



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:46 PM UTC

PDB ID : 5X60 / pdb_00005x60
Title : Crystal structure of LSD1-CoREST in complex with peptide 9
Authors : Kikuchi, M.; Amano, Y.; Sato, S.; Yokoyama, S.; Umezawa, N.; Higuchi, T.; Umehara, T.
Deposited on : 2017-02-20
Resolution : 2.69 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

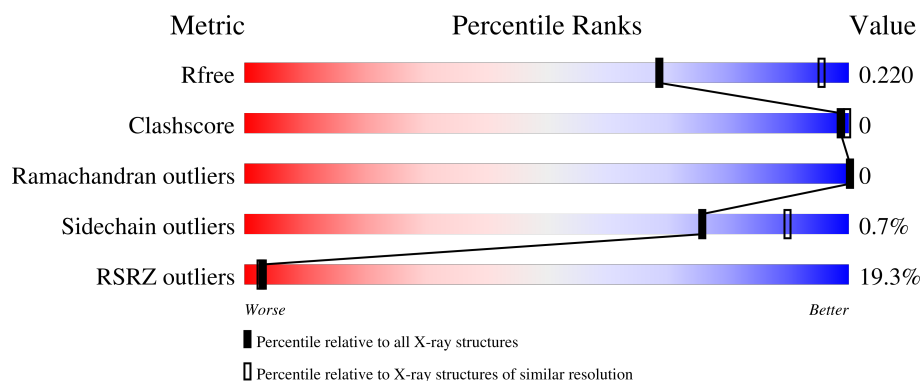
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	669	14% 97% ..
2	B	140	46% 92% 6%
3	C	20	5% 75% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6494 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	662	Total	C	N	O	S	0	3	0
			5198	3307	907	965	19			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	GLY	-	expression tag	UNP O60341
A	166	PRO	-	expression tag	UNP O60341
A	167	LEU	-	expression tag	UNP O60341
A	168	GLY	-	expression tag	UNP O60341
A	169	SER	-	expression tag	UNP O60341
A	170	HIS	-	expression tag	UNP O60341
A	171	MET	-	expression tag	UNP O60341

- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	1	0
			1057	665	185	204	3			

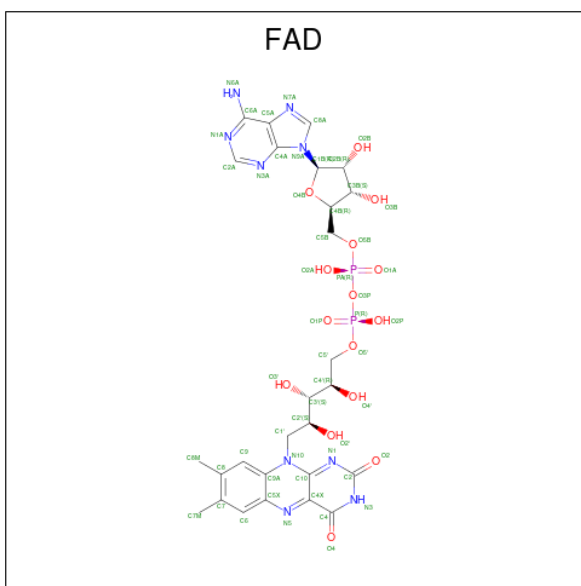
There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	301	GLY	-	expression tag	UNP Q9UKL0
B	302	SER	-	expression tag	UNP Q9UKL0
B	303	SER	-	expression tag	UNP Q9UKL0
B	304	GLY	-	expression tag	UNP Q9UKL0
B	305	SER	-	expression tag	UNP Q9UKL0
B	306	ALA	-	expression tag	UNP Q9UKL0
B	307	SER	-	expression tag	UNP Q9UKL0

- Molecule 3 is a protein called PEPTIDE SRTMQTARKSTGGKAPRKQL.

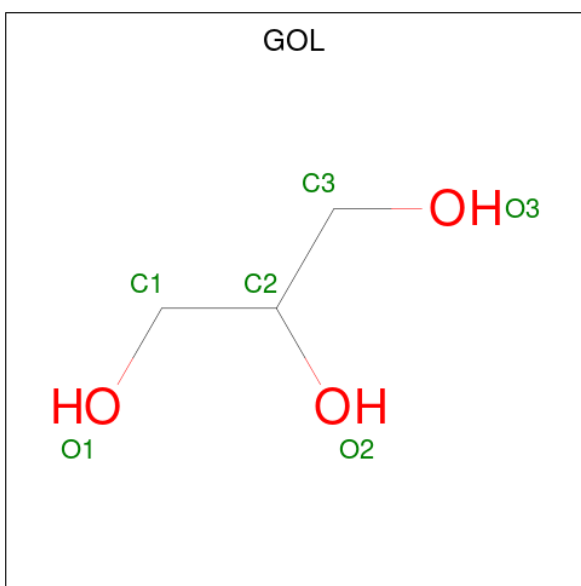
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	15	Total	C	N	O	S	0	0	0
			108	62	24	21	1			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		

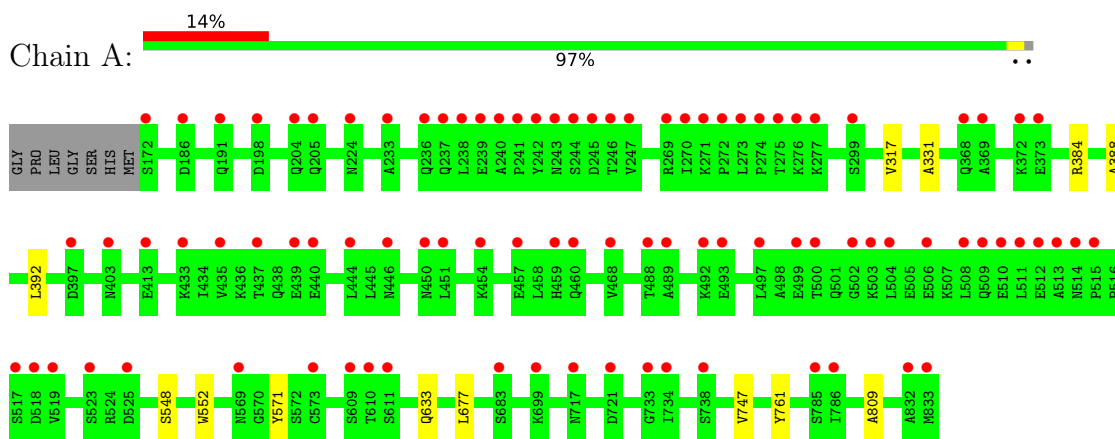
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	58	Total	O	0	0
			58	58		
6	B	1	Total	O	0	0
			1	1		
6	C	1	Total	O	0	0
			1	1		

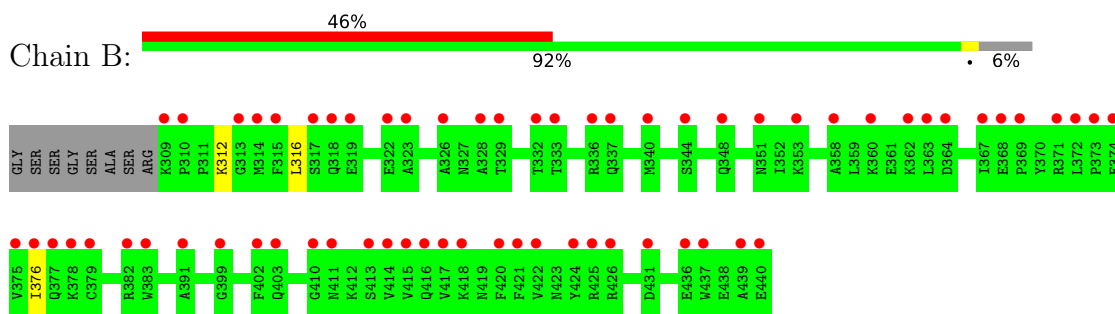
3 Residue-property plots

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.

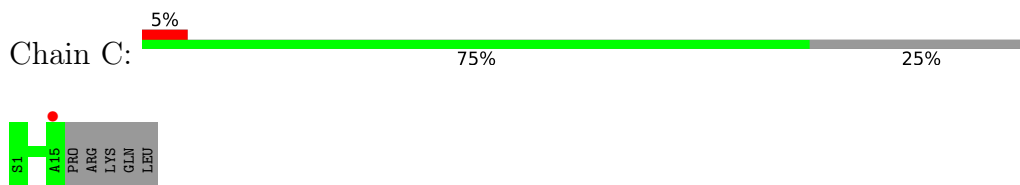
- Molecule 1: Lysine-specific histone demethylase 1A



- Molecule 2: REST corepressor 1



- Molecule 3: PEPTIDE SRTMQTARKSTGGKAPRKQL



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	122.00Å 180.36Å 233.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.69 50.00 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.69) 99.3 (50.00-2.69)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.09 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.221 , 0.236 0.211 , 0.220	Depositor DCC
R_{free} test set	1376 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å ²)	60.5	Xtriage
Anisotropy	0.776	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6494	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: GOL, 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	0.51	0/5313	0.76	0/7210
2	B	0.57	0/1072	0.81	0/1450
3	C	0.56	0/107	0.81	0/139
All	All	0.52	0/6492	0.77	0/8799

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 [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	5198	0	5216	6	0
2	B	1057	0	1050	2	0
3	C	108	0	118	0	0
4	A	53	0	31	1	0
5	A	18	0	24	0	0
6	A	58	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
All	All	6494	0	6439	6	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 0.

All (6) 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:384:ARG:NH1	2:B:312:LYS:O	2.49	0.45
1:A:331:ALA:HA	4:A:901:FAD:C4X	2.48	0.43
1:A:317:VAL:HG13	1:A:571:TYR:HB3	2.01	0.43
1:A:388:ALA:HB1	2:B:316:LEU:HD11	2.01	0.42
1:A:548:SER:O	1:A:552:TRP:HB3	2.21	0.41
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.57	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	663/669 (99%)	649 (98%)	14 (2%)	0	100	100
2	B	131/140 (94%)	125 (95%)	6 (5%)	0	100	100
3	C	13/20 (65%)	13 (100%)	0	0	100	100
All	All	807/829 (97%)	787 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	562/567 (99%)	558 (99%)	4 (1%)	76	90
2	B	114/121 (94%)	113 (99%)	1 (1%)	70	87
3	C	11/16 (69%)	11 (100%)	0	100	100
All	All	687/704 (98%)	682 (99%)	5 (1%)	76	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	LEU
1	A	633	GLN
1	A	677	LEU
1	A	747	VAL
2	B	376	ILE

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	243	ASN
1	A	422	HIS
1	A	633	GLN
1	A	742	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
5	GOL	A	904	-	5,5,5	0.32	0	5,5,5	0.25	0
4	FAD	A	901	-	58,58,58	1.56	12 (20%)	85,89,89	1.62	18 (21%)
5	GOL	A	903	-	5,5,5	0.39	0	5,5,5	0.33	0
5	GOL	A	902	-	5,5,5	0.36	0	5,5,5	0.51	0

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
5	GOL	A	904	-	-	0/4/4/4	-
4	FAD	A	901	-	-	2/34/50/50	0/6/6/6
5	GOL	A	903	-	-	1/4/4/4	-
5	GOL	A	902	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	FAD	C9A-C5X	5.82	1.50	1.41
4	A	901	FAD	C5A-C4A	4.60	1.47	1.39
4	A	901	FAD	C8-C7	3.37	1.49	1.40
4	A	901	FAD	C5A-C6A	2.60	1.48	1.41
4	A	901	FAD	C5A-N7A	-2.56	1.34	1.39
4	A	901	FAD	P-O3P	2.44	1.62	1.59
4	A	901	FAD	C4A-N9A	-2.38	1.32	1.37
4	A	901	FAD	C4-N3	-2.31	1.34	1.38
4	A	901	FAD	C8A-N7A	2.28	1.36	1.31
4	A	901	FAD	C5X-N5	-2.27	1.35	1.39
4	A	901	FAD	C4X-N5	2.20	1.35	1.30
4	A	901	FAD	C10-N10	2.01	1.41	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	FAD	C5A-C4A-N3A	-5.00	119.83	126.72
4	A	901	FAD	N3A-C2A-N1A	-3.95	122.61	128.58
4	A	901	FAD	N3A-C4A-N9A	3.91	133.81	127.17
4	A	901	FAD	C2A-N3A-C4A	3.63	120.69	111.83
4	A	901	FAD	C4A-C5A-N7A	-3.33	106.78	110.58
4	A	901	FAD	C4A-N9A-C8A	2.75	108.62	105.74
4	A	901	FAD	C4X-C10-N1	-2.63	118.13	124.59
4	A	901	FAD	C4-C4X-N5	2.62	121.83	118.21
4	A	901	FAD	C5'-C4'-C3'	-2.57	107.37	112.22
4	A	901	FAD	O4-C4-C4X	-2.55	119.80	126.53
4	A	901	FAD	C5A-N7A-C8A	2.40	107.22	103.45
4	A	901	FAD	O2-C2-N1	-2.40	117.82	121.80
4	A	901	FAD	C10-N1-C2	2.39	122.03	116.85
4	A	901	FAD	C6A-C5A-N7A	2.35	136.62	132.09
4	A	901	FAD	C2A-N1A-C6A	2.30	122.52	118.73
4	A	901	FAD	C4X-C10-N10	2.20	119.63	116.48
4	A	901	FAD	C4X-C4-N3	2.15	118.73	113.25
4	A	901	FAD	N9A-C8A-N7A	-2.05	111.03	113.94

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	902	GOL	C1-C2-C3-O3
5	A	902	GOL	O2-C2-C3-O3
4	A	901	FAD	C2'-C3'-C4'-O4'
5	A	903	GOL	O1-C1-C2-O2
4	A	901	FAD	C2'-C3'-C4'-C5'

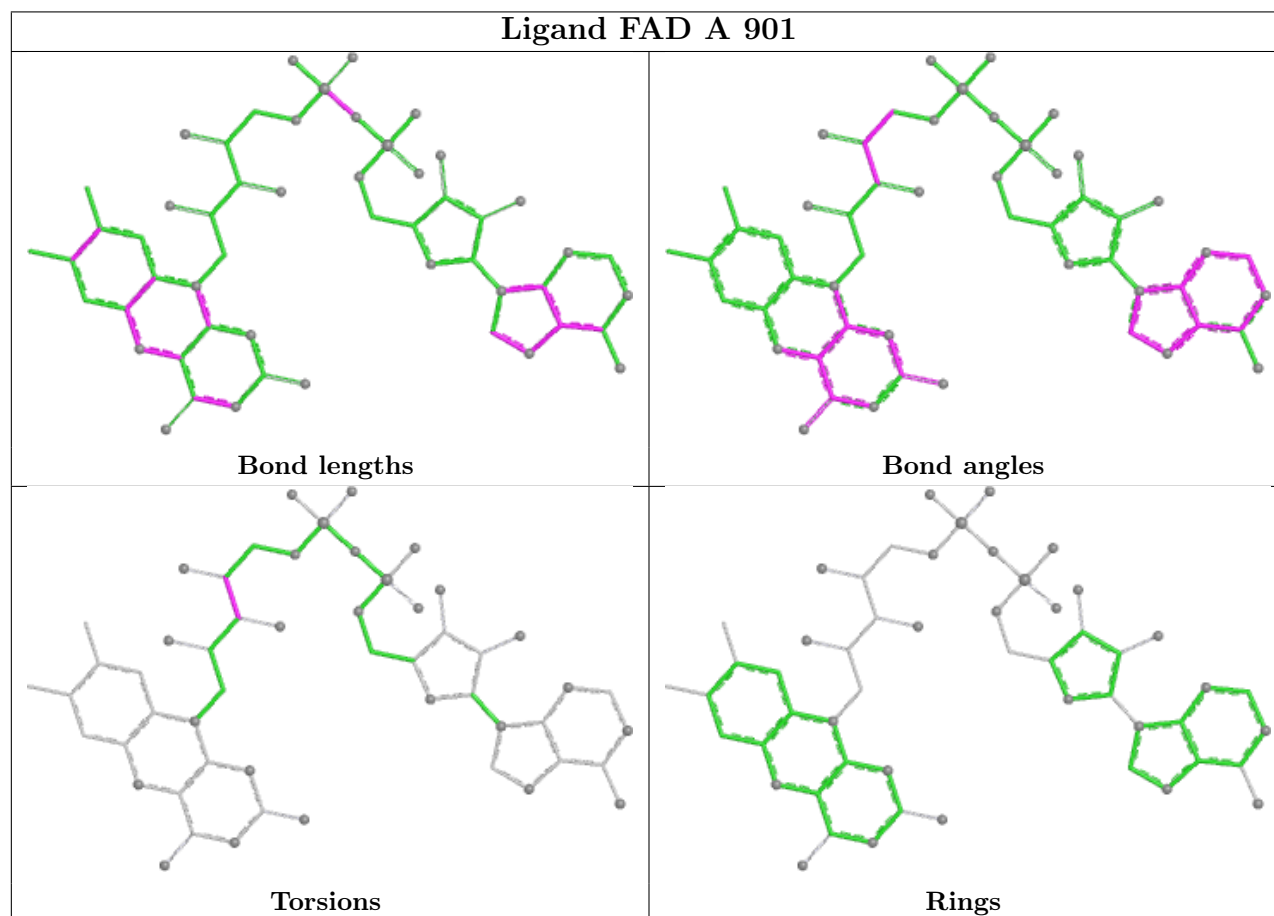
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	FAD	1	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 ⓘ

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	662/669 (98%)	0.77	91 (13%) 6 5	26, 68, 104, 134	3 (0%)
2	B	132/140 (94%)	2.23	64 (48%) 0 0	45, 102, 128, 158	1 (0%)
3	C	15/20 (75%)	0.84	1 (6%) 24 21	59, 62, 88, 99	0
All	All	809/829 (97%)	1.01	156 (19%) 3 3	26, 73, 116, 158	4 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	309	LYS	8.7
1	A	833	MET	7.7
2	B	375	VAL	6.6
3	C	15	ALA	6.5
2	B	376	ILE	5.8
2	B	332	THR	5.8
1	A	271	LYS	5.7
1	A	275	THR	5.6
2	B	340	MET	5.6
2	B	313	GLY	5.5
2	B	415	VAL	5.4
1	A	403	ASN	5.4
1	A	272	PRO	5.3
2	B	379	CYS	5.2
2	B	329	THR	4.8
2	B	372	LEU	4.6
2	B	426	ARG	4.4
2	B	382	ARG	4.4
2	B	414	VAL	4.4
1	A	832	ALA	4.3
2	B	418	LYS	4.3
2	B	378	LYS	4.3
1	A	241	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	274	PRO	4.3
1	A	373	GLU	4.3
2	B	422	VAL	4.3
1	A	240	ALA	4.1
2	B	399	GLY	4.0
2	B	351[A]	ASN	4.0
2	B	373	PRO	3.9
2	B	337	GLN	3.8
1	A	733	GLY	3.8
1	A	511	LEU	3.6
1	A	497	LEU	3.6
1	A	502	GLY	3.6
1	A	514	ASN	3.6
1	A	269	ARG	3.5
1	A	233	ALA	3.5
1	A	270	ILE	3.5
1	A	488	THR	3.5
1	A	506	GLU	3.5
2	B	383	TRP	3.4
1	A	508	LEU	3.4
1	A	236	GLN	3.3
1	A	721	ASP	3.3
2	B	315	PHE	3.3
2	B	368	GLU	3.3
1	A	454	LYS	3.3
2	B	333	THR	3.2
1	A	510	GLU	3.2
2	B	310	PRO	3.2
1	A	172	SER	3.2
1	A	224	ASN	3.2
1	A	446	ASN	3.2
2	B	417	VAL	3.1
1	A	786	ILE	3.0
1	A	519	VAL	3.0
1	A	515	PRO	3.0
2	B	421	PHE	3.0
1	A	499	GLU	3.0
2	B	362	LYS	2.9
1	A	186	ASP	2.9
1	A	503	LYS	2.9
1	A	717	ASN	2.9
1	A	437	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	322	GLU	2.9
1	A	504	LEU	2.9
1	A	273	LEU	2.8
1	A	513	ALA	2.8
1	A	439	GLU	2.8
1	A	205	GLN	2.8
2	B	318	GLN	2.8
2	B	348	GLN	2.8
1	A	699	LYS	2.8
1	A	450	ASN	2.8
2	B	369	PRO	2.8
1	A	433	LYS	2.8
1	A	244	SER	2.7
1	A	239	GLU	2.7
1	A	489	ALA	2.7
2	B	420	PHE	2.7
2	B	377	GLN	2.7
1	A	609	SER	2.7
1	A	518	ASP	2.7
1	A	204	GLN	2.6
1	A	512	GLU	2.6
1	A	198	ASP	2.6
1	A	509	GLN	2.6
1	A	413	GLU	2.5
1	A	569	ASN	2.5
2	B	353	LYS	2.5
1	A	191	GLN	2.5
2	B	326	ALA	2.5
1	A	500	THR	2.5
1	A	276	LYS	2.5
1	A	397	ASP	2.5
2	B	360	LYS	2.5
2	B	437	TRP	2.5
1	A	435	VAL	2.5
1	A	369	ALA	2.5
1	A	372	LYS	2.5
2	B	336	ARG	2.4
2	B	440	GLU	2.4
2	B	403	GLN	2.4
1	A	451	LEU	2.4
2	B	344	SER	2.4
1	A	493	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	328	ALA	2.4
1	A	683	SER	2.4
1	A	738	SER	2.4
1	A	785	SER	2.4
2	B	317	SER	2.4
1	A	525	ASP	2.4
2	B	431	ASP	2.4
1	A	277	LYS	2.4
1	A	573	CYS	2.4
1	A	368	GLN	2.4
1	A	460	GLN	2.4
1	A	457	GLU	2.3
1	A	459	HIS	2.3
1	A	610	THR	2.3
1	A	299	SER	2.3
2	B	367	ILE	2.3
2	B	314	MET	2.3
2	B	364	ASP	2.3
2	B	402	PHE	2.3
1	A	243	ASN	2.3
2	B	410	GLY	2.2
1	A	247	VAL	2.2
1	A	734	ILE	2.2
2	B	439	ALA	2.2
1	A	245	ASP	2.2
2	B	371	ARG	2.2
1	A	611	SER	2.2
2	B	363	LEU	2.2
2	B	416	GLN	2.1
1	A	523	SER	2.1
2	B	323	ALA	2.1
1	A	238	LEU	2.1
2	B	424	TYR	2.1
2	B	391	ALA	2.1
1	A	440	GLU	2.1
2	B	374	GLU	2.1
1	A	492	LYS	2.1
1	A	242	TYR	2.1
2	B	436	GLU	2.1
1	A	444	LEU	2.1
2	B	411	ASN	2.1
2	B	319	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	425	ARG	2.0
2	B	358	ALA	2.0
1	A	517	SER	2.0
2	B	413	SER	2.0
1	A	246	THR	2.0
1	A	237	GLN	2.0
1	A	468	VAL	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](#)

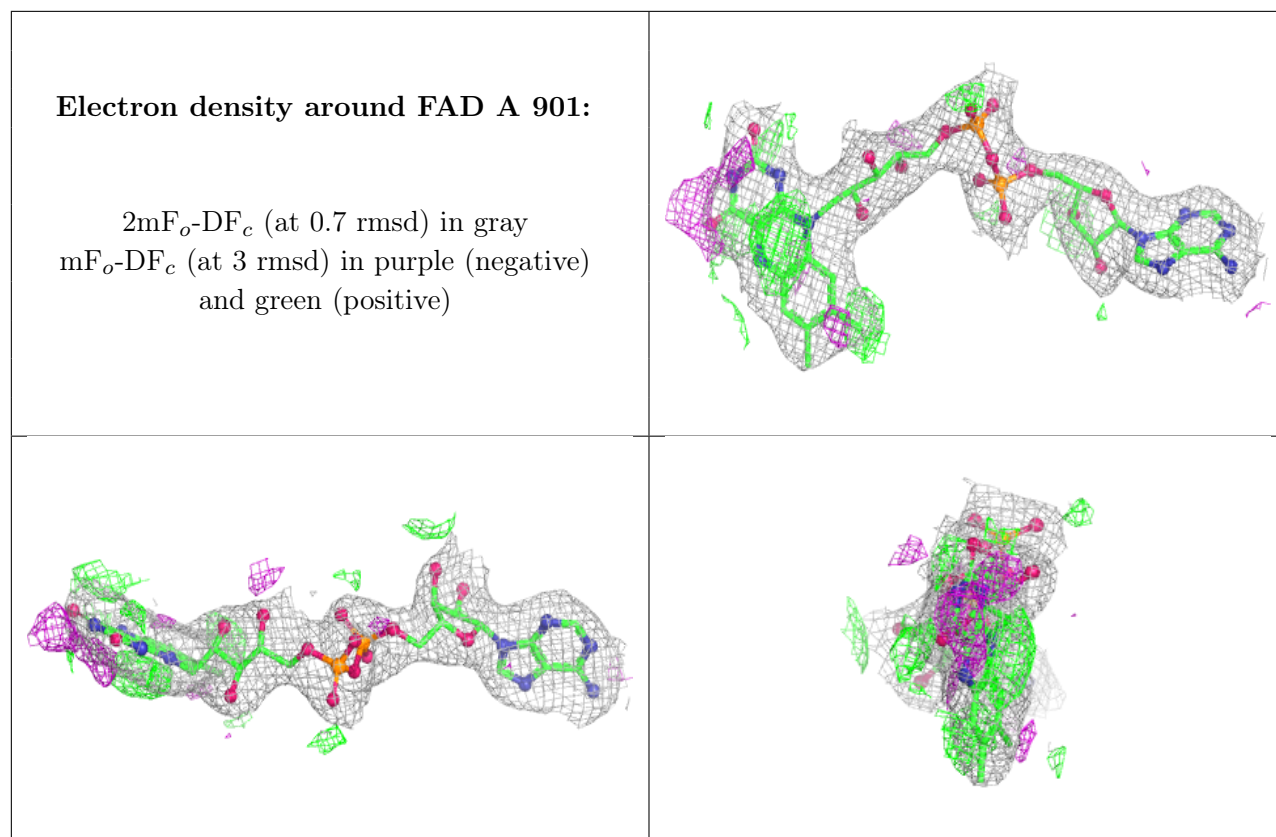
There are no oligosaccharides in this entry.

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
5	GOL	A	903	6/6	0.80	0.29	108,109,110,111	0
5	GOL	A	902	6/6	0.89	0.19	69,70,73,77	0
5	GOL	A	904	6/6	0.94	0.15	76,79,85,88	0
4	FAD	A	901	53/53	0.97	0.08	38,43,54,57	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.