



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:29 PM UTC

PDB ID : 8Q1H / pdb_00008q1h
Title : LSD1 Y391K-CoREST bound to Histone H3 N-terminal tail
Authors : Barone, M.; Mattevi, A.
Deposited on : 2023-07-31
Resolution : 2.90 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

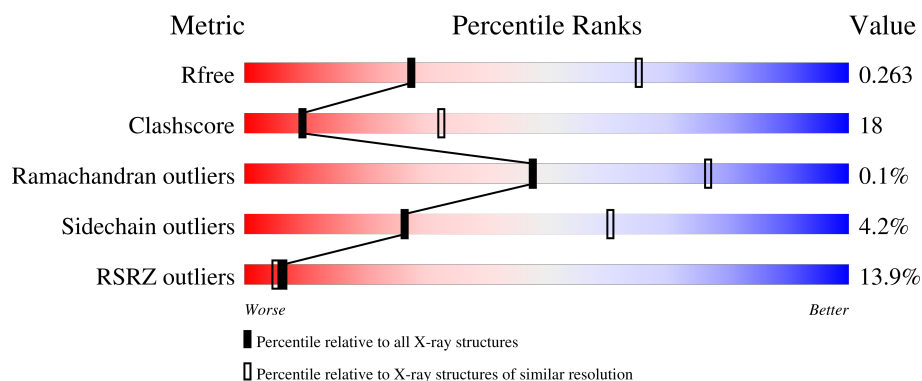
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	10% 60% 29% 9%
2	B	178	20% 48% 24% 27%
3	C	21	24% 33% 29% 10% 5% 24%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6430 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	666	Total	C	N	O	S	0	0	0
			5214	3321	907	966	20			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	391	LYS	TYR	conflict	UNP O60341

- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	S	0	0	0
			1049	659	187	200	3			

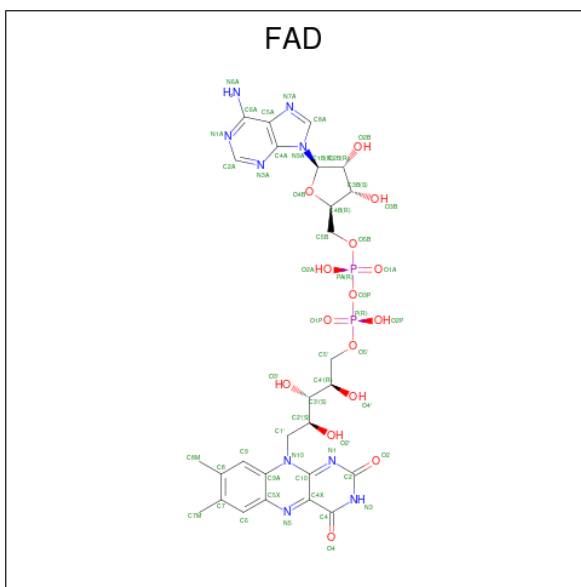
- Molecule 3 is a protein called Histone H3.3C.

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

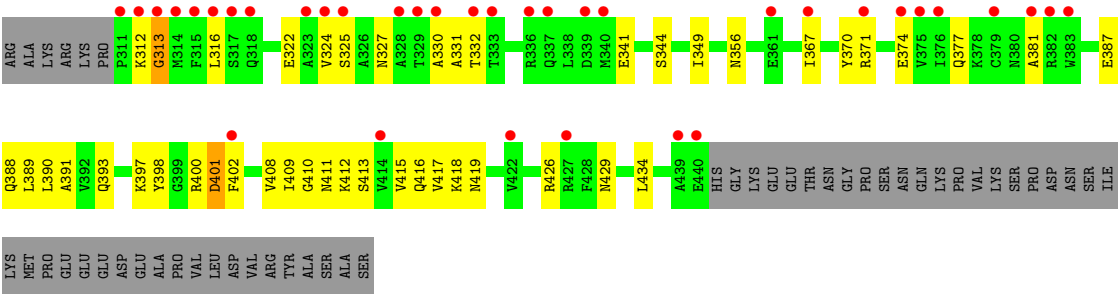
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	LYS	conflict	UNP Q6NXT2

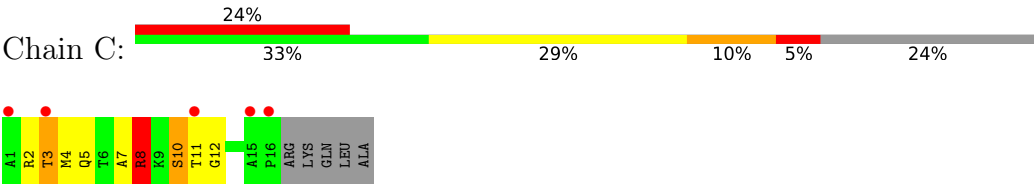
- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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



● Molecule 3: Histone H3.3C



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	118.06Å 179.35Å 233.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 2.90 48.86 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.86-2.90) 99.1 (48.86-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, R_{free}	0.233 , 0.254 0.241 , 0.263	Depositor DCC
R_{free} test set	2000 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	81.0	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6430	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	0.44	0/5327	0.83	19/7225 (0.3%)
2	B	0.32	0/1063	0.80	2/1433 (0.1%)
3	C	0.63	0/114	1.92	5/150 (3.3%)
All	All	0.42	0/6504	0.85	26/8808 (0.3%)

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
1	A	0	2
3	C	0	1
All	All	0	3

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ASN	CB-CA-C	-19.79	82.90	111.80
2	B	401	ASP	N-CA-C	-15.53	87.41	110.24
1	A	611	SER	N-CA-C	12.43	127.66	111.75
2	B	401	ASP	CB-CA-C	11.78	127.50	109.84
1	A	690	GLU	N-CA-C	11.23	126.60	108.63
3	C	11	THR	N-CA-CB	-10.96	96.01	110.59
3	C	10	SER	CB-CA-C	-10.93	92.02	109.84
1	A	610	THR	CB-CA-C	9.93	130.18	110.42
1	A	690	GLU	CB-CA-C	-9.89	95.05	110.88
1	A	793	ILE	CB-CA-C	-9.52	94.03	111.36
1	A	793	ILE	N-CA-C	8.69	127.66	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	THR	CB-CA-C	8.61	127.55	110.42
1	A	350	ASN	N-CA-C	-8.49	97.31	109.96
1	A	375	ASP	CB-CA-C	-8.30	93.89	110.42
1	A	611	SER	CB-CA-C	-7.99	94.95	110.46
1	A	468	VAL	N-CA-C	-7.53	99.44	109.30
1	A	612	GLN	N-CA-C	7.51	120.65	108.63
1	A	350	ASN	CB-CA-C	7.26	120.61	110.16
1	A	591	ARG	CB-CG-CD	-6.10	97.28	111.30
1	A	375	ASP	N-CA-C	6.08	123.75	110.80
1	A	514	ASN	N-CA-C	-5.88	96.84	109.01
3	C	11	THR	CA-C-N	-5.71	114.44	119.92
3	C	11	THR	C-N-CA	-5.71	114.44	119.92
1	A	468	VAL	CB-CA-C	5.58	120.52	111.71
1	A	313	VAL	CA-C-N	-5.43	111.28	120.79
1	A	313	VAL	C-N-CA	-5.43	111.28	120.79

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	485	ARG	Sidechain
1	A	792	PRO	Peptide
3	C	8	ARG	Sidechain

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	5214	0	5255	200	1
2	B	1049	0	1059	47	0
3	C	114	0	125	12	0
4	A	53	0	31	5	0
All	All	6430	0	6470	230	1

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:667:ASP:HB3	1:A:744:LYS:CE	1.29	1.61
1:A:667:ASP:CB	1:A:744:LYS:HE3	1.57	1.32
1:A:667:ASP:CB	1:A:744:LYS:CE	2.21	1.07
1:A:667:ASP:HB3	1:A:744:LYS:NZ	1.76	0.99
1:A:667:ASP:HB3	1:A:744:LYS:HE3	0.93	0.92
1:A:374:LYS:NZ	1:A:525:ASP:OD1	2.02	0.92
1:A:478:PHE:HE1	2:B:408:VAL:HG11	1.39	0.88
1:A:269:ARG:HH12	1:A:273:LEU:CD2	1.86	0.87
1:A:667:ASP:HB3	1:A:744:LYS:HE2	1.57	0.86
1:A:269:ARG:HH12	1:A:273:LEU:HD23	1.40	0.84
1:A:269:ARG:NH1	1:A:273:LEU:CD2	2.42	0.82
1:A:667:ASP:CB	1:A:744:LYS:HZ1	1.93	0.82
1:A:667:ASP:CB	1:A:744:LYS:NZ	2.40	0.82
1:A:592:GLN:HG3	1:A:638:GLN:HB3	1.61	0.82
1:A:401:LEU:HD21	2:B:325:SER:HB2	1.60	0.81
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.44	0.81
1:A:667:ASP:CA	1:A:744:LYS:HE3	2.11	0.81
1:A:478:PHE:CE1	2:B:408:VAL:HG11	2.17	0.80
1:A:269:ARG:NH1	1:A:273:LEU:HD23	2.00	0.77
1:A:216:ARG:HH11	1:A:219:GLN:HE21	1.32	0.76
1:A:291:LEU:HD21	1:A:313:VAL:HG11	1.66	0.76
1:A:188:MET:HB2	1:A:200:ILE:HD11	1.68	0.75
2:B:381:ALA:O	2:B:412:LYS:NZ	2.20	0.75
2:B:377:GLN:NE2	2:B:410:GLY:O	2.20	0.75
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.69	0.73
2:B:377:GLN:HE22	2:B:411:ASN:HA	1.55	0.72
1:A:444:LEU:HD21	1:A:501:GLN:HB2	1.72	0.72
1:A:216:ARG:NH1	1:A:219:GLN:HE21	1.89	0.71
1:A:331:ALA:HA	4:A:901:FAD:C4X	2.20	0.71
1:A:269:ARG:NH1	1:A:273:LEU:HD21	2.06	0.71
1:A:291:LEU:HD21	1:A:313:VAL:CG1	2.22	0.70
1:A:325:TYR:OH	1:A:744:LYS:HD2	1.91	0.69
1:A:593:VAL:HG22	1:A:602:VAL:HG22	1.75	0.68
1:A:526:ARG:NH1	1:A:530:ASP:OD1	2.26	0.67
1:A:609:SER:O	1:A:610:THR:C	2.38	0.67
1:A:331:ALA:HA	4:A:901:FAD:N5	2.09	0.66
1:A:313:VAL:HG12	1:A:313:VAL:O	1.96	0.66
1:A:280:LYS:N	1:A:619:ASP:OD2	2.29	0.66
1:A:495:ASP:OD1	2:B:371:ARG:NH2	2.29	0.65
1:A:349:VAL:HG12	1:A:350:ASN:O	1.97	0.65
1:A:522:SER:N	1:A:525:ASP:OD2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ASN:O	1:A:454:LYS:HG3	1.98	0.62
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.82	0.62
1:A:214:ARG:O	1:A:218:LEU:HD12	2.00	0.61
2:B:400:ARG:O	2:B:401:ASP:C	2.38	0.61
1:A:364:GLU:HA	1:A:681:VAL:HB	1.81	0.61
1:A:188:MET:CB	1:A:200:ILE:HD11	2.32	0.60
1:A:310:ARG:NH2	1:A:754:ASP:OD2	2.35	0.59
1:A:757:ALA:O	1:A:758:ARG:HB2	2.02	0.59
2:B:416:GLN:N	2:B:416:GLN:OE1	2.36	0.59
3:C:2:ARG:NH2	3:C:12:GLY:O	2.35	0.59
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.37	0.59
1:A:474:ILE:HG23	2:B:393:GLN:NE2	2.19	0.58
1:A:380:GLN:O	1:A:384:ARG:HG3	2.04	0.58
1:A:556:ASP:OD2	3:C:2:ARG:HD2	2.03	0.58
1:A:667:ASP:O	1:A:668:ARG:CG	2.52	0.58
1:A:216:ARG:O	1:A:220:LEU:HD12	2.04	0.58
1:A:385:LEU:HD23	1:A:415:VAL:HG12	1.84	0.58
1:A:647:LYS:O	1:A:651:VAL:HG23	2.04	0.57
1:A:755:PRO:HA	1:A:758:ARG:NH1	2.18	0.57
2:B:397:LYS:HG2	2:B:398:TYR:CD1	2.39	0.57
2:B:341:GLU:O	2:B:344:SER:OG	2.14	0.57
1:A:456:LYS:HA	2:B:370:TYR:HE2	1.70	0.57
2:B:389:LEU:O	2:B:393:GLN:HG3	2.04	0.57
1:A:542:THR:OG1	1:A:546:THR:OG1	2.23	0.57
1:A:498:ALA:HA	1:A:501:GLN:HB3	1.86	0.57
1:A:349:VAL:CG1	1:A:350:ASN:O	2.53	0.57
1:A:266:ILE:HD11	1:A:578:LEU:HD23	1.87	0.56
1:A:435:VAL:HG12	2:B:349:ILE:HG13	1.86	0.56
1:A:235:LEU:HD13	1:A:249:VAL:HG11	1.88	0.56
1:A:288:VAL:HA	1:A:291:LEU:HD12	1.87	0.56
1:A:421:LYS:NZ	1:A:425:ASP:OD1	2.39	0.56
2:B:416:GLN:HA	2:B:419:ASN:HB2	1.88	0.56
1:A:374:LYS:O	1:A:378:VAL:HG23	2.06	0.55
1:A:214:ARG:HG2	1:A:218:LEU:HD11	1.88	0.55
1:A:671:TRP:O	1:A:673:PRO:HD3	2.07	0.55
1:A:220:LEU:HD12	1:A:220:LEU:H	1.72	0.54
2:B:397:LYS:HG2	2:B:398:TYR:CE1	2.42	0.54
1:A:536:LEU:HD12	3:C:5:GLN:HE22	1.71	0.54
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.35	0.54
1:A:794:PRO:HD2	1:A:828:GLN:HG2	1.89	0.54
1:A:360:CYS:O	3:C:8:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:ALA:HB2	1:A:803:THR:HB	1.90	0.53
1:A:221:TRP:CD1	1:A:262:ILE:HA	2.44	0.53
1:A:808:PRO:O	1:A:810:THR:HG23	2.08	0.53
1:A:539:ALA:HB2	3:C:5:GLN:HG3	1.90	0.52
1:A:670:PHE:HZ	1:A:731:LEU:HD13	1.74	0.52
2:B:391:ALA:HB2	2:B:409:ILE:HD11	1.89	0.52
1:A:518:ASP:OD1	1:A:518:ASP:N	2.41	0.52
1:A:594:ARG:HB2	1:A:601:GLU:HG3	1.91	0.52
1:A:456:LYS:HA	2:B:370:TYR:CE2	2.44	0.52
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.45	0.52
1:A:417:GLN:HB3	2:B:324:VAL:HG11	1.91	0.51
1:A:594:ARG:CZ	1:A:640:VAL:HG11	2.40	0.51
1:A:255:TYR:CD1	1:A:256:LEU:HD23	2.45	0.51
1:A:667:ASP:O	1:A:668:ARG:HG3	2.10	0.51
1:A:444:LEU:HD23	1:A:445:LEU:HD23	1.93	0.51
2:B:413:SER:O	2:B:417:VAL:HG23	2.11	0.51
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.24	0.51
1:A:366:ASN:HD21	1:A:368:GLN:HB2	1.76	0.51
1:A:614:PHE:O	1:A:615:ILE:HD13	2.11	0.51
1:A:287:GLY:HA3	4:A:901:FAD:O5B	2.11	0.50
1:A:667:ASP:CA	1:A:744:LYS:CE	2.81	0.50
1:A:313:VAL:CG1	1:A:313:VAL:O	2.58	0.50
1:A:660:ASN:OD1	1:A:749:SER:OG	2.28	0.50
1:A:315:GLY:HA2	4:A:901:FAD:H3B	1.94	0.50
1:A:375:ASP:OD1	3:C:8:ARG:NH1	2.45	0.50
3:C:2:ARG:O	3:C:3:THR:C	2.55	0.50
1:A:664:LEU:HD11	1:A:727:CYS:SG	2.52	0.49
1:A:672:ASP:HB3	1:A:675:VAL:HG12	1.93	0.49
2:B:324:VAL:HG13	2:B:331:ALA:HA	1.93	0.49
1:A:672:ASP:HB3	1:A:675:VAL:CG1	2.42	0.49
1:A:536:LEU:HD12	3:C:5:GLN:NE2	2.28	0.49
1:A:320:PHE:CD2	1:A:747:VAL:HG21	2.48	0.49
1:A:289:SER:HB3	1:A:814:ALA:HB1	1.95	0.48
1:A:817:SER:HB2	1:A:820:ARG:NH2	2.28	0.48
2:B:381:ALA:C	2:B:412:LYS:NZ	2.71	0.48
1:A:384:ARG:NH1	2:B:312:LYS:HG2	2.29	0.48
1:A:594:ARG:HA	1:A:640:VAL:O	2.14	0.48
1:A:520:TYR:O	1:A:521:LEU:HD23	2.14	0.47
1:A:780:ILE:HB	1:A:796:LEU:HB3	1.96	0.47
2:B:434:LEU:HD23	2:B:434:LEU:HA	1.66	0.47
1:A:474:ILE:HG21	2:B:389:LEU:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:PRO:HD2	1:A:374:LYS:HB2	1.94	0.47
1:A:441:LEU:HB3	2:B:356:ASN:ND2	2.29	0.47
2:B:367:ILE:CD1	2:B:371:ARG:HE	2.27	0.47
1:A:501:GLN:O	1:A:505:GLU:HB2	2.13	0.47
1:A:230:THR:HG23	1:A:270:ILE:HD12	1.96	0.47
1:A:319:THR:OG1	1:A:572:SER:HB3	2.14	0.47
1:A:632:GLN:O	1:A:633:GLN:NE2	2.48	0.47
1:A:667:ASP:HB2	1:A:744:LYS:HZ1	1.77	0.47
1:A:198:ASP:OD1	1:A:198:ASP:N	2.48	0.47
1:A:342:MET:HG2	1:A:812:HIS:HB3	1.97	0.47
1:A:667:ASP:CA	1:A:744:LYS:NZ	2.78	0.47
2:B:322:GLU:HA	2:B:325:SER:OG	2.15	0.47
1:A:333:VAL:HA	1:A:565:LEU:O	2.15	0.46
1:A:428:ILE:O	1:A:432:LYS:HB2	2.15	0.46
1:A:205:GLN:O	1:A:209:VAL:HG23	2.15	0.46
1:A:329:LEU:HD21	1:A:747:VAL:HG12	1.97	0.46
1:A:667:ASP:HA	1:A:744:LYS:NZ	2.30	0.46
1:A:695:TRP:HE3	1:A:697:LEU:HD11	1.78	0.46
1:A:832:ALA:O	1:A:835:THR:HG22	2.16	0.46
1:A:667:ASP:CG	1:A:744:LYS:HE3	2.33	0.46
1:A:541:ALA:O	1:A:657:GLY:HA3	2.15	0.46
2:B:416:GLN:H	2:B:416:GLN:CD	2.22	0.46
2:B:387:GLU:HA	2:B:390:LEU:HD12	1.98	0.45
1:A:467:GLU:O	1:A:468:VAL:C	2.58	0.45
1:A:182:ARG:NH1	1:A:341:PRO:HD3	2.32	0.45
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.99	0.45
1:A:474:ILE:HG23	2:B:393:GLN:HE22	1.81	0.45
1:A:536:LEU:HD11	3:C:10:SER:OG	2.17	0.45
1:A:667:ASP:N	1:A:744:LYS:HE3	2.32	0.45
1:A:678:PHE:CD1	1:A:678:PHE:C	2.95	0.45
1:A:423:VAL:HG21	1:A:520:TYR:HA	1.98	0.44
1:A:200:ILE:HD12	1:A:200:ILE:HG23	1.60	0.44
1:A:677:LEU:CD1	3:C:7:ALA:HB2	2.46	0.44
1:A:385:LEU:HD23	1:A:415:VAL:CG1	2.47	0.44
1:A:758:ARG:HD3	1:A:758:ARG:HA	1.87	0.44
1:A:627:LEU:CD1	1:A:656:PHE:HB2	2.48	0.44
1:A:269:ARG:HH12	1:A:273:LEU:HD21	1.68	0.44
1:A:371:PRO:O	1:A:374:LYS:N	2.49	0.44
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.63	0.44
1:A:361:PRO:HB2	1:A:363:TYR:CE1	2.52	0.44
1:A:671:TRP:HA	1:A:735:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.76	0.44
1:A:282:ILE:HD13	1:A:305:THR:HB	1.99	0.44
1:A:609:SER:C	1:A:611:SER:N	2.76	0.43
1:A:568:ARG:NH1	1:A:699:LYS:HG2	2.33	0.43
1:A:200:ILE:HD13	1:A:200:ILE:HA	1.85	0.43
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.87	0.43
1:A:340:ASN:HA	1:A:560:PHE:CZ	2.53	0.43
1:A:411:ALA:HB2	1:A:549:LEU:HD22	1.99	0.43
1:A:388:ALA:HB1	2:B:316:LEU:HD11	1.99	0.43
1:A:442:LYS:N	2:B:356:ASN:HD21	2.17	0.43
1:A:258:ARG:NH1	1:A:827:ASP:OD1	2.52	0.43
2:B:377:GLN:HE22	2:B:411:ASN:CA	2.29	0.43
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.49	0.43
1:A:732:LYS:HG2	1:A:737:SER:HA	2.01	0.43
2:B:418:LYS:HB3	2:B:418:LYS:HE3	1.53	0.43
1:A:606:ASN:HD21	1:A:608:ARG:HH21	1.66	0.43
1:A:418:LEU:HD12	2:B:324:VAL:HG21	2.00	0.42
1:A:550:LYS:HB3	1:A:551:HIS:CD2	2.54	0.42
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.85	0.42
1:A:340:ASN:CG	1:A:342:MET:HB2	2.45	0.42
2:B:400:ARG:O	2:B:402:PHE:N	2.52	0.42
1:A:670:PHE:CD1	1:A:670:PHE:C	2.98	0.42
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.34	0.42
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.93	0.42
1:A:349:VAL:HG12	1:A:350:ASN:C	2.43	0.42
1:A:384:ARG:HH11	2:B:312:LYS:HG2	1.84	0.42
1:A:391:LYS:NZ	2:B:313:GLY:HA3	2.35	0.42
1:A:569:ASN:OD1	1:A:569:ASN:N	2.46	0.42
1:A:667:ASP:N	1:A:667:ASP:OD1	2.42	0.42
1:A:188:MET:HG2	1:A:210:PHE:CE1	2.54	0.42
2:B:312:LYS:O	2:B:313:GLY:C	2.63	0.42
1:A:552:TRP:CZ3	3:C:2:ARG:HB2	2.54	0.42
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.81	0.42
2:B:377:GLN:OE1	2:B:411:ASN:HB3	2.20	0.42
1:A:221:TRP:CZ3	1:A:225:PRO:HA	2.55	0.42
1:A:291:LEU:HD11	1:A:313:VAL:HG12	2.02	0.42
1:A:188:MET:HE3	1:A:210:PHE:CE1	2.55	0.42
1:A:308:GLU:HB3	1:A:586:LEU:HD23	2.02	0.42
4:A:901:FAD:C4	3:C:4:MET:HE1	2.50	0.42
1:A:351:MET:HE3	1:A:574:VAL:HG21	2.02	0.41
1:A:592:GLN:HB3	1:A:603:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLN:HG2	1:A:384:ARG:HE	1.85	0.41
1:A:385:LEU:HD22	1:A:416:ILE:HG13	2.02	0.41
1:A:627:LEU:HD12	1:A:656:PHE:HB2	2.02	0.41
1:A:441:LEU:HD12	1:A:441:LEU:HA	1.89	0.41
1:A:609:SER:O	1:A:611:SER:N	2.53	0.41
1:A:392:LEU:HD23	1:A:398:PHE:HD2	1.85	0.41
1:A:325:TYR:HH	1:A:744:LYS:HD2	1.84	0.41
1:A:401:LEU:HD12	1:A:401:LEU:HA	1.86	0.41
1:A:609:SER:O	1:A:609:SER:OG	2.34	0.41
1:A:633:GLN:OE1	1:A:635:PRO:HD3	2.21	0.41
1:A:715:MET:HB3	1:A:723:ILE:HD11	2.01	0.41
1:A:235:LEU:HD12	1:A:235:LEU:HA	1.74	0.41
1:A:408:LEU:HD12	1:A:408:LEU:HA	1.82	0.41
1:A:222:LEU:HA	1:A:222:LEU:HD23	1.83	0.41
1:A:389:THR:HA	1:A:392:LEU:HD13	2.02	0.41
1:A:632:GLN:NE2	1:A:636:ALA:HB2	2.35	0.41
1:A:691:LEU:HA	1:A:691:LEU:HD23	1.80	0.41
1:A:731:LEU:HD23	1:A:731:LEU:HA	1.91	0.41
2:B:426:ARG:O	2:B:429:ASN:ND2	2.54	0.41
2:B:367:ILE:HD11	2:B:371:ARG:HH21	1.86	0.40
1:A:192:GLU:HG2	1:A:255:TYR:CZ	2.56	0.40
1:A:649:SER:HB3	1:A:653:ARG:NH1	2.35	0.40
1:A:793:ILE:H	1:A:793:ILE:HG13	1.58	0.40
1:A:805:ARG:O	1:A:808:PRO:HD3	2.21	0.40
1:A:262:ILE:HD12	1:A:263:ASN:ND2	2.35	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:NH1	1:A:611:SER:O[2_565]	2.18	0.02

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	664/730 (91%)	617 (93%)	47 (7%)	0	100	100
2	B	128/178 (72%)	118 (92%)	9 (7%)	1 (1%)	16	44
3	C	14/21 (67%)	13 (93%)	1 (7%)	0	100	100
All	All	806/929 (87%)	748 (93%)	57 (7%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	313	GLY

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	566/623 (91%)	542 (96%)	24 (4%)	26	60
2	B	114/156 (73%)	110 (96%)	4 (4%)	32	66
3	C	11/15 (73%)	10 (91%)	1 (9%)	9	28
All	All	691/794 (87%)	662 (96%)	29 (4%)	26	60

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ILE
1	A	281	VAL
1	A	333	VAL
1	A	346	SER
1	A	395	GLN
1	A	429	GLU
1	A	466	SER
1	A	469	LYS
1	A	475	THR

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Mol	Chain	Res	Type
1	A	485	ARG
1	A	525	ASP
1	A	536	LEU
1	A	598	SER
1	A	613	THR
1	A	624	THR
1	A	627	LEU
1	A	633	GLN
1	A	659	LEU
1	A	690	GLU
1	A	727	CYS
1	A	749	SER
1	A	768	SER
1	A	785	SER
1	A	815	LEU
2	B	332	THR
2	B	374	GLU
2	B	388	GLN
2	B	415	VAL
3	C	8	ARG

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	191	GLN
1	A	219	GLN
1	A	259	HIS
1	A	399	ASN
1	A	402	ASN
1	A	410	GLN
1	A	501	GLN
1	A	551	HIS
1	A	592	GLN
1	A	606	ASN
1	A	632	GLN
1	A	806	ASN
2	B	327	ASN
2	B	377	GLN
2	B	429	ASN
2	B	435	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 ⓘ

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	901	-	58,58,58	0.30	0	85,89,89	0.63	3 (3%)

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	901	-	-	1/34/50/50	0/6/6/6

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	FAD	O2P-P-O5'	2.63	119.51	107.57
4	A	901	FAD	O2A-PA-O1A	2.56	124.34	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	FAD	O5'-P-O1P	-2.37	99.55	108.94

There are no chirality outliers.

All (1) torsion outliers are listed below:

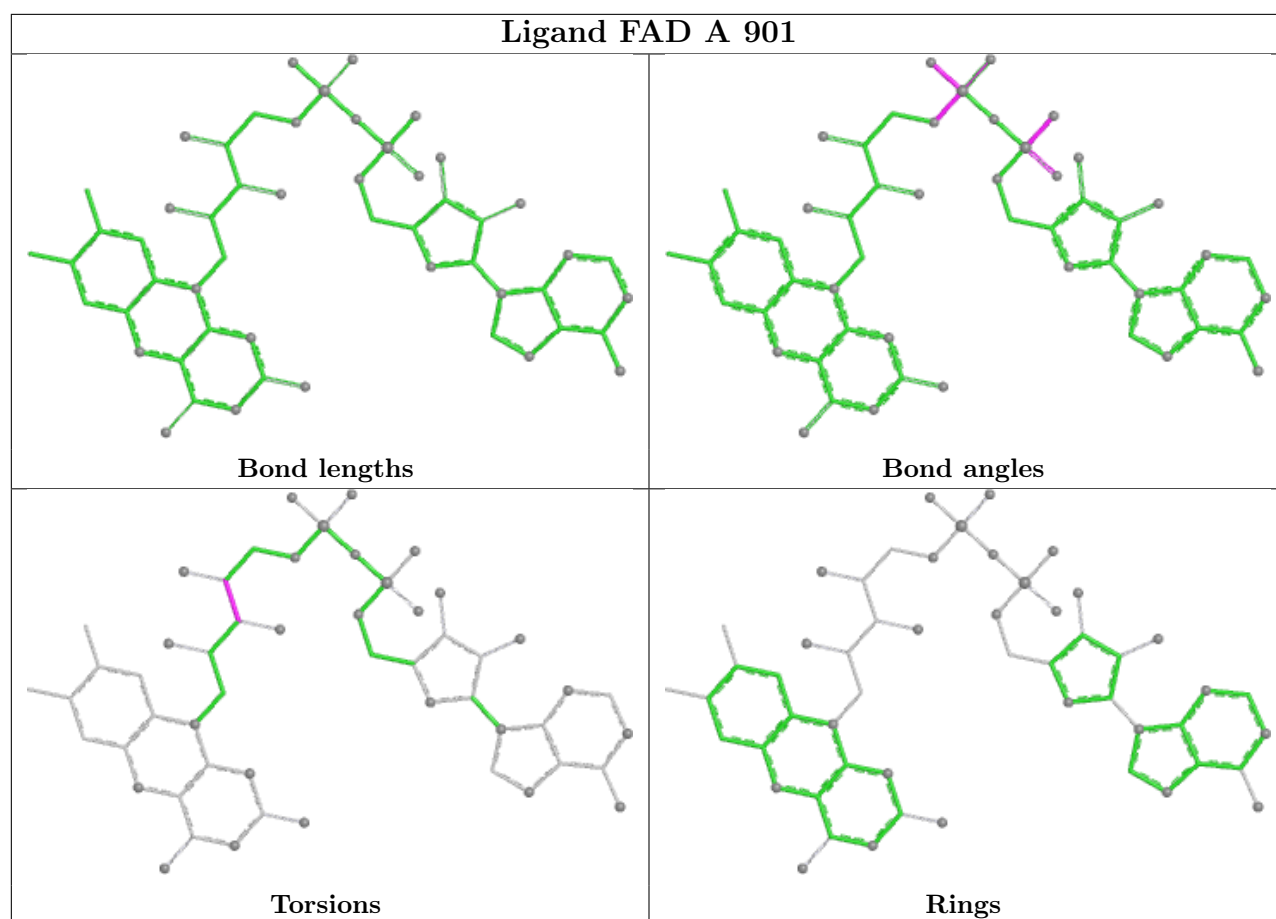
Mol	Chain	Res	Type	Atoms
4	A	901	FAD	C2'-C3'-C4'-O4'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	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	666/730 (91%)	0.97	72 (10%) 11 9	55, 85, 120, 145	0
2	B	130/178 (73%)	1.48	36 (27%) 1 1	86, 118, 145, 147	0
3	C	16/21 (76%)	1.70	5 (31%) 1 1	71, 82, 120, 127	0
All	All	812/929 (87%)	1.07	113 (13%) 6 5	55, 90, 129, 147	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	311	PRO	8.5
1	A	770	GLY	5.6
1	A	834	TYR	5.1
2	B	332	THR	5.0
1	A	373	GLU	5.0
1	A	836	LEU	4.8
2	B	376	ILE	4.8
1	A	674	SER	4.7
3	C	15	ALA	4.7
1	A	557	ASP	4.7
1	A	833	MET	4.5
3	C	16	PRO	4.4
1	A	715	MET	4.3
2	B	315	PHE	4.3
1	A	398	PHE	4.3
2	B	329	THR	4.2
3	C	3	THR	4.1
2	B	312	LYS	4.1
2	B	328	ALA	4.0
2	B	383	TRP	4.0
1	A	832	ALA	4.0
1	A	527	GLN	3.9
1	A	171	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	191	GLN	3.7
1	A	668	ARG	3.7
2	B	440	GLU	3.6
1	A	275	THR	3.6
1	A	273	LEU	3.6
1	A	377	MET	3.6
1	A	611	SER	3.6
1	A	774	ASP	3.6
1	A	523	SER	3.5
1	A	556	ASP	3.5
2	B	336	ARG	3.5
2	B	427	ARG	3.5
2	B	324	VAL	3.5
1	A	555	ASP	3.3
1	A	558	PHE	3.3
2	B	371	ARG	3.2
2	B	340	MET	3.2
1	A	786	ILE	3.1
2	B	374	GLU	3.1
2	B	414	VAL	3.1
1	A	610	THR	3.1
1	A	768	SER	3.1
1	A	403	ASN	3.0
1	A	806	ASN	3.0
1	A	194	ALA	3.0
1	A	519	VAL	3.0
1	A	835	THR	2.9
3	C	1	ALA	2.9
1	A	791	GLN	2.9
2	B	382	ARG	2.9
1	A	684	THR	2.9
1	A	232	GLU	2.8
1	A	440	GLU	2.8
1	A	478	PHE	2.8
2	B	317	SER	2.8
1	A	744	LYS	2.8
1	A	467	GLU	2.8
2	B	379	CYS	2.7
1	A	400	VAL	2.7
1	A	365	ALA	2.7
1	A	399	ASN	2.7
1	A	242	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	350	ASN	2.6
2	B	323	ALA	2.6
2	B	375	VAL	2.6
1	A	785	SER	2.6
1	A	827	ASP	2.6
1	A	226	LYS	2.5
1	A	247	VAL	2.4
2	B	402	PHE	2.4
2	B	422	VAL	2.4
1	A	544	LEU	2.4
1	A	525	ASP	2.4
2	B	337	GLN	2.4
2	B	314	MET	2.4
2	B	339	ASP	2.4
2	B	318	GLN	2.4
2	B	325	SER	2.3
1	A	773	TYR	2.3
1	A	269	ARG	2.3
1	A	453	GLU	2.3
1	A	793	ILE	2.3
1	A	503	LYS	2.3
1	A	771	ASN	2.3
2	B	439	ALA	2.3
1	A	772	ASP	2.3
3	C	11	THR	2.3
1	A	579	ALA	2.2
2	B	361	GLU	2.2
1	A	404	LYS	2.2
1	A	262	ILE	2.2
2	B	333	THR	2.2
1	A	699	LYS	2.2
1	A	702	ILE	2.2
1	A	336	GLY	2.2
1	A	563	SER	2.2
2	B	316	LEU	2.2
1	A	195	CYS	2.1
1	A	769	SER	2.1
1	A	469	LYS	2.1
1	A	805	ARG	2.1
1	A	447	LYS	2.1
1	A	516	PRO	2.1
2	B	330	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	381	ALA	2.1
2	B	313	GLY	2.0
2	B	367	ILE	2.0
1	A	276	LYS	2.0
1	A	585	LYS	2.0
1	A	739	ALA	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](#)

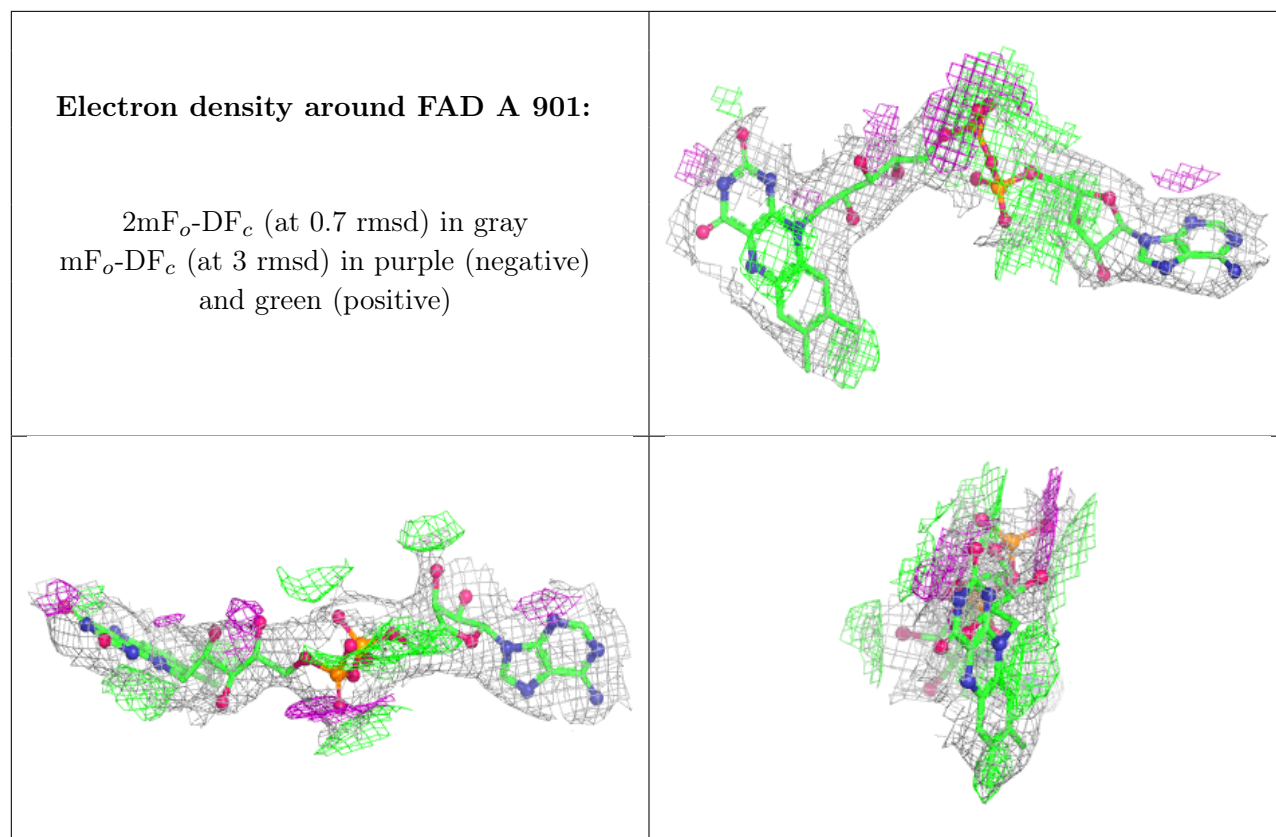
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
4	FAD	A	901	53/53	0.93	0.12	53,67,78,84	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.