



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:15 PM EST

PDB ID : 5LGN  
Title : Thieno[3,2-b]pyrrole-5-carboxamides as Novel Reversible Inhibitors of Histone Lysine Demethylase KDM1A/LSD1: Compound 19  
Authors : Mattevi, A.; Ciossani, G.  
Deposited on : 2016-07-07  
Resolution : 3.20 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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-20028442

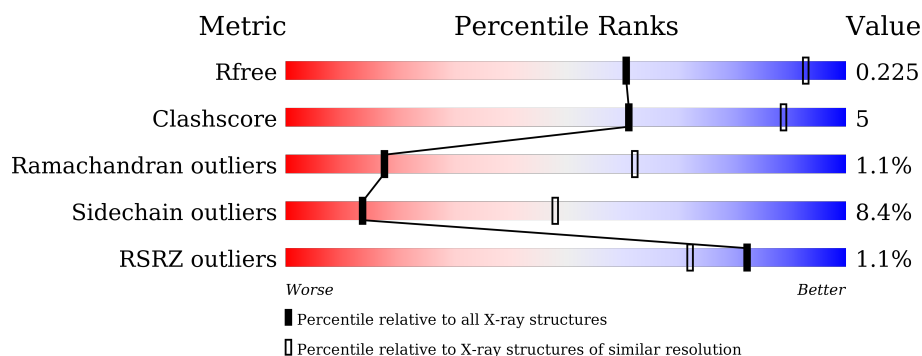
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	670	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 82%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>82%</span> <span>16%</span> <span>.</span> </div> </div>
2	B	133	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 25%, green 72%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>72%</span> <span>25%</span> <span>.</span> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6399 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 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	0	0	0
			5249	3343	911	975	20			

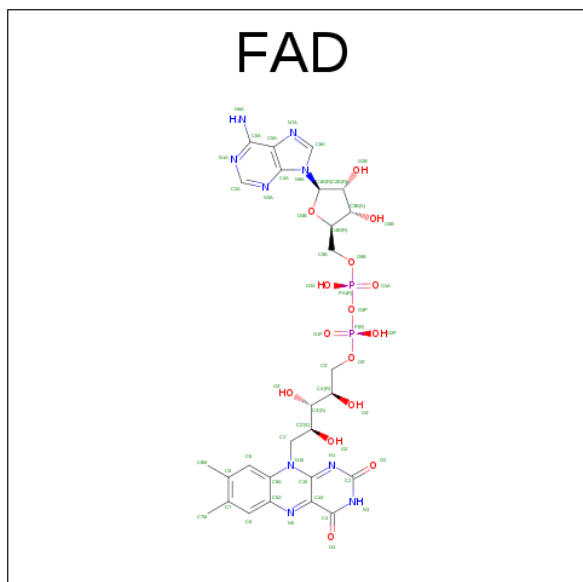
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	PRO	-	expression tag	UNP O60341
A	371	ASP	THR	conflict	UNP O60341

- Molecule 2 is a protein called REST corepressor 1.

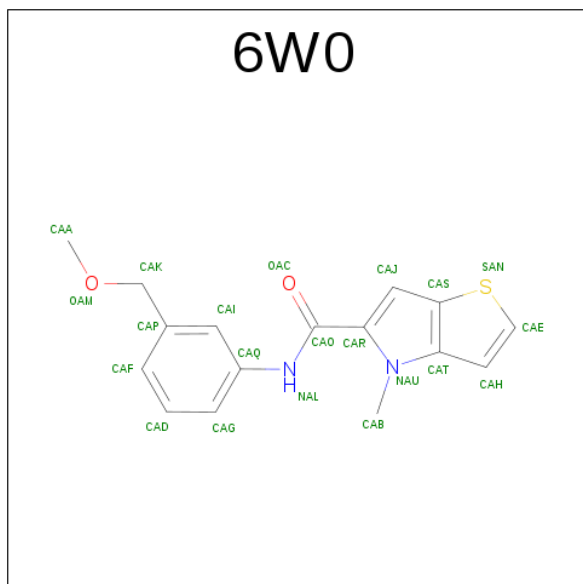
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 4 is {N}-[3-(methoxymethyl)phenyl]-4-methyl-thieno[3,2-b]pyrrole-5-carboxamide (three-letter code: 6W0) (formula: C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub>S).

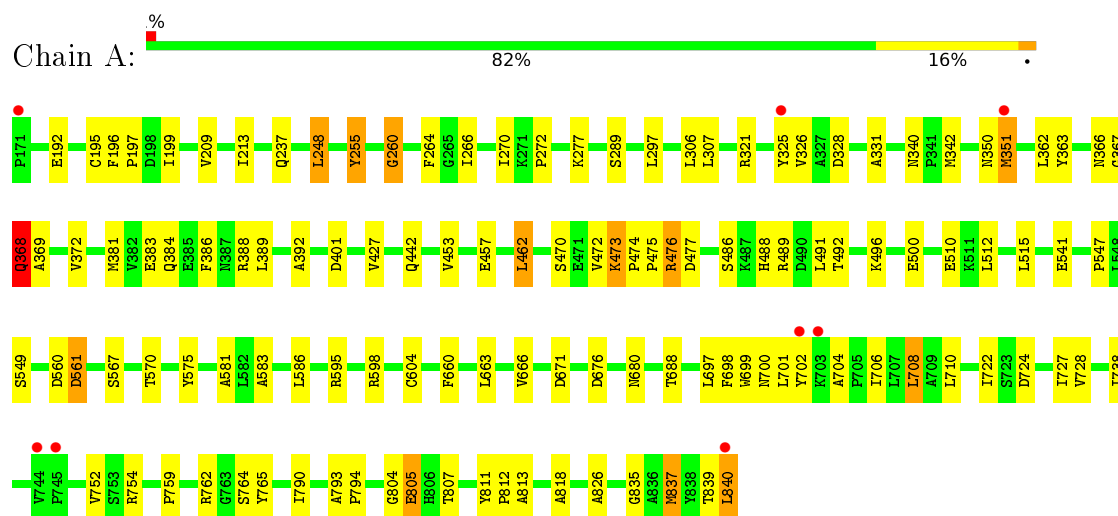


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			21	16	2	2	1		

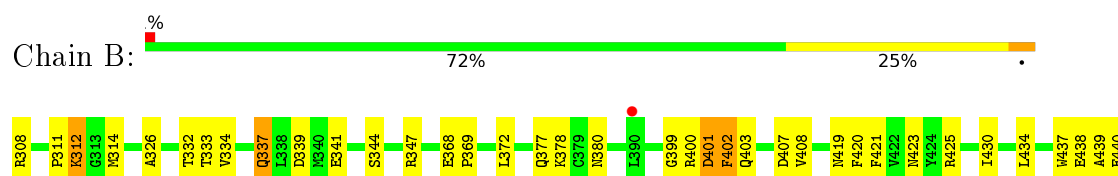
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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 1A



- Molecule 2: REST corepressor 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	120.51Å 180.44Å 235.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 3.20 100.21 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.8 (80.00-3.20) 97.9 (100.21-3.20)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.193 , 0.220 0.200 , 0.225	Depositor DCC
$R_{free}$ test set	811 reflections (1.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	111.9	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 86.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6W0, 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	0.46	0/5363	0.67	0/7275
2	B	0.41	0/1091	0.64	0/1471
All	All	0.45	0/6454	0.66	0/8746

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5249	0	5282	58	0
2	B	1076	0	1091	17	0
3	A	53	0	31	3	0
4	A	21	0	0	0	0
All	All	6399	0	6404	70	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 5.

All (70) 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:699:TRP:CZ2	1:A:710:LEU:HD21	2.24	0.72
1:A:366:ASN:HB3	1:A:369:ALA:HB3	1.76	0.67
1:A:331:ALA:HA	3:A:901:FAD:N5	2.08	0.67
1:A:488:HIS:CD2	2:B:372:LEU:HD13	2.32	0.64
1:A:804:GLY:O	1:A:807:THR:OG1	2.18	0.58
1:A:270:ILE:O	1:A:272:PRO:HD3	2.04	0.57
1:A:805:GLU:CG	1:A:813:ALA:HA	2.35	0.57
1:A:765:TYR:CD1	1:A:813:ALA:HB1	2.41	0.55
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.88	0.55
1:A:663:LEU:HD12	1:A:663:LEU:C	2.27	0.54
1:A:811:TYR:N	1:A:812:PRO:CD	2.72	0.53
2:B:400:ARG:O	2:B:402:PHE:N	2.37	0.53
1:A:388:ARG:NH1	2:B:312:LYS:O	2.37	0.53
1:A:759:PRO:HA	1:A:762:ARG:NH1	2.24	0.53
2:B:401:ASP:O	2:B:403:GLN:N	2.43	0.52
1:A:196:PHE:N	1:A:197:PRO:CD	2.72	0.51
1:A:325:TYR:HB3	1:A:706:ILE:HD11	1.92	0.51
1:A:805:GLU:HG3	1:A:813:ALA:HA	1.92	0.50
2:B:337:GLN:HA	2:B:337:GLN:HE21	1.77	0.49
1:A:722:ILE:HG22	1:A:727:ILE:HG13	1.93	0.49
1:A:297:LEU:HD21	1:A:826:ALA:HA	1.94	0.49
1:A:541:GLU:OE2	1:A:547:PRO:HA	2.13	0.48
1:A:473:LYS:HA	1:A:473:LYS:HE3	1.95	0.48
1:A:561:ASP:OD1	1:A:561:ASP:N	2.47	0.48
1:A:350:ASN:OD1	1:A:351:MET:N	2.47	0.47
1:A:583:ALA:HA	1:A:586:LEU:HD12	1.97	0.47
1:A:462:LEU:HB3	1:A:491:LEU:HD13	1.97	0.46
2:B:368:GLU:N	2:B:369:PRO:CD	2.78	0.46
1:A:489:ARG:HD3	2:B:408:VAL:HG23	1.98	0.45
1:A:389:LEU:O	1:A:392:ALA:HB3	2.16	0.45
1:A:362:LEU:C	1:A:363:TYR:CD1	2.90	0.45
1:A:472:VAL:O	1:A:476:ARG:NH1	2.49	0.45
1:A:793:ALA:HB1	1:A:794:PRO:CD	2.47	0.45
1:A:260:GLY:O	1:A:264:PHE:CD2	2.70	0.45
1:A:722:ILE:O	1:A:754:ARG:NH2	2.50	0.45
1:A:289:SER:HB3	1:A:818:ALA:HB1	1.98	0.45
2:B:401:ASP:O	2:B:402:PHE:C	2.55	0.44
1:A:367:GLY:O	1:A:368:GLN:HB3	2.17	0.44
1:A:837:MET:HA	1:A:840:LEU:HD13	2.00	0.44
1:A:704:ALA:HB1	1:A:706:ILE:HD12	1.99	0.43
1:A:199:ILE:HD11	1:A:248:LEU:HD11	2.00	0.43
1:A:764:SER:HB2	3:A:901:FAD:HM83	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:VAL:HG13	1:A:752:VAL:HG22	2.00	0.43
1:A:805:GLU:HG2	1:A:813:ALA:HA	1.99	0.43
1:A:192:GLU:HG3	1:A:255:TYR:OH	2.19	0.43
2:B:419:ASN:O	2:B:420:PHE:C	2.55	0.43
1:A:660:PHE:CE1	1:A:765:TYR:HA	2.53	0.43
1:A:266:ILE:HD11	1:A:581:ALA:C	2.39	0.42
1:A:363:TYR:CD2	1:A:738:ILE:HG23	2.54	0.42
1:A:676:ASP:OD1	1:A:676:ASP:C	2.58	0.42
1:A:321:ARG:HG2	1:A:326:VAL:HG22	2.01	0.42
1:A:489:ARG:HG3	2:B:407:ASP:HB2	2.01	0.42
1:A:698:PHE:HA	1:A:708:LEU:O	2.18	0.42
1:A:388:ARG:HB3	2:B:314:MET:CE	2.50	0.42
2:B:333:THR:HG22	2:B:334:VAL:N	2.35	0.41
2:B:421:PHE:HE2	2:B:434:LEU:HD11	1.86	0.41
1:A:724:ASP:O	1:A:728:VAL:HG23	2.21	0.41
2:B:430:ILE:HG22	2:B:434:LEU:HD12	2.03	0.41
1:A:340:ASN:OD1	1:A:342:MET:N	2.41	0.41
1:A:266:ILE:HD13	1:A:581:ALA:HB1	2.02	0.41
1:A:700:ASN:O	1:A:701:LEU:HG	2.21	0.41
1:A:701:LEU:HB3	1:A:702:TYR:CE1	2.56	0.41
2:B:400:ARG:O	2:B:402:PHE:CD1	2.73	0.41
1:A:306:LEU:C	1:A:307:LEU:HD23	2.40	0.41
1:A:474:PRO:HA	1:A:475:PRO:C	2.42	0.41
2:B:399:GLY:HA3	2:B:437:TRP:CE3	2.55	0.41
1:A:383:GLU:O	1:A:386:PHE:HB3	2.20	0.40
1:A:697:LEU:HD12	1:A:698:PHE:H	1.86	0.40
1:A:331:ALA:HA	3:A:901:FAD:C5X	2.52	0.40
2:B:438:GLU:C	2:B:440:GLU:H	2.25	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	668/670 (100%)	601 (90%)	64 (10%)	3 (0%)	39 80
2	B	131/133 (98%)	110 (84%)	15 (12%)	6 (5%)	3 23
All	All	799/803 (100%)	711 (89%)	79 (10%)	9 (1%)	17 62

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	GLY
1	A	368	GLN
1	A	835	GLY
2	B	326	ALA
2	B	425	ARG
2	B	401	ASP
2	B	402	PHE
2	B	439	ALA
2	B	311	PRO

### 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	570/570 (100%)	524 (92%)	46 (8%)	15 51
2	B	117/117 (100%)	105 (90%)	12 (10%)	9 36
All	All	687/687 (100%)	629 (92%)	58 (8%)	14 48

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	195	CYS
1	A	237	GLN
1	A	248	LEU
1	A	255	TYR
1	A	277	LYS
1	A	328	ASP
1	A	351	MET

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Mol	Chain	Res	Type
1	A	368	GLN
1	A	372	VAL
1	A	381	MET
1	A	384	GLN
1	A	401	ASP
1	A	427	VAL
1	A	442	GLN
1	A	453	VAL
1	A	457	GLU
1	A	462	LEU
1	A	470	SER
1	A	473	LYS
1	A	476	ARG
1	A	477	ASP
1	A	486	SER
1	A	492	THR
1	A	496	LYS
1	A	500	GLU
1	A	510	GLU
1	A	512	LEU
1	A	515	LEU
1	A	549	SER
1	A	560	ASP
1	A	561	ASP
1	A	567	SER
1	A	570	THR
1	A	575	TYR
1	A	595	ARG
1	A	598	ARG
1	A	604	CYS
1	A	671	ASP
1	A	680	ASN
1	A	688	THR
1	A	708	LEU
1	A	790	ILE
1	A	805	GLU
1	A	837	MET
1	A	839	THR
1	A	840	LEU
2	B	308	ARG
2	B	312	LYS
2	B	332	THR

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Mol	Chain	Res	Type
2	B	337	GLN
2	B	339	ASP
2	B	341	GLU
2	B	344	SER
2	B	347	ARG
2	B	377	GLN
2	B	378	LYS
2	B	380	ASN
2	B	423	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	399	GLN
1	A	426	HIS
1	A	488	HIS
1	A	539	ASN
1	A	637	GLN
2	B	337	GLN
2	B	350	GLN
2	B	380	ASN
2	B	403	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	FAD	A	901	-	52,58,58	1.35	7 (13%)	52,89,89	2.60	17 (32%)
4	6W0	A	902	-	19,23,23	2.15	5 (26%)	21,32,32	1.91	4 (19%)

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
3	FAD	A	901	-	-	0/30/50/50	0/6/6/6
4	6W0	A	902	-	-	0/8/11/11	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	6W0	CAJ-CAR	-6.27	1.33	1.38
4	A	902	6W0	CAK-CAP	-3.78	1.41	1.50
4	A	902	6W0	CAQ-NAL	-3.46	1.35	1.41
4	A	902	6W0	CAR-CAO	-2.72	1.33	1.50
4	A	902	6W0	CAJ-CAS	-2.39	1.32	1.42
3	A	901	FAD	C6-C5X	-2.24	1.38	1.41
3	A	901	FAD	C10-N10	2.50	1.42	1.39
3	A	901	FAD	C5A-C4A	2.79	1.46	1.40
3	A	901	FAD	C8-C7	2.92	1.48	1.41
3	A	901	FAD	C9A-N10	3.43	1.43	1.38
3	A	901	FAD	C9A-C5X	3.63	1.50	1.42
3	A	901	FAD	C4X-C10	3.95	1.48	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FAD	N3A-C2A-N1A	-7.55	122.94	128.87
3	A	901	FAD	C4X-C4-N3	-4.01	118.28	123.52
3	A	901	FAD	C4B-O4B-C1B	-3.94	105.47	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FAD	C1B-N9A-C4A	-3.84	122.52	126.81
3	A	901	FAD	N3-C2-N1	-3.68	121.49	127.69
3	A	901	FAD	C4X-C10-N10	-3.66	117.86	120.52
3	A	901	FAD	C6-C5X-N5	-2.94	115.25	118.92
4	A	902	6W0	CAJ-CAR-CAO	-2.62	122.94	129.81
3	A	901	FAD	C4-C4X-C10	-2.45	118.37	119.94
3	A	901	FAD	O4B-C1B-N9A	2.02	111.92	108.11
3	A	901	FAD	C4X-N5-C5X	2.02	119.10	116.72
3	A	901	FAD	O2A-PA-O1A	2.13	123.64	112.56
4	A	902	6W0	CAJ-CAS-CAT	2.99	108.84	106.24
3	A	901	FAD	O4'-C4'-C3'	2.99	116.66	108.96
3	A	901	FAD	N6A-C6A-N1A	3.25	123.97	118.52
3	A	901	FAD	C5X-C9A-N10	3.76	120.40	117.58
3	A	901	FAD	C6-C5X-C9A	4.15	123.68	119.11
4	A	902	6W0	CAE-SAN-CAS	4.20	96.25	91.56
3	A	901	FAD	C1'-N10-C9A	4.87	124.48	118.83
4	A	902	6W0	CAB-NAU-CAR	5.21	131.38	124.51
3	A	901	FAD	C4-N3-C2	9.19	122.83	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [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, 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	670/670 (100%)	0.32	8 (1%) 81 69	66, 107, 152, 216	0
2	B	133/133 (100%)	0.13	1 (0%) 87 80	94, 138, 167, 185	0
All	All	803/803 (100%)	0.29	9 (1%) 82 72	66, 112, 156, 216	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	4.6
1	A	703	LYS	2.7
1	A	325	TYR	2.7
1	A	840	LEU	2.6
1	A	351	MET	2.2
1	A	744	VAL	2.2
2	B	390	LEU	2.1
1	A	702	TYR	2.0
1	A	745	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 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(Å <sup>2</sup> )	Q<0.9
4	6W0	A	902	21/21	0.96	0.29	-0.17	88,103,133,136	0
3	FAD	A	901	53/53	0.98	0.26	-0.64	67,79,96,102	0

## 6.5 Other polymers

There are no such residues in this entry.