



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:26 AM UTC

PDB ID : 7ZRY / pdb_00007zry
Title : Structure of the 2a splicing variant of the full-length human LSD1 bound to CoREST (delta305)
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2022-05-06
Resolution : 2.70 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

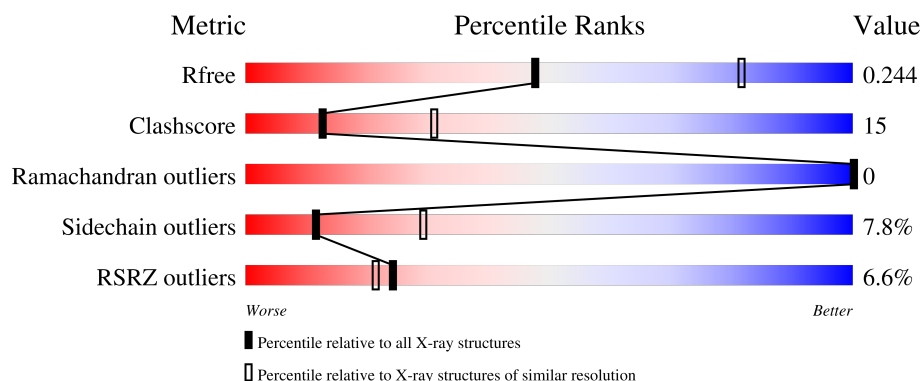
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	872	4% 56% 18% • 24%
2	B	178	11% 49% 22% • 25%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6339 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.

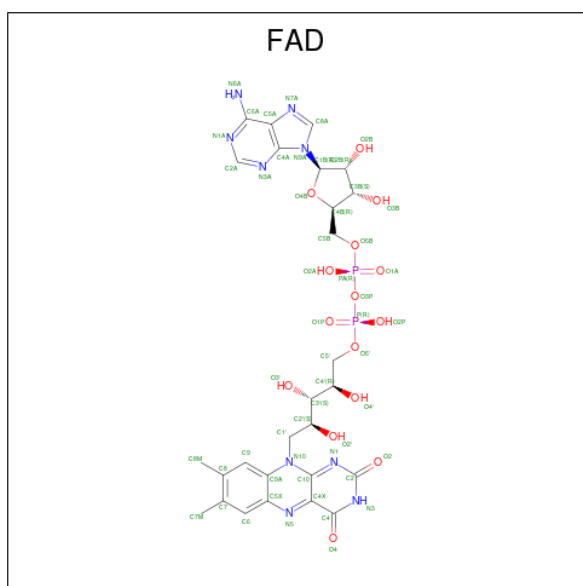
- Molecule 1 is a protein called Isoform of Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	665	Total	C	N	O	S	0	0	0
			5210	3319	905	966	20			

- 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 (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).

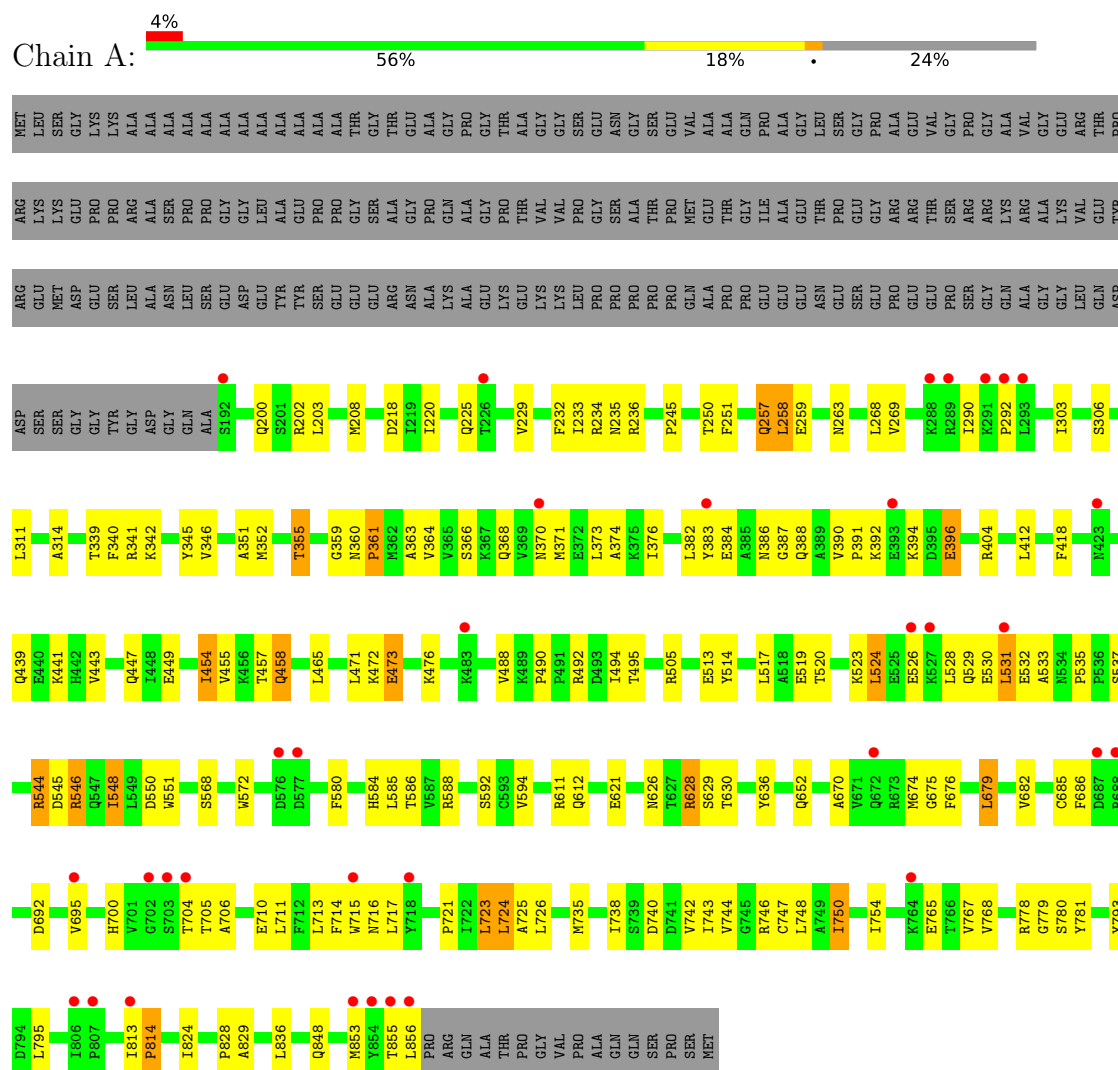


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

3 Residue-property plots

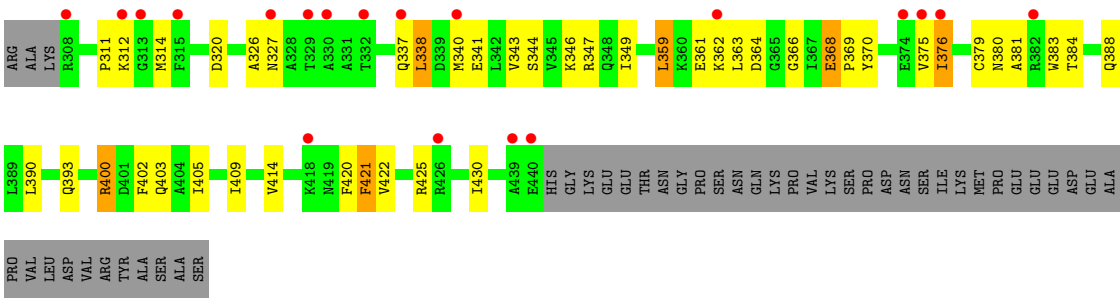
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Isoform of 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	119.75Å 179.75Å 234.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.12 – 2.70 49.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.12-2.70) 85.5 (49.12-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.41 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.220 , 0.241 0.229 , 0.244	Depositor DCC
R_{free} test set	1997 reflections (2.87%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6339	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 ⓘ

5.1 Standard geometry ⓘ

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	0.75	4/5323 (0.1%)	0.92	3/7221 (0.0%)
2	B	0.71	0/1091	1.03	3/1471 (0.2%)
All	All	0.75	4/6414 (0.1%)	0.94	6/8692 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	675	GLY	CA-C	-6.61	1.47	1.52
1	A	490	PRO	C-O	-6.25	1.17	1.24
1	A	814	PRO	C-O	-5.79	1.17	1.23
1	A	361	PRO	C-O	-5.55	1.17	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	421	PHE	CB-CA-C	-5.85	101.08	110.79
1	A	391	PRO	CB-CA-C	-5.17	104.20	110.98
2	B	362	LYS	CA-C-N	-5.11	114.47	122.95
2	B	362	LYS	C-N-CA	-5.11	114.47	122.95
1	A	257	GLN	CA-C-N	-5.10	115.05	122.65
1	A	257	GLN	C-N-CA	-5.10	115.05	122.65

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	5210	0	5244	166	0
2	B	1076	0	1091	38	0
3	A	53	0	31	5	0
All	All	6339	0	6366	193	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 15.

All (193) 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:412:LEU:CD2	1:A:418:PHE:HB3	2.03	0.88
1:A:258:LEU:HD12	1:A:263:ASN:HB3	1.54	0.88
1:A:258:LEU:CD1	1:A:263:ASN:HB3	2.03	0.88
1:A:458:GLN:CD	1:A:528:LEU:HD21	2.00	0.87
2:B:400:ARG:HH11	2:B:400:ARG:HG3	1.40	0.86
1:A:715:TRP:HB3	1:A:717:LEU:HD23	1.56	0.86
1:A:457:THR:OG1	1:A:528:LEU:HD11	1.75	0.85
1:A:704:THR:HG22	1:A:706:ALA:H	1.44	0.82
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.64	0.79
1:A:546:ARG:HH11	1:A:546:ARG:HG3	1.48	0.79
1:A:692:ASP:HB3	1:A:695:VAL:HG12	1.63	0.78
1:A:412:LEU:CD2	1:A:418:PHE:CB	2.63	0.76
1:A:458:GLN:OE1	1:A:528:LEU:CD2	2.34	0.76
1:A:531:LEU:HD23	1:A:531:LEU:N	2.00	0.75
1:A:458:GLN:OE1	1:A:528:LEU:HD23	1.86	0.75
2:B:376:ILE:HD12	2:B:376:ILE:O	1.87	0.74
1:A:544:ARG:HG2	1:A:544:ARG:NH1	2.02	0.74
1:A:458:GLN:CD	1:A:528:LEU:CD2	2.60	0.74
1:A:679:LEU:C	1:A:679:LEU:HD12	2.12	0.74
1:A:711:LEU:HD22	1:A:747:CYS:SG	2.28	0.74
2:B:363:LEU:O	2:B:363:LEU:HD12	1.87	0.74
1:A:458:GLN:HG2	1:A:528:LEU:HD21	1.69	0.73
2:B:338:LEU:N	2:B:338:LEU:HD23	2.03	0.73
1:A:258:LEU:HD12	1:A:258:LEU:C	2.12	0.73
1:A:473:GLU:OE2	1:A:473:GLU:HA	1.87	0.73
1:A:544:ARG:HG2	1:A:544:ARG:HH11	1.52	0.73
1:A:458:GLN:CG	1:A:528:LEU:HD21	2.19	0.72
1:A:384:GLU:OE1	1:A:544:ARG:NH2	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:LEU:N	1:A:524:LEU:HD23	2.06	0.69
1:A:546:ARG:HH11	1:A:546:ARG:CG	2.04	0.69
1:A:404:ARG:NH2	2:B:312:LYS:O	2.25	0.69
1:A:258:LEU:HD11	1:A:263:ASN:CA	2.24	0.68
1:A:361:PRO:HG3	1:A:836:LEU:HD11	1.74	0.68
1:A:700:HIS:CD2	1:A:750:ILE:CG2	2.77	0.68
1:A:412:LEU:HD22	1:A:418:PHE:HB3	1.75	0.67
1:A:710:GLU:OE2	1:A:746:ARG:NH1	2.28	0.67
1:A:351:ALA:HA	3:A:901:FAD:N5	2.11	0.66
2:B:403:GLN:NE2	2:B:403:GLN:HA	2.11	0.65
2:B:421:PHE:O	2:B:425:ARG:HB2	1.95	0.65
1:A:258:LEU:HD12	1:A:258:LEU:O	1.96	0.65
1:A:361:PRO:HG3	1:A:836:LEU:CD1	2.26	0.65
1:A:726:LEU:HD12	1:A:726:LEU:N	2.12	0.65
1:A:258:LEU:HD11	1:A:263:ASN:HB3	1.79	0.64
1:A:404:ARG:HB3	2:B:314:MET:HE3	1.80	0.64
1:A:711:LEU:CD2	1:A:747:CYS:SG	2.85	0.64
1:A:711:LEU:HD23	1:A:725:ALA:HB1	1.80	0.63
1:A:715:TRP:CD1	1:A:726:LEU:HD11	2.33	0.63
1:A:245:PRO:O	1:A:368:GLN:NE2	2.32	0.62
1:A:465:LEU:HB2	2:B:359:LEU:HD12	1.81	0.62
2:B:400:ARG:HG3	2:B:400:ARG:NH1	2.14	0.62
1:A:386:ASN:OD1	1:A:387:GLY:N	2.34	0.61
1:A:682:VAL:HG13	1:A:768:VAL:HG22	1.83	0.61
1:A:390:VAL:HG21	1:A:548:ILE:HD13	1.84	0.60
1:A:258:LEU:HD11	1:A:263:ASN:CB	2.32	0.59
2:B:425:ARG:HA	2:B:430:ILE:HD12	1.84	0.59
1:A:746:ARG:O	1:A:750:ILE:HG12	2.03	0.58
1:A:584:HIS:C	1:A:585:LEU:HD12	2.27	0.58
1:A:488:VAL:HG12	1:A:488:VAL:O	2.02	0.58
2:B:370:TYR:N	2:B:370:TYR:CD1	2.72	0.58
1:A:824:ILE:O	1:A:824:ILE:HG23	2.03	0.58
1:A:713:LEU:HD12	1:A:714:PHE:H	1.68	0.58
1:A:670:ALA:O	1:A:674:MET:HG3	2.04	0.57
1:A:704:THR:HG22	1:A:706:ALA:N	2.15	0.57
2:B:380:ASN:OD1	2:B:381:ALA:N	2.34	0.57
1:A:392:LYS:O	1:A:396:GLU:HG3	2.04	0.57
1:A:472:LYS:HE3	2:B:366:GLY:O	2.05	0.56
1:A:232:PHE:CE1	1:A:236:ARG:HB2	2.40	0.56
1:A:495:THR:HA	2:B:393:GLN:HE22	1.71	0.56
1:A:404:ARG:HB3	2:B:314:MET:CE	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:LEU:C	1:A:533:ALA:H	2.15	0.56
1:A:202:ARG:NH1	1:A:361:PRO:HD3	2.21	0.55
1:A:355:THR:O	1:A:355:THR:OG1	2.17	0.55
1:A:386:ASN:OD1	1:A:388:GLN:N	2.39	0.55
1:A:813:ILE:HG23	1:A:848:GLN:CD	2.32	0.55
1:A:412:LEU:HD21	1:A:418:PHE:CB	2.36	0.55
1:A:692:ASP:HB3	1:A:695:VAL:CG1	2.36	0.55
1:A:412:LEU:HD21	1:A:418:PHE:CG	2.42	0.54
1:A:700:HIS:CD2	1:A:750:ILE:HG23	2.42	0.54
1:A:203:LEU:HD13	1:A:234:ARG:HD2	1.88	0.54
1:A:306:SER:O	1:A:311:LEU:HD11	2.06	0.54
2:B:420:PHE:C	2:B:420:PHE:CD1	2.85	0.54
1:A:629:SER:O	1:A:629:SER:OG	2.21	0.54
1:A:544:ARG:HH11	1:A:544:ARG:CG	2.20	0.54
1:A:780:SER:HB2	3:A:901:FAD:HM83	1.89	0.54
1:A:781:TYR:CD1	1:A:829:ALA:HB1	2.43	0.53
1:A:412:LEU:HD23	1:A:412:LEU:O	2.08	0.53
2:B:346:LYS:O	2:B:349:ILE:HB	2.09	0.53
1:A:258:LEU:HD11	1:A:263:ASN:HA	1.90	0.53
1:A:814:PRO:HD2	1:A:848:GLN:OE1	2.09	0.53
1:A:439:GLN:NE2	2:B:314:MET:HA	2.24	0.53
1:A:373:LEU:HB3	1:A:585:LEU:HD23	1.90	0.52
1:A:531:LEU:N	1:A:531:LEU:CD2	2.72	0.52
1:A:371:MET:HE3	1:A:594:VAL:HG21	1.92	0.52
1:A:374:ALA:HB2	1:A:588:ARG:HD2	1.91	0.51
1:A:394:LYS:NZ	1:A:545:ASP:OD1	2.41	0.51
1:A:454:ILE:HG22	2:B:349:ILE:CD1	2.40	0.51
1:A:345:TYR:CE2	1:A:685:CYS:HB3	2.45	0.51
1:A:471:LEU:HD23	1:A:514:TYR:HB2	1.92	0.51
1:A:738:ILE:HG22	1:A:743:ILE:HG13	1.92	0.51
1:A:686:PHE:O	1:A:721:PRO:HG2	2.11	0.50
1:A:251:PHE:HE1	1:A:269:VAL:HG12	1.76	0.50
1:A:363:ALA:O	1:A:366:SER:OG	2.27	0.49
1:A:340:PHE:CE1	1:A:767:VAL:HG21	2.47	0.49
1:A:341:ARG:HG2	1:A:346:VAL:HG22	1.94	0.49
1:A:303:ILE:HD12	1:A:314:ALA:HB2	1.93	0.49
1:A:550:ASP:OD2	1:A:705:THR:HA	2.12	0.49
2:B:326:ALA:O	2:B:327:ASN:OD1	2.31	0.49
1:A:218:ASP:OD1	1:A:218:ASP:N	2.46	0.49
1:A:232:PHE:HE1	1:A:236:ARG:HB2	1.78	0.49
1:A:855:THR:HG23	1:A:856:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LYS:CE	2:B:366:GLY:O	2.61	0.48
1:A:443:VAL:O	1:A:447:GLN:HG3	2.13	0.48
1:A:531:LEU:C	1:A:533:ALA:N	2.72	0.48
2:B:400:ARG:NH1	2:B:400:ARG:CG	2.73	0.48
1:A:311:LEU:HD12	1:A:311:LEU:H	1.79	0.48
1:A:351:ALA:HA	3:A:901:FAD:C4X	2.43	0.48
1:A:813:ILE:CG2	1:A:814:PRO:CD	2.92	0.48
2:B:402:PHE:N	2:B:402:PHE:CD1	2.79	0.47
2:B:368:GLU:N	2:B:369:PRO:CD	2.78	0.47
1:A:258:LEU:CD1	1:A:258:LEU:C	2.85	0.47
1:A:535:PRO:HG2	1:A:535:PRO:O	2.15	0.47
1:A:364:VAL:O	1:A:368:GLN:HG3	2.14	0.46
2:B:383:TRP:CH2	2:B:420:PHE:CD2	3.03	0.46
1:A:200:GLN:HA	1:A:359:GLY:HA2	1.96	0.46
1:A:441:LYS:NZ	2:B:320:ASP:OD1	2.48	0.46
1:A:586:THR:HG21	1:A:717:LEU:HG	1.96	0.46
1:A:342:LYS:HE2	1:A:765:GLU:CD	2.41	0.46
1:A:710:GLU:CD	1:A:735:MET:HE3	2.41	0.46
2:B:402:PHE:CB	2:B:414:VAL:HG13	2.45	0.46
1:A:376:ILE:HD11	1:A:586:THR:CG2	2.47	0.45
1:A:746:ARG:O	1:A:750:ILE:CG1	2.63	0.45
1:A:390:VAL:HG21	1:A:548:ILE:CD1	2.47	0.45
1:A:676:PHE:CE2	1:A:779:GLY:HA3	2.52	0.45
2:B:368:GLU:OE2	2:B:368:GLU:HA	2.10	0.45
2:B:402:PHE:HB3	2:B:414:VAL:HG13	1.98	0.45
1:A:780:SER:O	3:A:901:FAD:HM81	2.16	0.45
1:A:290:ILE:O	1:A:292:PRO:HD3	2.16	0.45
1:A:742:VAL:O	1:A:746:ARG:HG3	2.17	0.45
1:A:652:GLN:CD	1:A:778:ARG:HE	2.25	0.44
1:A:412:LEU:CD2	1:A:418:PHE:CD2	3.00	0.44
2:B:383:TRP:CZ2	2:B:420:PHE:HD2	2.36	0.44
1:A:404:ARG:NH1	2:B:312:LYS:O	2.50	0.44
1:A:626:ASN:HD22	1:A:629:SER:H	1.63	0.44
1:A:692:ASP:O	1:A:695:VAL:HG12	2.17	0.44
1:A:740:ASP:O	1:A:744:VAL:HG23	2.18	0.44
2:B:376:ILE:H	2:B:376:ILE:HG13	1.49	0.44
1:A:621:GLU:HA	1:A:636:TYR:O	2.18	0.44
1:A:258:LEU:CD1	1:A:263:ASN:CB	2.82	0.44
1:A:208:MET:HE1	1:A:220:ILE:HA	1.99	0.44
1:A:225:GLN:O	1:A:229:VAL:HG23	2.18	0.44
1:A:251:PHE:CE1	1:A:269:VAL:HG12	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:LEU:HD23	1:A:723:LEU:HA	1.73	0.44
1:A:710:GLU:OE1	1:A:735:MET:HE3	2.19	0.43
1:A:412:LEU:HD21	1:A:418:PHE:CD2	2.53	0.43
1:A:514:TYR:CD1	1:A:514:TYR:O	2.70	0.43
1:A:229:VAL:O	1:A:233:ILE:HG13	2.18	0.43
1:A:546:ARG:CG	1:A:546:ARG:NH1	2.73	0.43
2:B:311:PRO:HG2	2:B:314:MET:CG	2.42	0.43
1:A:780:SER:HB2	3:A:901:FAD:C8M	2.47	0.43
2:B:369:PRO:HB2	2:B:370:TYR:CE1	2.54	0.43
1:A:232:PHE:CD1	1:A:232:PHE:C	2.97	0.43
1:A:340:PHE:CD1	1:A:767:VAL:HG21	2.53	0.43
1:A:339:THR:HB	1:A:592:SER:HB3	2.01	0.42
1:A:208:MET:HE1	1:A:220:ILE:CA	2.49	0.42
1:A:412:LEU:HD23	1:A:418:PHE:HB3	1.96	0.42
1:A:711:LEU:HD21	1:A:747:CYS:SG	2.60	0.42
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.84	0.42
1:A:513:GLU:O	1:A:517:LEU:HD13	2.20	0.42
1:A:568:SER:O	1:A:572:TRP:HB3	2.19	0.42
1:A:382:LEU:HD11	1:A:551:TRP:CE2	2.54	0.42
1:A:505:ARG:HD3	1:A:505:ARG:C	2.44	0.42
1:A:795:LEU:HD23	1:A:795:LEU:HA	1.79	0.41
1:A:716:ASN:C	1:A:717:LEU:HD22	2.46	0.41
1:A:715:TRP:HD1	1:A:726:LEU:HD11	1.79	0.41
1:A:793:TYR:CE2	1:A:828:PRO:HB3	2.55	0.41
1:A:360:ASN:HB2	1:A:580:PHE:CD2	2.55	0.41
1:A:628:ARG:H	1:A:628:ARG:HG3	1.55	0.41
1:A:679:LEU:C	1:A:679:LEU:CD1	2.85	0.41
1:A:383:TYR:CG	1:A:754:ILE:HD12	2.55	0.41
1:A:714:PHE:HA	1:A:724:LEU:O	2.21	0.41
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.82	0.41
1:A:352:MET:HE3	1:A:715:TRP:CZ3	2.56	0.41
1:A:735:MET:HE1	1:A:746:ARG:NH1	2.36	0.41
1:A:813:ILE:HG23	1:A:814:PRO:CD	2.50	0.41
1:A:814:PRO:CD	1:A:848:GLN:OE1	2.69	0.41
1:A:250:THR:HG23	1:A:290:ILE:HD12	2.02	0.40
1:A:412:LEU:CD2	1:A:418:PHE:CG	3.03	0.40
1:A:457:THR:OG1	1:A:528:LEU:CD1	2.56	0.40
1:A:494:ILE:HD12	1:A:494:ILE:HA	1.87	0.40
1:A:234:ARG:HG2	1:A:235:ASN:OD1	2.21	0.40
1:A:412:LEU:HD23	1:A:412:LEU:C	2.46	0.40
2:B:384:THR:O	2:B:388:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:LEU:HD23	1:A:748:LEU:HA	1.85	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	663/872 (76%)	645 (97%)	18 (3%)	0	100	100
2	B	131/178 (74%)	123 (94%)	8 (6%)	0	100	100
All	All	794/1050 (76%)	768 (97%)	26 (3%)	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	565/710 (80%)	530 (94%)	35 (6%)	16	39
2	B	117/156 (75%)	99 (85%)	18 (15%)	2	7
All	All	682/866 (79%)	629 (92%)	53 (8%)	11	29

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	GLN
1	A	258	LEU
1	A	259	GLU
1	A	355	THR
1	A	370	ASN
1	A	396	GLU
1	A	449	GLU
1	A	454	ILE
1	A	455	VAL
1	A	458	GLN
1	A	473	GLU
1	A	476	LYS
1	A	492	ARG
1	A	519	GLU
1	A	520	THR
1	A	523	LYS
1	A	524	LEU
1	A	526	GLU
1	A	529	GLN
1	A	530	GLU
1	A	531	LEU
1	A	532	GLU
1	A	537	SER
1	A	544	ARG
1	A	546	ARG
1	A	548	ILE
1	A	611	ARG
1	A	612	GLN
1	A	628	ARG
1	A	630	THR
1	A	679	LEU
1	A	723	LEU
1	A	724	LEU
1	A	750	ILE
1	A	853	MET
2	B	337	GLN
2	B	338	LEU
2	B	340	MET
2	B	341	GLU
2	B	343	VAL
2	B	344	SER
2	B	347	ARG
2	B	359	LEU

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Mol	Chain	Res	Type
2	B	361	GLU
2	B	364	ASP
2	B	368	GLU
2	B	375	VAL
2	B	376	ILE
2	B	379	CYS
2	B	400	ARG
2	B	405	ILE
2	B	409	ILE
2	B	422	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	403	ASN
1	A	504	HIS
1	A	534	ASN
1	A	626	ASN
1	A	658	GLN
1	A	700	HIS
1	A	762	GLN
1	A	832	HIS
2	B	318	GLN
2	B	356	ASN
2	B	377	GLN
2	B	393	GLN
2	B	403	GLN
2	B	419	ASN
2	B	429	ASN

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

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
3	FAD	A	901	-	58,58,58	1.52	13 (22%)	85,89,89	0.82	1 (1%)

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	-	-	8/34/50/50	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	FAD	PA-O3P	-3.62	1.55	1.59
3	A	901	FAD	C2-N3	-3.58	1.31	1.39
3	A	901	FAD	C1'-C2'	-3.34	1.48	1.52
3	A	901	FAD	P-O3P	-3.17	1.56	1.59
3	A	901	FAD	O2'-C2'	-2.92	1.37	1.43
3	A	901	FAD	C8A-N9A	-2.63	1.33	1.37
3	A	901	FAD	C4X-C4	-2.41	1.35	1.44
3	A	901	FAD	O3'-C3'	-2.34	1.37	1.43
3	A	901	FAD	O2-C2	-2.25	1.19	1.24
3	A	901	FAD	C6-C7	-2.15	1.36	1.39
3	A	901	FAD	C2-N1	-2.08	1.31	1.36
3	A	901	FAD	PA-O2A	-2.02	1.46	1.55
3	A	901	FAD	C5X-N5	-2.00	1.35	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FAD	C4-N3-C2	-2.11	121.89	125.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

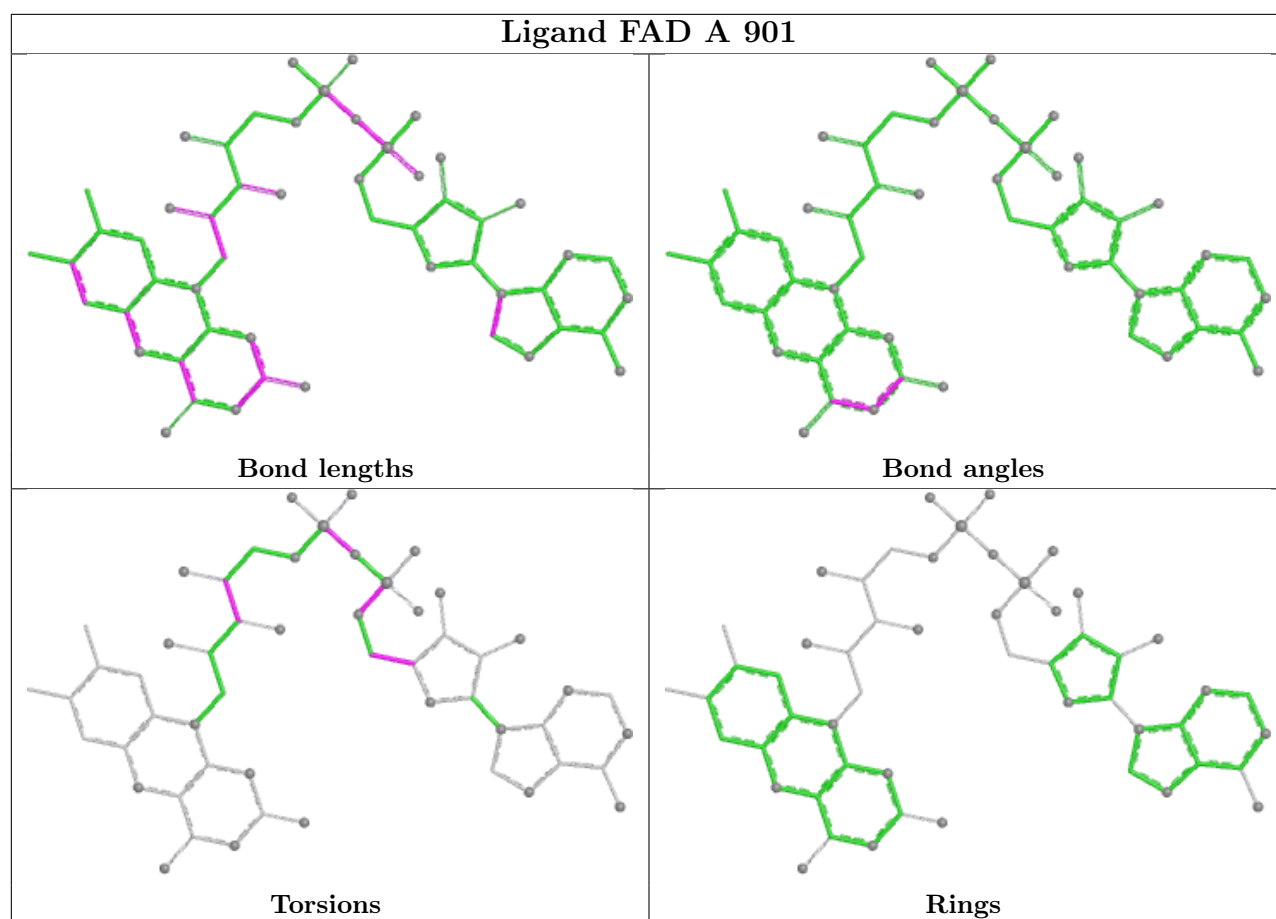
Mol	Chain	Res	Type	Atoms
3	A	901	FAD	C5B-O5B-PA-O1A
3	A	901	FAD	O3'-C3'-C4'-C5'
3	A	901	FAD	PA-O3P-P-O5'
3	A	901	FAD	C2'-C3'-C4'-O4'
3	A	901	FAD	C2'-C3'-C4'-C5'
3	A	901	FAD	O3'-C3'-C4'-O4'
3	A	901	FAD	C5B-O5B-PA-O3P
3	A	901	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	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

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%)	0.42	34 (5%) 33 29	63, 92, 122, 143	0
2	B	133/178 (74%)	1.04	19 (14%) 6 5	88, 121, 138, 149	0
All	All	798/1050 (76%)	0.52	53 (6%) 24 21	63, 98, 131, 149	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	856	LEU	6.8
2	B	376	ILE	5.0
2	B	327	ASN	4.7
2	B	440	GLU	4.3
1	A	293	LEU	4.1
2	B	375	VAL	4.0
1	A	288	LYS	3.9
1	A	855	THR	3.6
1	A	715	TRP	3.6
1	A	853	MET	3.5
1	A	531	LEU	3.5
2	B	439	ALA	3.2
1	A	813	ILE	3.2
2	B	315	PHE	3.1
1	A	687	ASP	3.0
1	A	192	SER	3.0
1	A	292	PRO	2.8
2	B	308	ARG	2.8
1	A	370	ASN	2.8
2	B	418	LYS	2.8
2	B	332	THR	2.8
1	A	526	GLU	2.8
1	A	806	ILE	2.7
1	A	393	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	764	LYS	2.6
1	A	688	ARG	2.6
1	A	718	TYR	2.6
1	A	577	ASP	2.5
1	A	289	ARG	2.5
1	A	483	LYS	2.5
2	B	312	LYS	2.5
2	B	340	MET	2.4
1	A	702	GLY	2.4
1	A	703	SER	2.4
2	B	313	GLY	2.3
2	B	382	ARG	2.3
1	A	672	GLN	2.3
2	B	337	GLN	2.3
1	A	704	THR	2.2
1	A	807	PRO	2.2
1	A	695	VAL	2.2
2	B	329	THR	2.2
1	A	383	TYR	2.2
1	A	527	LYS	2.2
2	B	330	ALA	2.1
1	A	226	THR	2.1
1	A	854	TYR	2.1
1	A	576	ASP	2.1
2	B	374	GLU	2.1
2	B	362	LYS	2.1
1	A	423	ASN	2.1
1	A	291	LYS	2.0
2	B	426	ARG	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](#)

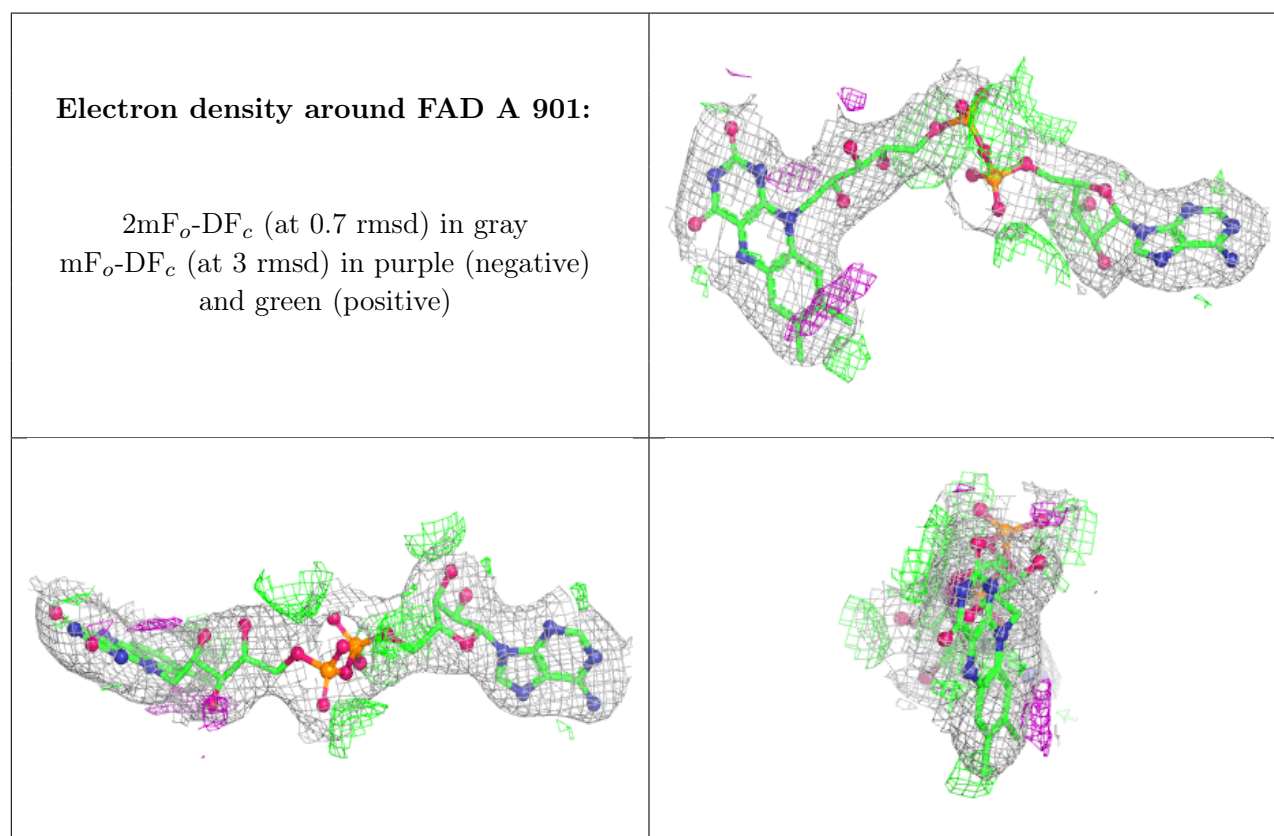
There are no oligosaccharides in this entry.

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
3	FAD	A	901	53/53	0.96	0.08	62,74,84,88	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.