



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:13 pm GMT

PDB ID : 3WE0  
Title : L-Amino acid oxidase/monooxygenase from Pseudomonas sp. AIU 813  
Authors : Im, D.H.; Matsui, D.; Fukuta, Y.; Fushinobu, S.; Isobe, K.; Asano, Y.  
Deposited on : 2013-06-26  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

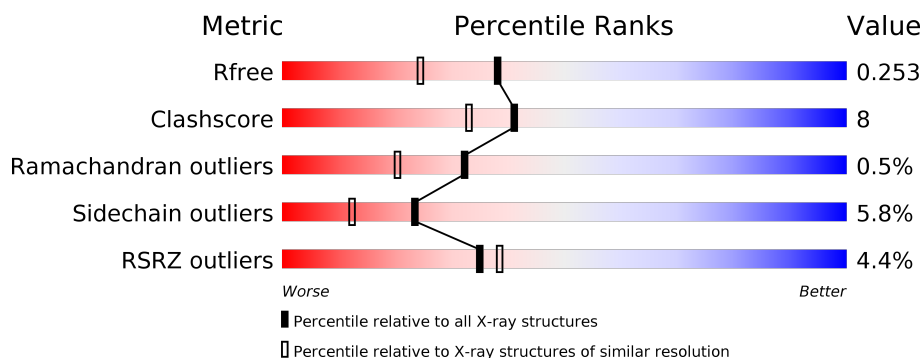
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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	580	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>• 7%</div> </div> </div>
1	B	580	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>•• 7%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8986 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 L-amino acid oxidase/monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	0	0
			4238	2706	732	779	21			
1	B	540	Total	C	N	O	S	0	0	0
			4238	2706	732	779	21			

- 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		

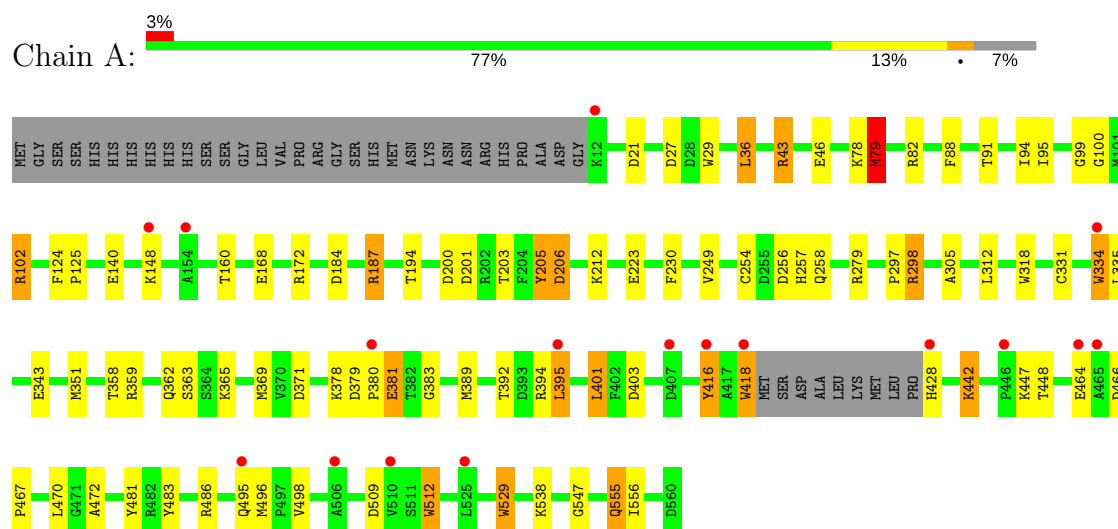
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	218	Total 218	O 218	0	0
3	B	186	Total 186	O 186	0	0

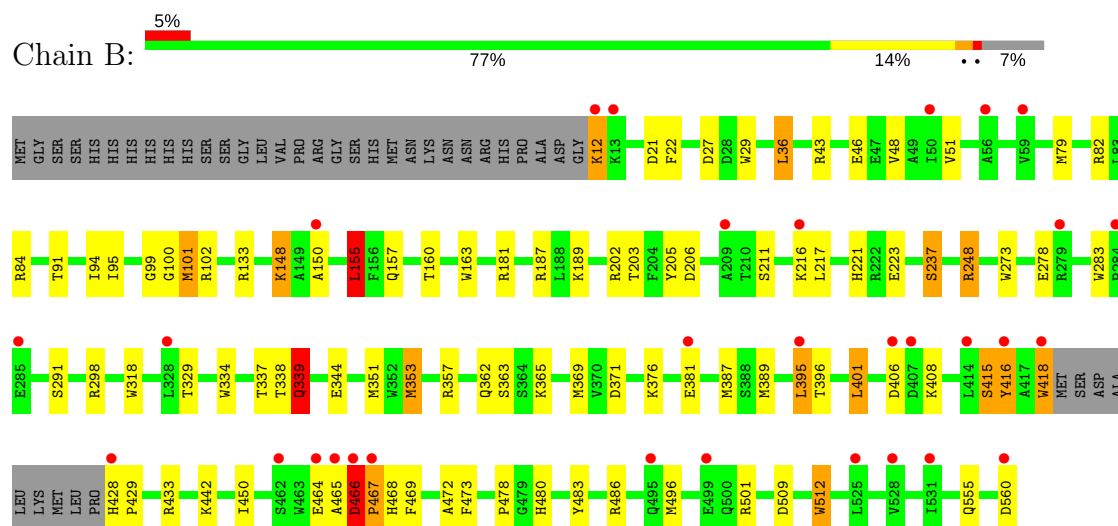
### 3 Residue-property plots [i](#)

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

- Molecule 1: L-amino acid oxidase/monooxygenase



- Molecule 1: L-amino acid oxidase/monooxygenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.93Å 141.35Å 75.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.38 – 1.90 30.38 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.38-1.90) 97.1 (30.38-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.21 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.209 , 0.254 0.209 , 0.253	Depositor DCC
$R_{free}$ test set	4899 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.13	7/4359 (0.2%)	1.05	18/5925 (0.3%)
1	B	1.12	9/4359 (0.2%)	1.05	16/5925 (0.3%)
All	All	1.12	16/8718 (0.2%)	1.05	34/11850 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	GLU	CD-OE1	9.18	1.35	1.25
1	A	29	TRP	CD2-CE2	7.51	1.50	1.41
1	B	418	TRP	CD2-CE2	6.91	1.49	1.41
1	B	334	TRP	CD2-CE2	6.71	1.49	1.41
1	A	334	TRP	CD2-CE2	6.22	1.48	1.41
1	B	512	TRP	CD2-CE2	5.99	1.48	1.41
1	B	318	TRP	CD2-CE2	5.97	1.48	1.41
1	B	163	TRP	CD2-CE2	5.82	1.48	1.41
1	A	418	TRP	CD2-CE2	5.62	1.48	1.41
1	A	318	TRP	CD2-CE2	5.60	1.48	1.41
1	B	283	TRP	CD2-CE2	5.58	1.48	1.41
1	A	529	TRP	CD2-CE2	5.47	1.48	1.41
1	B	29	TRP	CD2-CE2	5.30	1.47	1.41
1	B	291	SER	CB-OG	-5.20	1.35	1.42
1	A	512	TRP	CD2-CE2	5.12	1.47	1.41
1	B	273	TRP	CD2-CE2	5.08	1.47	1.41

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	ARG	NE-CZ-NH2	8.87	124.73	120.30
1	B	248	ARG	NE-CZ-NH1	-8.79	115.91	120.30
1	A	187	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	A	79	MET	CG-SD-CE	-8.48	86.63	100.20
1	A	298	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	B	401	LEU	CB-CG-CD1	8.10	124.76	111.00
1	A	298	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	A	43	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	B	466	ASP	C-N-CD	-7.56	103.97	120.60
1	B	101	MET	CG-SD-CE	-7.51	88.19	100.20
1	A	43	ARG	NE-CZ-NH2	6.94	123.77	120.30
1	A	27	ASP	CB-CG-OD1	6.53	124.17	118.30
1	B	187	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	B	155	LEU	CB-CG-CD2	-6.42	100.09	111.00
1	B	371	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	206	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	395	LEU	CA-CB-CG	6.23	129.62	115.30
1	A	509	ASP	CB-CA-C	-6.17	98.06	110.40
1	A	496	MET	CG-SD-CE	-6.12	90.40	100.20
1	A	200	ASP	CB-CG-OD1	6.06	123.76	118.30
1	B	468	HIS	N-CA-C	5.97	127.13	111.00
1	A	36	LEU	CB-CG-CD2	5.81	120.88	111.00
1	B	36	LEU	CB-CG-CD2	5.68	120.66	111.00
1	B	298	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	84	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	B	501	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	172	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	A	401	LEU	CB-CG-CD1	5.49	120.32	111.00
1	A	205	TYR	CB-CA-C	-5.46	99.47	110.40
1	A	312	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	A	403	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	371	ASP	CB-CG-OD1	5.09	122.89	118.30
1	B	27	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	496	MET	CG-SD-CE	-5.03	92.14	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	415	SER	Peptide



## 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	4238	0	4091	64	0
1	B	4238	0	4091	77	0
2	A	53	0	31	8	0
2	B	53	0	31	3	0
3	A	218	0	0	2	0
3	B	186	0	0	3	0
All	All	8986	0	8244	137	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 8.

All (137) 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:B:22:PHE:HB2	1:B:555:GLN:OE1	1.25	1.26
1:B:467:PRO:HA	1:B:469:PHE:H	1.22	1.03
1:A:94:ILE:HG21	1:A:369:MET:CE	1.91	1.00
1:B:94:ILE:HG21	1:B:369:MET:HE2	1.45	0.95
1:B:362:GLN:OE1	1:B:464:GLU:HG3	1.67	0.94
1:A:362:GLN:OE1	1:A:464:GLU:HG3	1.68	0.93
1:B:94:ILE:HG21	1:B:369:MET:CE	2.01	0.90
1:A:94:ILE:HG21	1:A:369:MET:HE2	1.54	0.89
1:A:94:ILE:CG2	1:A:369:MET:CE	2.51	0.87
1:B:338:THR:O	1:B:339:GLN:HB2	1.74	0.85
1:A:464:GLU:CD	1:A:464:GLU:H	1.77	0.84
1:A:94:ILE:HG21	1:A:369:MET:HE3	1.60	0.84
1:B:486:ARG:HD2	3:B:747:HOH:O	1.77	0.83
1:A:555:GLN:H	1:A:555:GLN:NE2	1.75	0.82
1:B:555:GLN:NE2	1:B:555:GLN:H	1.75	0.82
1:B:22:PHE:CB	1:B:555:GLN:OE1	2.20	0.81
1:B:467:PRO:HA	1:B:469:PHE:N	1.96	0.80
1:A:378:LYS:HE3	1:A:383:GLY:O	1.84	0.78
1:B:133:ARG:HH21	1:B:376:LYS:HE2	1.50	0.74
1:A:362:GLN:HA	1:A:362:GLN:OE1	1.90	0.72
1:B:133:ARG:HE	1:B:376:LYS:HG2	1.52	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:TRP:CZ2	1:B:555:GLN:HG2	2.24	0.72
1:A:94:ILE:CG2	1:A:369:MET:HE3	2.16	0.71
1:B:202:ARG:NH2	1:B:206:ASP:OD2	2.22	0.71
1:B:338:THR:O	1:B:339:GLN:CB	2.39	0.71
1:B:465:ALA:O	1:B:466:ASP:HB3	1.91	0.71
1:A:486:ARG:HD2	3:A:740:HOH:O	1.90	0.70
1:A:94:ILE:CG2	1:A:369:MET:HE2	2.20	0.70
1:A:256:ASP:OD2	1:A:257:HIS:ND1	2.22	0.69
1:A:362:GLN:OE1	1:A:464:GLU:CG	2.41	0.69
1:B:101:MET:HE2	1:B:416:TYR:HE2	1.57	0.67
1:B:101:MET:CE	1:B:416:TYR:HE2	2.07	0.66
1:B:95:ILE:C	1:B:95:ILE:HD12	2.16	0.66
1:B:91:THR:HG21	1:B:369:MET:CE	2.26	0.65
1:B:101:MET:CE	1:B:416:TYR:CE2	2.80	0.64
1:B:387:MET:HE1	1:B:450:ILE:HD13	1.78	0.64
1:B:21:ASP:HB3	1:B:555:GLN:HG3	1.79	0.64
1:B:43:ARG:NH1	1:B:46:GLU:OE1	2.31	0.64
1:B:465:ALA:O	1:B:466:ASP:CB	2.46	0.63
1:B:203:THR:OG1	1:B:205:TYR:HB2	1.97	0.63
1:B:217:LEU:HB3	1:B:221:HIS:ND1	2.14	0.63
1:B:155:LEU:HD12	1:B:221:HIS:CD2	2.34	0.62
1:B:387:MET:HE3	1:B:450:ILE:HD11	1.80	0.62
1:B:512:TRP:HZ2	1:B:555:GLN:HG2	1.66	0.61
1:B:21:ASP:OD2	1:B:248:ARG:HD3	2.01	0.61
1:A:88:PHE:HB2	1:A:369:MET:HE1	1.83	0.60
1:B:155:LEU:CD1	1:B:221:HIS:HD2	2.14	0.60
1:B:157:GLN:O	1:B:160:THR:HG22	2.03	0.59
1:B:418:TRP:CZ3	1:B:473:PHE:CZ	2.91	0.59
1:A:223:GLU:OE2	1:B:483:TYR:OH	2.20	0.59
1:A:362:GLN:CD	1:A:464:GLU:HG3	2.22	0.59
1:B:101:MET:HE1	1:B:416:TYR:CE2	2.38	0.58
1:A:512:TRP:HZ2	1:A:555:GLN:HG3	1.69	0.58
1:A:555:GLN:CD	1:A:555:GLN:H	2.06	0.57
1:B:91:THR:HG21	1:B:369:MET:HE3	1.85	0.57
1:B:472:ALA:HB1	2:B:601:FAD:HM83	1.85	0.57
1:B:101:MET:HE2	1:B:416:TYR:CE2	2.39	0.57
1:A:100:GLY:HA2	2:A:601:FAD:C5X	2.36	0.56
1:A:395:LEU:H	1:A:395:LEU:CD1	2.19	0.55
1:B:555:GLN:CD	1:B:555:GLN:H	2.09	0.55
1:B:387:MET:CE	1:B:450:ILE:CD1	2.85	0.54
1:B:387:MET:CE	1:B:450:ILE:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:OG1	1:A:205:TYR:HB2	2.07	0.54
1:B:12:LYS:HE3	1:B:181:ARG:CZ	2.37	0.54
1:A:249:VAL:HG13	1:A:254:CYS:HB2	1.91	0.52
1:B:12:LYS:HE3	1:B:181:ARG:NH2	2.25	0.52
1:A:331:CYS:HB2	1:A:335:LEU:HD12	1.91	0.52
1:B:396:THR:O	1:B:416:TYR:O	2.29	0.51
1:B:466:ASP:O	1:B:467:PRO:CB	2.55	0.51
1:B:387:MET:HE1	1:B:450:ILE:CD1	2.40	0.51
1:A:512:TRP:CZ2	1:A:555:GLN:HG3	2.45	0.51
1:A:442:LYS:HE3	1:A:448:THR:O	2.10	0.50
1:A:395:LEU:HD13	1:A:395:LEU:H	1.76	0.50
1:B:94:ILE:CG2	1:B:369:MET:HE3	2.42	0.49
1:A:82:ARG:O	1:A:99:GLY:HA3	2.13	0.49
1:B:100:GLY:HA2	2:B:601:FAD:C5X	2.42	0.49
1:B:362:GLN:CD	1:B:464:GLU:HG3	2.29	0.49
1:B:472:ALA:CB	2:B:601:FAD:HM83	2.43	0.49
1:A:95:ILE:C	1:A:95:ILE:HD12	2.33	0.48
1:B:94:ILE:CG2	1:B:369:MET:CE	2.82	0.48
1:B:155:LEU:CD1	1:B:221:HIS:CD2	2.94	0.48
1:A:206:ASP:OD2	1:B:206:ASP:HB2	2.12	0.48
1:A:100:GLY:HA2	2:A:601:FAD:N5	2.28	0.48
1:A:481:TYR:OH	1:A:555:GLN:HB2	2.14	0.48
1:A:184:ASP:OD2	1:A:187:ARG:NH2	2.44	0.48
1:A:102:ARG:HB2	1:A:258:GLN:HB3	1.95	0.48
1:B:338:THR:OG1	1:B:338:THR:O	2.30	0.47
1:B:466:ASP:O	1:B:467:PRO:HB3	2.14	0.47
1:A:124:PHE:CG	1:A:125:PRO:HD2	2.50	0.47
1:B:148:LYS:HB2	1:B:148:LYS:HE2	1.33	0.47
1:B:82:ARG:O	1:B:99:GLY:HA3	2.15	0.47
1:A:392:THR:HG23	1:A:394:ARG:N	2.30	0.46
1:B:555:GLN:N	1:B:555:GLN:CD	2.68	0.46
1:A:529:TRP:CD2	1:A:547:GLY:HA3	2.51	0.46
3:A:825:HOH:O	1:B:223:GLU:HG2	2.15	0.46
1:B:429:PRO:O	1:B:433:ARG:HG3	2.15	0.46
1:B:365:LYS:HD2	1:B:416:TYR:CE1	2.50	0.45
1:A:472:ALA:HB1	2:A:601:FAD:HM83	1.98	0.45
1:A:94:ILE:CB	1:A:369:MET:HE2	2.46	0.45
1:A:392:THR:HG23	1:A:394:ARG:H	1.82	0.44
1:B:353:MET:CE	1:B:357:ARG:HH11	2.30	0.44
1:A:79:MET:HB2	1:A:79:MET:HE3	1.08	0.44
1:A:91:THR:HG21	1:A:369:MET:CE	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:TYR:OH	1:B:223:GLU:OE2	2.21	0.44
1:A:140:GLU:OE2	1:B:353:MET:HG2	2.18	0.44
1:A:555:GLN:CD	1:A:555:GLN:N	2.68	0.43
1:B:509:ASP:HB2	3:B:862:HOH:O	2.18	0.43
1:A:334:TRP:HB3	1:A:470:LEU:HD13	2.01	0.43
1:B:237:SER:HB3	3:B:784:HOH:O	2.18	0.43
1:B:351:MET:SD	1:B:486:ARG:HG3	2.59	0.43
1:A:305:ALA:HA	1:A:343:GLU:HB2	1.99	0.43
1:B:94:ILE:HB	1:B:369:MET:HE3	2.01	0.43
1:A:472:ALA:HA	2:A:601:FAD:HM83	2.01	0.42
1:A:82:ARG:HD2	2:A:601:FAD:HM81	2.01	0.42
1:B:51:VAL:HB	1:B:329:THR:HA	2.01	0.42
1:A:379:ASP:HA	1:A:380:PRO:HD2	1.83	0.42
1:A:43:ARG:HD2	1:A:46:GLU:OE2	2.19	0.42
1:A:466:ASP:OD1	1:A:467:PRO:HD2	2.20	0.42
1:A:79:MET:HE1	1:A:297:PRO:CG	2.50	0.42
1:A:362:GLN:CD	1:A:464:GLU:CG	2.86	0.42
1:A:94:ILE:HG22	1:A:369:MET:HE3	1.99	0.42
1:B:365:LYS:HA	1:B:415:SER:O	2.19	0.42
1:B:148:LYS:NZ	1:B:150:ALA:H	2.18	0.41
1:A:472:ALA:CA	2:A:601:FAD:HM83	2.50	0.41
1:A:21:ASP:HB3	1:A:555:GLN:OE1	2.20	0.41
1:A:416:TYR:CE1	1:A:418:TRP:CZ2	3.09	0.41
1:A:472:ALA:CB	2:A:601:FAD:HM83	2.51	0.41
1:B:95:ILE:C	1:B:95:ILE:CD1	2.89	0.41
1:A:358:THR:O	1:A:359:ARG:HD3	2.21	0.41
1:A:351:MET:SD	1:A:486:ARG:HG3	2.61	0.41
1:A:529:TRP:CE3	1:A:547:GLY:HA3	2.56	0.41
1:B:94:ILE:CB	1:B:369:MET:HE3	2.51	0.41
1:A:102:ARG:HG2	2:A:601:FAD:O4	2.22	0.40
1:A:160:THR:OG1	1:A:230:PHE:HB2	2.21	0.40
1:B:337:THR:OG1	1:B:338:THR:HG23	2.22	0.40
1:B:365:LYS:HD2	1:B:416:TYR:CZ	2.56	0.40
1:B:203:THR:HG22	1:B:478:PRO:HG3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	536/580 (92%)	522 (97%)	13 (2%)	1 (0%)	51	41
1	B	536/580 (92%)	518 (97%)	14 (3%)	4 (1%)	25	13
All	All	1072/1160 (92%)	1040 (97%)	27 (2%)	5 (0%)	32	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	339	GLN
1	B	467	PRO
1	A	381	GLU
1	B	406	ASP
1	B	466	ASP

### 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	440/474 (93%)	415 (94%)	25 (6%)	24	13
1	B	440/474 (93%)	414 (94%)	26 (6%)	23	12
All	All	880/948 (93%)	829 (94%)	51 (6%)	23	12

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU

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Mol	Chain	Res	Type
1	A	78	LYS
1	A	79	MET
1	A	102	ARG
1	A	148	LYS
1	A	194	THR
1	A	201	ASP
1	A	212	LYS
1	A	279	ARG
1	A	298	ARG
1	A	363	SER
1	A	365	LYS
1	A	381	GLU
1	A	389	MET
1	A	395	LEU
1	A	401	LEU
1	A	416	TYR
1	A	428	HIS
1	A	442	LYS
1	A	447	LYS
1	A	495	GLN
1	A	498	VAL
1	A	538	LYS
1	A	555	GLN
1	A	556	ILE
1	B	12	LYS
1	B	36	LEU
1	B	48	VAL
1	B	79	MET
1	B	102	ARG
1	B	148	LYS
1	B	155	LEU
1	B	189	LYS
1	B	211	SER
1	B	216	LYS
1	B	237	SER
1	B	278	GLU
1	B	339	GLN
1	B	344	GLU
1	B	353	MET
1	B	363	SER
1	B	381	GLU
1	B	389	MET

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Mol	Chain	Res	Type
1	B	395	LEU
1	B	401	LEU
1	B	408	LYS
1	B	416	TYR
1	B	428	HIS
1	B	442	LYS
1	B	480	HIS
1	B	560	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

2 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	601	-	51,58,58	1.86	15 (29%)	54,89,89	3.16	17 (31%)
2	FAD	B	601	-	51,58,58	1.90	10 (19%)	54,89,89	2.92	23 (42%)

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	601	-	-	0/28/50/50	0/6/6/6
2	FAD	B	601	-	-	0/28/50/50	0/6/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C2-N1	-3.58	1.31	1.38
2	A	601	FAD	C4'-C3'	-2.88	1.47	1.53
2	B	601	FAD	C5X-N5	-2.48	1.31	1.35
2	B	601	FAD	C4'-C3'	-2.39	1.48	1.53
2	A	601	FAD	C2-N1	-2.28	1.33	1.38
2	A	601	FAD	C6-C5X	-2.20	1.38	1.41
2	B	601	FAD	C2A-N1A	2.10	1.37	1.33
2	A	601	FAD	C9A-N10	2.13	1.41	1.38
2	A	601	FAD	C7M-C7	2.13	1.55	1.51
2	B	601	FAD	C5A-C4A	2.23	1.45	1.40
2	A	601	FAD	C2A-N1A	2.26	1.38	1.33
2	A	601	FAD	C3B-C4B	2.29	1.59	1.53
2	A	601	FAD	C5'-C4'	2.86	1.56	1.51
2	A	601	FAD	C8-C7	2.89	1.48	1.41
2	A	601	FAD	O4B-C1B	2.90	1.45	1.41
2	B	601	FAD	C2A-N3A	2.92	1.37	1.32
2	A	601	FAD	C1'-N10	3.21	1.51	1.48
2	A	601	FAD	C2B-C1B	3.33	1.58	1.53
2	B	601	FAD	C9A-C5X	3.42	1.49	1.42
2	B	601	FAD	C8-C7	3.77	1.50	1.41
2	A	601	FAD	C4X-C10	3.80	1.47	1.41
2	A	601	FAD	C9A-C5X	3.85	1.50	1.42
2	A	601	FAD	C2A-N3A	4.66	1.39	1.32
2	B	601	FAD	C4X-C10	5.09	1.50	1.41
2	B	601	FAD	C1'-N10	6.78	1.55	1.48

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	N3A-C2A-N1A	-13.22	117.35	128.86
2	B	601	FAD	N3A-C2A-N1A	-10.49	119.72	128.86
2	A	601	FAD	C4X-C10-N10	-5.58	116.64	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4-C4X-C10	-5.44	115.56	119.96
2	B	601	FAD	C4X-C10-N10	-4.35	117.50	120.52
2	B	601	FAD	C4-C4X-C10	-4.21	116.56	119.96
2	A	601	FAD	C4X-C4-N3	-3.89	117.94	123.48
2	B	601	FAD	C1'-C2'-C3'	-3.57	99.61	109.82
2	B	601	FAD	C4X-C4-N3	-3.45	118.57	123.48
2	A	601	FAD	O3'-C3'-C4'	-3.35	100.52	108.82
2	A	601	FAD	C9A-C5X-N5	-3.33	117.28	122.24
2	B	601	FAD	C9A-C5X-N5	-3.17	117.52	122.24
2	B	601	FAD	C4A-C5A-N7A	-3.13	106.39	109.41
2	B	601	FAD	C1'-N10-C10	-3.00	115.43	118.50
2	A	601	FAD	C4A-C5A-N7A	-2.99	106.52	109.41
2	B	601	FAD	O2'-C2'-C1'	-2.83	103.24	109.79
2	B	601	FAD	C4B-O4B-C1B	-2.58	107.03	109.77
2	A	601	FAD	C4B-O4B-C1B	-2.46	107.15	109.77
2	B	601	FAD	O4'-C4'-C5'	-2.24	105.00	110.00
2	A	601	FAD	C1B-N9A-C4A	-2.21	122.81	126.64
2	A	601	FAD	O2'-C2'-C1'	-2.21	104.68	109.79
2	B	601	FAD	C8M-C8-C7	-2.17	116.16	120.72
2	B	601	FAD	O2A-PA-O1A	2.10	123.14	112.28
2	B	601	FAD	C7M-C7-C6	2.11	125.62	120.34
2	A	601	FAD	C6-C5X-N5	2.12	121.45	118.97
2	B	601	FAD	C9-C8-C7	2.45	124.33	119.95
2	A	601	FAD	O2P-P-O1P	2.66	126.06	112.28
2	A	601	FAD	O2A-PA-O1A	2.69	126.21	112.28
2	A	601	FAD	C4-C4X-N5	2.70	121.64	118.68
2	B	601	FAD	C6-C5X-C9A	2.73	122.54	119.00
2	B	601	FAD	O2P-P-O1P	2.81	126.80	112.28
2	B	601	FAD	C4-C4X-N5	2.86	121.82	118.68
2	B	601	FAD	C5X-C9A-N10	3.07	119.94	117.66
2	B	601	FAD	C2A-N1A-C6A	4.01	125.79	118.77
2	A	601	FAD	C4X-N5-C5X	4.39	121.39	116.76
2	B	601	FAD	C4X-N5-C5X	5.08	122.12	116.76
2	A	601	FAD	C2A-N1A-C6A	5.28	128.01	118.77
2	B	601	FAD	C1'-N10-C9A	6.83	124.61	118.35
2	B	601	FAD	C4-N3-C2	8.18	122.31	115.16
2	A	601	FAD	C4-N3-C2	11.03	124.80	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	8	0
2	B	601	FAD	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	540/580 (93%)	0.11	17 (3%)	49 53	15, 26, 47, 77	0
1	B	540/580 (93%)	0.21	31 (5%)	24 28	16, 26, 47, 72	0
All	All	1080/1160 (93%)	0.16	48 (4%)	35 38	15, 26, 47, 77	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	LYS	6.1
1	A	428	HIS	5.1
1	B	465	ALA	5.1
1	B	428	HIS	4.7
1	B	381	GLU	4.2
1	B	279	ARG	4.2
1	A	465	ALA	4.2
1	B	12	LYS	3.8
1	B	464	GLU	3.7
1	B	407	ASP	3.6
1	A	380	PRO	3.4
1	B	285	GLU	3.3
1	B	467	PRO	3.1
1	B	50	ILE	3.1
1	A	407	ASP	3.1
1	B	495	GLN	3.0
1	B	418	TRP	2.9
1	B	328	LEU	2.8
1	B	395	LEU	2.8
1	B	209	ALA	2.6
1	B	284	PRO	2.6
1	B	216	LYS	2.6
1	A	464	GLU	2.6
1	B	56	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	560	ASP	2.5
1	A	154	ALA	2.5
1	A	416	TYR	2.5
1	B	406	ASP	2.4
1	A	148	LYS	2.4
1	A	525	LEU	2.4
1	B	528	VAL	2.4
1	B	525	LEU	2.3
1	B	462	SER	2.3
1	B	416	TYR	2.2
1	B	59	VAL	2.2
1	A	334	TRP	2.2
1	A	506	ALA	2.2
1	B	150	ALA	2.2
1	B	499	GLU	2.2
1	A	446	PRO	2.2
1	A	495	GLN	2.2
1	A	510	VAL	2.1
1	B	531	ILE	2.1
1	A	418	TRP	2.1
1	A	395	LEU	2.1
1	B	13	LYS	2.1
1	B	466	ASP	2.0
1	B	414	LEU	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
2	FAD	A	601	53/53	0.97	0.11	-0.33	13,17,21,23	0
2	FAD	B	601	53/53	0.97	0.10	-0.75	14,19,22,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.