



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 10:53 PM EDT

PDB ID : 3ZMS
Title : LSD1-CoREST in complex with INSM1 peptide
Authors : Tortorici, M.; Borrello, M.T.; Tardugno, M.; Chiarelli, L.R.; Pilotto, S.; Ciossani, G.; Vellore, N.A.; Cowan, J.; O'Connell, M.; Mai, A.; Baron, R.; Ganesan, A.; Mattevi, A.
Deposited on : 2013-02-12
Resolution : 2.96 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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.36.2
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) : 2.36.2

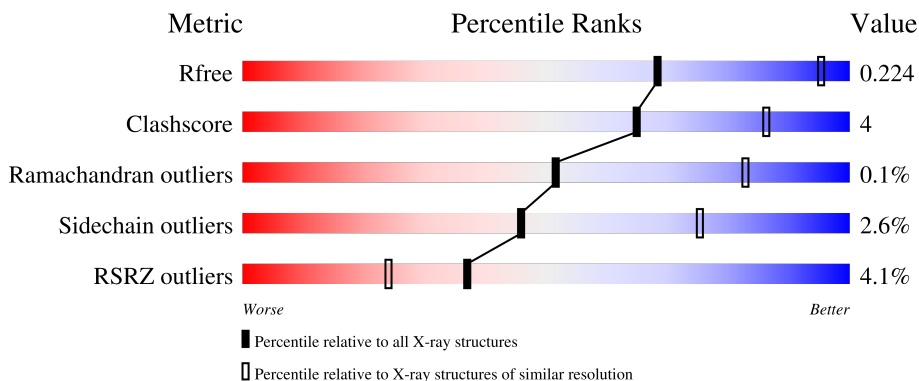
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	872	 2% 67% 9% 24%
2	B	482	 3% 26% 72%
3	C	509	 98%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6407 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
			Total	C	N	O	S			
1	A	665	5210	3319	905	966	20	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	PRO	ALA	conflict	UNP O60341
A	?	-	ASP	deletion	UNP O60341
A	?	-	THR	deletion	UNP O60341
A	?	-	VAL	deletion	UNP O60341
A	?	-	LYS	deletion	UNP O60341

- 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 INSULINOMA-ASSOCIATED PROTEIN 1.

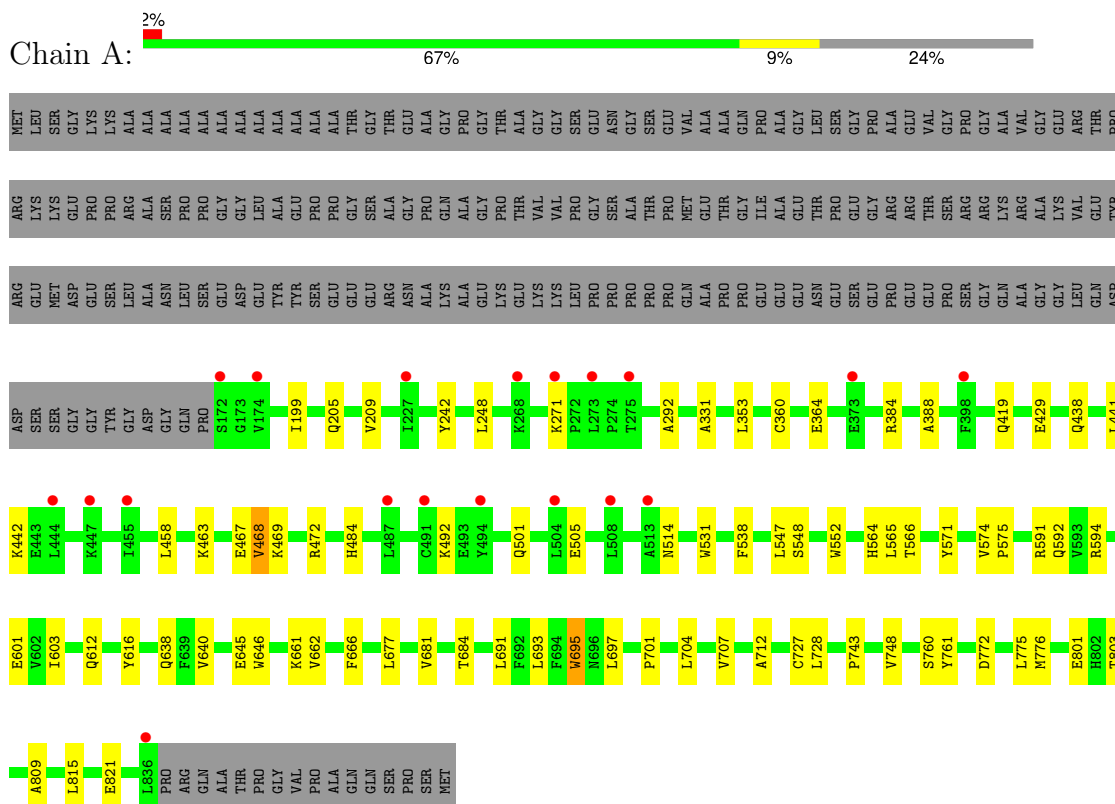
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	8	68	45	15	8	0	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).

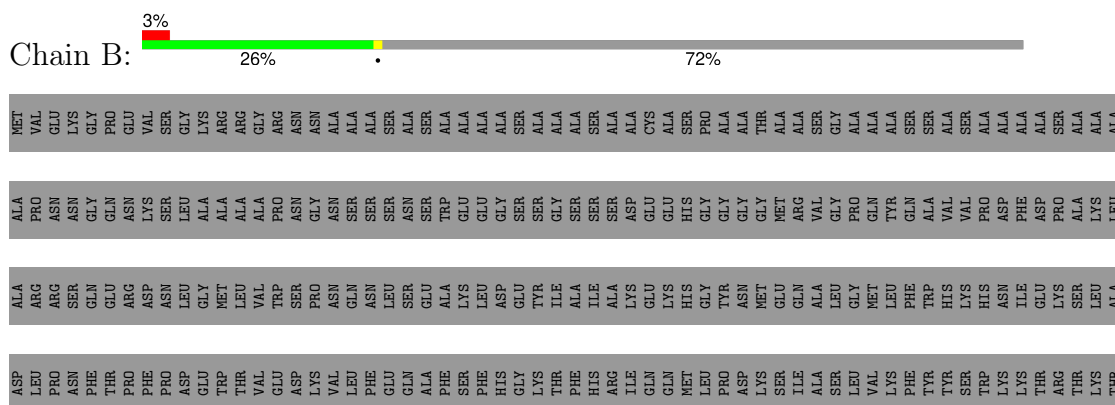
3 Residue-property plots i

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 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, α , β , γ	119.13Å 181.82Å 233.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.45 – 2.96 50.36 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.2 (63.45-2.96) 99.2 (50.36-2.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.96Å)	Xtrriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.215 , 0.227 0.215 , 0.224	Depositor DCC
R_{free} test set	1025 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	84.4	Xtrriage
Anisotropy	0.048	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6407	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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	0.43	3/5323 (0.1%)	0.49	0/7221
2	B	0.38	0/1091	0.46	0/1471
3	C	2.71	2/69 (2.9%)	1.31	2/89 (2.2%)
All	All	0.50	5/6483 (0.1%)	0.50	2/8781 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	6	VAL	C-N	-19.00	0.90	1.34
3	C	7	LYS	C-N	-11.71	1.07	1.34
1	A	646	TRP	CD2-CE2	5.26	1.47	1.41
1	A	531	TRP	CD2-CE2	5.10	1.47	1.41
1	A	695	TRP	CD2-CE2	5.01	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	7	LYS	O-C-N	-8.22	109.54	122.70
3	C	7	LYS	CA-C-N	5.72	129.79	117.20

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	5210	0	5244	48	0
2	B	1076	0	1091	8	0
3	C	68	0	78	10	0
4	A	53	0	31	4	0
All	All	6407	0	6444	52	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 4.

All (52) 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:760:SER:HB2	4:A:900:FAD:HM83	1.62	0.81
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.73	0.69
3:C:6:VAL:HG12	3:C:7:LYS:N	2.10	0.67
1:A:384:ARG:HB3	2:B:314:MET:HE3	1.76	0.67
1:A:384:ARG:HB3	2:B:314:MET:CE	2.26	0.66
1:A:677:LEU:HD11	3:C:6:VAL:HG13	1.80	0.64
1:A:801:GLU:HG2	1:A:809:ALA:H	1.62	0.64
3:C:2:ARG:HG2	3:C:8:ARG:HH22	1.64	0.61
1:A:677:LEU:HD11	3:C:6:VAL:CG1	2.32	0.59
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.85	0.59
1:A:419:GLN:HE22	2:B:315:PHE:H	1.51	0.58
1:A:331:ALA:HA	4:A:900:FAD:N5	2.19	0.58
1:A:574:VAL:HB	1:A:575:PRO:HD3	1.85	0.57
3:C:6:VAL:CG1	3:C:7:LYS:N	2.66	0.55
1:A:666:PHE:O	1:A:701:PRO:HG2	2.08	0.54
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.90	0.54
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.90	0.54
1:A:548:SER:O	1:A:552:TRP:HB3	2.08	0.53
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.44	0.52
1:A:501:GLN:O	1:A:505:GLU:HB2	2.10	0.52
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.46	0.51
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.76	0.51
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.50	0.50
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.95	0.49
3:C:8:ARG:HG3	3:C:8:ARG:O	2.13	0.48
1:A:601:GLU:HA	1:A:616:TYR:O	2.13	0.48
1:A:331:ALA:HA	4:A:900:FAD:C4X	2.45	0.47
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.97	0.46
1:A:463:LYS:O	1:A:467:GLU:HG2	2.16	0.46
1:A:821:GLU:OE1	1:A:821:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:ARG:HG2	1:A:640:VAL:HB	1.98	0.46
1:A:801:GLU:HG2	1:A:809:ALA:N	2.30	0.45
1:A:809:ALA:HB3	3:C:1:PRO:HD3	1.98	0.45
1:A:760:SER:CB	4:A:900:FAD:HM83	2.41	0.45
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.98	0.44
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.99	0.44
1:A:728:LEU:HD21	1:A:743:PRO:HD3	2.00	0.44
1:A:364:GLU:HA	1:A:681:VAL:HB	2.00	0.43
1:A:353:LEU:HB3	1:A:565:LEU:HD22	2.00	0.43
1:A:360:CYS:O	3:C:7:LYS:HE3	2.19	0.43
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.99	0.43
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.54	0.43
1:A:468:VAL:O	1:A:472:ARG:NH1	2.52	0.42
1:A:292:ALA:HB2	1:A:815:LEU:HD22	2.02	0.42
1:A:776:MET:HB3	1:A:803:THR:HG22	2.02	0.42
1:A:388:ALA:HB2	2:B:314:MET:HG2	2.00	0.41
1:A:677:LEU:CD1	3:C:6:VAL:HG11	2.50	0.41
1:A:772:ASP:HA	1:A:775:LEU:HD12	2.02	0.41
1:A:205:GLN:O	1:A:209:VAL:HG23	2.20	0.41
1:A:693:LEU:HD21	3:C:6:VAL:HG21	2.03	0.41
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.85	0.41
1:A:547:LEU:HD22	1:A:552:TRP:HB2	2.02	0.41

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	663/872 (76%)	642 (97%)	20 (3%)	1 (0%)	47	79
2	B	131/482 (27%)	125 (95%)	6 (5%)	0	100	100
3	C	6/509 (1%)	4 (67%)	2 (33%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	800/1863 (43%)	771 (96%)	28 (4%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	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	565/711 (80%)	550 (97%)	15 (3%)	44 74
2	B	117/395 (30%)	115 (98%)	2 (2%)	60 83
3	C	7/372 (2%)	6 (86%)	1 (14%)	3 13
All	All	689/1478 (47%)	671 (97%)	18 (3%)	46 75

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	271	LYS
1	A	429	GLU
1	A	438	GLN
1	A	458	LEU
1	A	469	LYS
1	A	492	LYS
1	A	514	ASN
1	A	538	PHE
1	A	564	HIS
1	A	571	TYR
1	A	591	ARG
1	A	612	GLN
1	A	638	GLN
1	A	645	GLU
1	A	684	THR

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Mol	Chain	Res	Type
2	B	316	LEU
2	B	337	GLN
3	C	7	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	191	GLN
1	A	419	GLN
1	A	438	GLN
1	A	742	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 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	900	-	54,58,58	1.36	8 (14%)	71,89,89	1.28	8 (11%)

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	900	-	-	0/30/50/50	0/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	FAD	C9A-C5X	5.50	1.50	1.41
4	A	900	FAD	C8-C7	3.54	1.49	1.40
4	A	900	FAD	C5X-N5	-2.34	1.35	1.39
4	A	900	FAD	P-O3P	2.31	1.62	1.59
4	A	900	FAD	C4-N3	-2.31	1.34	1.38
4	A	900	FAD	C10-N10	2.18	1.42	1.37
4	A	900	FAD	C4X-N5	2.07	1.35	1.30
4	A	900	FAD	PA-O3P	2.06	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	FAD	N3A-C2A-N1A	-4.37	122.74	128.67
4	A	900	FAD	O4-C4-C4X	-2.64	119.57	126.53
4	A	900	FAD	C4X-C10-N1	-2.61	118.18	124.59
4	A	900	FAD	C5'-C4'-C3'	-2.50	107.50	112.22
4	A	900	FAD	C1B-N9A-C4A	-2.41	122.40	126.64
4	A	900	FAD	C4A-C5A-N7A	-2.16	107.05	109.34
4	A	900	FAD	C10-N1-C2	2.13	121.46	116.85
4	A	900	FAD	C4X-C4-N3	2.12	118.66	113.25

There are no chirality outliers.

There are no torsion outliers.

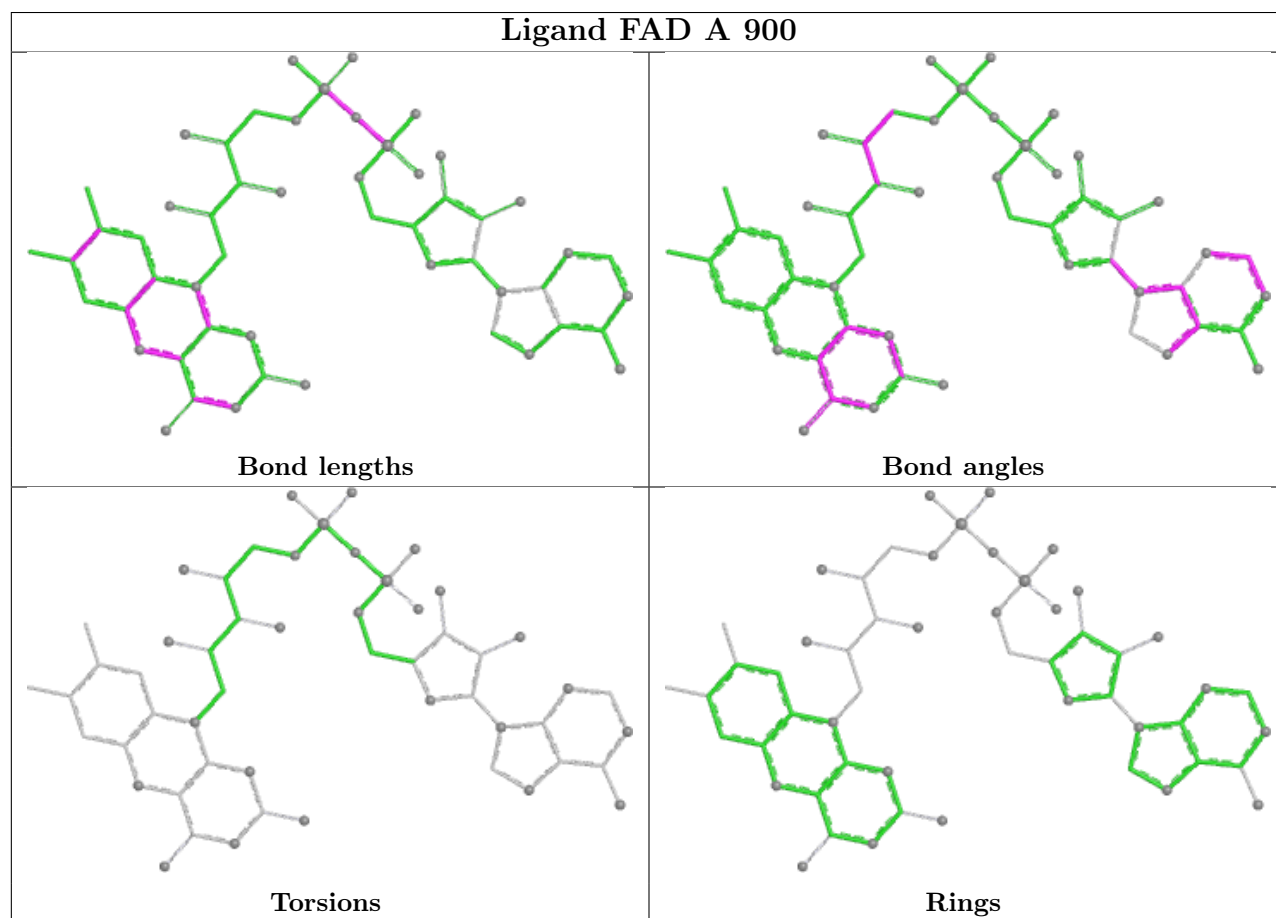
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	900	FAD	4	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	7:LYS	C	8:ARG	N	1.07
1	C	6:VAL	C	7:LYS	N	0.90

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, 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	665/872 (76%)	0.40	19 (2%) 51 35	52, 86, 123, 151	0
2	B	133/482 (27%)	0.72	14 (10%) 6 4	83, 119, 140, 159	0
3	C	8/509 (1%)	0.27	0 100 100	70, 83, 105, 132	0
All	All	806/1863 (43%)	0.45	33 (4%) 37 24	52, 92, 133, 159	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	376	ILE	4.9
1	A	172	SER	3.8
2	B	309	LYS	3.7
2	B	312	LYS	3.7
1	A	836	LEU	3.3
2	B	374	GLU	3.2
1	A	273	LEU	3.0
1	A	373	GLU	3.0
2	B	308	ARG	2.9
2	B	313	GLY	2.8
1	A	508	LEU	2.8
1	A	174	VAL	2.8
1	A	227	ILE	2.7
2	B	363	LEU	2.6
1	A	275	THR	2.5
2	B	399	GLY	2.5
1	A	487	LEU	2.5
1	A	398	PHE	2.5
1	A	271	LYS	2.4
2	B	378	LYS	2.4
2	B	375	VAL	2.4
1	A	268	LYS	2.4
1	A	494	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	455	ILE	2.3
2	B	418	LYS	2.3
1	A	444	LEU	2.2
1	A	504	LEU	2.2
2	B	367	ILE	2.2
2	B	321	VAL	2.1
1	A	447	LYS	2.1
1	A	513	ALA	2.1
1	A	491	CYS	2.0
2	B	372	LEU	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](#)

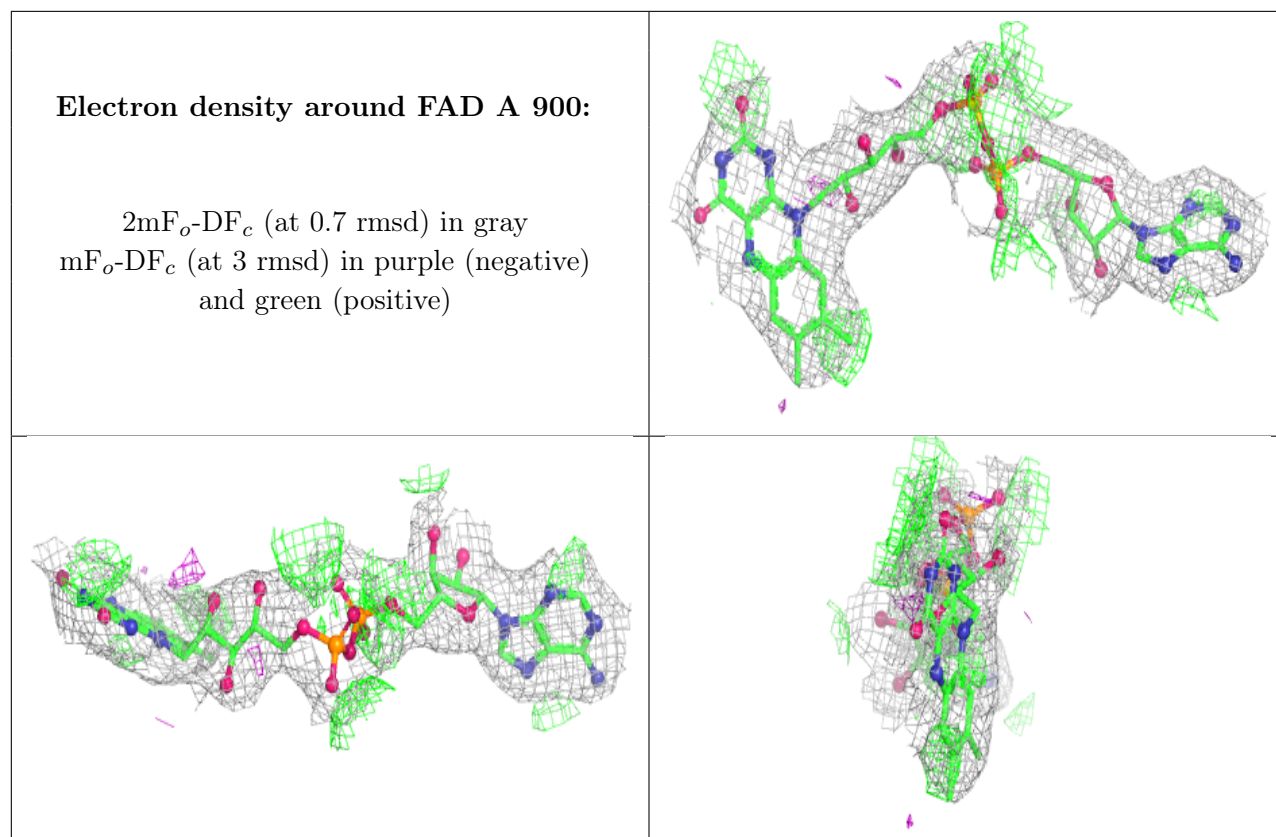
There are no monosaccharides in this entry.

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(Å ²)	Q<0.9
4	FAD	A	900	53/53	0.96	0.23	56,63,78,79	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.