



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:04 pm GMT

PDB ID : 1GV4  
Title : MURINE APOPTOSIS-INDUCING FACTOR (AIF)  
Authors : Mate, M.J.; Alzari, P.M.  
Deposited on : 2002-02-05  
Resolution : 2.00 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

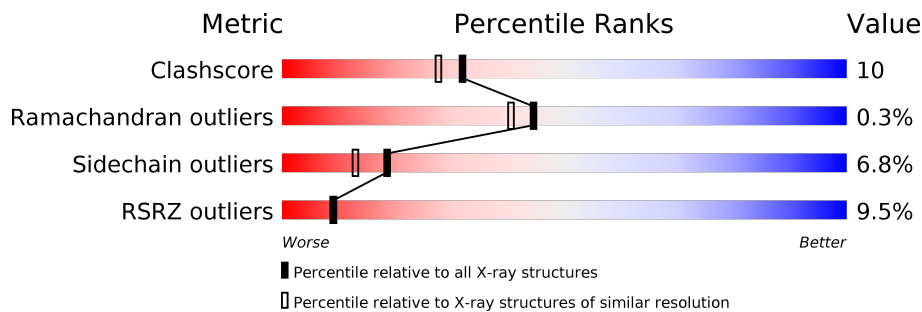
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.00 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))
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

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	528	 7% 71% 18% • • 7%
1	B	528	 10% 71% 18% • • 7%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8064 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 PROGRAMED CELL DEATH PROTEIN 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	27	0	0
			3759	2379	666	703	11			
1	B	490	Total	C	N	O	S	37	0	0
			3759	2379	666	703	11			

- 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		

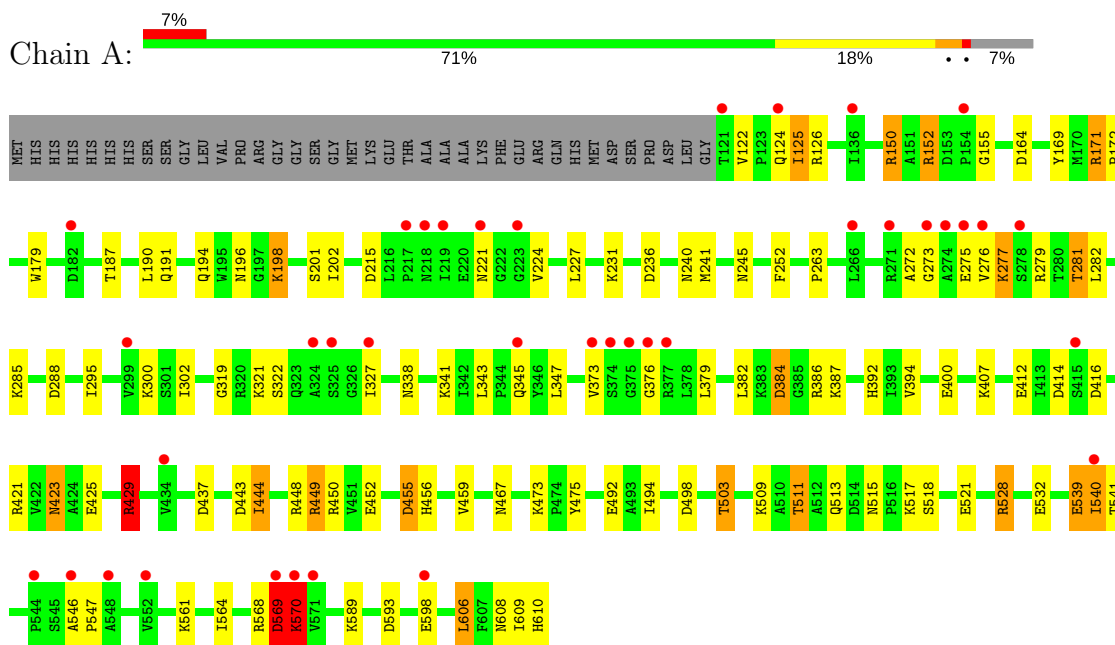
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	214	Total 214	O 214	0	0
3	B	226	Total 226	O 226	0	0

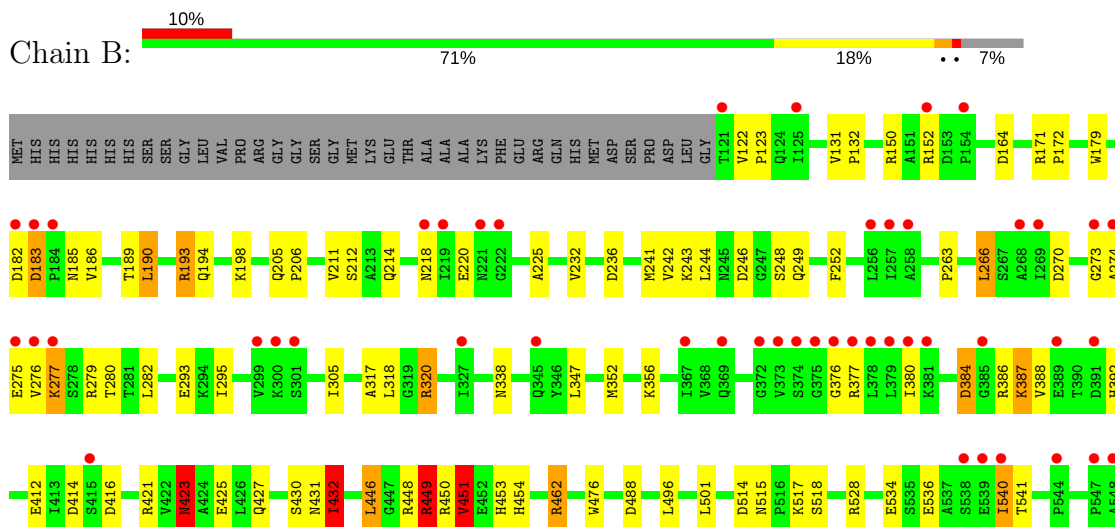
### 3 Residue-property plots

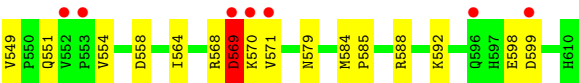
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: PROGRAMED CELL DEATH PROTEIN 8



#### • Molecule 1: PROGRAMED CELL DEATH PROTEIN 8





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.27Å 109.91Å 114.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 40.15 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (15.00-2.00) 96.1 (40.15-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.49 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.216 , 0.257 0.229 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.4	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.19 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.8122e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.78	2/3836 (0.1%)	0.99	22/5194 (0.4%)
1	B	0.83	3/3836 (0.1%)	1.09	32/5194 (0.6%)
All	All	0.81	5/7672 (0.1%)	1.04	54/10388 (0.5%)

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	1	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	569	ASP	C-N	-20.33	0.87	1.34
1	A	539	GLU	CA-CB	-11.82	1.27	1.53
1	B	568	ARG	C-N	11.21	1.59	1.34
1	B	451	VAL	CB-CG2	-5.30	1.41	1.52
1	A	452	GLU	CD-OE2	-5.23	1.19	1.25

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	569	ASP	O-C-N	-25.02	82.67	122.70
1	B	569	ASP	CA-C-N	15.22	150.67	117.20
1	B	569	ASP	CB-CA-C	12.95	136.29	110.40
1	A	150	ARG	NE-CZ-NH1	-11.85	114.38	120.30
1	A	449	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	B	432	ILE	CG1-CB-CG2	-9.35	90.82	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	A	449	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	277	LYS	CB-CG-CD	7.94	132.24	111.60
1	A	416	ASP	CB-CG-OD2	7.66	125.20	118.30
1	B	164	ASP	CB-CG-OD2	7.56	125.10	118.30
1	A	455	ASP	CB-CG-OD2	7.05	124.65	118.30
1	A	150	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	B	569	ASP	C-N-CA	6.83	138.77	121.70
1	B	449	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	449	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	462	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	437	ASP	CB-CG-OD2	6.53	124.18	118.30
1	B	488	ASP	CB-CG-OD2	6.46	124.12	118.30
1	B	414	ASP	CB-CG-OD2	6.43	124.09	118.30
1	B	384	ASP	CB-CG-OD2	6.33	124.00	118.30
1	B	214	GLN	CB-CA-C	-6.24	97.91	110.40
1	B	568	ARG	C-N-CA	-6.22	106.15	121.70
1	B	183	ASP	CB-CG-OD2	6.17	123.86	118.30
1	B	599	ASP	CB-CG-OD2	6.08	123.78	118.30
1	B	462	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	150	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	B	246	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	215	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	569	ASP	CB-CG-OD2	5.83	123.55	118.30
1	B	270	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	171	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	A	288	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	236	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	150	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	384	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	606	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	416	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	387	LYS	CB-CA-C	5.43	121.27	110.40
1	A	236	ASP	CB-CG-OD2	5.43	123.19	118.30
1	B	570	LYS	CB-CA-C	5.42	121.23	110.40
1	B	387	LYS	CB-CA-C	5.41	121.23	110.40
1	B	198	LYS	CB-CA-C	5.41	121.22	110.40
1	B	598	GLU	CB-CA-C	5.40	121.20	110.40
1	B	275	GLU	CB-CA-C	5.38	121.16	110.40
1	B	423	ASN	CB-CA-C	-5.35	99.70	110.40
1	B	570	LYS	CA-C-N	-5.32	105.50	117.20
1	A	394	VAL	CB-CA-C	-5.25	101.42	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	570	LYS	CA-C-N	-5.24	105.68	117.20
1	A	443	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	182	ASP	CB-CG-OD2	5.11	122.90	118.30
1	B	558	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	498	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	164	ASP	CB-CG-OD2	5.03	122.83	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	569	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	569	ASP	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	3759	0	3789	77	0
1	B	3759	0	3788	78	0
2	A	53	0	31	1	0
2	B	53	0	31	0	0
3	A	214	0	0	10	0
3	B	226	0	0	8	0
All	All	8064	0	7639	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (152) 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:274:ALA:HA	1:B:277:LYS:CE	1.51	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ALA:CA	1:B:277:LYS:HE2	1.49	1.37
1:A:272:ALA:HB1	1:A:276:VAL:HG21	1.44	0.98
1:B:273:GLY:O	1:B:277:LYS:HG3	1.64	0.97
1:B:421:ARG:NH2	3:B:2126:HOH:O	1.92	0.93
1:A:429:ARG:HD2	1:B:425:GLU:OE2	1.71	0.91
1:B:279:ARG:NH2	1:B:376:GLY:O	2.07	0.86
1:A:152:ARG:HG3	1:A:152:ARG:HH21	1.38	0.86
1:A:279:ARG:NH2	1:A:376:GLY:O	2.13	0.82
1:A:152:ARG:NH2	1:A:152:ARG:HG3	1.95	0.80
1:B:384:ASP:OD1	1:B:386:ARG:NH2	2.16	0.79
1:A:281:THR:CG2	1:A:392:HIS:NE2	2.48	0.76
1:B:273:GLY:O	1:B:277:LYS:CG	2.33	0.75
1:A:412:GLU:OE2	1:A:421:ARG:HD3	1.86	0.75
1:A:467:ASN:HD21	1:A:473:LYS:H	1.34	0.75
1:B:320:ARG:HG3	1:B:320:ARG:HH21	1.49	0.75
1:B:446:LEU:HD13	3:B:2210:HOH:O	1.85	0.75
1:B:273:GLY:C	1:B:277:LYS:HD3	2.08	0.74
1:A:570:LYS:O	3:A:2196:HOH:O	2.05	0.74
1:A:569:ASP:O	1:A:570:LYS:HB2	1.89	0.71
1:B:193:ARG:HH21	1:B:193:ARG:HG3	1.57	0.69
1:A:196:ASN:HD21	1:A:198:LYS:NZ	1.90	0.69
1:A:444:ILE:O	1:A:444:ILE:HG13	1.93	0.69
1:A:423:ASN:HD22	1:A:423:ASN:C	1.96	0.69
1:B:536:GLU:HG2	1:B:588:ARG:HB3	1.73	0.68
1:A:150:ARG:CD	3:A:2014:HOH:O	2.40	0.68
1:B:266:LEU:HD21	1:B:305:ILE:HG21	1.76	0.68
1:A:272:ALA:CB	1:A:276:VAL:HG21	2.21	0.66
1:B:183:ASP:HB3	1:B:186:VAL:HG23	1.75	0.66
1:A:517:LYS:O	1:A:521:GLU:HG3	1.96	0.65
1:B:276:VAL:O	1:B:280:THR:HG23	1.97	0.65
1:A:150:ARG:HD2	3:A:2014:HOH:O	1.96	0.65
1:A:421:ARG:HH11	1:A:448:ARG:HD2	1.62	0.64
1:A:155:GLY:HA2	1:A:221:ASN:O	1.98	0.64
1:A:569:ASP:O	1:A:570:LYS:CB	2.45	0.63
1:B:462:ARG:NH2	1:B:534:GLU:OE1	2.31	0.63
1:A:515:ASN:ND2	1:A:518:SER:H	1.96	0.63
1:A:272:ALA:HB1	1:A:276:VAL:CG2	2.26	0.63
1:A:196:ASN:HD21	1:A:198:LYS:HZ1	1.44	0.62
1:B:273:GLY:O	1:B:277:LYS:CD	2.48	0.61
1:A:302:ILE:HG13	1:A:327:ILE:HD11	1.83	0.60
1:A:338:ASN:H	1:A:338:ASN:HD22	1.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ARG:CD	1:B:425:GLU:OE2	2.45	0.60
1:A:467:ASN:ND2	1:A:473:LYS:H	1.99	0.60
1:B:131:VAL:O	1:B:252:PHE:HA	2.01	0.60
1:A:414:ASP:HB2	1:A:421:ARG:HG3	1.84	0.60
1:A:152:ARG:CG	1:A:152:ARG:HH21	2.11	0.59
1:A:382:LEU:HD12	1:A:386:ARG:HB2	1.84	0.59
1:A:281:THR:HG22	1:A:392:HIS:NE2	2.16	0.59
1:B:384:ASP:OD2	1:B:386:ARG:HD3	2.04	0.58
1:A:150:ARG:HD3	3:A:2014:HOH:O	2.02	0.58
1:B:122:VAL:HB	1:B:123:PRO:CD	2.33	0.58
1:B:320:ARG:CG	1:B:320:ARG:HH21	2.17	0.58
1:A:421:ARG:NH1	1:A:448:ARG:HD2	2.19	0.57
1:B:449:ARG:HG3	1:B:450:ARG:N	2.19	0.57
1:B:273:GLY:O	1:B:277:LYS:HD3	2.05	0.57
1:B:549:VAL:O	1:B:551:GLN:HG2	2.04	0.56
1:B:451:VAL:CG2	1:B:453:HIS:CE1	2.89	0.56
1:A:343:LEU:HD22	1:A:347:LEU:HD23	1.87	0.56
1:B:185:ASN:O	1:B:189:THR:HG23	2.06	0.56
1:B:122:VAL:HB	1:B:123:PRO:HD2	1.89	0.55
1:B:205:GLN:NE2	1:B:206:PRO:HD2	2.22	0.55
1:A:400:GLU:HG3	3:A:2108:HOH:O	2.06	0.54
1:A:423:ASN:ND2	1:A:425:GLU:H	2.06	0.54
1:A:540:ILE:HG22	1:A:540:ILE:O	2.08	0.54
1:A:231:LYS:H	1:A:245:ASN:HD22	1.54	0.54
1:B:427:GLN:NE2	3:B:2130:HOH:O	2.42	0.53
1:A:455:ASP:O	1:A:459:VAL:HG23	2.09	0.53
1:B:569:ASP:C	1:B:571:VAL:H	2.10	0.53
1:A:194:GLN:NE2	1:A:198:LYS:HE2	2.25	0.52
1:A:384:ASP:OD1	1:A:386:ARG:HD3	2.08	0.52
1:B:451:VAL:HG22	1:B:453:HIS:CE1	2.45	0.52
1:A:194:GLN:HE22	1:A:198:LYS:HE2	1.75	0.52
1:A:263:PRO:HB2	1:A:282:LEU:HB3	1.91	0.52
1:B:263:PRO:HB2	1:B:282:LEU:HB3	1.92	0.51
1:B:476:TRP:CZ2	3:B:2167:HOH:O	2.63	0.51
1:A:179:TRP:O	1:A:321:LYS:HE2	2.10	0.51
1:B:274:ALA:C	1:B:277:LYS:HE2	2.27	0.51
1:A:511:THR:HG23	1:A:513:GLN:H	1.76	0.50
1:B:193:ARG:HH21	1:B:193:ARG:CG	2.24	0.50
1:B:320:ARG:CG	1:B:320:ARG:NH2	2.73	0.50
1:B:412:GLU:OE1	1:B:421:ARG:HD3	2.11	0.50
1:A:528:ARG:HD3	3:A:2181:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:LEU:HD22	1:A:564:ILE:HD11	1.94	0.50
1:A:275:GLU:HB3	1:A:373:VAL:HG21	1.93	0.49
1:B:320:ARG:HG3	1:B:320:ARG:NH2	2.23	0.49
1:B:584:MET:N	1:B:585:PRO:CD	2.76	0.49
1:B:515:ASN:ND2	1:B:518:SER:H	2.11	0.49
1:A:423:ASN:ND2	1:A:423:ASN:C	2.66	0.48
1:A:568:ARG:O	1:A:569:ASP:HB2	2.12	0.48
1:B:540:ILE:HG22	1:B:541:THR:N	2.28	0.48
1:B:423:ASN:HB3	1:B:425:GLU:H	1.78	0.48
1:A:589:LYS:HE3	1:A:593:ASP:OD2	2.14	0.48
1:A:191:GLN:HE22	1:A:201:SER:HB2	1.78	0.47
1:A:281:THR:HG23	1:A:392:HIS:NE2	2.29	0.47
1:B:347:LEU:HD22	1:B:564:ILE:HD11	1.95	0.47
1:A:503:THR:HG23	3:A:2098:HOH:O	2.14	0.47
1:B:430:SER:O	1:B:431:ASN:HB2	2.15	0.47
1:B:454:HIS:HD2	3:B:2007:HOH:O	1.96	0.47
1:B:536:GLU:HG2	1:B:588:ARG:CB	2.43	0.47
1:A:285:LYS:HE3	1:A:285:LYS:HB2	1.70	0.46
1:B:446:LEU:CD1	3:B:2210:HOH:O	2.54	0.46
1:B:277:LYS:HB2	1:B:277:LYS:HE3	1.68	0.46
1:A:275:GLU:CB	1:A:373:VAL:HG21	2.45	0.45
1:A:319:GLY:O	1:A:322:SER:HB3	2.15	0.45
1:A:231:LYS:H	1:A:245:ASN:ND2	2.15	0.45
1:B:189:THR:O	1:B:190:LEU:HB2	2.16	0.45
1:A:429:ARG:HD3	1:B:425:GLU:HG3	1.99	0.45
1:A:171:ARG:N	1:A:172:PRO:CD	2.80	0.44
1:B:171:ARG:N	1:B:172:PRO:CD	2.80	0.44
1:B:449:ARG:HD3	3:B:2149:HOH:O	2.16	0.44
1:A:608:ASN:OD1	1:A:610:HIS:HE1	2.00	0.44
1:B:446:LEU:HD11	1:B:496:LEU:HB2	2.00	0.44
1:B:515:ASN:ND2	1:B:517:LYS:HB3	2.33	0.44
1:B:514:ASP:HB3	1:B:579:ASN:O	2.17	0.44
1:A:546:ALA:HB1	1:A:547:PRO:HD2	2.00	0.43
1:A:540:ILE:HG12	1:A:589:LYS:HG3	1.99	0.43
1:B:352:MET:O	1:B:356:LYS:HG3	2.18	0.43
1:A:125:ILE:HA	3:A:2002:HOH:O	2.17	0.43
1:B:152:ARG:HA	1:B:152:ARG:HD3	1.69	0.43
1:A:240:ASN:HB3	1:A:252:PHE:O	2.19	0.43
1:A:273:GLY:O	1:A:276:VAL:HG22	2.19	0.43
1:B:432:ILE:HG23	1:B:432:ILE:HD13	1.07	0.43
1:A:503:THR:CG2	3:A:2098:HOH:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLU:OE1	1:A:532:GLU:OE1	2.37	0.42
1:B:295:ILE:HD13	1:B:392:HIS:CD2	2.54	0.42
1:B:347:LEU:HD12	1:B:347:LEU:HA	1.79	0.42
1:A:125:ILE:HG12	1:A:125:ILE:H	1.10	0.42
1:B:380:ILE:HB	1:B:388:VAL:HB	2.00	0.42
1:B:211:VAL:O	1:B:225:ALA:HA	2.19	0.42
1:B:515:ASN:HD21	1:B:517:LYS:HB3	1.84	0.42
1:B:432:ILE:HD12	1:B:432:ILE:HG21	1.32	0.42
1:A:285:LYS:HD3	3:A:2019:HOH:O	2.20	0.41
1:A:456:HIS:HD2	1:A:475:TYR:OH	2.03	0.41
1:B:318:LEU:HA	1:B:318:LEU:HD23	1.94	0.41
1:B:243:LYS:HG2	1:B:249:GLN:HG2	2.03	0.41
1:B:338:ASN:H	1:B:338:ASN:HD22	1.69	0.41
1:A:150:ARG:HD2	1:A:224:VAL:HG23	2.02	0.41
1:A:169:TYR:HB2	1:A:202:ILE:HG12	2.03	0.41
1:A:561:LYS:HE3	1:A:609:ILE:HD13	2.02	0.41
1:B:179:TRP:CG	1:B:317:ALA:HB1	2.55	0.41
1:A:421:ARG:NH1	1:B:421:ARG:HD2	2.36	0.41
1:B:384:ASP:CG	1:B:386:ARG:HH21	2.23	0.41
1:A:276:VAL:HG23	1:A:277:LYS:N	2.35	0.40
1:A:295:ILE:HD13	1:A:392:HIS:CE1	2.55	0.40
1:B:232:VAL:HG13	1:B:242:VAL:HB	2.03	0.40
1:B:277:LYS:H	1:B:277:LYS:HG3	1.53	0.40
2:A:1611:FAD:H9	2:A:1611:FAD:H1'1	1.79	0.40
1:B:131:VAL:HA	1:B:132:PRO:HD3	1.90	0.40
1:B:193:ARG:CG	1:B:193:ARG:NH2	2.85	0.40
1:B:244:LEU:HD12	1:B:248:SER:OG	2.21	0.40
1:B:194:GLN:HB3	3:B:2032:HOH:O	2.20	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	488/528 (92%)	471 (96%)	15 (3%)	2 (0%)	38	33
1	B	488/528 (92%)	469 (96%)	18 (4%)	1 (0%)	51	48
All	All	976/1056 (92%)	940 (96%)	33 (3%)	3 (0%)	44	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	569	ASP
1	A	570	LYS
1	B	569	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	402/432 (93%)	371 (92%)	31 (8%)	15	9
1	B	402/432 (93%)	378 (94%)	24 (6%)	22	17
All	All	804/864 (93%)	749 (93%)	55 (7%)	18	13

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	124	GLN
1	A	125	ILE
1	A	126	ARG
1	A	152	ARG
1	A	187	THR
1	A	190	LEU
1	A	198	LYS
1	A	227	LEU
1	A	241	MET
1	A	281	THR
1	A	300	LYS
1	A	341	LYS

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Mol	Chain	Res	Type
1	A	345	GLN
1	A	379	LEU
1	A	407	LYS
1	A	423	ASN
1	A	429	ARG
1	A	444	ILE
1	A	449	ARG
1	A	450	ARG
1	A	494	ILE
1	A	503	THR
1	A	509	LYS
1	A	511	THR
1	A	528	ARG
1	A	539	GLU
1	A	540	ILE
1	A	541	THR
1	A	598	GLU
1	A	606	LEU
1	B	190	LEU
1	B	193	ARG
1	B	212	SER
1	B	218	ASN
1	B	220	GLU
1	B	241	MET
1	B	266	LEU
1	B	277	LYS
1	B	293	GLU
1	B	320	ARG
1	B	377	ARG
1	B	387	LYS
1	B	423	ASN
1	B	432	ILE
1	B	446	LEU
1	B	448	ARG
1	B	449	ARG
1	B	451	VAL
1	B	501	LEU
1	B	528	ARG
1	B	540	ILE
1	B	554	VAL
1	B	569	ASP
1	B	592	LYS



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	194	GLN
1	A	196	ASN
1	A	205	GLN
1	A	245	ASN
1	A	323	GLN
1	A	338	ASN
1	A	345	GLN
1	A	365	ASN
1	A	402	ASN
1	A	423	ASN
1	A	453	HIS
1	A	456	HIS
1	A	467	ASN
1	A	478	GLN
1	A	515	ASN
1	A	522	GLN
1	A	597	HIS
1	A	610	HIS
1	B	205	GLN
1	B	221	ASN
1	B	338	ASN
1	B	392	HIS
1	B	427	GLN
1	B	431	ASN
1	B	454	HIS
1	B	515	ASN

### 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	1611	-	51,58,58	1.39	7 (13%)	54,89,89	2.06	13 (24%)
2	FAD	B	1611	-	51,58,58	1.47	9 (17%)	54,89,89	2.21	10 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	1611	-	-	0/28/50/50	0/6/6/6
2	FAD	B	1611	-	-	0/28/50/50	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1611	FAD	O2B-C2B	-2.16	1.38	1.43
2	B	1611	FAD	C2A-N1A	2.12	1.37	1.33
2	A	1611	FAD	C2A-N1A	2.19	1.38	1.33
2	A	1611	FAD	C9A-N10	2.30	1.41	1.38
2	A	1611	FAD	C5X-N5	2.47	1.39	1.35
2	B	1611	FAD	C5X-N5	2.76	1.39	1.35
2	B	1611	FAD	C5'-C4'	2.82	1.56	1.51
2	B	1611	FAD	C1'-N10	3.12	1.51	1.48
2	A	1611	FAD	C2A-N3A	3.42	1.37	1.32
2	B	1611	FAD	C4X-N5	3.49	1.38	1.33
2	B	1611	FAD	C4-N3	3.51	1.39	1.33
2	A	1611	FAD	C4X-N5	3.55	1.38	1.33
2	B	1611	FAD	C10-N1	3.63	1.38	1.33
2	A	1611	FAD	C10-N1	3.72	1.38	1.33
2	A	1611	FAD	C4-N3	3.77	1.39	1.33
2	B	1611	FAD	C2A-N3A	4.20	1.39	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1611	FAD	N3A-C2A-N1A	-11.22	119.08	128.86
2	A	1611	FAD	N3A-C2A-N1A	-7.62	122.22	128.86
2	A	1611	FAD	O4'-C4'-C5'	-3.77	101.60	110.00
2	A	1611	FAD	O3B-C3B-C4B	-2.71	103.17	111.09
2	B	1611	FAD	C4X-C4-N3	-2.68	119.67	123.48
2	A	1611	FAD	C1B-N9A-C4A	-2.34	122.60	126.64
2	A	1611	FAD	C4X-C4-N3	-2.32	120.19	123.48
2	A	1611	FAD	C9A-C5X-N5	-2.30	118.82	122.24
2	B	1611	FAD	O5B-C5B-C4B	-2.09	101.61	109.00
2	B	1611	FAD	C4X-N5-C5X	2.01	118.88	116.76
2	A	1611	FAD	O4'-C4'-C3'	2.03	114.14	109.09
2	B	1611	FAD	C2A-N1A-C6A	2.04	122.33	118.77
2	A	1611	FAD	C4B-O4B-C1B	2.20	112.11	109.77
2	A	1611	FAD	C4-C4X-N5	2.30	121.20	118.68
2	B	1611	FAD	C4-C4X-N5	2.77	121.72	118.68
2	B	1611	FAD	C4B-O4B-C1B	3.05	113.02	109.77
2	B	1611	FAD	C5X-C9A-N10	3.31	120.12	117.66
2	A	1611	FAD	C5X-C9A-N10	3.97	120.60	117.66
2	B	1611	FAD	C1'-N10-C9A	3.97	121.99	118.35
2	A	1611	FAD	C4X-N5-C5X	4.33	121.34	116.76
2	A	1611	FAD	C1'-N10-C10	4.52	123.14	118.50
2	A	1611	FAD	C4-N3-C2	6.05	120.45	115.16
2	B	1611	FAD	C4-N3-C2	6.23	120.61	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1611	FAD	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	490/528 (92%)	0.67	38 (7%)	14 14	8, 13, 23, 30	6 (1%)
1	B	490/528 (92%)	0.77	55 (11%)	6 6	8, 13, 23, 30	9 (1%)
All	All	980/1056 (92%)	0.72	93 (9%)	9 9	8, 13, 23, 30	15 (1%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	570	LYS	5.8
1	B	539	GLU	5.6
1	A	373	VAL	5.1
1	B	374	SER	5.0
1	B	121	THR	4.9
1	B	273	GLY	4.9
1	B	376	GLY	4.9
1	B	375	GLY	4.9
1	A	221	ASN	4.8
1	B	569	ASP	4.6
1	A	275	GLU	4.5
1	A	376	GLY	4.5
1	B	182	ASP	4.4
1	B	219	ILE	4.4
1	A	121	THR	3.9
1	B	385	GLY	3.8
1	B	218	ASN	3.8
1	A	276	VAL	3.7
1	A	182	ASP	3.6
1	B	222	GLY	3.5
1	A	273	GLY	3.5
1	A	274	ALA	3.5
1	B	373	VAL	3.4
1	B	345	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	381	LYS	3.4
1	A	569	ASP	3.3
1	A	219	ILE	3.3
1	A	374	SER	3.3
1	B	268	ALA	3.3
1	B	274	ALA	3.2
1	A	375	GLY	3.2
1	A	278	SER	3.2
1	B	548	ALA	3.2
1	B	570	LYS	3.1
1	A	218	ASN	3.1
1	A	154	PRO	3.1
1	B	369	GLN	3.0
1	B	540	ILE	3.0
1	B	553	PRO	3.0
1	B	379	LEU	2.9
1	B	571	VAL	2.8
1	B	275	GLU	2.8
1	B	372	GLY	2.8
1	B	221	ASN	2.7
1	A	540	ILE	2.7
1	B	544	PRO	2.7
1	A	415	SER	2.7
1	A	546	ALA	2.6
1	B	300	LYS	2.5
1	A	327	ILE	2.5
1	B	538	SER	2.5
1	B	327	ILE	2.5
1	B	183	ASP	2.4
1	B	599	ASP	2.4
1	A	325	SER	2.4
1	B	184	PRO	2.4
1	B	276	VAL	2.4
1	A	271	ARG	2.4
1	B	154	PRO	2.3
1	B	389	GLU	2.3
1	A	217	PRO	2.3
1	B	415	SER	2.3
1	A	434	VAL	2.3
1	B	367	ILE	2.3
1	B	299	VAL	2.3
1	B	552	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	277	LYS	2.2
1	A	299	VAL	2.2
1	B	380	ILE	2.2
1	A	324	ALA	2.2
1	A	598	GLU	2.2
1	A	345	GLN	2.2
1	A	377	ARG	2.2
1	B	547	PRO	2.2
1	A	136	ILE	2.2
1	A	552	VAL	2.2
1	A	571	VAL	2.1
1	B	596	GLN	2.1
1	B	152	ARG	2.1
1	B	256	LEU	2.1
1	A	548	ALA	2.1
1	B	125	ILE	2.1
1	B	269	ILE	2.1
1	A	223	GLY	2.1
1	A	266	LEU	2.1
1	B	301	SER	2.1
1	A	124	GLN	2.1
1	B	378	LEU	2.0
1	B	258	ALA	2.0
1	B	377	ARG	2.0
1	A	544	PRO	2.0
1	B	257	ILE	2.0
1	B	391	ASP	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	B	1611	53/53	0.95	0.22	1.49	13,17,22,25	0
2	FAD	A	1611	53/53	0.94	0.21	1.43	12,16,19,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.