



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:07 AM GMT

PDB ID : 2FON  
Title : X-ray crystal structure of LeACX1, an acyl-CoA oxidase from *Lycopersicon esculentum* (tomato)  
Authors : Garavito, R.M.; Powers, R.A.  
Deposited on : 2006-01-13  
Resolution : 2.74 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 (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

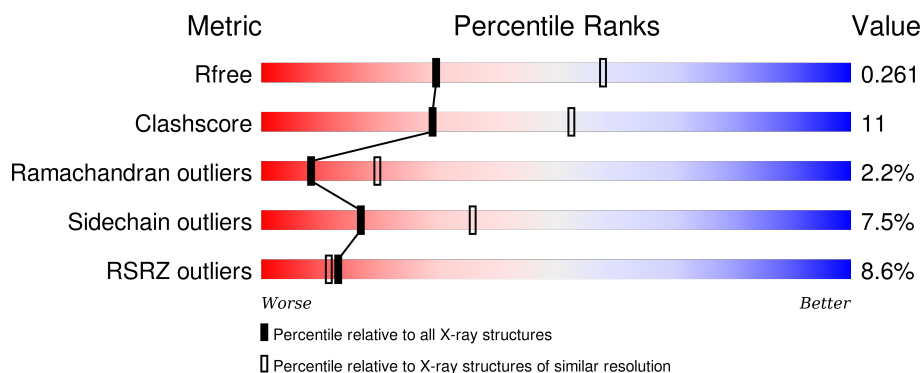
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.74 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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	683	<div> <div>4%</div> <div>69%</div> <div>23%</div> <div>• • •</div> </div>
1	B	683	<div> <div>3%</div> <div>71%</div> <div>21%</div> <div>• •</div> </div>
1	C	683	<div> <div>18%</div> <div>70%</div> <div>22%</div> <div>• •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14949 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 peroxisomal acyl-CoA oxidase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	0	0	0
			5010	3180	873	932	25			
1	B	656	Total	C	N	O	S	0	0	0
			5040	3198	878	939	25			
1	C	653	Total	C	N	O	S	0	0	0
			4704	2960	828	892	24			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	CLONING ARTIFACT	UNP Q5D8D3
A	-17	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
A	-16	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
A	-15	SER	-	CLONING ARTIFACT	UNP Q5D8D3
A	-14	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-13	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-12	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-11	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-10	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-9	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-8	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
A	-7	SER	-	CLONING ARTIFACT	UNP Q5D8D3
A	-6	ALA	-	CLONING ARTIFACT	UNP Q5D8D3
A	-5	CYS	-	CLONING ARTIFACT	UNP Q5D8D3
A	-4	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
A	-3	LEU	-	CLONING ARTIFACT	UNP Q5D8D3
A	-2	VAL	-	CLONING ARTIFACT	UNP Q5D8D3
A	-1	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
A	0	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
B	-18	MET	-	CLONING ARTIFACT	UNP Q5D8D3
B	-17	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
B	-16	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
B	-15	SER	-	CLONING ARTIFACT	UNP Q5D8D3

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-13	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-12	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-11	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-10	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-9	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-8	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
B	-7	SER	-	CLONING ARTIFACT	UNP Q5D8D3
B	-6	ALA	-	CLONING ARTIFACT	UNP Q5D8D3
B	-5	CYS	-	CLONING ARTIFACT	UNP Q5D8D3
B	-4	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
B	-3	LEU	-	CLONING ARTIFACT	UNP Q5D8D3
B	-2	VAL	-	CLONING ARTIFACT	UNP Q5D8D3
B	-1	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
B	0	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
C	-18	MET	-	CLONING ARTIFACT	UNP Q5D8D3
C	-17	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
C	-16	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
C	-15	SER	-	CLONING ARTIFACT	UNP Q5D8D3
C	-14	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-13	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-12	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-11	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-10	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-9	HIS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-8	GLY	-	CLONING ARTIFACT	UNP Q5D8D3
C	-7	SER	-	CLONING ARTIFACT	UNP Q5D8D3
C	-6	ALA	-	CLONING ARTIFACT	UNP Q5D8D3
C	-5	CYS	-	CLONING ARTIFACT	UNP Q5D8D3
C	-4	GLU	-	CLONING ARTIFACT	UNP Q5D8D3
C	-3	LEU	-	CLONING ARTIFACT	UNP Q5D8D3
C	-2	VAL	-	CLONING ARTIFACT	UNP Q5D8D3
C	-1	ARG	-	CLONING ARTIFACT	UNP Q5D8D3
C	0	GLU	-	CLONING ARTIFACT	UNP Q5D8D3

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

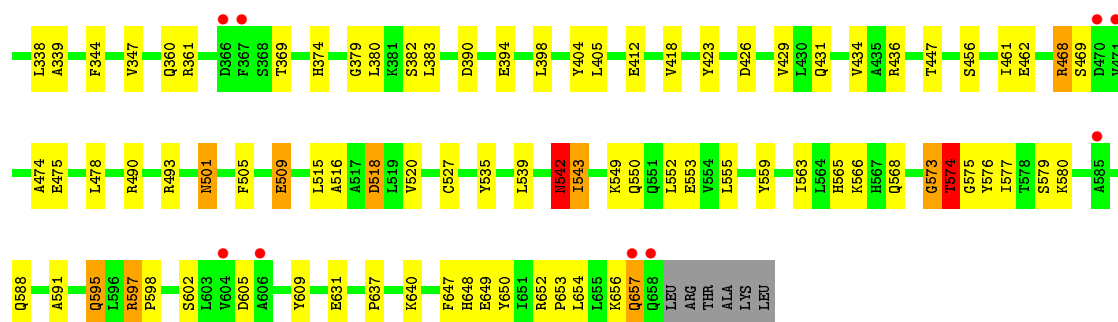


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

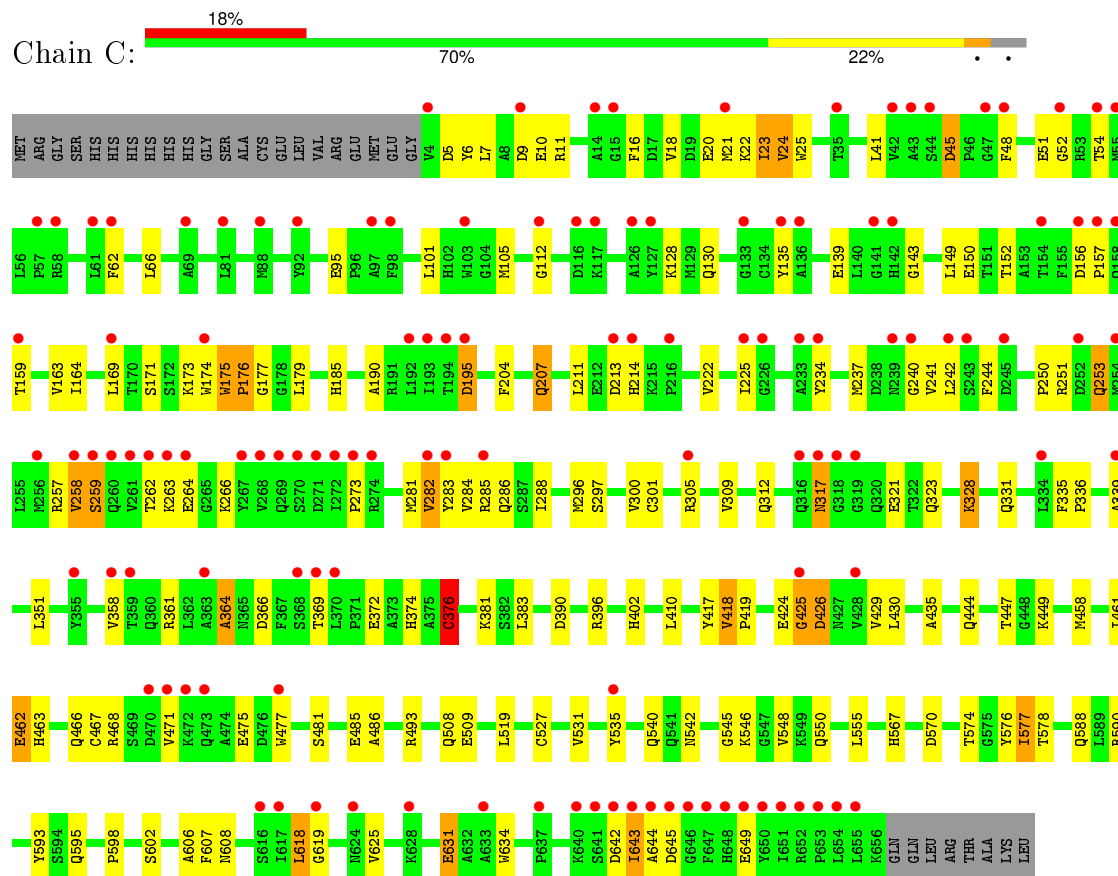
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	22	Total	O	0	0
			22	22		





- Molecule 1: peroxisomal acyl-CoA oxidase 1A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.20 Å   240.33 Å   89.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	30.00 – 2.74 29.82 – 2.74	Depositor EDS
% Data completeness (in resolution range)	92.9 (30.00-2.74) 92.8 (29.82-2.74)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 2.72 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.212   ,   0.267 0.205   ,   0.261	Depositor DCC
$R_{free}$ test set	3221 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.6	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 63.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	3 of 63840 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.28% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.99	2/5120 (0.0%)	1.00	18/6948 (0.3%)
1	B	0.94	4/5150 (0.1%)	0.96	12/6988 (0.2%)
1	C	0.61	1/4803 (0.0%)	0.70	2/6552 (0.0%)
All	All	0.87	7/15073 (0.0%)	0.90	32/20488 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	300	VAL	CB-CG1	-6.60	1.39	1.52
1	B	243	SER	CA-CB	6.01	1.61	1.52
1	B	404	TYR	CD2-CE2	-5.64	1.30	1.39
1	C	376	CYS	CB-SG	-5.43	1.73	1.81
1	A	100	ASP	CB-CG	5.28	1.62	1.51
1	A	376	CYS	CB-SG	-5.13	1.73	1.81
1	B	631	GLU	CG-CD	5.12	1.59	1.51

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	67	ARG	NE-CZ-NH2	-10.09	115.26	120.30
1	B	53	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	53	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	B	101	LEU	CA-CB-CG	-7.94	97.04	115.30
1	A	345	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	A	101	LEU	CA-CB-CG	-7.71	97.58	115.30
1	A	100	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	611	ASP	CB-CG-OD1	7.57	125.11	118.30
1	B	53	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	333	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	B	390	ASP	CB-CG-OD2	-6.50	112.45	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	LEU	CA-CB-CG	-6.36	100.67	115.30
1	B	222	VAL	CB-CA-C	-5.98	100.03	111.40
1	A	217	LEU	CA-CB-CG	5.90	128.87	115.30
1	A	67	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	213	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	217	LEU	CA-CB-CG	5.60	128.18	115.30
1	B	390	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	333	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	C	618	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	100	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	B	209	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	41	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	B	605	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	222	VAL	CB-CA-C	-5.31	101.32	111.40
1	A	622	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	80	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	163	VAL	CB-CA-C	5.15	121.19	111.40
1	A	468	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	B	9	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	611	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	645	ASP	CB-CG-OD1	-5.04	113.77	118.30

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	5010	0	4838	122	0
1	B	5040	0	4884	112	0
1	C	4704	0	4258	98	0
2	A	53	0	31	7	0
2	B	53	0	31	6	0
2	C	53	0	31	5	0
3	A	14	0	0	0	0
3	B	22	0	0	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14949	0	14073	329	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 11.

All (329) 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:A:29:ARG:HH11	1:A:29:ARG:HG3	1.15	1.07
1:C:361:ARG:HD2	1:C:369:THR:HG21	1.47	0.97
1:A:29:ARG:HH11	1:A:29:ARG:CG	1.77	0.96
1:B:361:ARG:HD3	1:B:369:THR:HG21	1.45	0.94
1:B:285:ARG:HG3	1:B:285:ARG:HH11	1.35	0.90
1:B:516:ALA:O	1:B:520:VAL:HG23	1.72	0.90
1:A:316:GLN:O	1:A:317:ASN:O	1.90	0.88
1:C:475:GLU:HA	1:C:588:GLN:NE2	1.90	0.87
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.40	0.85
1:A:29:ARG:NH1	1:A:29:ARG:HG3	1.92	0.84
1:A:412:GLU:O	1:A:416:VAL:HG12	1.78	0.84
1:B:539:LEU:HD13	1:B:553:GLU:HG3	1.61	0.81
1:A:317:ASN:O	1:A:319:GLY:N	2.13	0.79
1:C:372:GLU:O	1:C:376:CYS:HB2	1.83	0.79
1:C:475:GLU:HA	1:C:588:GLN:HE22	1.48	0.78
1:A:442:ILE:O	1:A:444:GLN:N	2.16	0.78
1:B:490:ARG:HD3	3:B:2013:HOH:O	1.84	0.76
1:A:113:GLN:O	1:A:257:ARG:HB2	1.86	0.75
1:A:333:ARG:HD2	1:A:394:GLU:OE2	1.85	0.75
1:B:595:GLN:O	1:B:598:PRO:HD2	1.85	0.74
1:B:637:PRO:O	1:B:640:LYS:HG3	1.87	0.74
1:A:516:ALA:HA	1:A:519:LEU:HD12	1.67	0.74
1:B:656:LYS:O	1:B:657:GLN:HG2	1.89	0.72
1:C:485:GLU:HG2	1:C:576:TYR:OH	1.89	0.72
1:C:286:GLN:HG2	1:C:351:LEU:HB3	1.70	0.71
1:C:631:GLU:HA	1:C:634:TRP:HD1	1.56	0.71
1:C:296:MET:O	1:C:300:VAL:HG23	1.91	0.71
1:B:333:ARG:HB2	1:B:398:LEU:HD21	1.73	0.70
1:B:34:LEU:HD23	1:B:88:MET:HG2	1.73	0.70
1:B:285:ARG:HG3	1:B:285:ARG:NH1	2.06	0.70
1:C:381:LYS:NZ	1:C:425:GLY:O	2.23	0.70
1:A:143:GLY:HA3	2:A:1000:FAD:O2P	1.92	0.69
1:B:91:ARG:HH11	1:B:91:ARG:HG3	1.58	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:HB3	1:C:240:GLY:HA3	1.75	0.69
1:A:568:GLN:NE2	1:A:582:GLY:HA3	2.08	0.68
1:C:105:MET:HB3	1:C:135:TYR:HB2	1.75	0.68
1:A:185:HIS:NE2	1:A:207:GLN:HG3	2.08	0.68
1:A:442:ILE:HD11	1:A:495:SER:HB3	1.73	0.68
1:C:20:GLU:HA	1:C:23:ILE:HD12	1.75	0.68
1:C:458:MET:HG2	1:C:461:ILE:HD11	1.75	0.68
1:A:101:LEU:HD23	1:A:105:MET:HG3	1.75	0.68
1:A:431:GLN:HG3	1:A:523:ALA:HB1	1.76	0.68
1:A:138:THR:OG1	2:A:1000:FAD:H1'1	1.94	0.67
1:A:502:LEU:HD12	1:A:515:LEU:HD12	1.77	0.67
1:C:284:VAL:HG12	1:C:288:ILE:HD11	1.76	0.67
1:A:502:LEU:HD12	1:A:515:LEU:CD1	2.24	0.66
1:B:118:GLN:NE2	1:B:254:MET:O	2.26	0.66
1:A:91:ARG:HG3	1:A:91:ARG:NH1	2.10	0.66
1:A:316:GLN:C	1:A:317:ASN:O	2.32	0.66
1:B:138:THR:OG1	2:B:2000:FAD:H1'1	1.96	0.66
1:C:339:ALA:HA	1:C:555:LEU:HD22	1.78	0.66
1:A:493:ARG:HD3	1:A:574:THR:HB	1.76	0.66
1:A:105:MET:HE2	1:A:105:MET:HA	1.79	0.65
1:B:174:TRP:C	1:B:176:PRO:HD3	2.17	0.64
1:B:176:PRO:HA	2:B:2000:FAD:C4	2.26	0.64
1:C:493:ARG:HD3	1:C:574:THR:HB	1.80	0.64
1:A:436:ARG:HG2	1:A:512:PHE:CZ	2.33	0.63
1:C:361:ARG:CD	1:C:369:THR:HG21	2.24	0.63
1:C:112:GLY:O	1:C:257:ARG:HD3	1.97	0.63
1:A:570:ASP:O	1:A:574:THR:HG23	1.98	0.63
1:C:174:TRP:O	1:C:175:TRP:HB2	2.00	0.62
1:C:242:LEU:HD21	1:C:244:PHE:CE1	2.35	0.62
1:A:47:GLY:O	1:A:67:ARG:NH2	2.32	0.62
1:B:361:ARG:CD	1:B:369:THR:HG21	2.24	0.62
1:A:283:TYR:HB2	1:A:355:TYR:CE1	2.36	0.61
1:A:88:MET:CE	1:A:91:ARG:HE	2.14	0.61
2:A:1000:FAD:H2'	2:A:1000:FAD:C9	2.30	0.61
1:A:282:VAL:O	1:A:286:GLN:HB2	2.01	0.60
1:A:595:GLN:O	1:A:598:PRO:HD2	2.01	0.60
1:C:527:CYS:O	1:C:531:VAL:HG23	2.02	0.60
1:B:209:ARG:HD3	1:B:214:HIS:O	2.01	0.60
1:C:618:LEU:HA	1:C:625:VAL:HG13	1.84	0.60
1:B:185:HIS:NE2	1:B:207:GLN:HG3	2.16	0.60
1:A:173:LYS:O	1:A:241:VAL:HA	2.02	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:648:HIS:HB3	3:B:2014:HOH:O	2.02	0.59
2:A:1000:FAD:H2'	2:A:1000:FAD:H9	1.84	0.59
1:A:264:GLU:CD	1:A:264:GLU:H	2.06	0.59
1:C:139:GLU:HG3	1:C:149:LEU:HD22	1.83	0.59
1:A:176:PRO:HA	2:A:1000:FAD:C4	2.32	0.59
1:C:284:VAL:O	1:C:288:ILE:HG13	2.03	0.59
2:B:2000:FAD:H2'	2:B:2000:FAD:C9	2.33	0.59
1:B:542:ASN:CG	1:B:543:ILE:H	2.06	0.58
1:B:262:THR:OG1	1:B:265:GLY:O	2.21	0.58
1:A:411:PRO:HB3	1:B:229:PHE:CD2	2.39	0.58
1:C:41:LEU:O	1:C:45:ASP:HB2	2.03	0.58
1:C:361:ARG:HA	1:C:364:ALA:HB3	1.86	0.58
1:C:297:SER:HB2	1:C:607:PHE:CZ	2.38	0.58
1:C:545:GLY:O	1:C:548:VAL:HB	2.05	0.57
1:B:574:THR:OG1	1:B:575:GLY:N	2.37	0.57
1:A:82:SER:OG	1:A:85:GLU:HG3	2.05	0.57
1:A:225:ILE:HD12	1:B:405:LEU:HD21	1.86	0.56
1:A:242:LEU:HD21	1:A:244:PHE:CZ	2.41	0.56
1:C:45:ASP:HB3	1:C:48:PHE:HD1	1.70	0.56
1:B:139:GLU:HG3	1:B:149:LEU:HD22	1.88	0.56
1:B:173:LYS:O	1:B:241:VAL:HA	2.06	0.56
1:C:396:ARG:HA	1:C:410:LEU:HD13	1.86	0.56
1:A:88:MET:HE1	1:A:91:ARG:HE	1.69	0.56
1:B:333:ARG:CZ	1:B:398:LEU:HD23	2.35	0.56
1:B:436:ARG:NH2	1:B:509:GLU:OE2	2.38	0.55
1:A:262:THR:OG1	1:A:264:GLU:OE1	2.19	0.55
1:B:139:GLU:HG2	1:B:173:LYS:HD3	1.87	0.55
1:A:568:GLN:HE22	1:A:582:GLY:HA3	1.72	0.55
1:C:590:ARG:HH11	1:C:590:ARG:HG3	1.71	0.55
1:A:150:GLU:HB2	1:A:171:SER:HB3	1.89	0.55
2:B:2000:FAD:H2'	2:B:2000:FAD:H9	1.89	0.55
1:C:185:HIS:HE2	1:C:207:GLN:HG2	1.71	0.55
1:B:493:ARG:HD3	1:B:574:THR:HB	1.89	0.54
1:C:418:VAL:N	1:C:419:PRO:HD2	2.22	0.54
1:C:173:LYS:HB2	1:C:242:LEU:HB3	1.88	0.54
1:C:374:HIS:C	1:C:374:HIS:CD2	2.81	0.54
1:A:636:ASP:CG	1:A:637:PRO:HD2	2.28	0.54
1:A:139:GLU:OE2	1:A:151:THR:OG1	2.15	0.54
1:C:185:HIS:NE2	1:C:207:GLN:HG2	2.23	0.54
1:B:256:MET:HB3	1:B:260:GLN:HB3	1.89	0.54
1:A:431:GLN:HG3	1:A:523:ALA:CB	2.38	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:VAL:HG22	1:B:6:TYR:CE1	2.43	0.54
1:C:435:ALA:HB1	1:C:519:LEU:HB3	1.90	0.54
1:B:382:SER:HB3	1:B:431:GLN:HE21	1.73	0.54
1:B:4:VAL:HG22	1:B:6:TYR:CZ	2.43	0.53
1:A:29:ARG:NH1	1:A:29:ARG:CG	2.48	0.53
1:B:329:THR:O	1:B:333:ARG:HG3	2.09	0.53
1:B:493:ARG:HH11	1:B:574:THR:HB	1.74	0.53
1:A:174:TRP:O	1:A:175:TRP:HB2	2.08	0.53
1:C:297:SER:HB2	1:C:607:PHE:CE2	2.45	0.52
1:A:221:THR:O	1:A:242:LEU:HA	2.09	0.52
1:C:7:LEU:HD21	1:C:309:VAL:HG22	1.91	0.52
1:C:361:ARG:HB2	1:C:366:ASP:HB3	1.92	0.52
1:A:283:TYR:HB2	1:A:355:TYR:HE1	1.74	0.52
1:C:152:THR:O	1:C:164:ILE:HA	2.10	0.52
1:A:335:PHE:CG	1:A:596:LEU:HD23	2.45	0.52
1:A:331:GLN:HG2	1:A:335:PHE:CE1	2.45	0.52
1:A:382:SER:HB3	1:A:431:GLN:OE1	2.10	0.51
1:B:174:TRP:O	1:B:175:TRP:HB2	2.10	0.51
1:C:486:ALA:HA	1:C:576:TYR:CE2	2.44	0.51
1:B:256:MET:HA	1:B:259:SER:O	2.10	0.51
1:C:471:VAL:HG11	1:C:477:TRP:NE1	2.25	0.51
1:B:475:GLU:O	1:B:478:LEU:HB2	2.11	0.51
1:C:234:TYR:O	1:C:237:MET:HB3	2.11	0.51
1:B:35:THR:OG1	1:B:88:MET:CE	2.58	0.51
1:B:518:ASP:N	1:B:518:ASP:OD2	2.44	0.51
1:C:467:CYS:HG	1:C:576:TYR:HE1	1.58	0.50
1:B:209:ARG:HD2	1:B:214:HIS:CE1	2.46	0.50
1:B:394:GLU:O	1:B:398:LEU:HG	2.12	0.50
1:A:67:ARG:HB2	1:B:650:TYR:CE1	2.46	0.50
1:B:18:VAL:O	1:B:22:LYS:HG3	2.10	0.50
1:B:53:ARG:HH22	1:B:412:GLU:CD	2.11	0.50
1:A:19:ASP:O	1:A:23:ILE:HD13	2.10	0.50
1:B:542:ASN:O	1:B:543:ILE:HB	2.12	0.50
1:A:551:GLN:HE21	1:A:603:LEU:HD11	1.77	0.50
2:C:3000:FAD:H8A	2:C:3000:FAD:O1A	2.12	0.49
1:C:174:TRP:HD1	1:C:175:TRP:CD1	2.30	0.49
1:A:273:PRO:C	1:A:275:GLN:H	2.15	0.49
1:B:559:TYR:O	1:B:563:ILE:HG12	2.11	0.49
1:B:175:TRP:N	1:B:176:PRO:HD3	2.27	0.49
1:A:651:ILE:HD13	1:B:66:LEU:HB3	1.94	0.49
1:A:471:VAL:HG21	1:A:477:TRP:CE2	2.46	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ARG:NH1	1:B:575:GLY:O	2.45	0.49
1:A:442:ILE:C	1:A:444:GLN:H	2.15	0.49
1:B:128:LYS:HD2	1:B:130:GLN:NE2	2.27	0.49
1:C:128:LYS:HB2	1:C:130:GLN:NE2	2.27	0.49
1:C:282:VAL:O	1:C:286:GLN:HB2	2.12	0.49
1:B:159:THR:HG21	1:B:161:GLU:OE1	2.12	0.49
1:B:474:ALA:HB1	1:B:588:GLN:HB2	1.94	0.49
1:B:505:PHE:HE1	1:B:515:LEU:HD11	1.77	0.49
1:C:417:TYR:C	1:C:419:PRO:HD2	2.33	0.49
1:C:16:PHE:HZ	1:C:602:SER:O	1.95	0.48
1:A:111:LYS:HZ1	1:A:127:TYR:HH	1.57	0.48
1:A:461:ILE:O	1:A:462:GLU:C	2.50	0.48
1:B:107:ILE:HB	1:B:108:PRO:HD3	1.95	0.48
1:A:88:MET:CE	1:A:91:ARG:NE	2.77	0.48
1:B:159:THR:CG2	1:B:161:GLU:OE1	2.60	0.48
1:A:535:TYR:CE2	1:A:556:CYS:HB2	2.48	0.48
1:B:379:GLY:HA3	1:B:527:CYS:SG	2.53	0.48
1:A:138:THR:HG1	2:A:1000:FAD:H1'1	1.76	0.48
1:A:187:VAL:HG12	1:A:189:TYR:CE1	2.47	0.48
1:A:648:HIS:HD2	1:A:652:ARG:HD2	1.79	0.48
1:C:331:GLN:OE1	1:C:593:TYR:HB3	2.12	0.48
1:C:361:ARG:HD3	1:C:366:ASP:OD2	2.14	0.48
1:C:25:TRP:CD1	1:C:607:PHE:HA	2.49	0.48
1:B:64:ASN:OD1	1:B:67:ARG:NH1	2.47	0.48
1:C:22:LYS:HA	1:C:606:ALA:O	2.12	0.48
1:A:382:SER:CB	1:A:431:GLN:OE1	2.62	0.47
1:B:493:ARG:HH11	1:B:574:THR:CB	2.27	0.47
1:B:175:TRP:N	1:B:176:PRO:CD	2.77	0.47
1:B:133:GLY:HA2	1:B:185:HIS:O	2.13	0.47
1:C:150:GLU:HB2	1:C:171:SER:HB3	1.96	0.47
1:A:106:PHE:CD1	1:A:133:GLY:HA3	2.48	0.47
1:A:420:ALA:HA	1:A:423:TYR:CE2	2.49	0.47
1:B:647:PHE:C	1:B:647:PHE:CD2	2.88	0.47
1:A:249:ILE:HG13	1:A:253:GLN:NE2	2.30	0.47
1:B:14:ALA:HB2	1:B:602:SER:OG	2.14	0.47
1:B:542:ASN:CG	1:B:543:ILE:N	2.68	0.47
1:B:169:LEU:O	1:B:172:SER:HB2	2.15	0.47
1:B:297:SER:OG	1:B:609:TYR:OH	2.17	0.47
1:B:447:THR:HG22	1:B:447:THR:O	2.15	0.47
1:B:426:ASP:HB3	1:B:429:VAL:HB	1.97	0.47
1:A:335:PHE:CD1	1:A:596:LEU:HD23	2.49	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:NZ	1:A:127:TYR:OH	2.35	0.46
2:A:1000:FAD:H2A	1:B:329:THR:OG1	2.16	0.46
1:A:178:GLY:O	1:A:183:SER:HB2	2.15	0.46
1:C:372:GLU:HG2	1:C:372:GLU:O	2.15	0.46
1:A:568:GLN:NE2	1:A:582:GLY:CA	2.78	0.46
1:A:179:LEU:HD23	1:A:240:GLY:HA3	1.98	0.46
1:B:111:LYS:O	1:B:119:GLN:NE2	2.48	0.46
1:B:474:ALA:C	1:B:588:GLN:HE21	2.19	0.46
1:A:284:VAL:O	1:A:287:SER:HB3	2.16	0.46
1:B:573:GLY:O	1:B:575:GLY:N	2.49	0.45
1:B:469:SER:HB2	1:B:576:TYR:CE2	2.51	0.45
1:C:10:GLU:OE2	1:C:323:GLN:NE2	2.49	0.45
1:A:114:GLY:O	1:A:257:ARG:HG3	2.16	0.45
1:C:328:LYS:HA	1:C:328:LYS:HD2	1.59	0.45
1:B:9:ASP:N	1:B:9:ASP:OD1	2.44	0.45
1:C:567:HIS:HB3	1:C:570:ASP:OD2	2.16	0.45
1:C:358:VAL:O	1:C:361:ARG:HG2	2.17	0.45
1:B:461:ILE:O	1:B:462:GLU:C	2.54	0.45
1:A:294:LEU:HD21	1:A:613:TYR:OH	2.16	0.45
1:B:313:PHE:O	1:B:321:GLU:HB3	2.17	0.45
1:C:52:GLY:C	1:C:54:THR:H	2.20	0.45
1:A:88:MET:CE	1:A:88:MET:HA	2.47	0.45
1:C:21:MET:HG3	1:C:606:ALA:HB1	1.98	0.45
1:B:339:ALA:HA	1:B:555:LEU:HD22	1.99	0.45
1:C:101:LEU:HD22	2:C:3000:FAD:O4	2.17	0.45
1:B:280:THR:O	1:B:284:VAL:HG23	2.17	0.44
1:A:521:GLU:CD	1:B:565:HIS:HE2	2.21	0.44
1:C:20:GLU:HB2	1:C:548:VAL:HG21	2.00	0.44
1:C:643:ILE:HG12	1:C:644:ALA:N	2.31	0.44
1:C:577:ILE:HG23	1:C:578:THR:O	2.16	0.44
1:C:176:PRO:HA	2:C:3000:FAD:C4	2.47	0.44
1:C:105:MET:HB3	1:C:135:TYR:CB	2.44	0.44
1:A:502:LEU:HD12	1:A:515:LEU:HD13	1.98	0.44
1:A:289:VAL:HG13	1:A:384:THR:HG21	1.99	0.44
1:C:301:CYS:O	1:C:305:ARG:HG3	2.18	0.44
1:A:314:GLY:O	1:A:315:SER:C	2.55	0.44
1:B:597:ARG:HB3	1:B:598:PRO:HD3	1.99	0.44
1:C:631:GLU:HG2	1:C:631:GLU:O	2.17	0.44
1:C:285:ARG:HA	1:C:288:ILE:HD12	1.99	0.44
1:B:75:ARG:HD2	1:B:75:ARG:HA	1.77	0.44
1:A:205:ILE:HB	1:A:253:GLN:HG2	1.99	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ILE:C	1:A:444:GLN:N	2.71	0.44
1:B:447:THR:O	1:B:447:THR:CG2	2.65	0.44
1:B:34:LEU:CD2	1:B:88:MET:HG2	2.45	0.44
1:A:311:ARG:HA	1:A:322:THR:O	2.17	0.44
1:A:479:LYS:HA	1:A:480:PRO:HD2	1.85	0.44
1:C:462:GLU:HG3	1:C:463:HIS:H	1.81	0.44
1:B:344:PHE:HA	1:B:347:VAL:HG12	2.00	0.44
1:A:312:GLN:O	1:A:313:PHE:HB2	2.18	0.44
1:B:74:LYS:O	1:B:78:GLU:HG3	2.18	0.44
1:C:425:GLY:HA3	1:C:430:LEU:HD21	1.99	0.43
1:A:27:GLY:O	1:A:28:SER:HB3	2.17	0.43
1:B:4:VAL:CG2	1:B:6:TYR:CZ	3.01	0.43
1:C:258:VAL:CG2	1:C:259:SER:N	2.81	0.43
1:A:559:TYR:O	1:A:563:ILE:HG12	2.18	0.43
1:C:447:THR:OG1	1:C:449:LYS:HB3	2.18	0.43
1:C:419:PRO:HB3	2:C:3000:FAD:HM71	2.00	0.43
1:A:186:ALA:HB2	1:A:208:LEU:HD11	1.99	0.43
1:A:381:LYS:O	1:A:385:THR:HG23	2.18	0.43
1:C:101:LEU:HD12	1:C:101:LEU:H	1.82	0.43
1:C:23:ILE:O	1:C:24:VAL:C	2.57	0.43
1:A:355:TYR:CD2	1:A:355:TYR:C	2.91	0.43
1:C:281:MET:O	1:C:283:TYR:N	2.52	0.43
1:B:335:PHE:CD2	1:B:335:PHE:N	2.85	0.43
1:A:104:GLY:O	1:A:105:MET:HE3	2.19	0.43
1:A:294:LEU:HD12	1:A:609:TYR:OH	2.19	0.43
1:C:5:ASP:OD1	1:C:11:ARG:NH1	2.52	0.43
1:B:189:TYR:HA	1:B:202:ASN:O	2.19	0.42
1:C:509:GLU:OE1	1:C:509:GLU:HA	2.19	0.42
1:B:113:GLN:O	1:B:255:LEU:HB3	2.19	0.42
1:B:138:THR:HG1	2:B:2000:FAD:H1'1	1.84	0.42
1:B:35:THR:O	1:B:39:SER:HB2	2.18	0.42
1:B:591:ALA:O	1:B:595:GLN:HG2	2.19	0.42
1:A:249:ILE:HG13	1:A:253:GLN:HE21	1.84	0.42
1:C:251:ARG:C	1:C:253:GLN:H	2.23	0.42
1:C:101:LEU:HD13	1:C:177:GLY:HA3	2.02	0.42
1:C:426:ASP:OD2	2:C:3000:FAD:H2B	2.19	0.42
1:B:501:ASN:HD22	1:B:501:ASN:HA	1.50	0.42
1:A:242:LEU:HD21	1:A:244:PHE:HZ	1.84	0.42
1:C:156:ASP:HA	1:C:157:PRO:HD3	1.82	0.42
1:C:262:THR:HG22	1:C:263:LYS:H	1.84	0.42
1:C:190:ALA:HB3	1:C:204:PHE:CE1	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:THR:OG1	1:B:88:MET:HE3	2.19	0.42
1:A:283:TYR:O	1:A:286:GLN:HB3	2.20	0.42
1:A:646:GLY:HA3	1:B:66:LEU:HD12	2.01	0.42
1:A:42:VAL:HG11	1:A:92:TYR:C	2.40	0.42
1:C:95:GLU:HA	1:C:95:GLU:OE1	2.19	0.42
1:A:597:ARG:C	1:A:597:ARG:HD2	2.40	0.42
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.60	0.42
1:B:155:PHE:HB2	1:B:162:PHE:CE2	2.55	0.42
1:C:195:ASP:OD1	1:C:195:ASP:N	2.52	0.42
1:A:222:VAL:HA	1:A:241:VAL:O	2.18	0.41
1:B:379:GLY:CA	1:B:434:VAL:HG21	2.50	0.41
1:A:83:GLN:HA	1:A:83:GLN:HE21	1.85	0.41
1:B:383:LEU:HD12	1:B:383:LEU:HA	1.80	0.41
1:C:176:PRO:HB2	1:C:179:LEU:HB2	2.02	0.41
1:A:381:LYS:HD2	1:A:430:LEU:CD1	2.50	0.41
1:A:184:THR:O	1:A:208:LEU:N	2.43	0.41
1:A:532:VAL:O	1:A:536:ILE:HD12	2.20	0.41
1:C:435:ALA:CB	1:C:519:LEU:HB3	2.48	0.41
1:B:65:THR:OG1	1:B:236:SER:HB2	2.21	0.41
1:C:595:GLN:O	1:C:598:PRO:HD2	2.21	0.41
1:A:273:PRO:C	1:A:275:GLN:N	2.73	0.41
1:A:647:PHE:CE1	1:B:214:HIS:CE1	3.09	0.41
1:A:357:ASP:O	1:A:361:ARG:HG3	2.20	0.41
1:A:450:LYS:HA	1:A:451:PRO:HD3	1.93	0.41
1:A:489:ALA:O	1:A:493:ARG:HD2	2.21	0.41
1:A:491:SER:O	1:A:492:ALA:C	2.58	0.41
1:C:312:GLN:HA	1:C:321:GLU:OE2	2.20	0.41
1:B:576:TYR:HD2	1:B:577:ILE:HG23	1.86	0.41
1:A:83:GLN:CA	1:A:83:GLN:HE21	2.34	0.41
1:B:552:LEU:HD23	1:B:552:LEU:HA	1.94	0.41
1:A:571:PHE:HB2	1:A:577:ILE:HD11	2.02	0.40
1:B:380:LEU:HD23	1:B:380:LEU:HA	1.85	0.40
1:A:232:GLY:O	1:A:233:ALA:C	2.59	0.40
1:C:383:LEU:HD22	1:C:527:CYS:HB2	2.02	0.40
1:B:652:ARG:O	1:B:653:PRO:C	2.59	0.40
1:B:374:HIS:CD2	1:B:374:HIS:C	2.94	0.40
1:A:146:VAL:O	1:A:149:LEU:HG	2.21	0.40
1:B:144:SER:HB2	2:B:2000:FAD:O1A	2.22	0.40
1:A:179:LEU:HD11	1:A:242:LEU:HD22	2.02	0.40
1:A:603:LEU:HD23	1:A:603:LEU:HA	1.84	0.40
1:C:335:PHE:N	1:C:336:PRO:CD	2.84	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:579:SER:O	1:B:580:LYS:C	2.58	0.40
1:B:539:LEU:O	1:B:549:LYS:HE3	2.21	0.40
1:B:436:ARG:HH22	1:B:509:GLU:CD	2.24	0.40
1:C:643:ILE:HG12	1:C:645:ASP:H	1.87	0.40
1:A:245:ASP:OD1	1:A:245:ASP:C	2.60	0.40
1:C:305:ARG:NH1	1:C:619:GLY:O	2.54	0.40
1:A:393:GLU:OE1	1:A:393:GLU:HA	2.21	0.40
1:A:321:GLU:OE1	1:B:142:HIS:NE2	2.38	0.40
1:C:62:PHE:O	1:C:66:LEU:HG	2.21	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	652/683 (96%)	591 (91%)	47 (7%)	14 (2%)	9	21
1	B	654/683 (96%)	617 (94%)	27 (4%)	10 (2%)	13	30
1	C	651/683 (95%)	560 (86%)	71 (11%)	20 (3%)	5	11
All	All	1957/2049 (96%)	1768 (90%)	145 (7%)	44 (2%)	8	20

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	THR
1	A	175	TRP
1	A	317	ASN
1	A	318	GLY
1	B	175	TRP
1	B	271	ASP
1	B	574	THR
1	C	23	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	175	TRP
1	C	266	LYS
1	C	273	PRO
1	C	282	VAL
1	C	546	LYS
1	A	12	LYS
1	A	53	ARG
1	A	273	PRO
1	A	442	ILE
1	A	443	SER
1	B	318	GLY
1	B	573	GLY
1	C	24	VAL
1	C	51	GLU
1	C	159	THR
1	C	214	HIS
1	C	468	ARG
1	B	317	ASN
1	B	542	ASN
1	C	317	ASN
1	C	364	ALA
1	C	424	GLU
1	A	28	SER
1	A	264	GLU
1	A	274	ARG
1	A	364	ALA
1	A	424	GLU
1	C	608	ASN
1	B	543	ILE
1	B	597	ARG
1	B	657	GLN
1	C	176	PRO
1	C	6	TYR
1	C	143	GLY
1	C	425	GLY
1	C	250	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/571 (89%)	470 (92%)	39 (8%)	16	34
1	B	516/571 (90%)	482 (93%)	34 (7%)	21	43
1	C	434/571 (76%)	397 (92%)	37 (8%)	13	28
All	All	1459/1713 (85%)	1349 (92%)	110 (8%)	17	36

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	VAL
1	A	29	ARG
1	A	40	LYS
1	A	67	ARG
1	A	83	GLN
1	A	88	MET
1	A	89	LEU
1	A	101	LEU
1	A	121	LYS
1	A	149	LEU
1	A	159	THR
1	A	183	SER
1	A	194	THR
1	A	222	VAL
1	A	229	PHE
1	A	234	TYR
1	A	249	ILE
1	A	256	MET
1	A	257	ARG
1	A	260	GLN
1	A	262	THR
1	A	264	GLU
1	A	312	GLN
1	A	359	THR
1	A	360	GLN
1	A	465	MET
1	A	468	ARG
1	A	501	ASN
1	A	502	LEU
1	A	512	PHE
1	A	535	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	536	ILE
1	A	550	GLN
1	A	560	SER
1	A	579	SER
1	A	597	ARG
1	A	601	VAL
1	A	645	ASP
1	A	649	GLU
1	B	4	VAL
1	B	9	ASP
1	B	39	SER
1	B	88	MET
1	B	101	LEU
1	B	147	GLN
1	B	159	THR
1	B	172	SER
1	B	183	SER
1	B	222	VAL
1	B	228	LYS
1	B	249	ILE
1	B	257	ARG
1	B	260	GLN
1	B	315	SER
1	B	333	ARG
1	B	338	LEU
1	B	360	GLN
1	B	418	VAL
1	B	423	TYR
1	B	456	SER
1	B	468	ARG
1	B	501	ASN
1	B	509	GLU
1	B	518	ASP
1	B	535	TYR
1	B	542	ASN
1	B	550	GLN
1	B	566	LYS
1	B	568	GLN
1	B	574	THR
1	B	595	GLN
1	B	649	GLU
1	B	654	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	9	ASP
1	C	18	VAL
1	C	45	ASP
1	C	169	LEU
1	C	195	ASP
1	C	207	GLN
1	C	211	LEU
1	C	213	ASP
1	C	222	VAL
1	C	225	ILE
1	C	241	VAL
1	C	253	GLN
1	C	258	VAL
1	C	259	SER
1	C	264	GLU
1	C	317	ASN
1	C	328	LYS
1	C	376	CYS
1	C	390	ASP
1	C	402	HIS
1	C	418	VAL
1	C	426	ASP
1	C	429	VAL
1	C	444	GLN
1	C	462	GLU
1	C	466	GLN
1	C	481	SER
1	C	508	GLN
1	C	535	TYR
1	C	540	GLN
1	C	542	ASN
1	C	550	GLN
1	C	577	ILE
1	C	631	GLU
1	C	642	ASP
1	C	643	ILE
1	C	649	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	202	ASN
1	A	253	GLN
1	A	444	GLN
1	A	473	GLN
1	A	501	ASN
1	A	567	HIS
1	A	568	GLN
1	A	588	GLN
1	A	648	HIS
1	B	130	GLN
1	B	202	ASN
1	B	260	GLN
1	B	374	HIS
1	B	444	GLN
1	B	501	ASN
1	B	542	ASN
1	B	588	GLN
1	C	202	ASN
1	C	360	GLN
1	C	374	HIS
1	C	466	GLN
1	C	501	ASN
1	C	541	GLN
1	C	550	GLN
1	C	588	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

3 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	1000	-	48,58,58	1.52	8 (16%)	54,89,89	2.72	14 (25%)
2	FAD	B	2000	-	48,58,58	1.46	7 (14%)	54,89,89	2.26	12 (22%)
2	FAD	C	3000	-	48,58,58	1.37	6 (12%)	54,89,89	2.08	8 (14%)

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	1000	-	-	0/30/50/50	0/6/6/6
2	FAD	B	2000	-	-	0/30/50/50	0/6/6/6
2	FAD	C	3000	-	-	0/30/50/50	0/6/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	FAD	C6-C5X	-3.26	1.36	1.41
2	B	2000	FAD	C10-N10	-2.98	1.35	1.39
2	B	2000	FAD	C6-C5X	-2.97	1.37	1.41
2	A	1000	FAD	O2'-C2'	-2.29	1.38	1.43
2	B	2000	FAD	O3B-C3B	-2.10	1.37	1.43
2	C	3000	FAD	O4B-C1B	2.02	1.43	1.41
2	C	3000	FAD	C5X-N5	2.10	1.38	1.35
2	A	1000	FAD	C4-N3	2.14	1.37	1.33
2	B	2000	FAD	C1'-N10	2.21	1.50	1.48
2	A	1000	FAD	C2A-N1A	2.22	1.38	1.33
2	B	2000	FAD	C4-N3	3.05	1.38	1.33
2	A	1000	FAD	C1'-N10	3.07	1.51	1.48
2	A	1000	FAD	C2A-N3A	3.15	1.37	1.32
2	C	3000	FAD	C2A-N1A	3.23	1.40	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	FAD	C9A-N10	3.31	1.43	1.38
2	B	2000	FAD	C2A-N3A	3.35	1.38	1.32
2	C	3000	FAD	C4-N3	3.45	1.39	1.33
2	C	3000	FAD	C4X-N5	3.89	1.39	1.33
2	A	1000	FAD	C4X-N5	4.14	1.39	1.33
2	B	2000	FAD	C4X-N5	4.21	1.39	1.33
2	C	3000	FAD	C2A-N3A	4.87	1.40	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	FAD	N3A-C2A-N1A	-13.20	118.79	128.89
2	B	2000	FAD	N3A-C2A-N1A	-11.72	119.92	128.89
2	C	3000	FAD	N3A-C2A-N1A	-10.32	120.99	128.89
2	C	3000	FAD	P-O3P-PA	-5.17	118.22	132.73
2	A	1000	FAD	C2B-C1B-N9A	-4.59	107.28	114.29
2	B	2000	FAD	P-O3P-PA	-4.28	120.72	132.73
2	A	1000	FAD	O2'-C2'-C3'	-3.80	99.46	109.02
2	A	1000	FAD	P-O3P-PA	-3.58	122.66	132.73
2	B	2000	FAD	C2B-C1B-N9A	-2.66	110.23	114.29
2	A	1000	FAD	O3P-PA-O5B	-2.65	95.91	102.94
2	C	3000	FAD	C4X-C4-N3	-2.61	120.03	123.59
2	B	2000	FAD	C7M-C7-C6	-2.32	113.97	120.28
2	B	2000	FAD	C1B-N9A-C4A	-2.28	123.50	126.94
2	B	2000	FAD	O2'-C2'-C3'	-2.26	103.34	109.02
2	A	1000	FAD	O5B-C5B-C4B	-2.19	101.04	109.12
2	B	2000	FAD	C4X-C4-N3	-2.19	120.59	123.59
2	A	1000	FAD	C4X-C4-N3	-2.18	120.61	123.59
2	A	1000	FAD	C9A-C5X-N5	-2.13	119.21	122.36
2	A	1000	FAD	O3B-C3B-C2B	-2.04	105.19	111.83
2	B	2000	FAD	C4X-N5-C5X	2.14	119.22	116.76
2	C	3000	FAD	O4B-C1B-N9A	2.17	112.63	108.10
2	C	3000	FAD	C1'-N10-C9A	2.36	121.52	118.86
2	C	3000	FAD	C4X-N5-C5X	2.38	119.50	116.76
2	B	2000	FAD	C4-C4X-N5	2.43	121.67	118.72
2	B	2000	FAD	C1'-C2'-C3'	3.02	118.46	109.82
2	C	3000	FAD	C5X-C9A-N10	3.04	119.93	117.62
2	B	2000	FAD	C1'-N10-C9A	3.21	122.47	118.86
2	A	1000	FAD	C1'-C2'-C3'	3.39	119.52	109.82
2	A	1000	FAD	C6-C5X-C9A	3.46	123.54	118.98
2	A	1000	FAD	C1'-N10-C9A	3.58	122.88	118.86
2	B	2000	FAD	C4-N3-C2	4.37	119.03	115.25

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	FAD	C4X-N5-C5X	5.04	122.57	116.76
2	C	3000	FAD	C4-N3-C2	5.62	120.10	115.25
2	A	1000	FAD	C4-N3-C2	6.67	121.01	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	FAD	7	0
2	B	2000	FAD	6	0
2	C	3000	FAD	5	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	654/683 (95%)	0.16	25 (3%) 44 46	49, 67, 78, 91	0
1	B	656/683 (96%)	0.19	19 (2%) 55 57	53, 67, 78, 85	0
1	C	653/683 (95%)	0.98	124 (18%) 2 1	55, 70, 89, 112	0
All	All	1963/2049 (95%)	0.44	168 (8%) 13 11	49, 68, 81, 112	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	GLY	8.3
1	C	646	GLY	6.8
1	C	273	PRO	6.4
1	C	159	THR	6.3
1	C	644	ALA	6.1
1	C	194	THR	6.0
1	C	126	ALA	5.9
1	C	470	ASP	5.9
1	C	245	ASP	5.8
1	C	645	ASP	5.8
1	C	42	VAL	5.6
1	C	650	TYR	5.4
1	C	112	GLY	5.3
1	C	617	ILE	5.3
1	C	318	GLY	5.2
1	C	158	GLN	5.2
1	C	127	TYR	5.0
1	C	471	VAL	5.0
1	C	62	PHE	5.0
1	C	653	PRO	4.9
1	C	192	LEU	4.9
1	C	619	GLY	4.7
1	C	48	PHE	4.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	157	PRO	4.6
1	C	261	VAL	4.6
1	C	156	ASP	4.6
1	C	651	ILE	4.6
1	C	363	ALA	4.5
1	C	15	GLY	4.5
1	C	655	LEU	4.3
1	C	92	TYR	4.2
1	C	268	VAL	4.1
1	C	272	ILE	4.0
1	A	271	ASP	4.0
1	C	97	ALA	4.0
1	C	477	TRP	4.0
1	A	270	SER	3.9
1	C	648	HIS	3.9
1	C	195	ASP	3.9
1	C	57	PRO	3.9
1	C	214	HIS	3.9
1	C	193	ILE	3.8
1	C	243	SER	3.6
1	C	654	LEU	3.6
1	C	624	ASN	3.6
1	C	55	MET	3.6
1	C	642	ASP	3.6
1	C	98	PHE	3.6
1	C	649	GLU	3.6
1	A	272	ILE	3.5
1	C	141	GLY	3.5
1	C	256	MET	3.5
1	C	616	SER	3.4
1	A	366	ASP	3.4
1	C	154	THR	3.4
1	B	470	ASP	3.4
1	C	14	ALA	3.4
1	C	267	TYR	3.4
1	B	265	GLY	3.4
1	C	355	TYR	3.3
1	C	262	THR	3.3
1	C	21	MET	3.3
1	C	44	SER	3.2
1	C	4	VAL	3.2
1	C	61	LEU	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	254	MET	3.2
1	C	81	LEU	3.2
1	C	117	LYS	3.1
1	A	273	PRO	3.1
1	C	339	ALA	3.1
1	C	263	LYS	3.1
1	C	282	VAL	3.1
1	C	213	ASP	3.0
1	C	368	SER	3.0
1	B	658	GLN	3.0
1	C	252	ASP	3.0
1	C	35	THR	3.0
1	C	369	THR	2.9
1	A	187	VAL	2.9
1	C	174	TRP	2.9
1	A	604	VAL	2.9
1	C	264	GLU	2.9
1	C	643	ILE	2.9
1	C	103	TRP	2.9
1	B	273	PRO	2.9
1	C	133	GLY	2.8
1	A	367	PHE	2.8
1	C	271	ASP	2.8
1	C	47	GLY	2.8
1	C	43	ALA	2.8
1	B	301	CYS	2.8
1	C	240	GLY	2.8
1	C	54	THR	2.8
1	A	195	ASP	2.8
1	A	365	ASN	2.7
1	A	276	LEU	2.7
1	C	334	LEU	2.7
1	C	472	LYS	2.7
1	B	267	TYR	2.7
1	A	318	GLY	2.7
1	C	116	ASP	2.7
1	C	269	GLN	2.6
1	A	315	SER	2.6
1	C	641	SER	2.6
1	C	359	THR	2.6
1	C	242	LEU	2.6
1	C	58	ARG	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	258	VAL	2.6
1	B	367	PHE	2.6
1	C	69	ALA	2.6
1	C	316	GLN	2.6
1	C	358	VAL	2.5
1	C	260	GLN	2.5
1	C	216	PRO	2.5
1	C	652	ARG	2.5
1	C	628	LYS	2.5
1	A	301	CYS	2.5
1	C	647	PHE	2.5
1	A	203	GLY	2.5
1	C	270	SER	2.5
1	A	585	ALA	2.4
1	B	471	VAL	2.4
1	B	585	ALA	2.4
1	C	239	ASN	2.4
1	B	606	ALA	2.4
1	C	169	LEU	2.4
1	B	3	GLY	2.4
1	C	637	PRO	2.4
1	A	186	ALA	2.4
1	B	187	VAL	2.4
1	C	640	LYS	2.4
1	C	283	TYR	2.3
1	C	285	ARG	2.3
1	B	366	ASP	2.3
1	C	135	TYR	2.3
1	A	297	SER	2.3
1	C	473	GLN	2.3
1	A	446	GLY	2.3
1	C	425	GLY	2.3
1	C	142	HIS	2.3
1	A	651	ILE	2.3
1	B	203	GLY	2.3
1	C	274	ARG	2.2
1	C	305	ARG	2.2
1	C	52	GLY	2.2
1	A	4	VAL	2.2
1	C	319	GLY	2.2
1	A	258	VAL	2.2
1	C	535	TYR	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	657	GLN	2.2
1	C	136	ALA	2.2
1	B	195	ASP	2.2
1	A	374	HIS	2.2
1	B	303	ALA	2.2
1	C	259	SER	2.1
1	C	9	ASP	2.1
1	C	88	MET	2.1
1	A	478	LEU	2.1
1	B	604	VAL	2.1
1	C	225	ILE	2.1
1	A	176	PRO	2.1
1	C	233	ALA	2.1
1	C	633	ALA	2.1
1	C	317	ASN	2.0
1	C	428	VAL	2.0
1	C	370	LEU	2.0
1	C	234	TYR	2.0
1	B	300	VAL	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	C	3000	53/53	0.79	0.35	1.65	87,99,107,107	0
2	FAD	A	1000	53/53	0.93	0.21	0.32	43,55,59,63	0
2	FAD	B	2000	53/53	0.94	0.18	-0.52	45,49,55,57	0



## 6.5 Other polymers

There are no such residues in this entry.