



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2024 – 03:09 pm BST

PDB ID : 8Q1H  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
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

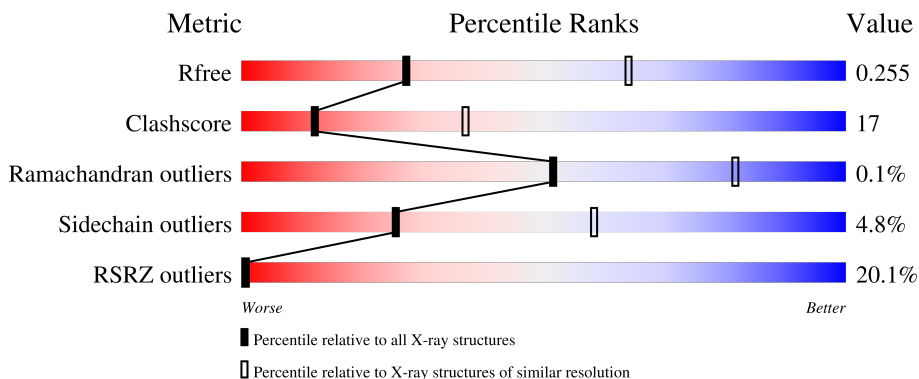
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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  $\geq 3$ , 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	
2	B	178	
3	C	21	

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	A	666	5214	3321	907	966	20	0	0	0

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
			Total	C	N	O	S			
2	B	130	1049	659	187	200	3	0	0	0

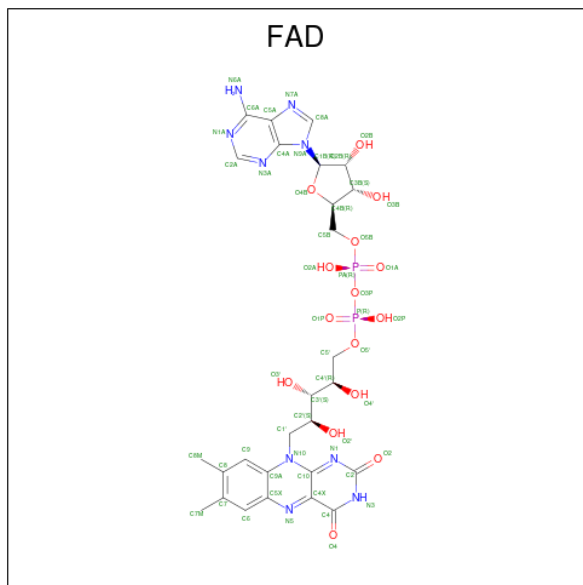
- Molecule 3 is a protein called Histone H3.3C.

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

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

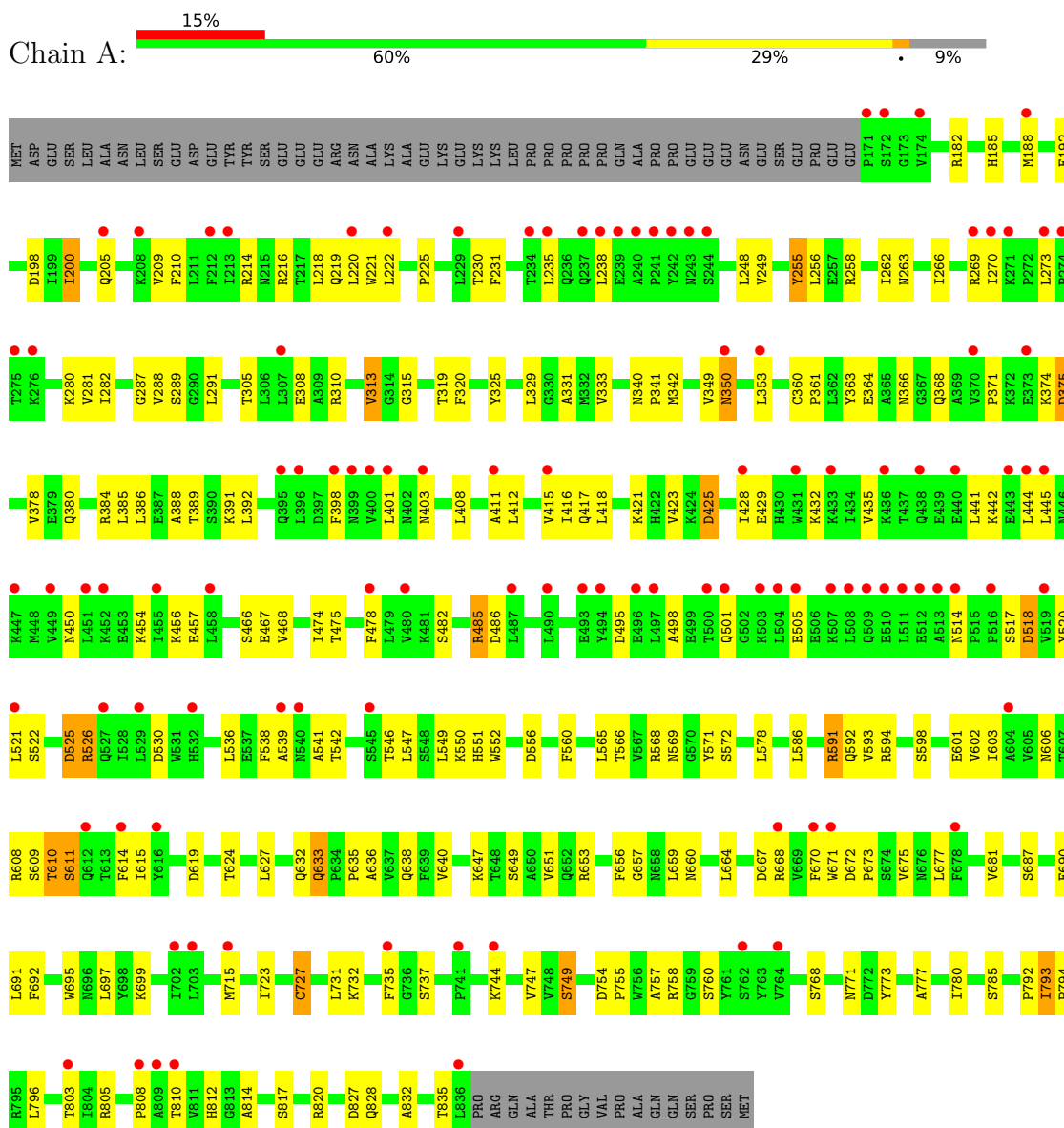


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	53	27	9	15	2	0	0

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

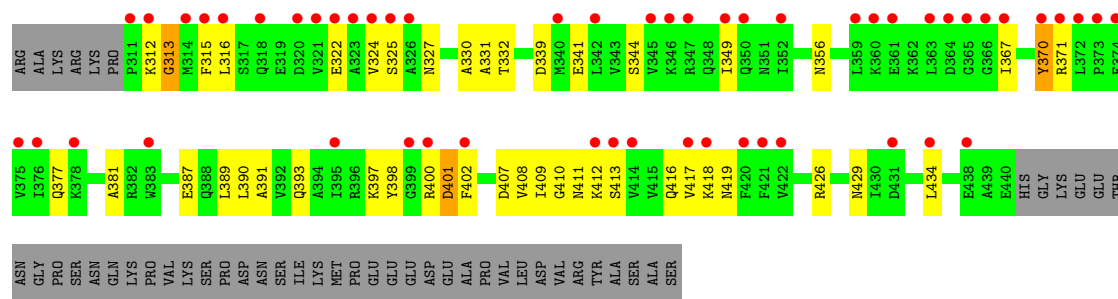
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

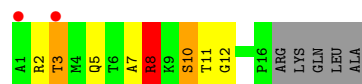


- Molecule 2: REST corepressor 1





- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, $R_{free}$	0.233 , 0.254 0.235 , 0.255	Depositor DCC
$R_{free}$ test set	1992 reflections (3.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.0	Xtrriage
Anisotropy	0.592	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 81.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6430	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtrriage'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.*

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

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

## 5 Model quality [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	0.49	0/5327	0.77	15/7225 (0.2%)
2	B	0.40	0/1063	0.73	2/1433 (0.1%)
3	C	0.53	0/114	1.36	3/150 (2.0%)
All	All	0.47	0/6504	0.78	20/8808 (0.2%)

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 (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ASN	CB-CA-C	-13.75	82.90	110.40
3	C	10	SER	CB-CA-C	-9.52	92.02	110.10
1	A	793	ILE	CB-CA-C	-8.79	94.03	111.60
2	B	401	ASP	N-CA-C	-8.74	87.41	111.00
2	B	401	ASP	CB-CA-C	8.55	127.50	110.40
1	A	375	ASP	CB-CA-C	-8.25	93.89	110.40
1	A	611	SER	CB-CA-C	-7.97	94.95	110.10
1	A	690	GLU	CB-CA-C	-7.68	95.05	110.40
3	C	11	THR	N-CA-CB	-7.52	96.01	110.30
1	A	610	THR	CB-CA-C	6.88	130.18	111.60
1	A	611	SER	N-CA-C	6.17	127.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	793	ILE	N-CA-C	6.17	127.66	111.00
3	C	3	THR	CB-CA-C	5.91	127.55	111.60
1	A	690	GLU	N-CA-C	5.78	126.60	111.00
1	A	591	ARG	CB-CG-CD	-5.51	97.28	111.60
1	A	200	ILE	CG1-CB-CG2	-5.35	99.64	111.40
1	A	313	VAL	C-N-CA	-5.25	111.28	122.30
1	A	514	ASN	N-CA-C	-5.25	96.84	111.00
1	A	350	ASN	CB-CA-C	5.11	120.61	110.40
1	A	350	ASN	N-CA-C	-5.07	97.31	111.00

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	193	1
2	B	1049	0	1059	46	0
3	C	114	0	125	11	0
4	A	53	0	31	5	0
All	All	6430	0	6470	221	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 17.

All (221) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:667:ASP:CB	1:A:744:LYS:HZ1	2.06	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
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

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<b>Atom-1</b>	<b>Atom-2</b>	<b>Interatomic distance (Å)</b>	<b>Clash overlap (Å)</b>
1:A:609:SER:O	1:A:610:THR:C	2.38	0.62
2:B:400:ARG:O	2:B:401:ASP:C	2.38	0.62
1:A:214:ARG:O	1:A:218:LEU:HD12	2.00	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: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:667:ASP:HB3	1:A:744:LYS:HZ1	1.64	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:421:LYS:NZ	1:A:425:ASP:OD1	2.39	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:667:ASP:HA	1:A:744:LYS:HZ2	1.73	0.53
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: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
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
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
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:541:ALA:O	1:A:657:GLY:HA3	2.15	0.46
1:A:667:ASP:HA	1:A:744:LYS:NZ	2.30	0.46
2:B:387:GLU:HA	2:B:390:LEU:HD12	1.98	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
3:C:2:ARG:O	3:C:3:THR:C	2.55	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: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
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
2:B:381:ALA:C	2:B:412:LYS:NZ	2.71	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:542:THR:HG1	1:A:546:THR:HG1	1.49	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
1:A:760:SER:HB2	4:A:901:FAD:HM83	2.00	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
2:B:400:ARG:O	2:B:402:PHE:N	2.52	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: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
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:308:GLU:HB3	1:A:586:LEU:HD23	2.02	0.42
1:A:592:GLN:HB3	1:A:603:ILE:CD1	2.50	0.41
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:401:LEU:HD12	1:A:401:LEU:HA	1.86	0.41
1:A:667:ASP:CG	1:A:744:LYS:HE3	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LEU:HD12	1:A:408:LEU:HA	1.82	0.41
2:B:416:GLN:H	2:B:416:GLN:CD	2.22	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:467:GLU:O	1:A:468:VAL:C	2.58	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 [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	664/730 (91%)	617 (93%)	47 (7%)	0	100	100
2	B	128/178 (72%)	118 (92%)	9 (7%)	1 (1%)	19	51
3	C	14/21 (67%)	13 (93%)	1 (7%)	0	100	100
All	All	806/929 (87%)	748 (93%)	57 (7%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	313	GLY

### 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	566/623 (91%)	539 (95%)	27 (5%)	25	58
2	B	114/156 (73%)	109 (96%)	5 (4%)	28	61
3	C	11/15 (73%)	10 (91%)	1 (9%)	9	28
All	All	691/794 (87%)	658 (95%)	33 (5%)	25	58

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	255	TYR
1	A	281	VAL
1	A	425	ASP
1	A	429	GLU
1	A	457	GLU
1	A	466	SER
1	A	475	THR
1	A	482	SER
1	A	485	ARG
1	A	517	SER
1	A	518	ASP
1	A	525	ASP
1	A	526	ARG
1	A	538	PHE
1	A	571	TYR
1	A	598	SER
1	A	624	THR
1	A	633	GLN
1	A	659	LEU

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Mol	Chain	Res	Type
1	A	687	SER
1	A	692	PHE
1	A	727	CYS
1	A	749	SER
1	A	768	SER
1	A	771	ASN
1	A	785	SER
2	B	315	PHE
2	B	332	THR
2	B	339	ASP
2	B	370	TYR
2	B	407	ASP
3	C	8	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	259	HIS
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 [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

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	-	53,58,58	0.44	0	68,89,89	0.77	4 (5%)

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	-	-	2/30/50/50	0/6/6/6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	FAD	O2P-P-O5'	2.53	119.51	107.75
4	A	901	FAD	O2A-PA-O1A	2.45	124.34	112.24
4	A	901	FAD	O5'-P-O1P	-2.44	99.55	109.07
4	A	901	FAD	C5A-C6A-N6A	2.11	123.56	120.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

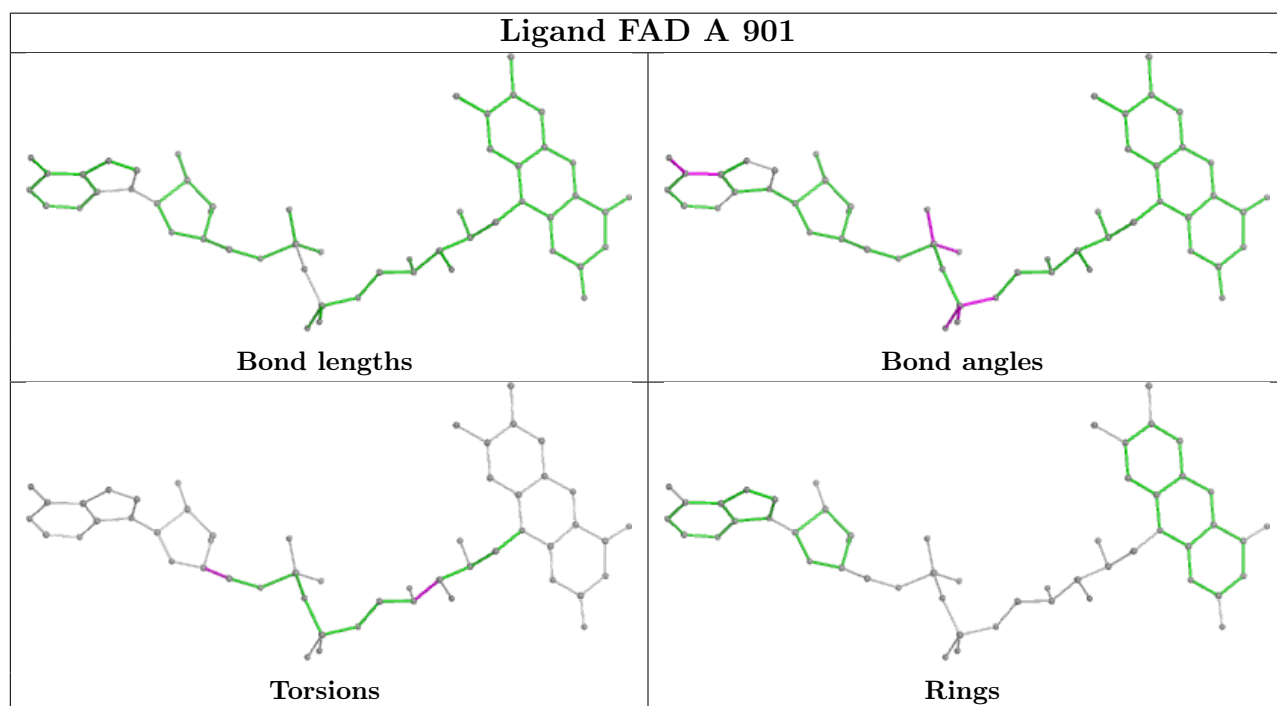
Mol	Chain	Res	Type	Atoms
4	A	901	FAD	C2'-C3'-C4'-O4'
4	A	901	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	666/730 (91%)	1.15	108 (16%) <b>1</b> <b>1</b>	55, 85, 120, 145	0
2	B	130/178 (73%)	1.97	53 (40%) <b>0</b> <b>0</b>	86, 118, 145, 147	0
3	C	16/21 (76%)	0.82	2 (12%) <b>3</b> <b>3</b>	71, 82, 120, 127	0
All	All	812/929 (87%)	1.27	163 (20%) <b>1</b> <b>0</b>	55, 90, 129, 147	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	311	PRO	9.9
2	B	367	ILE	8.2
1	A	398	PHE	7.5
1	A	242	TYR	7.3
1	A	171	PRO	6.3
2	B	402	PHE	6.3
2	B	325	SER	6.1
1	A	174	VAL	5.7
1	A	509	GLN	5.7
2	B	374	GLU	5.4
1	A	273	LEU	5.0
1	A	238	LEU	5.0
1	A	494	TYR	4.8
1	A	431	TRP	4.7
2	B	324	VAL	4.7
2	B	312	LYS	4.7
2	B	323	ALA	4.6
2	B	371	ARG	4.5
1	A	497	LEU	4.5
2	B	376	ILE	4.4
2	B	321	VAL	4.4
2	B	363	LEU	4.4
2	B	420	PHE	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	314	MET	4.3
1	A	512	GLU	4.3
2	B	372	LEU	4.2
1	A	508	LEU	4.2
2	B	316	LEU	4.2
1	A	744	LYS	4.2
1	A	715	MET	4.2
2	B	395	ILE	4.1
2	B	400	ARG	4.1
1	A	172	SER	4.1
2	B	315	PHE	4.1
2	B	421	PHE	4.1
1	A	447	LYS	4.0
1	A	212	PHE	4.0
2	B	414	VAL	4.0
2	B	375	VAL	3.9
1	A	510	GLU	3.9
1	A	505	GLU	3.7
1	A	490	LEU	3.7
1	A	239	GLU	3.7
1	A	396	LEU	3.7
1	A	519	VAL	3.6
2	B	347	ARG	3.6
1	A	504	LEU	3.5
2	B	349	ILE	3.5
1	A	234	THR	3.5
1	A	440	GLU	3.5
2	B	378	LYS	3.5
2	B	360	LYS	3.5
1	A	503	LYS	3.5
2	B	320	ASP	3.4
2	B	318	GLN	3.4
1	A	511	LEU	3.4
1	A	270	ILE	3.3
1	A	208	LYS	3.3
1	A	668	ARG	3.3
2	B	431	ASP	3.2
1	A	241	PRO	3.2
1	A	449	VAL	3.1
1	A	235	LEU	3.1
1	A	487	LEU	3.1
2	B	418	LYS	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	516	PRO	3.1
1	A	438	GLN	3.1
2	B	326	ALA	3.1
1	A	436	LYS	3.1
2	B	399	GLY	3.1
1	A	445	LEU	3.0
1	A	671	TRP	3.0
1	A	271	LYS	2.9
2	B	352	ILE	2.9
1	A	353	LEU	2.9
1	A	702	ILE	2.9
1	A	604	ALA	2.9
1	A	274	PRO	2.9
1	A	444	LEU	2.9
1	A	370	VAL	2.8
2	B	422	VAL	2.8
1	A	275	THR	2.8
1	A	415	VAL	2.8
1	A	458	LEU	2.8
1	A	480	VAL	2.8
1	A	762	SER	2.8
1	A	501	GLN	2.7
1	A	809	ALA	2.7
1	A	496	GLU	2.7
1	A	240	ALA	2.7
1	A	237	GLN	2.7
1	A	400	VAL	2.7
2	B	361	GLU	2.7
1	A	836	LEU	2.6
2	B	413	SER	2.6
1	A	735	PHE	2.6
1	A	703	LEU	2.6
1	A	478	PHE	2.6
2	B	383	TRP	2.6
2	B	340	MET	2.5
1	A	401	LEU	2.5
2	B	359	LEU	2.5
1	A	307	LEU	2.5
2	B	342	LEU	2.5
2	B	434	LEU	2.5
1	A	433	LYS	2.5
2	B	322	GLU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	373	PRO	2.4
1	A	213	ILE	2.4
1	A	808	PRO	2.4
2	B	438	GLU	2.4
1	A	678	PHE	2.4
1	A	612	GLN	2.4
1	A	395	GLN	2.4
1	A	507	LYS	2.4
1	A	244	SER	2.4
1	A	529	LEU	2.4
1	A	205	GLN	2.4
1	A	276	LYS	2.4
2	B	345	VAL	2.3
1	A	373	GLU	2.3
1	A	810	THR	2.3
1	A	493	GLU	2.3
1	A	514	ASN	2.3
1	A	741	PRO	2.3
3	C	1	ALA	2.3
1	A	540	ASN	2.3
1	A	188	MET	2.3
2	B	365	GLY	2.3
2	B	364	ASP	2.2
2	B	412	LYS	2.2
2	B	370	TYR	2.2
1	A	443	GLU	2.2
1	A	500	THR	2.2
1	A	455	ILE	2.2
1	A	616	TYR	2.2
1	A	399	ASN	2.2
1	A	350	ASN	2.2
3	C	3	THR	2.2
1	A	532	HIS	2.2
2	B	346	LYS	2.2
1	A	428	ILE	2.2
1	A	513	ALA	2.2
2	B	417	VAL	2.2
1	A	220	LEU	2.2
1	A	451	LEU	2.2
1	A	614	PHE	2.1
1	A	269	ARG	2.1
1	A	803	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	229	LEU	2.1
1	A	670	PHE	2.1
1	A	527	GLN	2.1
1	A	545	SER	2.1
1	A	764	VAL	2.1
1	A	539	ALA	2.1
2	B	350	GLN	2.1
1	A	222	LEU	2.0
1	A	243	ASN	2.0
1	A	521	LEU	2.0
1	A	411	ALA	2.0
2	B	366	GLY	2.0
1	A	452	LYS	2.0
1	A	403	ASN	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.

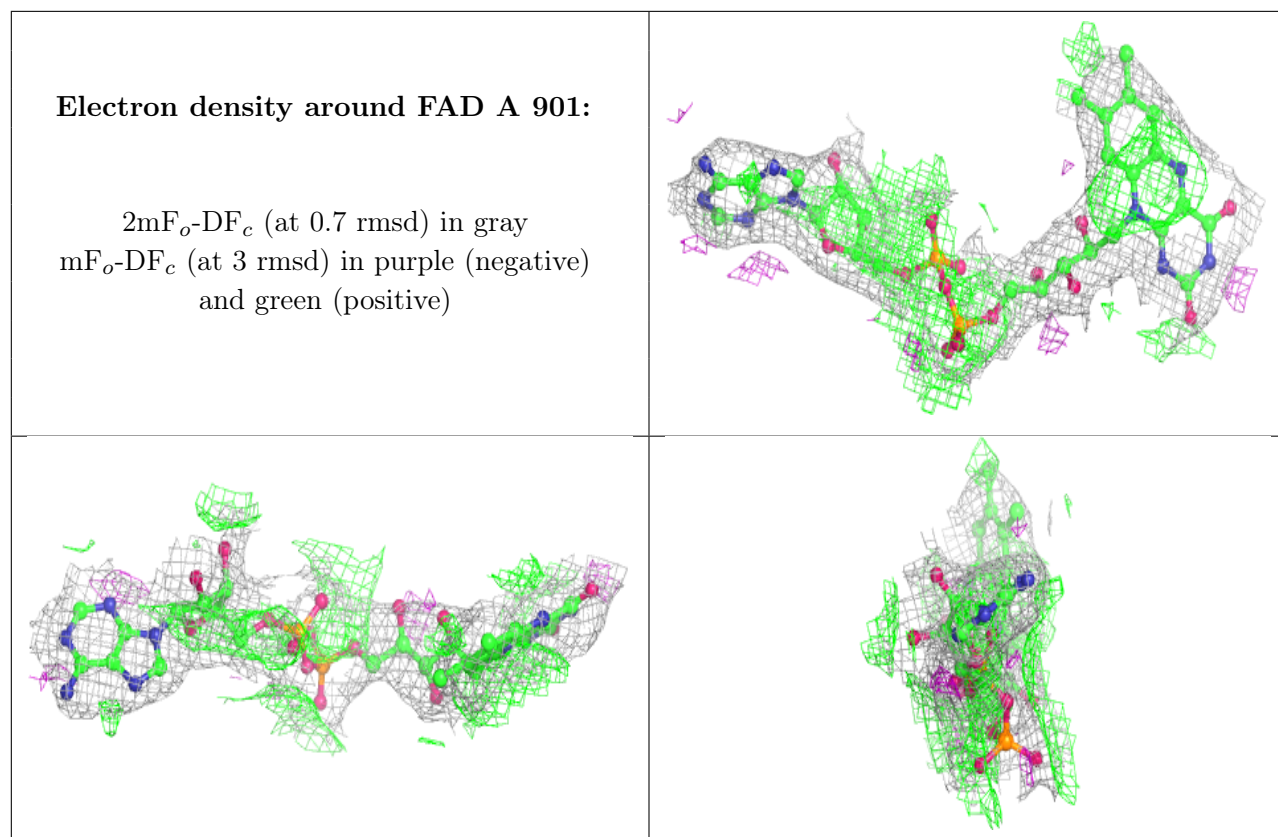
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FAD	A	901	53/53	0.92	0.28	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.