:HOH:O	2.41	0.52
1:A:9:ARG:HG2	4:A:581:HOH:O	2.10	0.52
1:A:32:PRO:CG	1:A:38:GLU:HG2	2.39	0.52
1:B:193:ARG:HD3	4:B:715:HOH:O	2.10	0.52
1:C:69:ARG:O	1:C:73:ILE:HD13	2.10	0.51
1:A:143:ALA:HB3	1:A:145:PHE:CE1	2.45	0.51
1:B:111:ILE:HD12	1:B:111:ILE:N	2.26	0.51
1:A:132:ALA:HB3	1:A:172:LYS:HE2	1.92	0.50
1:A:157:PRO:HG3	1:A:228:ASN:HB2	1.93	0.50
1:A:16:LEU:HD11	1:A:290:LEU:HD23	1.92	0.50
1:C:47:ARG:HG2	1:C:47:ARG:HH11	1.75	0.50
1:B:238:MET:HG3	1:B:252:VAL:CG1	2.40	0.50
1:A:47:ARG:HH21	1:A:47:ARG:HG2	1.76	0.50
1:C:36:GLU:CD	1:C:36:GLU:H	2.14	0.50
1:C:138:LEU:HD23	1:C:138:LEU:C	2.32	0.50
1:C:74:ILE:HG13	1:C:87:PRO:HB3	1.94	0.49
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.77	0.49
1:B:266:ARG:NH2	1:C:189:GLU:HB2	2.27	0.49
1:C:118:ARG:HD3	1:C:121:LEU:HD21	1.94	0.49
1:A:90:THR:HA	1:A:117:LEU:O	2.13	0.49
1:A:138:LEU:O	1:A:142:VAL:HG23	2.13	0.49
1:C:277:LEU:HD13	3:C:497:4HF:HG1	1.95	0.48
1:C:238:MET:HG3	1:C:252:VAL:CG1	2.42	0.48
1:B:26:SER:OG	1:B:273:HIS:HD2	1.96	0.48
1:C:47:ARG:HG2	1:C:47:ARG:NH1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASN:HD21	1:B:262:LYS:HZ1	1.61	0.48
1:A:63:ASN:O	1:A:67:ARG:HG3	2.14	0.48
1:C:140:LYS:HD3	1:C:147:ILE:HD12	1.95	0.48
1:A:63:ASN:HD22	1:A:64:SER:H	1.60	0.48
1:A:63:ASN:ND2	1:A:64:SER:N	2.62	0.47
1:B:47:ARG:HH11	1:B:47:ARG:HG2	1.79	0.47
1:A:138:LEU:HD23	1:A:138:LEU:C	2.34	0.47
1:A:179:ARG:HH11	1:A:179:ARG:HG2	1.79	0.47
1:C:112:ARG:CG	1:C:112:ARG:HH11	2.25	0.47
1:C:26:SER:OG	1:C:273:HIS:HD2	1.97	0.47
1:A:54:LYS:HD3	1:A:54:LYS:O	2.15	0.47
1:B:156:HIS:ND1	1:B:158:GLU:HB2	2.30	0.47
1:C:106:TYR:HD1	1:C:111:ILE:HG13	1.80	0.47
1:C:293:ARG:HB3	1:C:294:PRO:HD2	1.95	0.46
1:A:60:TYR:HD1	1:A:70:THR:HG21	1.81	0.46
1:B:9:ARG:HD2	1:B:9:ARG:O	2.16	0.46
1:A:173:VAL:HA	1:A:177:VAL:CG2	2.45	0.46
1:A:69:ARG:O	1:A:73:ILE:HG13	2.16	0.46
1:B:104:ARG:HG2	1:B:142:VAL:HG13	1.97	0.45
1:C:120:ASP:O	1:C:122:PRO:HD3	2.17	0.45
1:A:132:ALA:O	1:A:136:VAL:HG23	2.17	0.45
1:C:92:ILE:HG21	1:C:122:PRO:HD2	1.99	0.44
1:C:106:TYR:CD1	1:C:111:ILE:HG13	2.53	0.44
1:B:187:ASP:OD2	1:B:230:ARG:NH2	2.50	0.44
1:A:149:VAL:CG1	1:A:172:LYS:HD3	2.48	0.44
1:A:33:ARG:HB2	1:A:37:MET:CE	2.47	0.44
1:B:45:ILE:HD13	1:B:77:ILE:HG12	2.00	0.43
1:A:215:SER:HB3	1:A:282:MET:CE	2.48	0.43
1:B:281:GLU:HB2	4:B:639:HOH:O	2.19	0.43
1:B:74:ILE:HG13	1:B:87:PRO:HB3	2.00	0.43
1:B:32:PRO:HD2	1:B:73:ILE:CD1	2.48	0.43
1:A:138:LEU:O	1:A:138:LEU:HD23	2.18	0.43
1:B:70:THR:O	1:B:74:ILE:HG12	2.19	0.43
1:B:90:THR:HA	1:B:117:LEU:O	2.19	0.43
1:C:193:ARG:HG3	1:C:193:ARG:NH2	2.33	0.42
1:C:112:ARG:HG3	1:C:112:ARG:NH1	2.31	0.42
1:A:188:VAL:HG12	1:A:192:LEU:HD22	2.02	0.42
1:A:130:MET:HB2	1:A:134:ASP:HB2	2.01	0.42
1:A:233:ALA:O	1:A:237:GLN:HG2	2.20	0.42
1:C:58:VAL:HG21	1:C:73:ILE:HG22	2.01	0.42
1:A:32:PRO:HD2	1:A:73:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLU:OE2	1:C:193:ARG:NH1	2.53	0.41
1:C:112:ARG:CG	1:C:112:ARG:NH1	2.81	0.41
1:A:9:ARG:NH2	1:C:260:MET:HG3	2.36	0.41
1:A:218:LYS:O	1:A:222:LYS:HG3	2.21	0.41
1:C:189:GLU:HB3	1:C:193:ARG:HH22	1.79	0.41
1:A:28:GLU:HB2	1:A:273:HIS:NE2	2.36	0.41
1:B:13:ASN:ND2	1:B:262:LYS:NZ	2.67	0.41
1:A:281:GLU:HG2	4:A:684:HOH:O	2.21	0.41
1:A:172:LYS:O	1:A:175:ALA:HB3	2.21	0.41
1:A:104:ARG:O	1:A:108:ASN:ND2	2.53	0.41
1:C:136:VAL:O	1:C:140:LYS:HG2	2.21	0.41
1:C:149:VAL:HG22	1:C:177:VAL:HG11	2.02	0.41
1:B:122:PRO:HA	1:B:123:PRO:HD3	1.96	0.40
1:A:149:VAL:HG11	1:A:172:LYS:HD3	2.03	0.40
1:A:179:ARG:NH1	1:A:179:ARG:HG2	2.35	0.40
1:A:62:ALA:HA	1:A:67:ARG:HH11	1.87	0.40
1:A:104:ARG:HB2	1:A:104:ARG:HE	1.60	0.40
1:C:65:GLY:O	1:C:66:GLU:HB2	2.21	0.40
1:C:214:VAL:O	1:C:253:GLY:HA3	2.21	0.40
1:B:170:LYS:HD2	1:B:201:ALA:O	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	284/304 (93%)	272 (96%)	11 (4%)	1 (0%)	39	28
1	B	283/304 (93%)	278 (98%)	3 (1%)	2 (1%)	26	15
1	C	267/304 (88%)	258 (97%)	8 (3%)	1 (0%)	39	28
All	All	834/912 (91%)	808 (97%)	22 (3%)	4 (0%)	34	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	PHE
1	C	155	VAL
1	A	155	VAL
1	B	155	VAL

### 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	228/259 (88%)	222 (97%)	6 (3%)	54	47
1	B	233/259 (90%)	226 (97%)	7 (3%)	48	41
1	C	216/259 (83%)	214 (99%)	2 (1%)	84	84
All	All	677/777 (87%)	662 (98%)	15 (2%)	60	53

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	63	ASN
1	A	171	ARG
1	A	192	LEU
1	A	195	ARG
1	A	247	GLU
1	B	54	LYS
1	B	112	ARG
1	B	163	GLN
1	B	228	ASN
1	B	259	ASP
1	B	281	GLU
1	B	290	LEU
1	C	237	GLN
1	C	290	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	43	ASN
1	A	63	ASN
1	A	108	ASN
1	A	168	ASN
1	A	219	GLN
1	A	228	ASN
1	B	13	ASN
1	B	14	GLN
1	B	20	GLN
1	B	24	ASN
1	B	109	ASN
1	B	163	GLN
1	B	273	HIS
1	C	39	GLN
1	C	163	GLN
1	C	237	GLN
1	C	273	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	395	-	48,58,58	2.06	11 (22%)	54,89,89	3.03	16 (29%)
3	4HF	A	495	-	22,33,33	1.64	5 (22%)	16,46,46	1.64	3 (18%)
2	FAD	B	396	-	48,58,58	2.01	10 (20%)	54,89,89	2.85	14 (25%)
3	4HF	B	496	-	22,33,33	1.69	5 (22%)	16,46,46	1.66	3 (18%)
2	FAD	C	397	-	48,58,58	2.08	8 (16%)	54,89,89	2.89	9 (16%)
3	4HF	C	497	-	22,33,33	1.67	5 (22%)	16,46,46	1.67	3 (18%)

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	395	-	-	0/30/50/50	0/6/6/6
3	4HF	A	495	-	-	0/13/31/31	0/3/3/3
2	FAD	B	396	-	-	0/30/50/50	0/6/6/6
3	4HF	B	496	-	-	0/13/31/31	0/3/3/3
2	FAD	C	397	-	-	0/30/50/50	0/6/6/6
3	4HF	C	497	-	-	0/13/31/31	0/3/3/3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	395	FAD	C8A-N7A	-2.15	1.30	1.34
2	A	395	FAD	P-O2P	-2.12	1.45	1.54
2	B	396	FAD	C9-C9A	2.01	1.45	1.40
2	A	395	FAD	C5X-N5	2.16	1.38	1.35
2	C	397	FAD	C6-C5X	2.19	1.45	1.41
3	A	495	4HF	C3'-S2'	2.23	1.78	1.73
2	A	395	FAD	C6-C5X	2.27	1.45	1.41
2	A	395	FAD	C9-C9A	2.28	1.45	1.40
3	C	497	4HF	C3'-S2'	2.46	1.78	1.73
2	B	396	FAD	C4-C4X	2.53	1.46	1.41
3	B	496	4HF	C3'-S2'	2.56	1.79	1.73
2	C	397	FAD	C8-C7	2.57	1.47	1.41
2	C	397	FAD	C5X-N5	2.58	1.39	1.35
2	A	395	FAD	C8-C7	2.58	1.47	1.41
3	A	495	4HF	C7-N8	2.59	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	396	FAD	C8-C7	2.66	1.48	1.41
3	B	496	4HF	C7-N8	2.69	1.49	1.46
3	A	495	4HF	C7-C6	2.79	1.55	1.53
3	C	497	4HF	C2-N3	2.97	1.40	1.35
3	C	497	4HF	C7-N8	3.02	1.50	1.46
2	B	396	FAD	C8M-C8	3.03	1.57	1.51
3	A	495	4HF	C2-N3	3.07	1.40	1.35
2	B	396	FAD	C7M-C7	3.07	1.57	1.51
2	C	397	FAD	C8M-C8	3.10	1.57	1.51
2	B	396	FAD	C5X-N5	3.14	1.40	1.35
3	B	496	4HF	C2-N3	3.21	1.41	1.35
2	A	395	FAD	O4B-C1B	3.24	1.45	1.41
2	C	397	FAD	C4-N3	3.35	1.39	1.33
3	B	496	4HF	C7-C6	3.37	1.56	1.53
3	C	497	4HF	C7-C6	3.43	1.56	1.53
2	B	396	FAD	C4-N3	3.44	1.39	1.33
2	A	395	FAD	C4-N3	3.91	1.40	1.33
2	C	397	FAD	C4X-N5	3.98	1.39	1.33
2	A	395	FAD	C4X-N5	4.22	1.40	1.33
3	C	497	4HF	C4-N3	4.28	1.41	1.33
3	B	496	4HF	C4-N3	4.39	1.41	1.33
3	A	495	4HF	C4-N3	4.54	1.41	1.33
2	B	396	FAD	C4X-N5	5.10	1.41	1.33
2	B	396	FAD	C9A-N10	6.19	1.47	1.38
2	C	397	FAD	C9A-N10	6.38	1.47	1.38
2	B	396	FAD	C10-N10	6.65	1.46	1.39
2	A	395	FAD	C9A-N10	7.03	1.48	1.38
2	A	395	FAD	C10-N10	7.09	1.47	1.39
2	C	397	FAD	C10-N10	8.31	1.48	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	397	FAD	C4X-C10-N10	-9.49	114.93	120.52
2	A	395	FAD	C4X-C10-N10	-9.24	115.07	120.52
2	B	396	FAD	C4X-C10-N10	-7.31	116.21	120.52
2	A	395	FAD	C4X-C4-N3	-7.11	113.86	123.59
2	B	396	FAD	C4X-C4-N3	-6.68	114.46	123.59
2	B	396	FAD	C4-C4X-C10	-6.26	115.94	119.94
2	C	397	FAD	C4X-C4-N3	-6.02	115.35	123.59
2	C	397	FAD	C4-C4X-C10	-5.10	116.68	119.94
2	C	397	FAD	C5X-C9A-N10	-5.04	113.79	117.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	395	FAD	C4-C4X-C10	-4.27	117.21	119.94
2	A	395	FAD	C5X-C9A-N10	-3.99	114.58	117.62
2	C	397	FAD	C1B-N9A-C4A	-3.93	121.02	126.94
3	C	497	4HF	N3-C2-N1	-3.79	119.32	125.53
2	A	395	FAD	O3P-P-O5'	-3.78	92.90	102.94
3	B	496	4HF	N3-C2-N1	-3.77	119.35	125.53
3	A	495	4HF	N3-C2-N1	-3.75	119.39	125.53
2	B	396	FAD	C5X-C9A-N10	-3.59	114.89	117.62
2	A	395	FAD	C1B-N9A-C4A	-3.15	122.18	126.94
2	C	397	FAD	O3P-P-O5'	-3.00	94.97	102.94
2	B	396	FAD	O3P-PA-O5B	-2.75	95.64	102.94
2	A	395	FAD	C6-C5X-N5	-2.66	115.54	118.96
2	B	396	FAD	C1B-N9A-C4A	-2.60	123.02	126.94
2	A	395	FAD	C2B-C1B-N9A	-2.58	110.36	114.29
2	A	395	FAD	C4-C4X-N5	-2.55	115.62	118.72
2	B	396	FAD	O3P-P-O5'	-2.17	97.17	102.94
2	A	395	FAD	O5B-C5B-C4B	2.00	116.51	109.12
2	C	397	FAD	O2P-P-O3P	2.02	114.25	105.09
2	B	396	FAD	C8M-C8-C7	2.02	125.17	120.73
2	C	397	FAD	O5B-C5B-C4B	2.06	116.73	109.12
2	B	396	FAD	C9A-C5X-N5	2.10	125.45	122.36
2	B	396	FAD	C1'-N10-C9A	2.11	121.22	118.86
2	B	396	FAD	C2B-C1B-N9A	2.12	117.53	114.29
2	B	396	FAD	O3'-C3'-C4'	2.15	114.18	108.75
2	A	395	FAD	C9A-C5X-N5	2.17	125.57	122.36
2	B	396	FAD	O2'-C2'-C3'	2.29	114.78	109.02
2	A	395	FAD	C8M-C8-C7	2.30	125.78	120.73
2	A	395	FAD	O2'-C2'-C3'	2.33	114.86	109.02
2	A	395	FAD	C1'-N10-C9A	2.33	121.47	118.86
2	A	395	FAD	C4A-C5A-N7A	2.47	111.75	109.48
3	A	495	4HF	C4-N3-C2	2.71	119.69	115.94
3	B	496	4HF	C4-N3-C2	2.86	119.91	115.94
3	C	497	4HF	C4-N3-C2	2.94	120.01	115.94
3	B	496	4HF	C2-N1-C8A	3.17	121.67	114.54
3	C	497	4HF	C2-N1-C8A	3.21	121.75	114.54
3	A	495	4HF	C2-N1-C8A	3.28	121.92	114.54
2	C	397	FAD	C4-N3-C2	13.65	127.04	115.25
2	B	396	FAD	C4-N3-C2	14.16	127.49	115.25
2	A	395	FAD	C4-N3-C2	15.01	128.22	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	497	4HF	1	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	288/304 (94%)	0.66	32 (11%) <b>7</b> <b>7</b>	21, 40, 65, 71	0
1	B	287/304 (94%)	0.08	5 (1%) <b>73</b> <b>78</b>	16, 30, 48, 58	0
1	C	271/304 (89%)	0.02	8 (2%) <b>54</b> <b>61</b>	18, 29, 43, 56	0
All	All	846/912 (92%)	0.26	45 (5%) <b>30</b> <b>34</b>	16, 32, 58, 71	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	LEU	9.1
1	A	295	GLY	7.8
1	A	64	SER	6.5
1	C	128	PRO	5.1
1	A	21	GLY	4.8
1	C	21	GLY	4.8
1	A	104	ARG	4.8
1	A	102	ILE	4.5
1	C	121	LEU	4.3
1	C	295	GLY	4.3
1	A	107	TRP	4.3
1	A	110	GLY	4.2
1	C	122	PRO	3.9
1	A	108	ASN	3.8
1	A	109	ASN	3.7
1	A	92	ILE	3.7
1	A	143	ALA	3.6
1	B	65	GLY	3.6
1	B	66	GLU	3.5
1	A	71	HIS	3.5
1	A	103	ALA	3.5
1	A	112	ARG	3.4
1	A	65	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	66	GLU	3.2
1	A	145	PHE	3.1
1	A	129	GLU	3.0
1	A	63	ASN	3.0
1	A	101	THR	3.0
1	B	92	ILE	2.8
1	A	93	ASP	2.7
1	A	144	ASP	2.7
1	C	22	GLN	2.6
1	C	65	GLY	2.6
1	A	3	PHE	2.5
1	A	114	ILE	2.4
1	A	79	ASP	2.4
1	A	97	ASP	2.4
1	A	122	PRO	2.3
1	A	181	ILE	2.3
1	B	60	TYR	2.3
1	B	5	HIS	2.2
1	A	70	THR	2.2
1	A	106	TYR	2.1
1	A	20	GLN	2.0
1	A	7	SER	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( $\text{\AA}^2$ )	Q<0.9
3	4HF	C	497	31/31	0.87	0.17	1.65	27,42,58,59	0
3	4HF	A	495	31/31	0.86	0.17	1.49	33,42,57,58	0
3	4HF	B	496	31/31	0.87	0.15	1.09	28,37,51,52	0
2	FAD	B	396	53/53	0.93	0.12	-0.36	20,24,40,40	0
2	FAD	C	397	53/53	0.95	0.10	-0.48	20,24,39,40	0
2	FAD	A	395	53/53	0.93	0.12	-0.52	28,31,47,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.