Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 08:47 PM GMT

PDB ID	:	4Z2U
Title	:	Crystal Structure of 2-hydroxybiphenyl 3-monooxygenase R242Q from Pseudomonas azelaica
Authors	:	Kanteev, M.; Bregman-Cohen, A.; Fishman, A.
Deposited on	:	2015-03-30
Resolution	:	2.50 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
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:

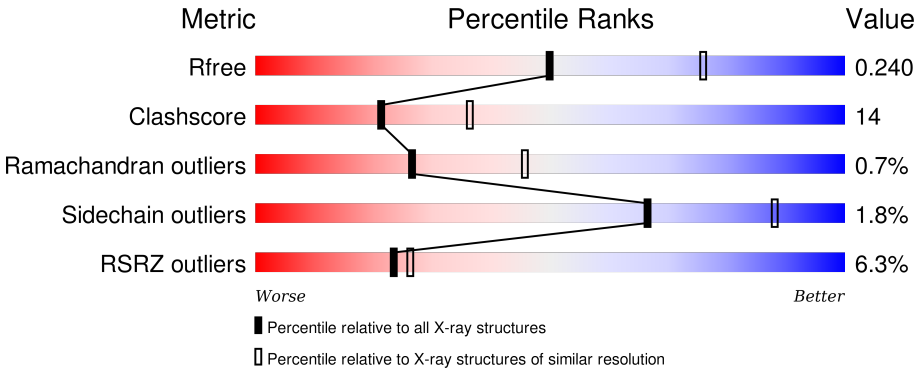
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 >=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 <=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	592	6%, 70%, 23%, 5%
1	B	592	6%, 76%, 18%, 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	601	X	-	-	-
2	FAD	B	601	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9413 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.

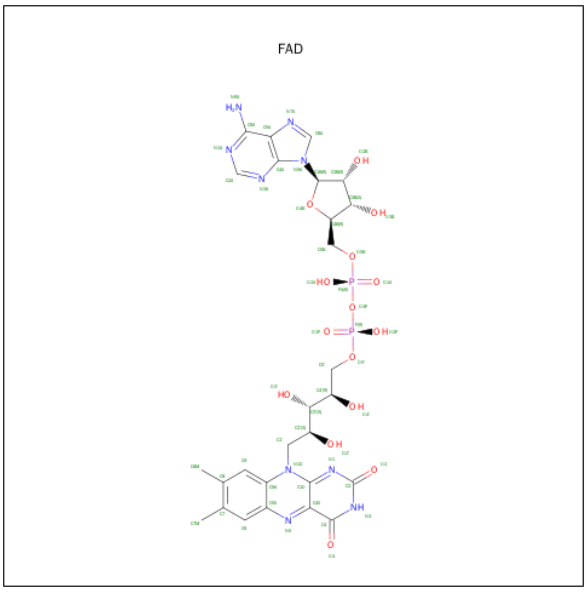
- Molecule 1 is a protein called 2-hydroxybiphenyl-3-monooxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4330	2737	759	814	20			
1	B	563	Total	C	N	O	S	0	0	0
			4330	2737	759	814	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP O06647
A	-4	HIS	-	expression tag	UNP O06647
A	-3	HIS	-	expression tag	UNP O06647
A	-2	HIS	-	expression tag	UNP O06647
A	-1	HIS	-	expression tag	UNP O06647
A	0	HIS	-	expression tag	UNP O06647
A	1	HIS	-	expression tag	UNP O06647
A	242	GLN	ARG	engineered mutation	UNP O06647
B	-5	MET	-	initiating methionine	UNP O06647
B	-4	HIS	-	expression tag	UNP O06647
B	-3	HIS	-	expression tag	UNP O06647
B	-2	HIS	-	expression tag	UNP O06647
B	-1	HIS	-	expression tag	UNP O06647
B	0	HIS	-	expression tag	UNP O06647
B	1	HIS	-	expression tag	UNP O06647
B	242	GLN	ARG	engineered mutation	UNP O06647

- 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.

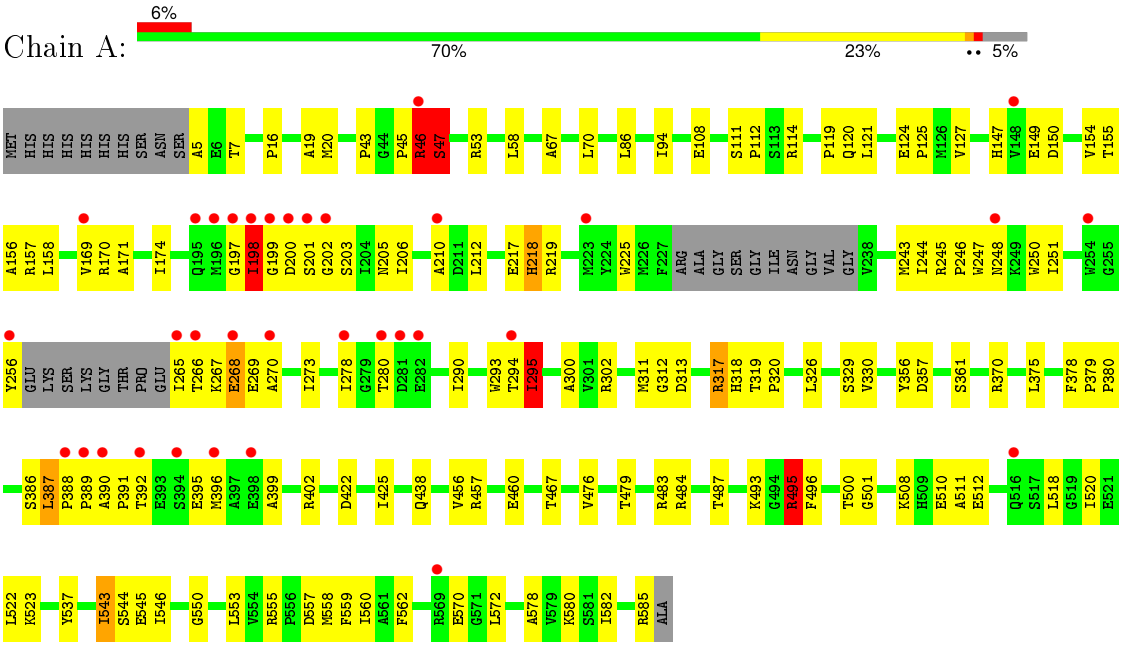
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	313	Total	O	0	0
			313	313		
3	B	334	Total	O	0	0
			334	334		

3 Residue-property plots (i)

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

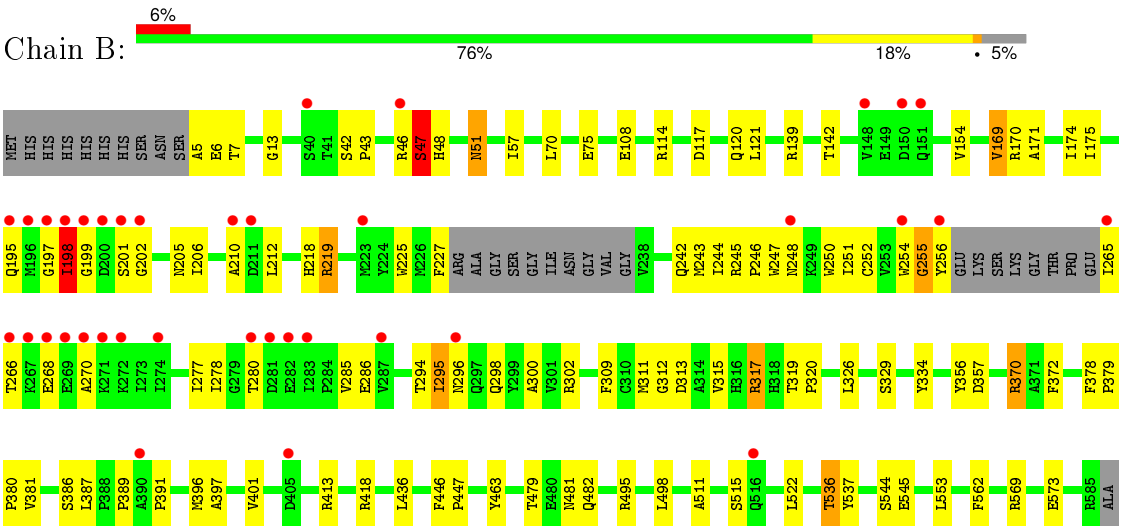
- Molecule 1: 2-hydroxybiphenyl-3-monooxygenase

Chain A:



- Molecule 1: 2-hydroxybiphenyl-3-monooxygenase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.14Å 131.54Å 79.00Å 90.00° 98.28° 90.00°	Depositor
Resolution (Å)	32.37 – 2.50 38.33 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.2 (32.37-2.50) 92.2 (38.33-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.67 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.204 , 0.237 0.213 , 0.240	Depositor DCC
R_{free} test set	2528 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	26.3	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 49675 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9413	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.55	4/4425 (0.1%)	0.74	11/5998 (0.2%)
1	B	0.50	3/4425 (0.1%)	0.60	2/5998 (0.0%)
All	All	0.52	7/8850 (0.1%)	0.67	13/11996 (0.1%)

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	A	0	5
1	B	0	1
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	255	GLY	C-N	-13.89	1.02	1.34
1	A	46	ARG	C-N	-11.98	1.06	1.34
1	A	149	GLU	C-N	-11.72	1.07	1.34
1	B	169	VAL	C-N	-7.39	1.17	1.34
1	A	218	HIS	C-N	-7.17	1.17	1.34
1	B	51	ASN	C-N	-7.09	1.17	1.34
1	A	217	GLU	C-N	-6.95	1.18	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	ARG	O-C-N	-16.09	96.96	122.70
1	A	150	ASP	O-C-N	-12.74	102.32	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	46	ARG	C-N-CA	11.94	151.55	121.70
1	A	218	HIS	O-C-N	-11.43	104.41	122.70
1	A	46	ARG	CA-C-N	10.58	140.49	117.20
1	A	295	ILE	N-CA-CB	-10.52	86.61	110.80
1	A	150	ASP	CA-C-N	9.10	137.23	117.20
1	B	169	VAL	O-C-N	-8.08	109.78	122.70
1	A	318	HIS	N-CA-CB	-7.91	96.36	110.60
1	A	218	HIS	CA-C-N	6.77	132.09	117.20
1	B	255	GLY	C-N-CA	6.72	138.49	121.70
1	A	543	ILE	O-C-N	6.57	133.21	122.70
1	A	47	SER	O-C-N	-5.94	113.19	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	HIS	Mainchain
1	A	46	ARG	Mainchain,Peptide
1	A	47	SER	Mainchain
1	A	495	ARG	Sidechain
1	B	255	GLY	Mainchain

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	4330	0	4274	141	0
1	B	4330	0	4275	104	0
2	A	53	0	30	8	0
2	B	53	0	30	8	0
3	A	313	0	0	3	4
3	B	334	0	0	1	5
All	All	9413	0	8609	246	6

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 14.

All (246) 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:201:SER:HB3	1:A:256:TYR:O	1.39	1.22
1:A:319:THR:CG2	1:A:320:PRO:HD2	1.71	1.21
1:A:319:THR:HG23	1:A:320:PRO:HD2	1.17	1.10
1:A:511:ALA:HB1	1:A:522:LEU:HD11	1.10	1.07
1:B:75:GLU:OE1	1:B:75:GLU:N	1.95	1.00
1:A:511:ALA:HB1	1:A:522:LEU:CD1	1.94	0.96
1:A:5:ALA:HB3	1:A:169:VAL:HG22	1.47	0.95
1:B:294:THR:O	1:B:295:ILE:HG22	1.69	0.92
1:A:511:ALA:CB	1:A:522:LEU:HD11	1.98	0.92
1:A:319:THR:CG2	1:A:320:PRO:CD	2.49	0.91
1:B:46:ARG:O	1:B:47:SER:HB3	1.70	0.90
1:B:108:GLU:HG3	1:B:114:ARG:NH2	1.86	0.90
1:B:46:ARG:HD3	2:B:601:FAD:C7	2.02	0.90
1:A:46:ARG:HD3	2:A:601:FAD:C8	2.04	0.87
1:B:370:ARG:HD3	1:B:370:ARG:O	1.74	0.87
1:A:206:ILE:HD13	1:A:270:ALA:HB1	1.57	0.86
1:B:511:ALA:HB1	1:B:522:LEU:HD11	1.58	0.85
1:A:370:ARG:O	1:A:370:ARG:HD3	1.75	0.85
1:B:205:ASN:HB3	1:B:251:ILE:HD11	1.59	0.84
1:A:154:VAL:HG21	1:A:174:ILE:HG13	1.60	0.84
1:A:202:GLY:O	1:A:256:TYR:HB3	1.78	0.84
1:B:511:ALA:HB1	1:B:522:LEU:CD1	2.08	0.82
1:A:225:TRP:HZ3	1:A:378:PHE:CE1	1.98	0.81
1:A:388:PRO:O	1:A:390:ALA:N	2.14	0.80
1:B:46:ARG:HD3	2:B:601:FAD:C8	2.13	0.78
1:A:46:ARG:HD3	2:A:601:FAD:C7	2.14	0.78
1:A:319:THR:HG22	1:A:320:PRO:CD	2.14	0.77
1:B:70:LEU:O	1:B:245:ARG:NH2	2.17	0.77
1:A:197:GLY:O	1:A:198:ILE:HB	1.85	0.76
1:A:154:VAL:O	1:A:170:ARG:HD2	1.86	0.76
1:A:379:PRO:HB2	1:A:380:PRO:HD3	1.64	0.76
1:B:202:GLY:O	1:B:256:TYR:C	2.24	0.76
1:A:370:ARG:C	1:A:370:ARG:HD3	2.06	0.76
1:B:370:ARG:HD3	1:B:370:ARG:C	2.08	0.73
1:A:70:LEU:O	1:A:245:ARG:NH2	2.19	0.73
1:A:94:ILE:HB	1:A:425:ILE:HD11	1.71	0.73
1:B:154:VAL:HG21	1:B:174:ILE:HG13	1.69	0.72
1:B:225:TRP:CZ3	1:B:378:PHE:CE1	2.77	0.72
1:A:201:SER:CB	1:A:256:TYR:O	2.29	0.71
1:B:244:ILE:O	1:B:245:ARG:HD3	1.90	0.71
1:A:5:ALA:CB	1:A:169:VAL:HG22	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:ILE:HD12	1:A:550:GLY:HA3	1.72	0.71
1:A:244:ILE:O	1:A:245:ARG:HD3	1.90	0.71
1:A:270:ALA:HA	1:A:273:ILE:HD12	1.73	0.70
1:A:267:LYS:HG3	1:A:268:GLU:H	1.56	0.70
1:B:295:ILE:HG23	1:B:295:ILE:O	1.92	0.70
1:A:225:TRP:CZ3	1:A:378:PHE:CE1	2.79	0.69
1:A:294:THR:O	1:A:294:THR:HG23	1.91	0.68
1:B:75:GLU:CD	1:B:75:GLU:H	1.95	0.68
1:A:205:ASN:HB3	1:A:251:ILE:HD11	1.76	0.68
1:A:319:THR:HG22	1:A:320:PRO:HD2	1.68	0.67
1:B:387:LEU:HD13	1:B:391:PRO:HG3	1.77	0.67
1:B:48:HIS:CD2	1:B:242:GLN:NE2	2.63	0.67
1:A:108:GLU:HG3	1:A:114:ARG:NH2	2.09	0.67
1:A:278:ILE:HG22	1:A:280:THR:HG22	1.77	0.66
1:A:555:ARG:HG3	1:A:559:PHE:O	1.95	0.66
1:A:387:LEU:HG	1:A:391:PRO:HB3	1.78	0.66
1:B:43:PRO:O	1:B:121:LEU:HD13	1.96	0.66
1:B:46:ARG:O	1:B:120:GLN:OE1	2.14	0.65
1:B:569:ARG:O	1:B:573:GLU:HG2	1.97	0.65
1:A:94:ILE:HB	1:A:425:ILE:CD1	2.28	0.64
1:A:147:HIS:HB3	1:A:156:ALA:HB2	1.79	0.63
1:B:397:ALA:O	1:B:401:VAL:HG23	1.99	0.63
1:B:498:LEU:HD23	1:B:498:LEU:C	2.19	0.63
1:B:379:PRO:HB2	1:B:380:PRO:HD3	1.81	0.62
1:B:46:ARG:O	1:B:47:SER:CB	2.45	0.62
1:B:225:TRP:HZ3	1:B:378:PHE:CE1	2.16	0.62
1:A:312:GLY:HA2	1:A:329:SER:OG	2.00	0.62
1:A:388:PRO:C	1:A:390:ALA:H	2.02	0.62
1:A:495:ARG:NH2	1:A:523:LYS:HD3	2.15	0.61
1:A:154:VAL:HG21	1:A:174:ILE:CG1	2.29	0.61
1:A:422:ASP:O	1:A:425:ILE:HG12	2.00	0.61
1:B:202:GLY:O	1:B:256:TYR:CA	2.49	0.61
1:A:391:PRO:CG	1:A:396:MET:HE2	2.32	0.60
1:B:202:GLY:O	1:B:256:TYR:HB3	2.02	0.59
1:A:46:ARG:O	2:A:601:FAD:C4	2.50	0.59
1:A:391:PRO:HG3	1:A:396:MET:CE	2.33	0.59
1:A:319:THR:HG22	1:A:320:PRO:N	2.16	0.59
1:A:46:ARG:O	2:A:601:FAD:C4X	2.50	0.59
1:A:94:ILE:HD12	1:A:425:ILE:HD13	1.83	0.59
1:A:243:MET:HA	1:A:250:TRP:CE3	2.38	0.59
1:A:518:LEU:HB2	1:A:520:ILE:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:THR:O	1:A:171:ALA:HA	2.03	0.59
1:A:391:PRO:HG3	1:A:396:MET:HE2	1.85	0.58
1:A:147:HIS:CB	1:A:156:ALA:HB2	2.34	0.58
1:B:225:TRP:CZ3	1:B:378:PHE:CZ	2.92	0.58
1:A:147:HIS:HA	1:A:156:ALA:HA	1.87	0.57
1:A:47:SER:HB3	1:A:120:GLN:OE1	2.04	0.57
1:B:46:ARG:CD	2:B:601:FAD:C8	2.82	0.57
1:A:267:LYS:C	1:A:269:GLU:H	2.08	0.57
1:A:280:THR:O	1:A:280:THR:HG23	2.04	0.57
1:A:557:ASP:O	1:A:558:MET:HB2	2.04	0.57
1:A:510:GLU:HG3	1:A:572:LEU:HD22	1.88	0.56
1:B:522:LEU:O	1:B:522:LEU:HD12	2.06	0.56
1:A:495:ARG:HH21	1:A:523:LYS:HD3	1.70	0.56
1:A:295:ILE:HG23	1:A:295:ILE:O	2.05	0.56
1:A:370:ARG:HH21	1:A:460:GLU:CD	2.08	0.56
1:B:46:ARG:HD3	2:B:601:FAD:C7M	2.36	0.55
1:B:295:ILE:O	1:B:295:ILE:CG2	2.55	0.55
1:A:295:ILE:CG2	1:A:295:ILE:O	2.54	0.55
1:A:544:SER:O	1:A:545:GLU:HB2	2.07	0.55
1:A:43:PRO:O	1:A:121:LEU:HD13	2.06	0.55
1:A:267:LYS:HG3	1:A:268:GLU:N	2.21	0.55
1:B:326:LEU:HD23	1:B:326:LEU:C	2.26	0.55
1:A:157:ARG:O	1:A:158:LEU:HD23	2.06	0.55
1:A:580:LYS:HG2	1:A:585:ARG:O	2.06	0.55
1:A:202:GLY:O	1:A:256:TYR:CB	2.53	0.54
1:B:391:PRO:HG2	1:B:396:MET:HE2	1.89	0.54
1:B:206:ILE:HD13	1:B:270:ALA:HB1	1.89	0.54
1:A:294:THR:CG2	1:A:294:THR:O	2.56	0.54
1:B:48:HIS:HB2	1:B:117:ASP:OD2	2.08	0.54
1:B:198:ILE:CG1	1:B:372:PHE:HE1	2.21	0.54
1:A:169:VAL:HG12	1:A:169:VAL:O	2.07	0.53
1:A:266:THR:CG2	1:A:290:ILE:HD13	2.39	0.53
1:A:311:MET:HB3	1:A:356:TYR:OH	2.08	0.53
1:B:296:ASN:O	1:B:298:GLN:HG3	2.08	0.53
1:A:45:PRO:O	1:A:120:GLN:HB2	2.08	0.53
1:A:388:PRO:C	1:A:390:ALA:N	2.60	0.52
1:A:313:ASP:O	1:A:317:ARG:HG3	2.09	0.52
1:B:57:ILE:HG12	1:B:334:TYR:CD2	2.44	0.52
1:A:266:THR:HG23	1:A:290:ILE:HD13	1.92	0.52
1:B:212:LEU:HD21	1:B:278:ILE:HD13	1.90	0.52
1:B:201:SER:O	1:B:294:THR:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:GLY:HA2	1:B:329:SER:OG	2.10	0.52
1:A:198:ILE:O	1:A:199:GLY:C	2.46	0.52
1:B:511:ALA:CB	1:B:522:LEU:HD11	2.37	0.52
1:B:391:PRO:CG	1:B:396:MET:HE2	2.40	0.52
1:B:294:THR:HG23	1:B:295:ILE:N	2.25	0.52
1:B:197:GLY:C	1:B:198:ILE:CG1	2.79	0.52
1:A:155:THR:O	1:A:155:THR:HG22	2.10	0.52
1:A:248:ASN:OD1	1:A:248:ASN:N	2.42	0.52
1:A:86:LEU:CD2	1:A:212:LEU:HD13	2.40	0.52
1:A:484:ARG:HD2	1:A:537:TYR:OH	2.10	0.51
1:B:47:SER:HB2	2:B:601:FAD:C2	2.40	0.51
1:A:387:LEU:HD21	1:A:396:MET:SD	2.50	0.51
1:B:5:ALA:HB3	1:B:169:VAL:HG22	1.91	0.51
1:A:543:ILE:O	3:A:703:HOH:O	2.19	0.51
1:B:294:THR:O	1:B:295:ILE:CG2	2.52	0.51
1:B:319:THR:HB	1:B:320:PRO:HD2	1.92	0.51
1:A:225:TRP:HZ3	1:A:378:PHE:CZ	2.29	0.50
2:A:601:FAD:O2A	3:A:704:HOH:O	2.19	0.50
1:A:496:PHE:O	1:A:522:LEU:HA	2.11	0.50
1:B:436:LEU:HB3	1:B:463:TYR:CD1	2.46	0.50
1:A:202:GLY:HA2	1:A:294:THR:HA	1.94	0.50
1:A:200:ASP:OD1	1:A:200:ASP:O	2.30	0.50
1:B:311:MET:HB3	1:B:356:TYR:OH	2.11	0.50
1:B:544:SER:O	1:B:545:GLU:HB2	2.12	0.49
1:A:265:ILE:HG22	1:A:266:THR:N	2.27	0.49
1:A:312:GLY:HA3	2:A:601:FAD:O1P	2.13	0.49
1:B:210:ALA:O	1:B:248:ASN:HA	2.11	0.49
1:A:225:TRP:CZ3	1:A:378:PHE:CZ	3.00	0.49
1:A:493:LYS:HD2	1:A:495:ARG:CZ	2.43	0.49
1:A:267:LYS:HB3	1:A:269:GLU:OE1	2.13	0.49
1:B:195:GLN:NE2	1:B:298:GLN:NE2	2.61	0.49
1:B:227:PHE:CE2	1:B:381:VAL:HG11	2.48	0.49
1:B:536:THR:HG22	1:B:537:TYR:CD2	2.48	0.49
1:B:202:GLY:O	1:B:256:TYR:CB	2.61	0.49
1:B:198:ILE:HD11	1:B:372:PHE:HE1	1.78	0.49
1:A:479:THR:HA	1:A:483:ARG:O	2.13	0.48
1:A:319:THR:HG21	1:A:375:LEU:HD21	1.94	0.48
1:A:210:ALA:O	1:A:248:ASN:HA	2.14	0.48
1:B:48:HIS:CD2	1:B:242:GLN:HE22	2.31	0.48
1:A:45:PRO:CB	1:A:119:PRO:HB3	2.44	0.48
1:A:200:ASP:CG	1:A:200:ASP:O	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:VAL:HG12	1:B:286:GLU:N	2.28	0.48
1:B:218:HIS:NE2	1:B:219:ARG:HD2	2.28	0.48
1:A:379:PRO:CB	1:A:380:PRO:HD3	2.40	0.47
1:A:246:PRO:HA	1:A:247:TRP:HA	1.56	0.47
1:A:570:GLU:H	1:A:570:GLU:CD	2.17	0.47
1:A:203:SER:N	1:A:293:TRP:O	2.46	0.47
1:A:19:ALA:HB1	1:A:127:VAL:HG12	1.97	0.47
1:B:302:ARG:HA	1:B:357:ASP:OD1	2.15	0.47
1:B:285:VAL:CG1	1:B:286:GLU:N	2.77	0.47
1:B:277:ILE:HG22	1:B:278:ILE:N	2.31	0.46
1:B:386:SER:OG	1:B:413:ARG:NH1	2.42	0.46
1:A:268:GLU:O	1:A:268:GLU:CG	2.64	0.46
1:A:399:ALA:HA	1:A:402:ARG:NH2	2.32	0.46
1:B:227:PHE:CZ	1:B:381:VAL:HG11	2.51	0.45
1:B:246:PRO:HA	1:B:247:TRP:HA	1.60	0.45
1:B:278:ILE:HG22	1:B:280:THR:HG22	1.99	0.45
1:A:476:VAL:HG23	1:A:487:THR:HG23	1.99	0.45
1:A:267:LYS:CB	1:A:269:GLU:OE1	2.65	0.45
1:A:243:MET:HA	1:A:250:TRP:CZ3	2.52	0.45
1:A:147:HIS:HB3	1:A:156:ALA:CB	2.47	0.45
1:A:295:ILE:HD13	3:A:924:HOH:O	2.17	0.44
1:B:198:ILE:HG22	1:B:199:GLY:H	1.82	0.44
1:A:124:GLU:N	1:A:125:PRO:HD2	2.32	0.44
1:B:387:LEU:HD13	1:B:391:PRO:CG	2.46	0.44
1:A:467:THR:HA	1:A:560:ILE:HD12	1.99	0.44
1:B:312:GLY:HA3	2:B:601:FAD:O1P	2.17	0.44
1:A:58:LEU:HD13	1:A:67:ALA:HB2	1.98	0.44
1:B:244:ILE:HD11	1:B:251:ILE:CG2	2.47	0.44
1:A:379:PRO:HB2	1:A:380:PRO:CD	2.41	0.43
1:A:300:ALA:HB1	1:A:302:ARG:O	2.18	0.43
1:A:425:ILE:HG12	1:A:425:ILE:H	1.68	0.43
1:B:265:ILE:HG13	1:B:266:THR:N	2.34	0.43
1:B:391:PRO:HG2	1:B:396:MET:CE	2.48	0.43
1:B:446:PHE:HA	1:B:447:PRO:HD3	1.91	0.43
1:B:243:MET:HA	1:B:250:TRP:CE3	2.53	0.43
1:B:6:GLU:HG3	1:B:170:ARG:HB3	1.99	0.43
1:A:357:ASP:O	1:A:361:SER:HB2	2.19	0.43
1:A:202:GLY:O	1:A:256:TYR:N	2.52	0.43
1:B:46:ARG:CD	2:B:601:FAD:C7	2.87	0.43
1:B:511:ALA:HB1	1:B:522:LEU:HD12	1.98	0.43
1:A:422:ASP:O	1:A:425:ILE:CG1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLY:HA2	2:B:601:FAD:O4B	2.19	0.43
1:A:280:THR:CG2	1:A:280:THR:O	2.67	0.43
1:B:5:ALA:O	1:B:169:VAL:HA	2.18	0.43
1:B:294:THR:CG2	1:B:295:ILE:N	2.82	0.42
1:A:267:LYS:C	1:A:269:GLU:N	2.71	0.42
1:A:295:ILE:H	1:A:295:ILE:HG22	1.47	0.42
1:A:553:LEU:HB3	1:A:562:PHE:HB3	2.00	0.42
1:A:46:ARG:O	2:A:601:FAD:N5	2.52	0.42
1:B:479:THR:HG23	1:B:536:THR:HB	2.01	0.42
1:B:48:HIS:HB2	1:B:117:ASP:CG	2.40	0.42
1:B:379:PRO:CB	1:B:380:PRO:HD3	2.49	0.42
1:A:392:THR:H	1:A:395:GLU:HB2	1.84	0.42
1:A:243:MET:CA	1:A:250:TRP:CZ3	3.02	0.42
1:A:16:PRO:HD2	2:A:601:FAD:O2P	2.20	0.42
1:A:20:MET:HG2	1:A:330:VAL:HG13	2.00	0.42
1:B:7:THR:O	1:B:171:ALA:HA	2.20	0.42
1:B:481:ASN:O	1:B:482:GLN:HB2	2.19	0.42
1:B:379:PRO:N	1:B:380:PRO:CD	2.83	0.42
1:A:510:GLU:CG	1:A:572:LEU:HD22	2.50	0.41
1:B:197:GLY:O	1:B:198:ILE:CG1	2.68	0.41
1:A:111:SER:OG	1:A:112:PRO:HD2	2.19	0.41
1:B:51:ASN:HB2	3:B:823:HOH:O	2.20	0.41
1:B:300:ALA:HB3	1:B:315:VAL:HB	2.01	0.41
1:B:197:GLY:O	1:B:198:ILE:HG13	2.21	0.41
1:A:326:LEU:C	1:A:326:LEU:HD23	2.40	0.41
1:B:553:LEU:HB3	1:B:562:PHE:HB3	2.02	0.41
1:B:418:ARG:O	1:B:418:ARG:HD3	2.21	0.41
1:A:198:ILE:CG2	1:A:199:GLY:N	2.82	0.41
1:B:198:ILE:CD1	1:B:372:PHE:HE1	2.34	0.41
1:A:202:GLY:O	1:A:256:TYR:CA	2.69	0.41
1:B:205:ASN:HA	1:B:252:CYS:O	2.21	0.41
1:B:175:ILE:HA	1:B:309:PHE:O	2.20	0.41
1:B:206:ILE:HD11	1:B:254:TRP:HH2	1.86	0.40
1:B:313:ASP:O	1:B:317:ARG:HG3	2.21	0.40
1:A:86:LEU:HD22	1:A:212:LEU:HD13	2.03	0.40
1:A:53:ARG:NH1	1:A:438:GLN:OE1	2.53	0.40
1:B:139:ARG:HG3	1:B:142:THR:OG1	2.21	0.40
1:A:456:VAL:HG22	1:A:457:ARG:HG3	2.03	0.40
1:A:500:THR:OG1	1:A:501:GLY:N	2.54	0.40
1:A:508:LYS:O	1:A:512:GLU:HG3	2.21	0.40
1:A:578:ALA:O	1:A:582:ILE:HG13	2.22	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:919:HOH:O	3:A:960:HOH:O[2_555]	1.92	0.28
3:A:935:HOH:O	3:B:849:HOH:O[4_445]	2.04	0.16
3:B:746:HOH:O	3:B:848:HOH:O[2_455]	2.06	0.14
3:A:1002:HOH:O	3:B:913:HOH:O[4_445]	2.08	0.12
3:A:975:HOH:O	3:B:911:HOH:O[4_445]	2.09	0.11
3:B:848:HOH:O	3:B:848:HOH:O[2_455]	2.19	0.01

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	557/592 (94%)	525 (94%)	29 (5%)	3 (0%)	34	55
1	B	557/592 (94%)	520 (93%)	32 (6%)	5 (1%)	21	37
All	All	1114/1184 (94%)	1045 (94%)	61 (6%)	8 (1%)	26	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	198	ILE
1	A	389	PRO
1	B	198	ILE
1	B	268	GLU
1	B	47	SER
1	B	295	ILE
1	A	268	GLU
1	B	389	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	451/473 (95%)	444 (98%)	7 (2%)	70 90
1	B	451/473 (95%)	442 (98%)	9 (2%)	63 86
All	All	902/946 (95%)	886 (98%)	16 (2%)	66 88

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ILE
1	A	219	ARG
1	A	295	ILE
1	A	317	ARG
1	A	386	SER
1	A	387	LEU
1	A	495	ARG
1	B	42	SER
1	B	47	SER
1	B	198	ILE
1	B	219	ARG
1	B	317	ARG
1	B	370	ARG
1	B	495	ARG
1	B	515	SER
1	B	536	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	275	HIS
1	B	242	GLN
1	B	296	ASN
1	B	298	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

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	-	52,58,58	2.43	15 (28%)	52,89,89	2.99	12 (23%)
2	FAD	B	601	-	52,58,58	2.35	15 (28%)	52,89,89	3.21	15 (28%)

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	-	1/1/9/9	0/30/50/50	0/6/6/6
2	FAD	B	601	-	1/1/9/9	0/30/50/50	0/6/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C2B-C1B	-3.65	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C2B-C1B	-3.63	1.47	1.53
2	B	601	FAD	C1'-N10	-3.24	1.44	1.48
2	A	601	FAD	O3'-C3'	-2.56	1.36	1.43
2	B	601	FAD	O3'-C3'	-2.45	1.37	1.43
2	A	601	FAD	O2B-C2B	-2.36	1.37	1.43
2	B	601	FAD	O2B-C2B	-2.23	1.37	1.43
2	A	601	FAD	O3B-C3B	-2.19	1.37	1.43
2	B	601	FAD	C2B-C3B	-2.15	1.47	1.53
2	B	601	FAD	C6A-N6A	2.08	1.42	1.34
2	A	601	FAD	C6A-N6A	2.19	1.43	1.34
2	A	601	FAD	C10-N10	2.28	1.41	1.39
2	B	601	FAD	C4-C4X	2.58	1.46	1.41
2	B	601	FAD	O2'-C2'	2.69	1.49	1.43
2	A	601	FAD	O2'-C2'	2.72	1.49	1.43
2	A	601	FAD	C4-C4X	2.77	1.46	1.41
2	A	601	FAD	C2A-N3A	2.86	1.37	1.32
2	B	601	FAD	C9A-N10	3.17	1.43	1.38
2	B	601	FAD	C2A-N3A	3.42	1.38	1.32
2	B	601	FAD	C4-N3	3.57	1.39	1.33
2	A	601	FAD	C4-N3	3.80	1.39	1.33
2	B	601	FAD	C2'-C3'	4.10	1.61	1.53
2	A	601	FAD	C9A-N10	4.45	1.45	1.38
2	B	601	FAD	C2-N1	4.67	1.47	1.38
2	A	601	FAD	C2-N1	4.77	1.48	1.38
2	A	601	FAD	C2'-C3'	4.84	1.63	1.53
2	A	601	FAD	C4X-C10	6.35	1.52	1.40
2	B	601	FAD	C4X-C10	6.55	1.53	1.40
2	B	601	FAD	C5X-N5	8.79	1.49	1.35
2	A	601	FAD	C5X-N5	9.10	1.49	1.35

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	FAD	N3A-C2A-N1A	-11.77	119.63	128.87
2	B	601	FAD	N3A-C2A-N1A	-11.06	120.18	128.87
2	B	601	FAD	O5'-P-O1P	-5.82	85.38	109.21
2	B	601	FAD	N3-C2-N1	-5.58	118.29	127.69
2	A	601	FAD	O5'-P-O1P	-5.49	86.73	109.21
2	B	601	FAD	C4X-C10-N10	-5.47	116.55	120.52
2	A	601	FAD	O2P-P-O5'	-5.25	83.22	108.24
2	A	601	FAD	N3-C2-N1	-5.19	118.95	127.69
2	B	601	FAD	C4X-C4-N3	-4.86	117.17	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	FAD	O2P-P-O5'	-4.73	85.71	108.24
2	A	601	FAD	C4X-C4-N3	-4.49	117.66	123.52
2	A	601	FAD	C4X-C10-N10	-3.70	117.83	120.52
2	B	601	FAD	C4-C4X-C10	-3.37	117.79	119.94
2	A	601	FAD	C1B-N9A-C4A	-2.09	124.47	126.81
2	B	601	FAD	O4B-C4B-C5B	2.03	116.55	109.29
2	A	601	FAD	O2'-C2'-C1'	2.62	116.40	109.93
2	B	601	FAD	C1'-C2'-C3'	3.07	118.60	109.82
2	B	601	FAD	O3'-C3'-C2'	3.56	117.95	108.73
2	B	601	FAD	O3'-C3'-C4'	3.76	118.48	108.73
2	B	601	FAD	O2'-C2'-C1'	3.87	119.49	109.93
2	B	601	FAD	O2'-C2'-C3'	4.06	119.41	108.96
2	A	601	FAD	O2P-P-O3P	4.24	123.42	105.27
2	A	601	FAD	C1'-C2'-C3'	4.26	122.00	109.82
2	A	601	FAD	O2'-C2'-C3'	4.27	119.96	108.96
2	B	601	FAD	O2P-P-O3P	4.53	124.69	105.27
2	A	601	FAD	C4-N3-C2	10.65	124.04	115.16
2	B	601	FAD	C4-N3-C2	12.37	125.48	115.16

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	601	FAD	C3'
2	A	601	FAD	C3'

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

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

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4
1	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	217:GLU	C	218:HIS	N	1.18
1	A	218:HIS	C	219:ARG	N	1.17
1	B	51:ASN	C	52:GLN	N	1.17
1	B	169:VAL	C	170:ARG	N	1.17
1	A	149:GLU	C	150:ASP	N	1.07
1	A	46:ARG	C	47:SER	N	1.06
1	B	255:GLY	C	256:TYR	N	1.02

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^{th} 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^2)	Q<0.9
1	A	563/592 (95%)	0.19	34 (6%)	25	28	6, 22, 62, 157	0
1	B	563/592 (95%)	0.07	37 (6%)	22	24	6, 22, 62, 157	0
All	All	1126/1184 (95%)	0.13	71 (6%)	23	26	6, 22, 62, 157	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	GLY	10.2
1	B	198	ILE	7.5
1	B	199	GLY	7.2
1	A	198	ILE	7.1
1	A	256	TYR	6.6
1	A	197	GLY	5.7
1	A	265	ILE	5.6
1	A	200	ASP	5.6
1	A	202	GLY	5.3
1	A	196	MET	5.3
1	A	201	SER	5.2
1	B	265	ILE	5.0
1	A	390	ALA	4.8
1	B	268	GLU	4.7
1	B	267	LYS	4.5
1	A	195	GLN	4.5
1	B	282	GLU	4.4
1	A	282	GLU	4.4
1	A	516	GLN	4.4
1	B	200	ASP	4.3
1	B	256	TYR	4.1
1	B	223	MET	4.1
1	A	280	THR	4.0
1	A	270	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	281	ASP	3.7
1	B	270	ALA	3.6
1	A	392	THR	3.6
1	A	388	PRO	3.6
1	B	196	MET	3.6
1	B	516	GLN	3.5
1	A	389	PRO	3.5
1	B	202	GLY	3.4
1	B	254	TRP	3.3
1	A	148	VAL	3.3
1	A	394	SER	3.2
1	B	197	GLY	3.2
1	B	272	LYS	3.2
1	A	169	VAL	3.2
1	B	210	ALA	3.1
1	A	223	MET	3.0
1	B	151	GLN	3.0
1	B	201	SER	2.8
1	B	148	VAL	2.8
1	A	268	GLU	2.8
1	A	210	ALA	2.7
1	B	266	THR	2.7
1	A	569	ARG	2.6
1	B	296	ASN	2.6
1	A	254	TRP	2.6
1	A	294	THR	2.5
1	B	281	ASP	2.5
1	B	287	VAL	2.5
1	B	280	THR	2.4
1	B	405	ASP	2.4
1	B	274	ILE	2.3
1	B	150	ASP	2.3
1	A	46	ARG	2.3
1	A	278	ILE	2.2
1	A	248	ASN	2.2
1	B	195	GLN	2.2
1	B	40	SER	2.2
1	B	283	ILE	2.2
1	B	248	ASN	2.2
1	B	390	ALA	2.2
1	A	266	THR	2.2
1	B	271	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	211	ASP	2.1
1	A	396	MET	2.1
1	A	398	GLU	2.1
1	B	46	ARG	2.1
1	B	269	GLU	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^{th} 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^2)	Q<0.9
2	FAD	B	601	53/53	0.95	0.13	-0.44	4,8,11,13	0
2	FAD	A	601	53/53	0.95	0.13	-0.58	4,8,11,13	0

6.5 Other polymers (i)

There are no such residues in this entry.