



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 06:16 pm GMT

PDB ID : 2V1D
Title : Structural basis of LSD1-CoREST selectivity in histone H3 recognition
Authors : Forneris, F.; Binda, C.; Adamo, A.; Battaglioli, E.; Mattevi, A.
Deposited on : 2007-05-23
Resolution : 3.10 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

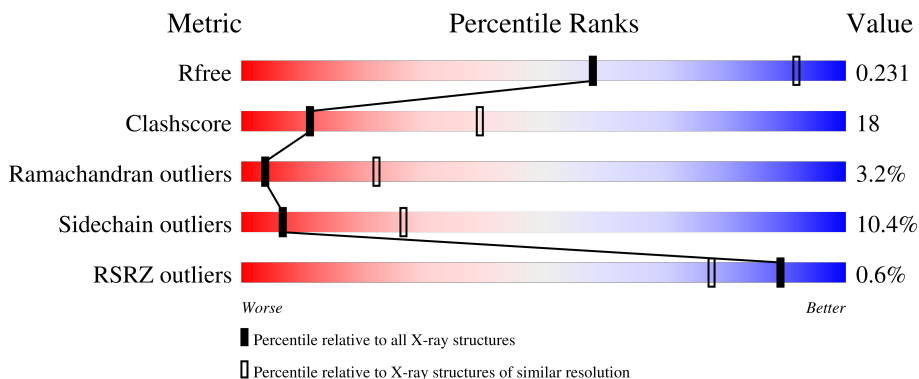
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	730	
2	B	178	
3	C	21	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6460 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 LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	5217	3324	906	967	20	0	0	0

- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	133	1076	676	194	203	3	0	0	0

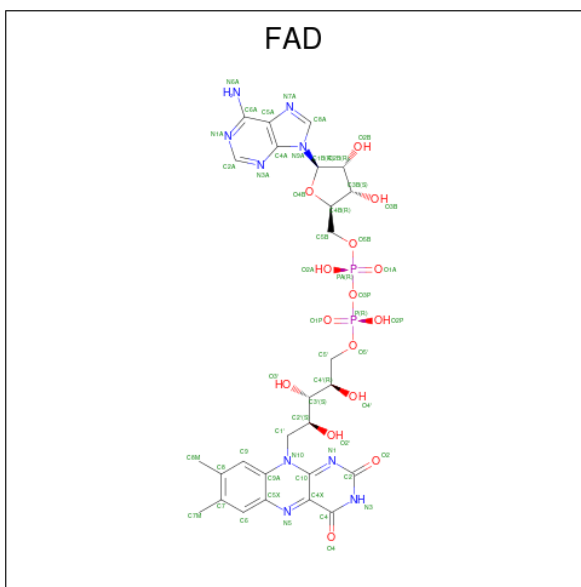
- Molecule 3 is a protein called HISTONE H3.1T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	16	114	67	25	21	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	LYS	engineered mutation	UNP Q16695

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

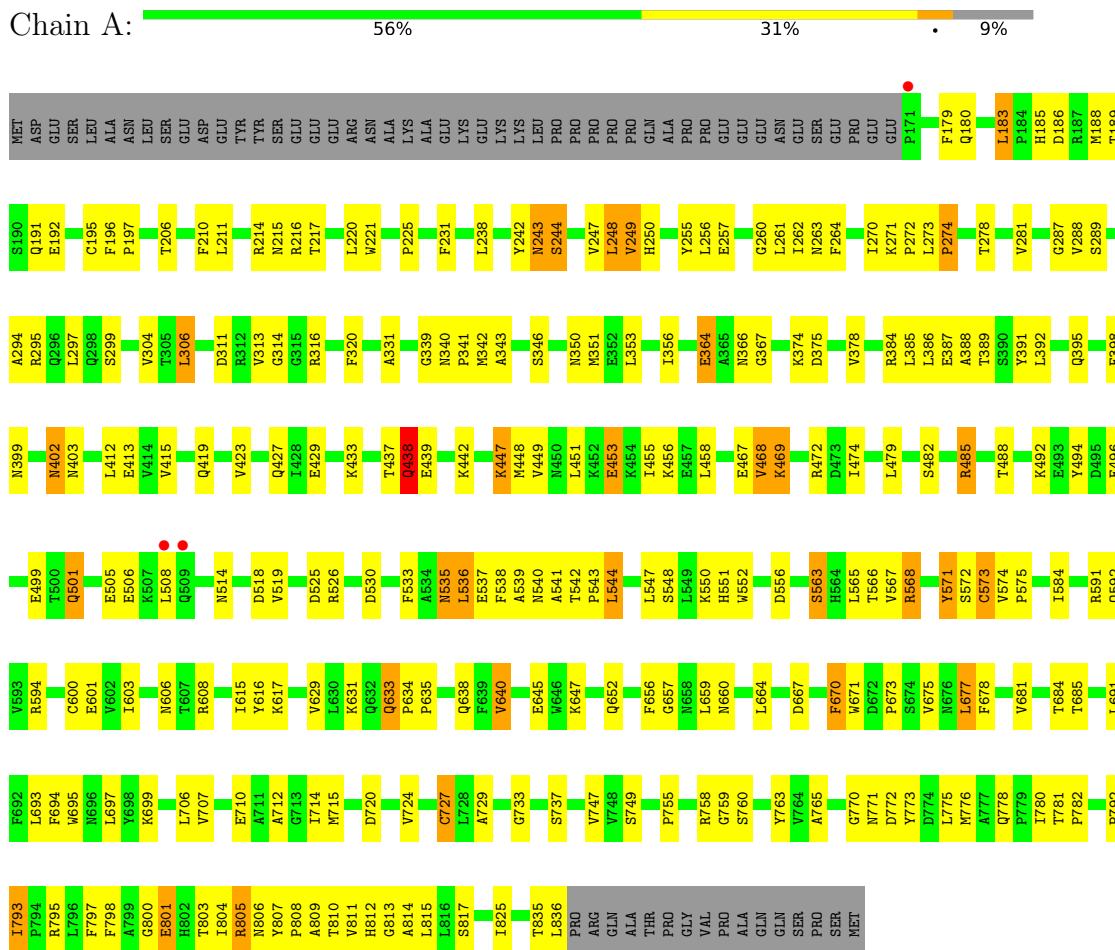


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	53	27	9	15	2	0	0

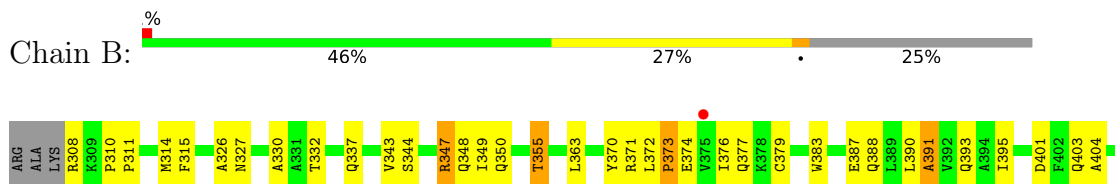
3 Residue-property plots

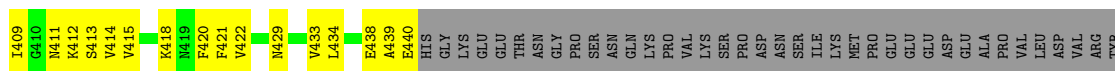
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1



• Molecule 2: REST COREPRESSOR 1





• Molecule 3: HISTONE H3.1T



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.06Å 180.50Å 233.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.03 – 3.10 75.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (76.03-3.10) 95.1 (75.92-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.13Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.239 0.213 , 0.231	Depositor DCC
R_{free} test set	860 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtrriage
Anisotropy	0.511	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6460	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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	0.76	2/5331 (0.0%)	0.82	2/7232 (0.0%)
2	B	0.52	0/1091	0.66	0/1471
3	C	1.11	1/114 (0.9%)	1.08	0/150
All	All	0.73	3/6536 (0.0%)	0.80	2/8853 (0.0%)

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
3	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	15	ALA	CA-CB	5.50	1.64	1.52
1	A	600	CYS	CB-SG	-5.14	1.73	1.81
1	A	447	LYS	CE-NZ	5.11	1.61	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	795	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	A	544	LEU	CB-CG-CD1	-5.19	102.17	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	15	ALA	Peptide

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	5217	0	5252	195	0
2	B	1076	0	1091	40	0
3	C	114	0	125	21	0
4	A	53	0	31	5	0
All	All	6460	0	6499	230	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 18.

All (230) 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:793:ILE:HD12	1:A:793:ILE:H	1.18	1.08
3:C:14:LYS:HB3	3:C:16:PRO:HD2	1.47	0.96
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.56	0.87
1:A:760:SER:HB2	4:A:1837:FAD:HM83	1.57	0.87
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.90	0.86
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.56	0.86
1:A:677:LEU:HD12	3:C:7:ALA:HB2	1.60	0.84
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.75	0.82
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.43	0.81
2:B:377:GLN:OE1	2:B:411:ASN:HB3	1.81	0.81
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.45	0.80
1:A:537:GLU:HG2	1:A:544:LEU:CD2	2.14	0.77
1:A:374:LYS:O	1:A:378:VAL:HG23	1.85	0.76
1:A:810:THR:HG22	3:C:4:MET:CE	2.16	0.75
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.21	0.74
1:A:793:ILE:H	1:A:793:ILE:CD1	1.85	0.74
1:A:385:LEU:HD23	1:A:415:VAL:CG1	2.20	0.71
2:B:403:GLN:OE1	2:B:403:GLN:HA	1.90	0.71
3:C:14:LYS:HB3	3:C:16:PRO:CD	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:HA	4:A:1837:FAD:N5	2.06	0.70
1:A:385:LEU:HD23	1:A:415:VAL:HG12	1.74	0.70
1:A:633:GLN:OE1	1:A:635:PRO:HD3	1.92	0.70
1:A:720:ASP:O	1:A:724:VAL:HG23	1.91	0.70
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.28	0.69
1:A:437:THR:HG22	1:A:508:LEU:HD21	1.73	0.69
1:A:810:THR:HG22	3:C:4:MET:HE1	1.73	0.69
1:A:793:ILE:HD12	1:A:793:ILE:N	2.02	0.69
1:A:770:GLY:O	1:A:805:ARG:HG3	1.93	0.68
1:A:670:PHE:HD1	1:A:670:PHE:O	1.76	0.68
1:A:395:GLN:HE22	2:B:308:ARG:HH12	1.42	0.67
1:A:270:ILE:O	1:A:272:PRO:HD3	1.95	0.67
1:A:603:ILE:HG23	1:A:615:ILE:HD13	1.77	0.67
1:A:693:LEU:HD12	1:A:694:PHE:N	2.10	0.66
1:A:677:LEU:N	1:A:677:LEU:HD23	2.11	0.65
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.79	0.65
1:A:469:LYS:HA	1:A:469:LYS:HE3	1.78	0.64
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.12	0.64
1:A:556:ASP:OD2	3:C:2:ARG:HD2	1.98	0.64
1:A:540:ASN:HB3	1:A:547:LEU:HD21	1.79	0.64
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.79	0.62
1:A:533:PHE:O	1:A:537:GLU:HG3	1.99	0.62
1:A:572:SER:O	1:A:574:VAL:N	2.32	0.62
3:C:2:ARG:HE	3:C:10:SER:HG	1.47	0.62
1:A:448:MET:HE2	2:B:363:LEU:HD13	1.80	0.62
1:A:395:GLN:HE22	2:B:308:ARG:NH1	1.98	0.61
1:A:195:CYS:HB2	1:A:196:PHE:CD1	2.35	0.61
3:C:14:LYS:C	3:C:16:PRO:HD2	2.20	0.61
1:A:474:ILE:HG23	2:B:393:GLN:NE2	2.16	0.60
1:A:537:GLU:HG2	1:A:544:LEU:HD23	1.80	0.60
1:A:671:TRP:O	1:A:673:PRO:HD3	2.01	0.60
1:A:331:ALA:HA	4:A:1837:FAD:C4X	2.32	0.59
1:A:231:PHE:HE1	1:A:249:VAL:CG1	2.13	0.58
1:A:255:TYR:CD2	1:A:256:LEU:HD23	2.38	0.58
1:A:809:ALA:O	3:C:4:MET:CE	2.52	0.58
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.39	0.58
1:A:656:PHE:CE2	1:A:759:GLY:HA3	2.39	0.58
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.34	0.58
1:A:801:GLU:CG	1:A:809:ALA:HA	2.33	0.57
1:A:437:THR:O	1:A:439:GLU:N	2.38	0.57
1:A:693:LEU:HD12	1:A:694:PHE:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:GLU:HA	1:A:616:TYR:O	2.04	0.57
1:A:485:ARG:HD2	2:B:404:ALA:HB1	1.87	0.57
1:A:530:ASP:OD2	1:A:685:THR:HA	2.05	0.56
1:A:763:TYR:CE1	1:A:765:ALA:HB2	2.40	0.56
2:B:347:ARG:HG3	2:B:348:GLN:N	2.19	0.56
1:A:494:TYR:CD2	1:A:494:TYR:O	2.58	0.56
1:A:537:GLU:HG2	1:A:544:LEU:HD21	1.86	0.56
2:B:374:GLU:OE2	2:B:374:GLU:HA	2.04	0.56
1:A:260:GLY:O	1:A:264:PHE:CD2	2.59	0.56
1:A:670:PHE:O	1:A:670:PHE:CD1	2.58	0.56
1:A:539:ALA:O	3:C:1:ALA:N	2.37	0.55
1:A:760:SER:CB	4:A:1837:FAD:HM83	2.33	0.55
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.88	0.55
1:A:540:ASN:CB	1:A:547:LEU:HD21	2.37	0.55
1:A:387:GLU:HG3	3:C:13:GLY:H	1.72	0.54
1:A:183:LEU:HD23	1:A:189:THR:HG21	1.88	0.54
1:A:399:ASN:ND2	1:A:550:LYS:HE2	2.22	0.54
2:B:418:LYS:O	2:B:421:PHE:HB2	2.08	0.54
1:A:539:ALA:HB2	3:C:5:GLN:HG3	1.89	0.53
1:A:346:SER:HA	1:A:351:MET:SD	2.48	0.53
1:A:402:ASN:O	1:A:403:ASN:HB2	2.08	0.53
3:C:1:ALA:O	3:C:4:MET:HB2	2.09	0.53
1:A:374:LYS:HE3	1:A:525:ASP:OD1	2.09	0.53
1:A:670:PHE:CD1	1:A:670:PHE:C	2.81	0.53
1:A:797:PHE:CG	1:A:825:ILE:HD11	2.43	0.53
1:A:660:ASN:OD1	1:A:749:SER:OG	2.22	0.52
1:A:437:THR:C	1:A:439:GLU:H	2.12	0.52
1:A:601:GLU:OE1	1:A:617:LYS:HE2	2.09	0.52
1:A:647:LYS:HE3	1:A:798:PHE:CE1	2.44	0.52
1:A:343:ALA:O	1:A:346:SER:OG	2.27	0.52
1:A:810:THR:HG22	3:C:4:MET:HE2	1.89	0.52
1:A:467:GLU:O	1:A:469:LYS:N	2.42	0.52
1:A:474:ILE:HG23	2:B:393:GLN:HE22	1.75	0.52
1:A:342:MET:HE2	1:A:571:TYR:OH	2.10	0.51
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.41	0.51
1:A:351:MET:HB3	1:A:567:VAL:HG13	1.93	0.51
1:A:385:LEU:O	1:A:388:ALA:HB3	2.11	0.51
1:A:574:VAL:HB	1:A:575:PRO:CD	2.41	0.51
1:A:640:VAL:HG12	1:A:640:VAL:O	2.10	0.51
1:A:342:MET:HG2	1:A:812:HIS:HB3	1.93	0.50
1:A:776:MET:HB3	1:A:803:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:2:ARG:NH2	3:C:12:GLY:O	2.44	0.50
2:B:391:ALA:HA	2:B:409:ILE:HD11	1.94	0.50
1:A:539:ALA:CB	3:C:5:GLN:HG3	2.42	0.50
1:A:710:GLU:HA	1:A:710:GLU:OE1	2.12	0.50
2:B:308:ARG:HH11	2:B:308:ARG:HA	1.77	0.50
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.93	0.50
1:A:385:LEU:CD2	1:A:415:VAL:HG12	2.41	0.50
1:A:366:ASN:OD1	1:A:367:GLY:N	2.45	0.49
1:A:537:GLU:CG	1:A:544:LEU:HD21	2.42	0.49
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.52	0.49
1:A:374:LYS:O	1:A:375:ASP:C	2.50	0.49
1:A:453:GLU:OE1	1:A:453:GLU:CA	2.54	0.49
1:A:677:LEU:N	1:A:677:LEU:CD2	2.75	0.49
1:A:391:TYR:O	1:A:395:GLN:HB2	2.11	0.49
1:A:437:THR:C	1:A:439:GLU:N	2.65	0.49
1:A:645:GLU:O	1:A:645:GLU:HG3	2.12	0.49
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.94	0.49
2:B:391:ALA:CA	2:B:409:ILE:HD11	2.43	0.49
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.33	0.49
3:C:11:THR:O	3:C:14:LYS:HB2	2.12	0.49
1:A:214:ARG:HD2	1:A:215:ASN:OD1	2.14	0.48
1:A:594:ARG:CZ	1:A:640:VAL:HG11	2.44	0.48
1:A:320:PHE:CD1	1:A:747:VAL:HG21	2.48	0.48
1:A:385:LEU:HD23	1:A:415:VAL:HG11	1.92	0.48
1:A:810:THR:CG2	3:C:4:MET:HE2	2.43	0.48
1:A:804:ILE:HG21	1:A:813:GLY:O	2.14	0.48
1:A:707:VAL:HG11	1:A:715:MET:HG3	1.95	0.48
2:B:387:GLU:HA	2:B:390:LEU:HD12	1.96	0.48
2:B:372:LEU:O	2:B:373:PRO:O	2.32	0.48
1:A:192:GLU:HG3	1:A:255:TYR:OH	2.13	0.47
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.96	0.47
2:B:391:ALA:HB2	2:B:409:ILE:HD11	1.95	0.47
1:A:273:LEU:HA	1:A:274:PRO:HD2	1.65	0.47
1:A:386:LEU:O	1:A:387:GLU:C	2.52	0.47
1:A:815:LEU:HD13	1:A:815:LEU:C	2.35	0.47
1:A:341:PRO:HG2	1:A:812:HIS:HB2	1.96	0.47
1:A:541:ALA:O	1:A:657:GLY:HA3	2.15	0.47
2:B:395:ILE:HG22	2:B:433:VAL:HG11	1.96	0.46
1:A:568:ARG:NH1	1:A:699:LYS:HG2	2.29	0.46
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.80	0.46
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:ASN:C	1:A:807:TYR:CD2	2.89	0.46
1:A:572:SER:C	1:A:574:VAL:N	2.68	0.46
1:A:221:TRP:CD1	1:A:262:ILE:HA	2.51	0.46
1:A:257:GLU:HG3	1:A:263:ASN:HD22	1.80	0.46
1:A:288:VAL:O	1:A:289:SER:C	2.54	0.46
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.51	0.46
1:A:771:ASN:HA	1:A:805:ARG:NH1	2.31	0.46
1:A:563:SER:O	1:A:565:LEU:HD12	2.15	0.46
1:A:248:LEU:O	1:A:249:VAL:C	2.54	0.45
1:A:548:SER:O	1:A:552:TRP:HB3	2.15	0.45
1:A:297:LEU:HB2	1:A:304:VAL:HG21	1.97	0.45
1:A:572:SER:C	1:A:574:VAL:H	2.20	0.45
1:A:448:MET:CE	2:B:363:LEU:HD13	2.46	0.45
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.77	0.45
1:A:772:ASP:HA	1:A:775:LEU:HD12	1.99	0.45
1:A:392:LEU:HD23	1:A:398:PHE:HD2	1.82	0.45
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.99	0.45
1:A:536:LEU:HD12	1:A:536:LEU:HA	1.72	0.45
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.57	0.45
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.51	0.45
1:A:412:LEU:HD13	1:A:533:PHE:CE1	2.52	0.45
2:B:388:GLN:O	2:B:391:ALA:HB3	2.17	0.45
1:A:386:LEU:O	1:A:389:THR:OG1	2.32	0.44
2:B:383:TRP:CD2	2:B:412:LYS:HE2	2.52	0.44
1:A:211:LEU:O	1:A:214:ARG:HB3	2.17	0.44
2:B:383:TRP:CE3	2:B:412:LYS:HE2	2.52	0.44
1:A:633:GLN:HA	1:A:634:PRO:HA	1.75	0.44
1:A:242:TYR:C	1:A:244:SER:H	2.21	0.44
1:A:438:GLN:NE2	1:A:508:LEU:HD13	2.33	0.44
1:A:770:GLY:O	1:A:773:TYR:HB2	2.16	0.44
1:A:606:ASN:HD21	1:A:608:ARG:HB2	1.81	0.44
1:A:629:VAL:C	1:A:631:LYS:N	2.69	0.44
3:C:7:ALA:O	3:C:8:ARG:C	2.56	0.44
1:A:255:TYR:HD2	1:A:256:LEU:HD23	1.82	0.44
1:A:455:ILE:HG22	1:A:456:LYS:N	2.32	0.44
1:A:306:LEU:HD13	1:A:584:ILE:HG12	2.00	0.43
1:A:811:VAL:HG12	1:A:812:HIS:N	2.32	0.43
1:A:340:ASN:HA	1:A:341:PRO:HD2	1.89	0.43
1:A:427:GLN:NE2	1:A:518:ASP:HA	2.34	0.43
1:A:438:GLN:HE21	1:A:438:GLN:HB2	1.58	0.43
1:A:592:GLN:HB3	1:A:603:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ILE:HD11	1:A:566:THR:HG23	2.00	0.43
2:B:403:GLN:OE1	2:B:403:GLN:CA	2.63	0.43
1:A:386:LEU:HD13	3:C:2:ARG:HH21	1.82	0.43
1:A:216:ARG:O	1:A:220:LEU:HD12	2.19	0.43
1:A:800:GLY:O	1:A:803:THR:N	2.45	0.43
1:A:677:LEU:O	1:A:678:PHE:HB3	2.19	0.42
1:A:494:TYR:CD2	1:A:494:TYR:C	2.92	0.42
1:A:535:ASN:HD22	1:A:535:ASN:HA	1.51	0.42
2:B:438:GLU:C	2:B:440:GLU:H	2.23	0.42
1:A:311:ASP:OD1	1:A:311:ASP:N	2.45	0.42
1:A:419:GLN:HE22	2:B:315:PHE:H	1.68	0.42
1:A:807:TYR:N	1:A:808:PRO:CD	2.83	0.42
2:B:413:SER:OG	2:B:415:VAL:HG12	2.19	0.42
1:A:506:GLU:C	1:A:508:LEU:H	2.23	0.42
1:A:707:VAL:HG12	1:A:712:ALA:HA	2.02	0.42
1:A:314:GLY:HA2	1:A:575:PRO:HB3	2.01	0.42
2:B:401:ASP:O	2:B:403:GLN:N	2.53	0.42
1:A:387:GLU:HB3	2:B:311:PRO:HG3	2.02	0.42
1:A:331:ALA:HA	4:A:1837:FAD:C5X	2.50	0.42
1:A:364:GLU:HA	1:A:681:VAL:HB	2.02	0.42
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.85	0.42
1:A:814:ALA:O	1:A:817:SER:N	2.45	0.42
1:A:217:THR:HA	1:A:220:LEU:HD12	2.02	0.41
1:A:221:TRP:CZ3	1:A:225:PRO:HA	2.55	0.41
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.55	0.41
2:B:391:ALA:HB2	2:B:409:ILE:CD1	2.49	0.41
1:A:542:THR:HA	1:A:543:PRO:HD2	1.92	0.41
1:A:256:LEU:CB	1:A:262:ILE:HG12	2.50	0.41
1:A:551:HIS:O	1:A:552:TRP:C	2.59	0.41
1:A:501:GLN:O	1:A:505:GLU:HB2	2.21	0.41
1:A:574:VAL:O	1:A:575:PRO:C	2.57	0.41
1:A:664:LEU:HD21	1:A:724:VAL:HG13	2.03	0.41
1:A:384:ARG:HB3	2:B:314:MET:HE1	2.03	0.41
1:A:496:GLU:O	1:A:499:GLU:HB3	2.21	0.41
1:A:782:PRO:O	1:A:792:PRO:HG2	2.20	0.41
2:B:391:ALA:CB	2:B:409:ILE:HD11	2.50	0.41
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.85	0.40
1:A:539:ALA:HB2	3:C:5:GLN:CG	2.50	0.40
1:A:629:VAL:C	1:A:631:LYS:H	2.24	0.40
2:B:350:GLN:HE21	2:B:350:GLN:HB2	1.58	0.40
1:A:468:VAL:O	1:A:472:ARG:NH1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LEU:HA	1:A:451:LEU:HD12	1.62	0.40
1:A:781:THR:HA	1:A:782:PRO:HD2	1.92	0.40
2:B:409:ILE:O	2:B:409:ILE:HG22	2.21	0.40
2:B:421:PHE:HE2	2:B:434:LEU:HD11	1.87	0.40
1:A:196:PHE:N	1:A:197:PRO:CD	2.85	0.40
1:A:294:ALA:O	1:A:295:ARG:C	2.60	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	664/730 (91%)	569 (86%)	78 (12%)	17 (3%)	5	26
2	B	131/178 (74%)	110 (84%)	14 (11%)	7 (5%)	2	12
3	C	14/21 (67%)	11 (79%)	1 (7%)	2 (14%)	0	1
All	All	809/929 (87%)	690 (85%)	93 (12%)	26 (3%)	4	22

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	GLU
1	A	438	GLN
1	A	468	VAL
1	A	573	CYS
2	B	373	PRO
3	C	8	ARG
1	A	243	ASN
1	A	274	PRO
1	A	805	ARG
2	B	326	ALA
2	B	429	ASN

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Mol	Chain	Res	Type
3	C	15	ALA
1	A	271	LYS
1	A	733	GLY
1	A	248	LEU
1	A	316	ARG
1	A	801	GLU
1	A	350	ASN
1	A	501	GLN
2	B	391	ALA
2	B	420	PHE
2	B	439	ALA
1	A	287	GLY
1	A	729	ALA
2	B	310	PRO
1	A	249	VAL

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	566/623 (91%)	509 (90%)	57 (10%)	7	28
2	B	117/156 (75%)	105 (90%)	12 (10%)	7	27
3	C	11/15 (73%)	8 (73%)	3 (27%)	0	1
All	All	694/794 (87%)	622 (90%)	72 (10%)	7	27

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	PHE
1	A	183	LEU
1	A	191	GLN
1	A	206	THR
1	A	244	SER
1	A	247	VAL
1	A	250	HIS

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Mol	Chain	Res	Type
1	A	278	THR
1	A	281	VAL
1	A	299	SER
1	A	306	LEU
1	A	313	VAL
1	A	402	ASN
1	A	413	GLU
1	A	423	VAL
1	A	429	GLU
1	A	433	LYS
1	A	438	GLN
1	A	447	LYS
1	A	449	VAL
1	A	453	GLU
1	A	458	LEU
1	A	469	LYS
1	A	482	SER
1	A	485	ARG
1	A	488	THR
1	A	492	LYS
1	A	514	ASN
1	A	519	VAL
1	A	526	ARG
1	A	535	ASN
1	A	536	LEU
1	A	538	PHE
1	A	563	SER
1	A	568	ARG
1	A	571	TYR
1	A	573	CYS
1	A	591	ARG
1	A	633	GLN
1	A	638	GLN
1	A	640	VAL
1	A	652	GLN
1	A	659	LEU
1	A	667	ASP
1	A	670	PHE
1	A	675	VAL
1	A	677	LEU
1	A	684	THR
1	A	706	LEU

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Mol	Chain	Res	Type
1	A	714	ILE
1	A	727	CYS
1	A	737	SER
1	A	778	GLN
1	A	780	ILE
1	A	793	ILE
1	A	835	THR
1	A	836	LEU
2	B	332	THR
2	B	337	GLN
2	B	343	VAL
2	B	344	SER
2	B	347	ARG
2	B	349	ILE
2	B	355	THR
2	B	371	ARG
2	B	376	ILE
2	B	379	CYS
2	B	414	VAL
2	B	422	VAL
3	C	4	MET
3	C	10	SER
3	C	14	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	395	GLN
1	A	419	GLN
1	A	422	HIS
1	A	438	GLN
1	A	535	ASN
1	A	632	GLN
2	B	350	GLN
2	B	423	ASN

5.3.3 RNA

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](#)

1 ligand is 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
4	FAD	A	1837	-	53,58,58	1.38	7 (13%)	68,89,89	1.69	16 (23%)

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
4	FAD	A	1837	-	-	3/30/50/50	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1837	FAD	C2A-N3A	3.93	1.38	1.32
4	A	1837	FAD	C2A-N1A	3.82	1.41	1.33
4	A	1837	FAD	C4X-N5	3.42	1.37	1.30
4	A	1837	FAD	C8A-N7A	2.88	1.39	1.34
4	A	1837	FAD	O4B-C4B	-2.55	1.39	1.45
4	A	1837	FAD	C10-N1	2.49	1.38	1.33
4	A	1837	FAD	C5'-C4'	2.05	1.54	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1837	FAD	N3A-C2A-N1A	-5.29	120.41	128.68
4	A	1837	FAD	O4B-C1B-C2B	-3.90	101.23	106.93
4	A	1837	FAD	C4-N3-C2	-3.63	118.94	125.64
4	A	1837	FAD	C4-C4X-C10	3.23	122.22	116.79
4	A	1837	FAD	C1B-N9A-C4A	-3.05	121.28	126.64
4	A	1837	FAD	C4X-C10-N1	-3.03	117.70	124.73
4	A	1837	FAD	P-O3P-PA	-2.97	122.65	132.83
4	A	1837	FAD	O4-C4-C4X	-2.87	119.00	126.60
4	A	1837	FAD	C4X-C4-N3	2.64	119.88	113.19
4	A	1837	FAD	O5'-C5'-C4'	2.53	116.11	109.36
4	A	1837	FAD	C5X-C9A-N10	2.39	120.42	117.95
4	A	1837	FAD	C4X-C10-N10	2.27	119.80	116.48
4	A	1837	FAD	C4'-C3'-C2'	-2.21	108.77	113.36
4	A	1837	FAD	C1'-C2'-C3'	2.20	115.94	109.79
4	A	1837	FAD	C5A-C6A-N6A	-2.12	117.14	120.35
4	A	1837	FAD	C6-C5X-C9A	2.05	121.84	118.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1837	FAD	PA-O3P-P-O5'
4	A	1837	FAD	C5B-O5B-PA-O2A
4	A	1837	FAD	O4B-C4B-C5B-O5B

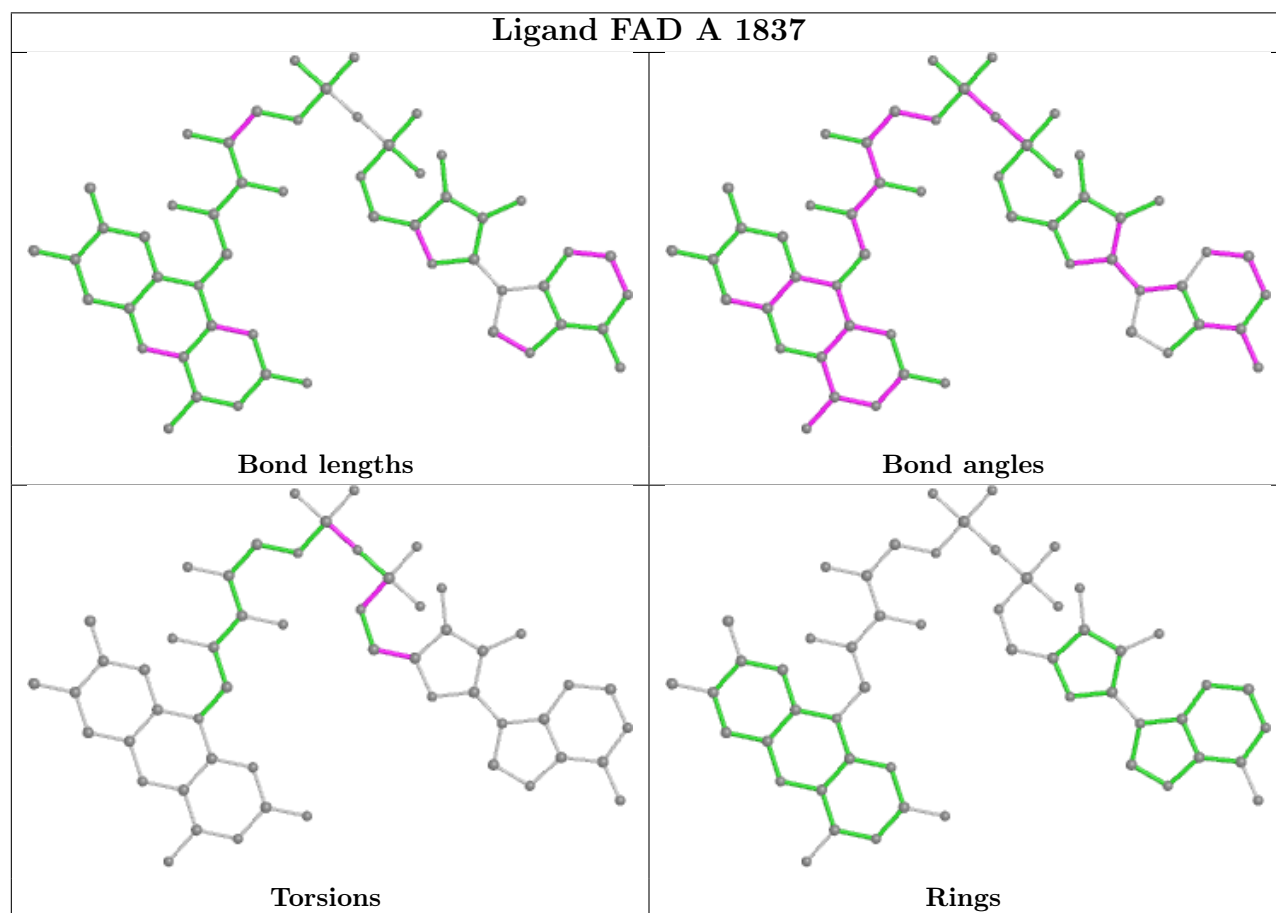
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1837	FAD	5	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	666/730 (91%)	0.03	3 (0%) 91 81	45, 76, 109, 125	0
2	B	133/178 (74%)	0.22	1 (0%) 86 72	81, 120, 138, 141	0
3	C	16/21 (76%)	0.20	1 (6%) 20 8	57, 65, 75, 78	0
All	All	815/929 (87%)	0.07	5 (0%) 89 78	45, 82, 126, 141	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	GLN	2.9
2	B	375	VAL	2.3
1	A	508	LEU	2.0
1	A	171	PRO	2.0
3	C	16	PRO	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](#)

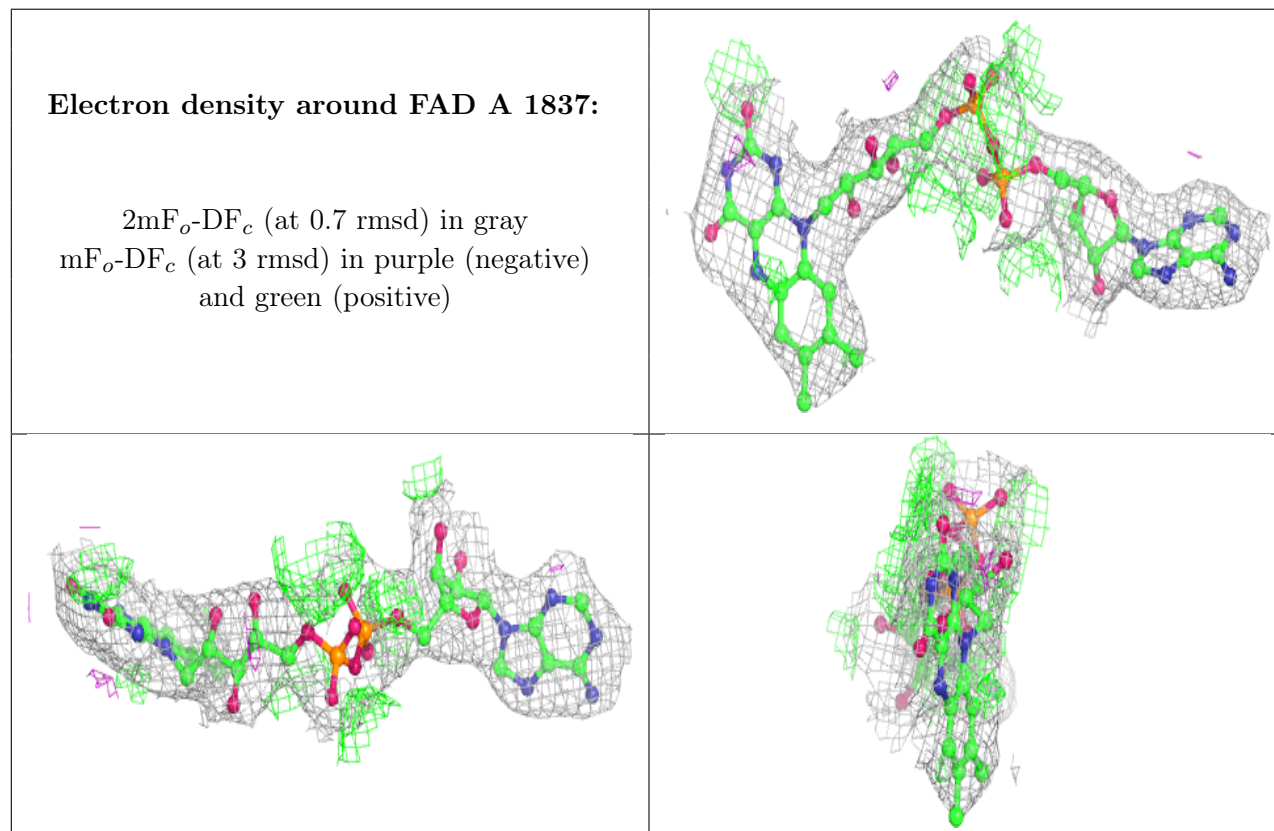
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
4	FAD	A	1837	53/53	0.98	0.21	39,53,64,65	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.