



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 04:58 PM EDT

PDB ID : 5L46
Title : Crystal structure of human dimethylglycine-dehydrogenase
Authors : Hromic, A.; Pavkov-Keller, T.; Gruber, K.
Deposited on : 2016-05-25
Resolution : 3.09 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

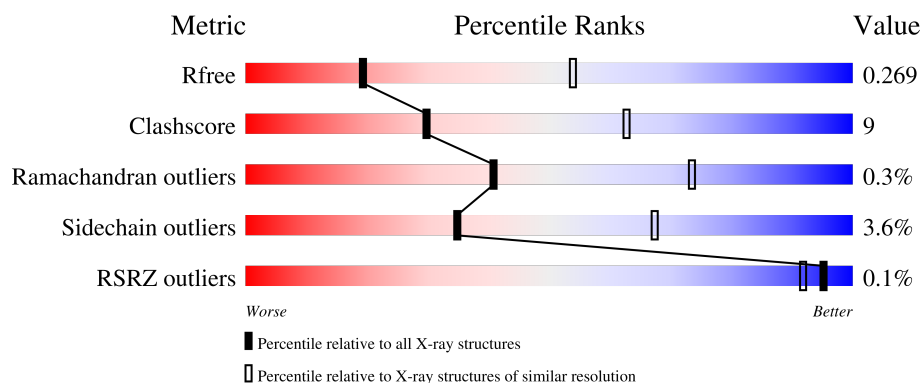
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	841	
1	B	841	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12894 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 Dimethylglycine dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	809	Total	C	N	O	S	0	0	0
			6398	4099	1090	1186	23			
1	B	808	Total	C	N	O	S	0	0	0
			6384	4088	1088	1185	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	initiating methionine	UNP Q9UI17
A	279	PRO	SER	conflict	UNP Q9UI17
A	867	ARG	-	expression tag	UNP Q9UI17
A	868	PRO	-	expression tag	UNP Q9UI17
B	28	MET	-	initiating methionine	UNP Q9UI17
B	279	PRO	SER	conflict	UNP Q9UI17
B	867	ARG	-	expression tag	UNP Q9UI17
B	868	PRO	-	expression tag	UNP Q9UI17

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

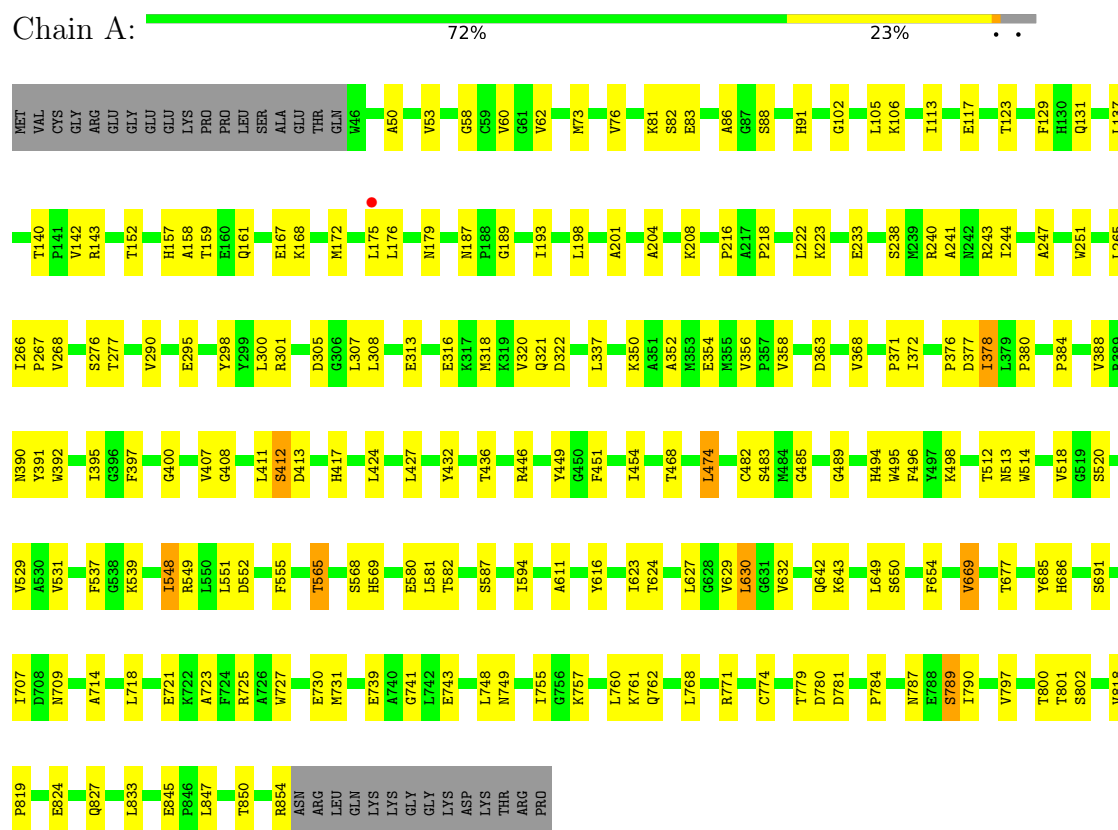
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	2	Total O 2 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Dimethylglycine dehydrogenase, mitochondrial



• Molecule 1: Dimethylglycine dehydrogenase, mitochondrial



V796	V797	T800	T801	S802	L813	A814	F815	V818	P819	L822	S823	E824	Q827	L833	L834	G835	K836	N837	I842	E845	P846	L847	L848	L849	T850	E851	P852	T853	R854	ASN	ARG	LEU	GLN	LYS	LYS	GLY	GLY	LYS	ASP	LYS	THR	ARG	PRO
R688	E689	D690	S691	F710	N716	R719	L720	E721	K722	R725	A726	W727	E730	N731	N732	C733	L738	E739	F745	V746	N749	Q758	A759	L760	K761	Q762	A765	L768	K769	L772	L775	T776	L777	D780	D781	P784	N787	I790	N793	G794	K795		
V562	T565	N566	I567	S568	T572	P573	K574	Y578	L581	S587	P588	I594	R605	V612	K621	T624	L627	L630	R638	K643	L644	S650	F654	L657	Q658	T659	K660	V664	I667	P668	V669	I672	W682	Y685	H686	R687							
D423	L424	Y432	T436	R446	E447	S448	Y449	G450	F451	N452	N453	I454	Y457	R462	R466	C482	G485	F486	H487	E491	Q492	P493	H494	W495	F496	P507	R511	T512	N513	W514	Q524	A530	V531	T532	F537	G538	K539	F540	N541	I542	L551	F555	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.38Å 119.87Å 86.47Å 90.00° 92.58° 90.00°	Depositor
Resolution (Å)	58.65 – 3.09 58.65 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.7 (58.65-3.09) 97.7 (58.65-3.09)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.179 , 0.269 0.182 , 0.269	Depositor DCC
R_{free} test set	1525 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.003 for l,k,-h 0.068 for h,-k,-l 0.030 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12894	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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	0.49	1/6558 (0.0%)	0.66	0/8895
1	B	0.50	0/6542	0.64	1/8872 (0.0%)
All	All	0.50	1/13100 (0.0%)	0.65	1/17767 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	774	CYS	CB-SG	-5.00	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	813	LEU	CA-CB-CG	5.69	128.39	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6398	0	6352	115	0
1	B	6384	0	6342	128	0
2	A	53	0	30	6	0
2	B	53	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	0	0	0
3	B	2	0	0	0	0
All	All	12894	0	12754	241	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 9.

All (241) 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:290:VAL:HG13	1:B:301:ARG:HB3	1.54	0.90
1:B:487:HIS:CD2	1:B:492:GLN:HE21	2.01	0.78
1:A:290:VAL:HG13	1:A:301:ARG:HB3	1.66	0.76
1:A:755:ILE:HD11	1:B:793:ASN:HD21	1.53	0.74
1:B:115:LEU:HA	1:B:118:LYS:HE2	1.71	0.72
1:A:73:MET:HG2	1:A:76:VAL:HG22	1.72	0.71
1:B:730:GLU:OE2	1:B:802:SER:OG	2.08	0.70
1:A:677:THR:HG22	1:A:718:LEU:HD13	1.76	0.68
1:B:143:ARG:NH2	1:B:453:ASN:O	2.28	0.67
1:B:73:MET:HG2	1:B:76:VAL:HG22	1.77	0.66
1:B:176:LEU:HD11	1:B:355:MET:HG3	1.78	0.65
1:B:687:ARG:HG3	1:B:689:GLU:HG2	1.80	0.64
1:A:277:THR:HG23	1:A:305:ASP:HB3	1.77	0.64
1:A:723:ALA:O	1:A:725:ARG:NH1	2.30	0.63
1:A:787:ASN:N	1:A:800:THR:O	2.29	0.63
1:A:337:LEU:HD11	1:A:368:VAL:HG13	1.80	0.63
1:A:152:THR:O	1:A:789:SER:OG	2.15	0.63
1:B:487:HIS:HD2	1:B:492:GLN:HE21	1.44	0.62
1:B:356:VAL:HG12	1:B:358:VAL:HG22	1.80	0.62
1:B:562:VAL:HG11	1:B:588:PRO:HG3	1.81	0.62
1:B:686:HIS:NE2	1:B:691:SER:OG	2.32	0.62
1:A:408:GLY:O	1:A:412:SER:HB3	2.01	0.61
1:A:413:ASP:O	1:A:417:HIS:ND1	2.32	0.61
1:A:739:GLU:HB3	1:A:768:LEU:HD22	1.82	0.61
1:A:251:TRP:CE3	2:A:901:FAD:H8A	2.36	0.60
1:A:267:PRO:HB2	1:A:321:GLN:HB2	1.83	0.60
1:A:721:GLU:HG2	1:A:847:LEU:HD23	1.83	0.59
1:A:313:GLU:HG2	1:A:449:TYR:HE2	1.68	0.59
1:B:137:LEU:HD11	1:B:176:LEU:HD21	1.85	0.58
1:B:234:THR:HG22	1:B:236:GLN:H	1.67	0.58
1:B:219:VAL:H	2:B:901:FAD:H61A	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:LEU:HD22	1:B:555:PHE:HE2	1.70	0.57
1:A:81:LYS:HG3	1:A:218:PRO:HB3	1.85	0.57
1:B:81:LYS:HG3	1:B:218:PRO:HB3	1.87	0.56
1:A:380:PRO:HG2	1:A:427:LEU:HD11	1.87	0.56
1:A:485:GLY:HA3	1:A:494:HIS:CE1	2.41	0.56
1:B:161:GLN:HG3	1:B:187:ASN:OD1	2.05	0.56
1:A:175:LEU:HD13	1:A:358:VAL:HG11	1.87	0.55
1:A:630:LEU:HD12	1:A:686:HIS:CE1	2.42	0.55
1:B:80:GLU:HA	2:B:901:FAD:H8A	1.89	0.55
1:B:300:LEU:HD21	1:B:307:LEU:HD22	1.87	0.55
1:A:850:THR:O	1:A:854:ARG:HG3	2.07	0.54
1:B:262:GLU:OE1	1:B:262:GLU:N	2.35	0.54
1:A:468:THR:OG1	1:A:489:GLY:O	2.26	0.54
1:B:716:ASN:O	1:B:719:ARG:HG3	2.08	0.54
1:A:397:PHE:HZ	1:A:407:VAL:HG11	1.73	0.54
1:A:581:LEU:HB2	1:A:594:ILE:O	2.08	0.54
1:A:356:VAL:HG12	1:A:358:VAL:HG22	1.89	0.53
1:B:638:ARG:HD3	1:B:650:SER:HA	1.90	0.53
1:A:784:PRO:HA	1:A:833:LEU:HD21	1.90	0.53
1:A:193:ILE:HG21	1:A:198:LEU:HD22	1.89	0.53
1:A:266:ILE:HD11	1:A:320:VAL:HB	1.89	0.53
1:B:277:THR:HG23	1:B:305:ASP:HB3	1.91	0.53
1:B:511:ARG:NH1	1:B:780:ASP:O	2.42	0.52
1:A:131:GLN:NE2	1:A:189:GLY:O	2.42	0.52
1:A:143:ARG:NE	1:A:295:GLU:OE2	2.29	0.52
1:A:83:GLU:HG3	1:A:86:ALA:HB2	1.92	0.52
1:A:137:LEU:HD11	1:A:176:LEU:HD21	1.92	0.52
1:B:787:ASN:N	1:B:800:THR:O	2.35	0.52
1:B:721:GLU:HG2	1:B:847:LEU:HD23	1.91	0.52
1:A:518:VAL:HG13	1:A:714:ALA:HA	1.92	0.51
1:B:228:GLY:O	1:B:390:ASN:ND2	2.30	0.51
1:B:244:ILE:HG13	1:B:391:TYR:HD1	1.73	0.51
1:B:836:LYS:HE3	1:B:837:ASN:H	1.74	0.51
1:B:245:VAL:HG22	1:B:392:TRP:HB2	1.91	0.51
1:B:482:CYS:HB3	1:B:496:PHE:CD1	2.46	0.51
1:A:161:GLN:HG3	1:A:187:ASN:OD1	2.11	0.51
1:B:259:ILE:HG13	1:B:261:LEU:HG	1.92	0.51
1:B:449:TYR:O	1:B:452:ASN:HB2	2.10	0.51
1:A:630:LEU:HD12	1:A:686:HIS:HE1	1.76	0.51
1:B:487:HIS:CE1	1:B:494:HIS:HE2	2.28	0.51
1:B:790:ILE:HD11	1:B:818:VAL:HG12	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:769:LYS:HB3	1:B:769:LYS:NZ	2.26	0.50
1:A:265:LEU:HD11	1:A:395:ILE:HD12	1.94	0.50
1:B:539:LYS:HD3	1:B:627:LEU:HB2	1.93	0.50
1:A:582:THR:HB	1:A:594:ILE:HB	1.94	0.50
1:B:268:VAL:HG12	1:B:320:VAL:HG12	1.93	0.50
1:A:432:TYR:HB3	1:A:436:THR:OG1	2.12	0.50
1:A:240:ARG:NH2	1:B:765:ALA:O	2.45	0.49
1:B:739:GLU:HB3	1:B:768:LEU:HD22	1.94	0.49
1:B:386:GLN:HB2	1:B:605:ARG:HB2	1.95	0.49
1:A:204:ALA:O	1:A:208:LYS:HB2	2.12	0.49
1:A:301:ARG:CZ	1:A:308:LEU:HD13	2.43	0.49
1:B:143:ARG:NE	1:B:295:GLU:OE2	2.40	0.49
1:B:539:LYS:HD2	1:B:624:THR:HA	1.94	0.49
1:B:313:GLU:HG2	1:B:449:TYR:HE2	1.78	0.49
1:A:498:LYS:HE3	1:A:520:SER:OG	2.12	0.49
1:B:276:SER:N	1:B:363:ASP:O	2.45	0.49
1:B:485:GLY:HA3	1:B:494:HIS:CE1	2.48	0.49
1:B:278:ILE:HG12	1:B:362:ALA:HB2	1.94	0.49
1:B:153:ARG:HA	1:B:787:ASN:O	2.13	0.49
1:B:827:GLN:HB3	1:B:842:ILE:HD12	1.93	0.49
1:A:669:VAL:HG23	1:A:686:HIS:HB3	1.94	0.49
1:B:524:GLN:HG2	1:B:530:ALA:HB2	1.94	0.48
1:A:244:ILE:HG13	1:A:391:TYR:HD1	1.78	0.48
1:A:569:HIS:CE1	1:A:580:GLU:HG3	2.48	0.48
1:A:548:ILE:O	1:A:552:ASP:HB2	2.13	0.48
1:B:154:THR:HG21	1:B:161:GLN:NE2	2.29	0.48
1:B:638:ARG:HG3	1:B:682:TRP:HH2	1.78	0.48
1:A:451:PHE:HA	1:A:454:ILE:HG23	1.94	0.48
1:B:432:TYR:HB3	1:B:436:THR:OG1	2.14	0.48
1:B:297:SER:HA	1:B:453:ASN:HD22	1.78	0.48
1:A:400:GLY:HA3	2:A:901:FAD:H4'	1.95	0.47
1:B:60:VAL:HG22	2:B:901:FAD:O2P	2.14	0.47
1:B:667:ILE:O	1:B:669:VAL:HG23	2.15	0.47
1:B:230:TRP:O	1:B:240:ARG:HA	2.15	0.47
1:B:664:VAL:O	1:B:667:ILE:HB	2.15	0.47
1:A:301:ARG:NH2	1:A:308:LEU:HD13	2.29	0.47
1:A:318:MET:SD	1:A:446:ARG:HG3	2.55	0.47
1:A:106:LYS:HD2	1:A:157:HIS:CE1	2.50	0.47
1:B:374:TYR:CE2	1:B:378:ILE:HG13	2.49	0.47
1:A:757:LYS:HE2	1:A:761:LYS:NZ	2.30	0.47
1:B:58:GLY:O	1:B:62:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:TRP:CE2	1:A:514:TRP:HB3	2.50	0.47
1:A:551:LEU:HD22	1:A:555:PHE:HE2	1.79	0.46
1:A:781:ASP:OD1	1:A:781:ASP:N	2.48	0.46
1:B:95:LEU:HD23	1:B:192:HIS:HB3	1.96	0.46
1:B:495:TRP:CE2	1:B:514:TRP:HB3	2.51	0.46
1:B:644:LEU:HB3	1:B:664:VAL:HG13	1.97	0.46
1:A:411:LEU:HA	1:A:411:LEU:HD23	1.71	0.46
1:B:781:ASP:OD1	1:B:781:ASP:N	2.48	0.46
1:B:797:VAL:O	1:B:819:PRO:HD3	2.16	0.46
1:A:482:CYS:HB3	1:A:496:PHE:CD1	2.50	0.46
1:B:411:LEU:HD23	1:B:411:LEU:HA	1.61	0.46
1:A:529:VAL:HG13	1:A:707:ILE:HG13	1.98	0.46
1:B:269:GLN:HB3	1:B:344:ARG:HH22	1.81	0.46
1:B:746:VAL:HG11	1:B:760:LEU:HD13	1.98	0.46
1:B:532:THR:HB	1:B:710:PHE:CE1	2.51	0.46
1:B:410:TYR:OH	1:B:424:LEU:HB2	2.17	0.45
1:A:790:ILE:HD11	1:A:818:VAL:HG12	1.98	0.45
1:B:572:THR:HG23	1:B:578:TYR:HB2	1.98	0.45
1:A:565:THR:HG23	1:A:582:THR:HG23	1.99	0.45
1:B:451:PHE:HA	1:B:454:ILE:HG23	1.99	0.45
1:B:581:LEU:HB2	1:B:594:ILE:O	2.17	0.45
1:A:730:GLU:OE2	1:A:802:SER:OG	2.22	0.45
1:B:845:GLU:H	1:B:845:GLU:HG2	1.55	0.45
1:A:222:LEU:O	1:A:223:LYS:HD2	2.17	0.45
1:A:424:LEU:HD13	1:A:427:LEU:HD22	1.98	0.45
1:A:376:PRO:HD2	1:A:432:TYR:CZ	2.52	0.45
1:B:168:LYS:O	1:B:172:MET:HG3	2.17	0.45
1:B:316:GLU:HG2	1:B:317:LYS:N	2.31	0.45
1:B:541:ASN:HB3	1:B:621:LYS:HG3	1.99	0.45
1:B:658:GLN:OE1	1:B:660:LYS:HE3	2.17	0.45
1:B:376:PRO:HD2	1:B:432:TYR:CZ	2.52	0.45
2:A:901:FAD:H1'2	2:A:901:FAD:H9	1.59	0.45
1:A:300:LEU:HD21	1:A:307:LEU:HD22	1.99	0.44
1:A:748:LEU:HD21	1:A:760:LEU:HD13	2.00	0.44
1:B:758:GLN:O	1:B:762:GLN:HG3	2.17	0.44
1:B:836:LYS:HE3	1:B:837:ASN:N	2.33	0.44
1:B:119:LEU:HD12	1:B:119:LEU:HA	1.79	0.44
1:B:300:LEU:HD12	1:B:309:PHE:HB3	1.99	0.44
1:A:780:ASP:HB3	1:A:781:ASP:OD1	2.18	0.44
1:A:384:PRO:HD3	1:A:392:TRP:CZ3	2.53	0.44
1:A:539:LYS:HD2	1:A:624:THR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.59	0.44
1:B:193:ILE:HD13	1:B:198:LEU:HD22	2.00	0.44
1:B:537:PHE:O	1:B:539:LYS:NZ	2.43	0.44
1:B:687:ARG:HG3	1:B:689:GLU:CG	2.47	0.43
1:A:268:VAL:O	1:A:371:PRO:HA	2.19	0.43
1:A:377:ASP:O	1:A:378:ILE:HG22	2.19	0.43
1:A:611:ALA:HA	1:A:616:TYR:HD2	1.84	0.43
1:A:797:VAL:O	1:A:819:PRO:HD3	2.18	0.43
1:B:137:LEU:HD13	1:B:181:VAL:HG22	1.99	0.43
1:B:313:GLU:OE2	1:B:344:ARG:NE	2.29	0.43
1:A:60:VAL:HG23	1:A:247:ALA:HB1	2.01	0.43
1:B:738:LEU:HG	1:B:760:LEU:HD22	2.00	0.43
1:B:419:GLU:OE1	1:B:574:LYS:HB2	2.18	0.43
1:A:58:GLY:O	1:A:62:VAL:HG23	2.19	0.43
1:A:233:GLU:OE2	1:A:238:SER:HB3	2.18	0.43
1:A:267:PRO:HA	1:A:372:ILE:O	2.19	0.43
1:A:741:GLY:HA2	1:A:743:GLU:OE2	2.18	0.43
1:B:565:THR:O	1:B:657:LEU:HD13	2.19	0.43
1:B:672:ILE:HD12	1:B:685:TYR:HE2	1.83	0.43
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.52	0.43
1:B:725:ARG:HD3	1:B:772:LEU:HD23	2.01	0.43
1:A:60:VAL:HG22	2:A:901:FAD:O1P	2.19	0.42
1:A:82:SER:HA	1:A:216:PRO:HB3	2.00	0.42
1:A:113:ILE:O	1:A:117:GLU:HG3	2.19	0.42
1:B:512:THR:OG1	1:B:513:ASN:N	2.52	0.42
1:B:288:LEU:HA	1:B:289:PRO:HD3	1.91	0.42
1:B:413:ASP:O	1:B:417:HIS:ND1	2.39	0.42
1:B:727:TRP:HA	1:B:731:MET:HG2	2.01	0.42
1:A:60:VAL:HG13	2:A:901:FAD:O1P	2.19	0.42
1:A:376:PRO:HD2	1:A:432:TYR:CE2	2.55	0.42
1:B:485:GLY:HA3	1:B:494:HIS:NE2	2.34	0.42
1:A:549:ARG:NH2	1:B:795:LYS:HE2	2.34	0.42
1:B:457:TYR:CG	1:B:507:PRO:HB2	2.54	0.42
1:A:50:ALA:O	1:A:241:ALA:HA	2.19	0.42
1:A:642:GLN:HA	1:A:649:LEU:HD12	2.01	0.42
1:A:727:TRP:HA	1:A:731:MET:HG2	2.02	0.42
1:A:168:LYS:O	1:A:172:MET:HB2	2.20	0.42
1:A:512:THR:OG1	1:A:513:ASN:N	2.48	0.42
1:B:214:LYS:HD2	1:B:214:LYS:HA	1.81	0.42
1:B:246:ASN:HB3	1:B:393:VAL:HG12	2.01	0.42
1:B:567:ILE:HB	1:B:745:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:THR:HG22	1:B:396:GLY:HA2	2.01	0.42
1:A:350:LYS:O	1:A:354:GLU:HG2	2.19	0.42
1:A:388:VAL:HG23	1:A:391:TYR:HB3	2.01	0.42
1:B:55:ILE:HG12	1:B:219:VAL:HG21	2.02	0.42
1:A:276:SER:N	1:A:363:ASP:O	2.50	0.42
1:A:611:ALA:HA	1:A:616:TYR:CD2	2.55	0.41
1:A:629:VAL:HG22	1:A:685:TYR:CD1	2.54	0.41
1:B:630:LEU:HD23	1:B:630:LEU:HA	1.94	0.41
1:B:851:GLU:HB3	1:B:852:PRO:HD3	2.01	0.41
1:A:123:THR:HG21	1:A:201:ALA:O	2.20	0.41
1:B:836:LYS:HD2	1:B:836:LYS:HA	1.64	0.41
1:A:739:GLU:HA	1:A:768:LEU:HD13	2.02	0.41
1:A:158:ALA:O	1:A:159:THR:C	2.58	0.41
1:B:466:ARG:NH2	1:B:491:GLU:OE1	2.50	0.41
1:B:103:ILE:HD11	1:B:153:ARG:CZ	2.50	0.41
1:B:727:TRP:CD1	1:B:731:MET:HG3	2.56	0.41
1:A:251:TRP:CD2	2:A:901:FAD:H8A	2.55	0.41
1:A:474:LEU:HA	1:A:474:LEU:HD23	1.86	0.41
1:B:555:PHE:CZ	1:B:581:LEU:HD11	2.55	0.41
1:A:298:TYR:CZ	1:A:352:ALA:HA	2.56	0.41
1:A:669:VAL:CG2	1:A:686:HIS:HB3	2.51	0.41
1:A:818:VAL:HG23	1:A:819:PRO:O	2.21	0.41
1:B:722:LYS:HD2	1:B:850:THR:HG22	2.03	0.41
1:A:140:THR:HG23	1:A:295:GLU:HG3	2.03	0.41
1:A:496:PHE:CE2	1:A:709:ASN:HB3	2.56	0.41
1:A:514:TRP:HE3	1:A:514:TRP:O	2.04	0.41
1:A:531:VAL:HG22	1:A:632:VAL:HG22	2.03	0.41
1:A:623:ILE:HG13	1:A:627:LEU:HD13	2.02	0.41
1:A:845:GLU:H	1:A:845:GLU:HG2	1.68	0.41
1:B:68:LEU:O	1:B:73:MET:HB3	2.21	0.41
1:B:79:LEU:HB3	1:B:217:ALA:O	2.21	0.41
1:B:165:GLU:HB3	1:B:167:GLU:OE2	2.21	0.41
1:B:389:ARG:CZ	1:B:612:VAL:HG11	2.51	0.41
1:B:451:PHE:HD2	1:B:462:ARG:HD3	1.86	0.41
1:A:168:LYS:HE2	1:A:168:LYS:HB2	1.88	0.41
1:B:318:MET:SD	1:B:446:ARG:HG2	2.61	0.40
1:B:822:LEU:O	1:B:827:GLN:HG2	2.22	0.40
1:B:846:PRO:HG2	1:B:849:LEU:HD23	2.03	0.40
1:A:53:VAL:HG23	1:A:241:ALA:HB2	2.04	0.40
1:B:278:ILE:HG21	1:B:358:VAL:HB	2.04	0.40
1:B:423:ASP:HB2	1:B:733:CYS:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:834:LEU:HD23	1:B:834:LEU:HA	1.71	0.40
1:A:88:SER:O	1:A:91:HIS:ND1	2.54	0.40
1:A:243:ARG:HA	1:A:390:ASN:HB3	2.04	0.40
1:A:824:GLU:HG2	1:A:827:GLN:HB2	2.03	0.40
1:B:784:PRO:HA	1:B:833:LEU:HD21	2.04	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	807/841 (96%)	765 (95%)	39 (5%)	3 (0%)	34	69
1	B	806/841 (96%)	756 (94%)	48 (6%)	2 (0%)	47	79
All	All	1613/1682 (96%)	1521 (94%)	87 (5%)	5 (0%)	41	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	ILE
1	B	378	ILE
1	A	537	PHE
1	B	102	GLY
1	A	102	GLY

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	682/709 (96%)	657 (96%)	25 (4%)	34	66
1	B	681/709 (96%)	657 (96%)	24 (4%)	36	68
All	All	1363/1418 (96%)	1314 (96%)	49 (4%)	35	67

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	PHE
1	A	142	VAL
1	A	167	GLU
1	A	179	ASN
1	A	316	GLU
1	A	322	ASP
1	A	412	SER
1	A	474	LEU
1	A	483	SER
1	A	548	ILE
1	A	565	THR
1	A	568	SER
1	A	587	SER
1	A	630	LEU
1	A	643	LYS
1	A	650	SER
1	A	654	PHE
1	A	669	VAL
1	A	691	SER
1	A	749	ASN
1	A	762	GLN
1	A	771	ARG
1	A	779	THR
1	A	789	SER
1	A	801	THR
1	B	108	ILE
1	B	129	PHE
1	B	163	LEU
1	B	254	GLU
1	B	316	GLU
1	B	320	VAL
1	B	322	ASP
1	B	448	SER
1	B	542	ILE

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Mol	Chain	Res	Type
1	B	568	SER
1	B	587	SER
1	B	643	LYS
1	B	654	PHE
1	B	691	SER
1	B	749	ASN
1	B	775	LEU
1	B	777	LEU
1	B	780	ASP
1	B	790	ILE
1	B	797	VAL
1	B	801	THR
1	B	815	PHE
1	B	824	GLU
1	B	836	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	ASN
1	A	494	HIS
1	B	487	HIS
1	B	793	ASN

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 monosaccharides 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	901	1	53,58,58	1.36	8 (15%)	68,89,89	1.85	18 (26%)
2	FAD	B	901	1	53,58,58	1.40	6 (11%)	68,89,89	1.53	14 (20%)

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	901	1	-	17/30/50/50	0/6/6/6
2	FAD	B	901	1	-	3/30/50/50	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	FAD	C9A-C5X	5.70	1.50	1.41
2	A	901	FAD	C9A-C5X	4.86	1.49	1.41
2	B	901	FAD	C8-C7	3.25	1.49	1.40
2	A	901	FAD	C8-C7	3.21	1.48	1.40
2	A	901	FAD	C10-N10	3.19	1.44	1.37
2	A	901	FAD	C4-N3	-3.07	1.33	1.38
2	B	901	FAD	C5A-C4A	2.97	1.48	1.40
2	B	901	FAD	C4-N3	-2.49	1.34	1.38
2	B	901	FAD	C5X-N5	-2.48	1.34	1.39
2	B	901	FAD	O4B-C1B	2.37	1.44	1.41
2	A	901	FAD	O4B-C1B	2.34	1.44	1.41
2	A	901	FAD	C4X-N5	2.28	1.35	1.30
2	A	901	FAD	C2-N3	-2.24	1.33	1.39
2	A	901	FAD	C5X-N5	-2.19	1.35	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	FAD	C1'-N10-C9A	-6.53	109.63	120.51
2	A	901	FAD	C5X-C9A-N10	4.36	122.45	117.95
2	A	901	FAD	C4X-C10-N1	-3.98	115.50	124.73
2	B	901	FAD	C1'-N10-C9A	3.64	126.58	120.51
2	A	901	FAD	N3A-C2A-N1A	-3.59	123.07	128.68
2	A	901	FAD	C5'-C4'-C3'	3.54	119.04	112.20
2	B	901	FAD	C1'-C2'-C3'	3.47	119.48	109.79
2	A	901	FAD	O4'-C4'-C5'	-3.45	102.16	109.92
2	B	901	FAD	C4X-C10-N10	3.32	121.34	116.48
2	A	901	FAD	C9A-N10-C10	-3.10	115.94	120.77
2	B	901	FAD	N3A-C2A-N1A	-3.00	123.99	128.68
2	A	901	FAD	C10-N1-C2	2.93	122.75	116.90
2	B	901	FAD	C9A-N10-C10	-2.92	116.22	120.77
2	B	901	FAD	N6A-C6A-N1A	2.78	124.35	118.57
2	B	901	FAD	C4X-C10-N1	-2.78	118.29	124.73
2	A	901	FAD	C9-C9A-N10	-2.70	118.19	121.84
2	A	901	FAD	O2'-C2'-C1'	2.68	116.28	109.80
2	A	901	FAD	N10-C10-N1	2.63	125.91	118.35
2	A	901	FAD	C9A-C5X-N5	-2.63	119.58	122.43
2	B	901	FAD	O2-C2-N1	-2.38	117.88	121.83
2	B	901	FAD	O4-C4-C4X	-2.37	120.31	126.60
2	B	901	FAD	O5'-C5'-C4'	2.28	115.45	109.36
2	A	901	FAD	C4-N3-C2	-2.27	121.45	125.64
2	B	901	FAD	C10-N1-C2	2.24	121.37	116.90
2	A	901	FAD	C4X-C4-N3	2.21	118.81	113.19
2	B	901	FAD	C1B-N9A-C4A	2.21	130.53	126.64
2	B	901	FAD	O4B-C1B-C2B	-2.14	103.80	106.93
2	A	901	FAD	O3'-C3'-C4'	2.10	113.88	108.81
2	A	901	FAD	C3B-C2B-C1B	2.10	104.13	100.98
2	A	901	FAD	O4-C4-C4X	-2.03	121.23	126.60
2	B	901	FAD	O3'-C3'-C4'	-2.02	103.93	108.81
2	A	901	FAD	N3-C2-N1	2.01	123.33	119.38

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	FAD	C5B-O5B-PA-O1A
2	A	901	FAD	C5B-O5B-PA-O2A
2	A	901	FAD	C5B-O5B-PA-O3P
2	A	901	FAD	C2'-C1'-N10-C9A
2	A	901	FAD	C2'-C1'-N10-C10
2	A	901	FAD	N10-C1'-C2'-O2'

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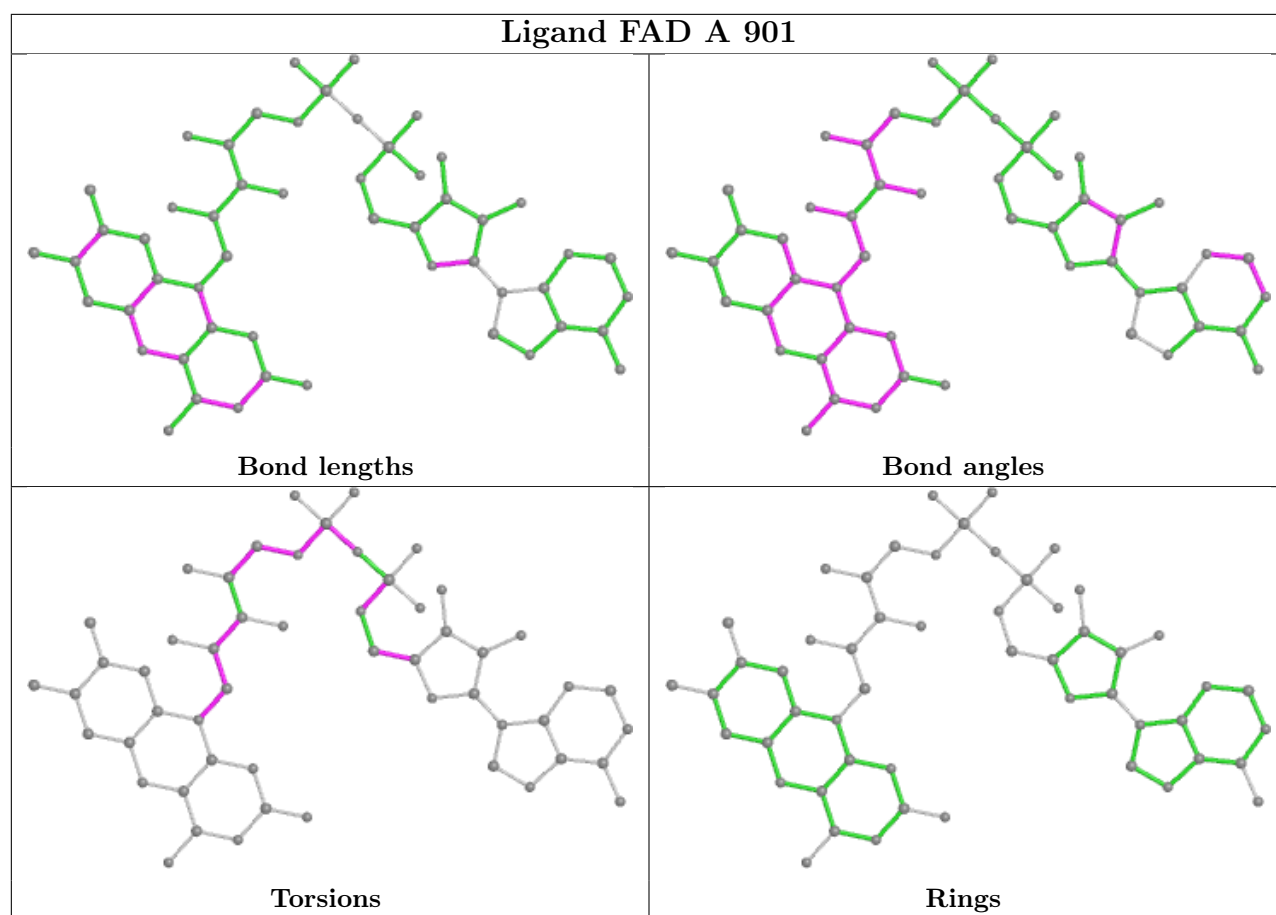
Mol	Chain	Res	Type	Atoms
2	A	901	FAD	N10-C1'-C2'-C3'
2	A	901	FAD	C3'-C4'-C5'-O5'
2	A	901	FAD	O4'-C4'-C5'-O5'
2	A	901	FAD	C5'-O5'-P-O3P
2	A	901	FAD	PA-O3P-P-O5'
2	B	901	FAD	C3'-C4'-C5'-O5'
2	B	901	FAD	PA-O3P-P-O5'
2	A	901	FAD	O4B-C4B-C5B-O5B
2	A	901	FAD	C3B-C4B-C5B-O5B
2	A	901	FAD	C4'-C5'-O5'-P
2	A	901	FAD	C5'-O5'-P-O1P
2	B	901	FAD	O4B-C4B-C5B-O5B
2	A	901	FAD	PA-O3P-P-O2P
2	A	901	FAD	C1'-C2'-C3'-O3'

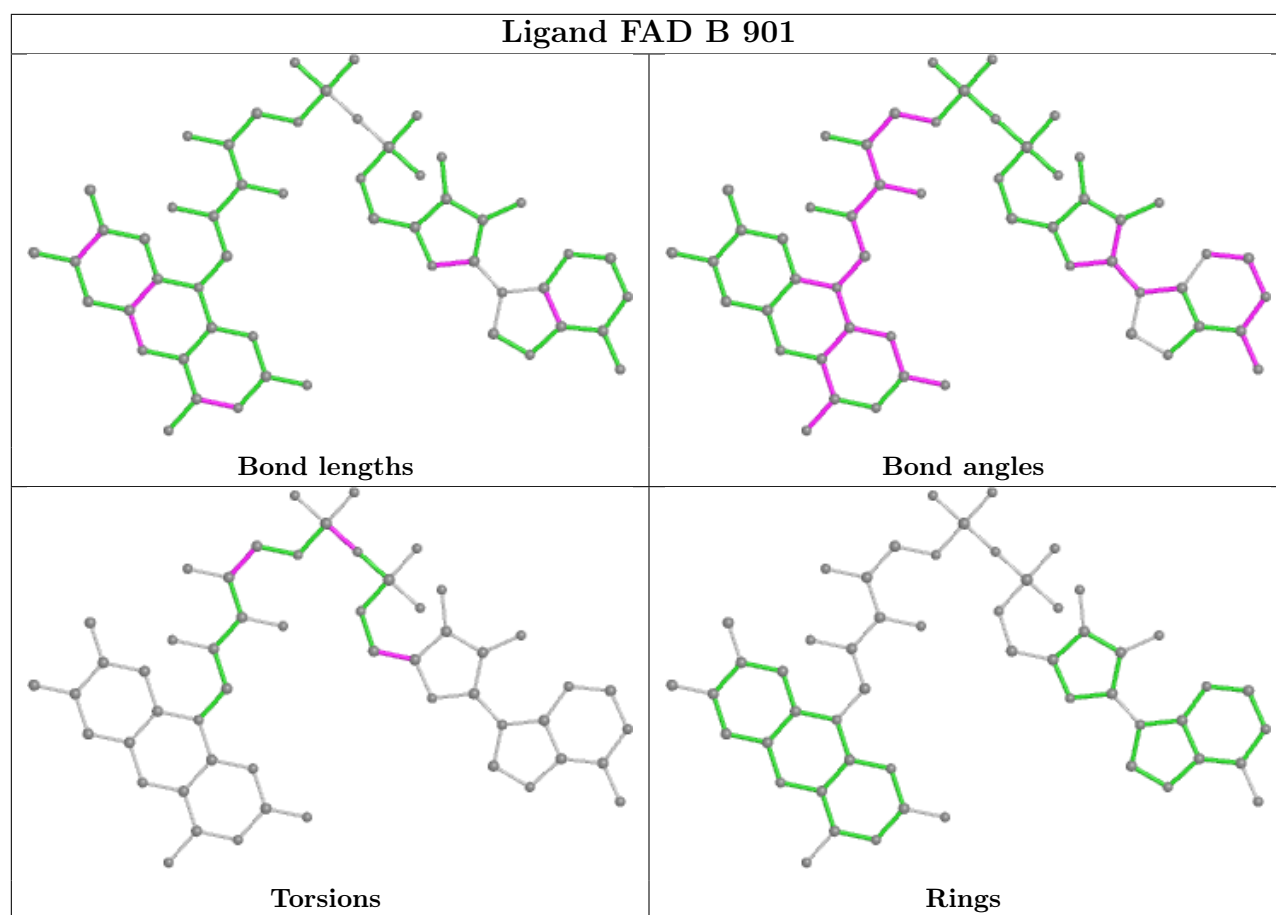
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	FAD	6	0
2	B	901	FAD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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	809/841 (96%)	-0.34	1 (0%) 95 92	7, 36, 61, 98	0
1	B	808/841 (96%)	-0.36	0 100 100	10, 36, 62, 105	0
All	All	1617/1682 (96%)	-0.35	1 (0%) 95 92	7, 36, 62, 105	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	LEU	2.2

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 monosaccharides in this entry.

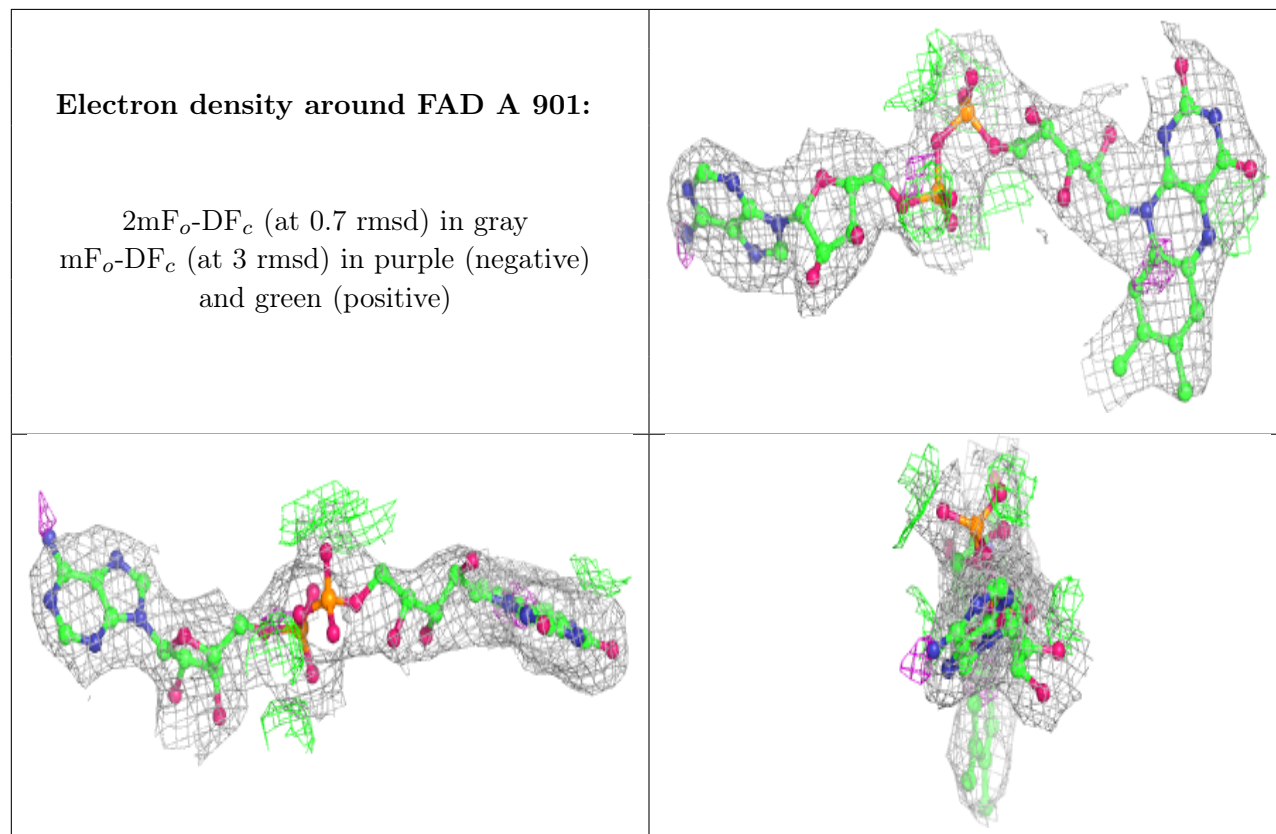
6.4 Ligands [i](#)

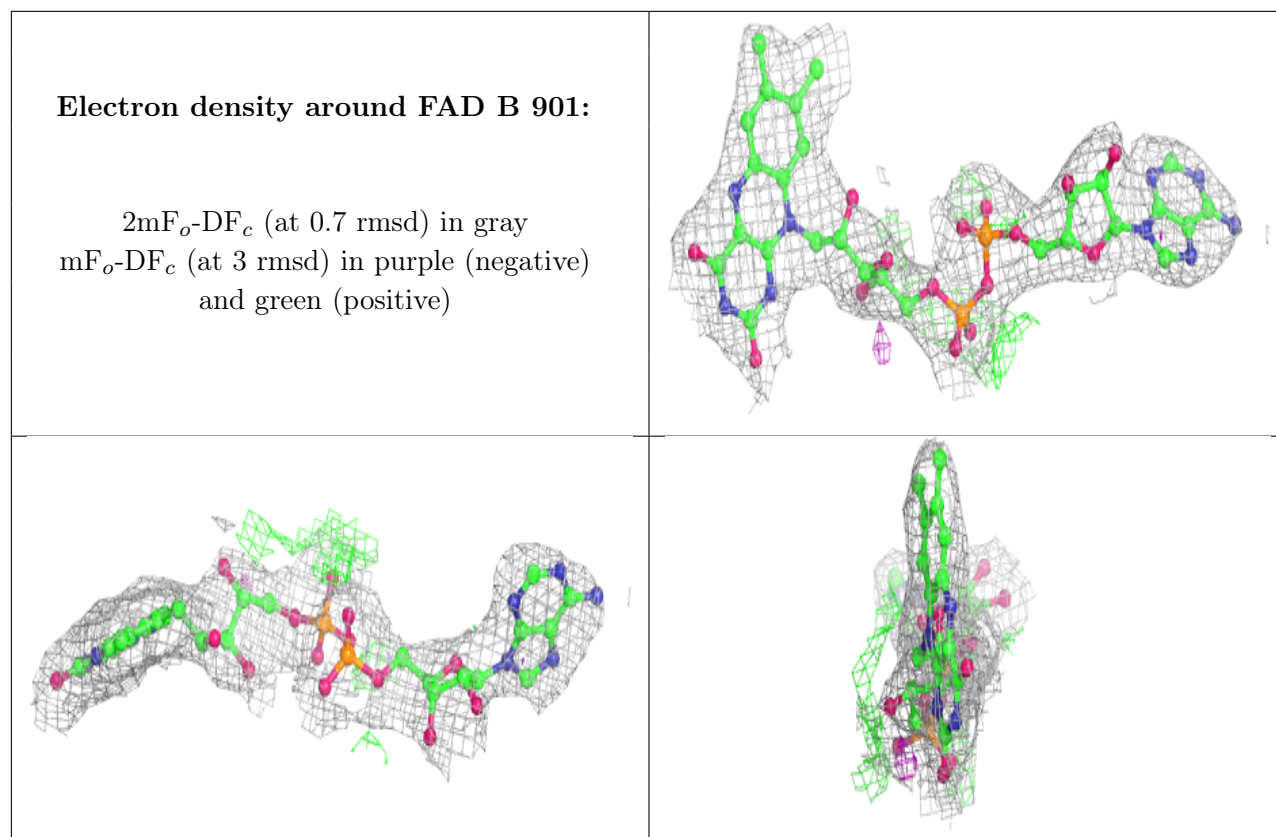
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	A	901	53/53	0.95	0.17	25,25,25,25	0
2	FAD	B	901	53/53	0.95	0.17	34,34,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.