



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2025 – 10:05 AM EDT

PDB ID : 9DBP / pdb\_00009dbp  
Title : Crystal structure of the LSD1/CoREST histone demethylase in complex with the cofactor FAD and the inhibitor GSK690  
Authors : An, S.; Engel, J.; Wang, Y.; Yu, L.; Cho, U.S.  
Deposited on : 2024-08-23  
Resolution : 2.66 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 : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

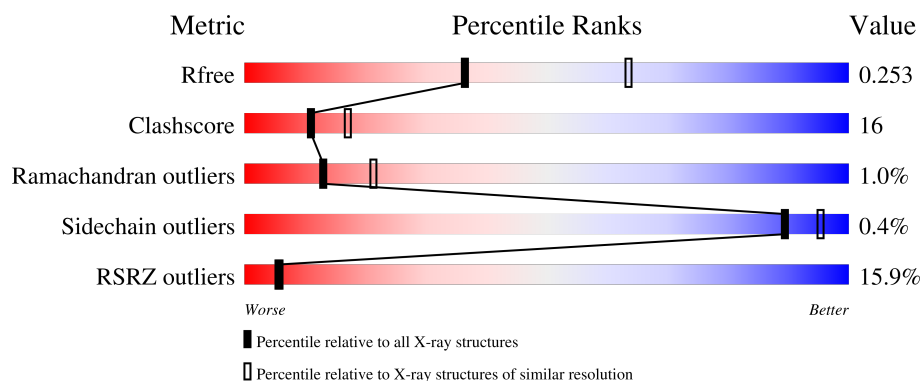
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.66 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))
$R_{free}$	164625	1003 (2.66-2.66)
Clashscore	180529	1063 (2.66-2.66)
Ramachandran outliers	177936	1052 (2.66-2.66)
Sidechain outliers	177891	1052 (2.66-2.66)
RSRZ outliers	164620	1003 (2.66-2.66)

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	660	<div> <div>12%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>
2	B	131	<div> <div>37%</div> <div>56%</div> <div>34%</div> <div>8%</div> <div>.</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12539 atoms, of which 6257 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	660	Total	C	H	N	O	S	0	0	0
			10303	3278	5155	894	957	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	269	ALA	ARG	engineered mutation	UNP O60341
A	469	ALA	LYS	engineered mutation	UNP O60341

- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	131	Total	C	H	N	O	S	0	0	0
			2072	654	1032	184	199	3			

There are 4 discrepancies between the modelled and reference sequences:

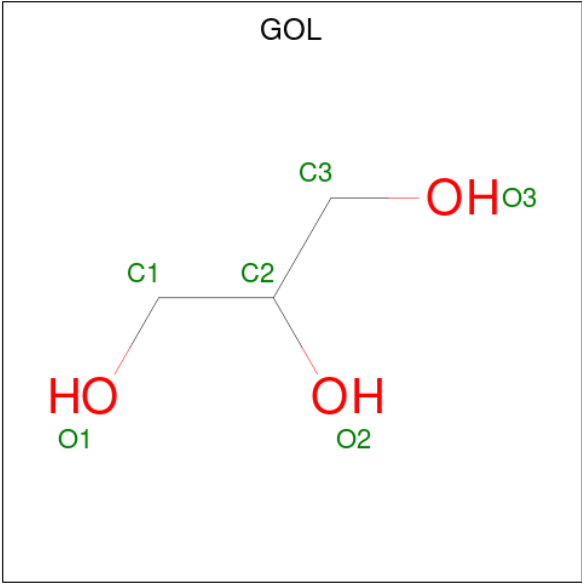
Chain	Residue	Modelled	Actual	Comment	Reference
B	312	ALA	LYS	engineered mutation	UNP Q9UKL0
B	378	ALA	LYS	engineered mutation	UNP Q9UKL0
B	422	ALA	VAL	engineered mutation	UNP Q9UKL0
B	425	ALA	ARG	engineered mutation	UNP Q9UKL0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

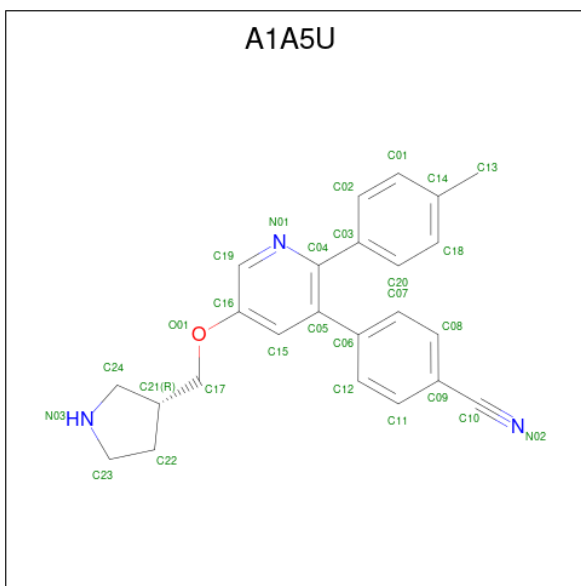
- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	A	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is 4-[2-(4-methylphenyl)-5-{(3R)-pyrrolidin-3-yl}methoxy}pyridin-3-yl]benzonitr

ile (CCD ID: A1A5U) (formula:  $C_{24}H_{23}N_3O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			51	24	23	3	1		

- Molecule 6 is water.

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

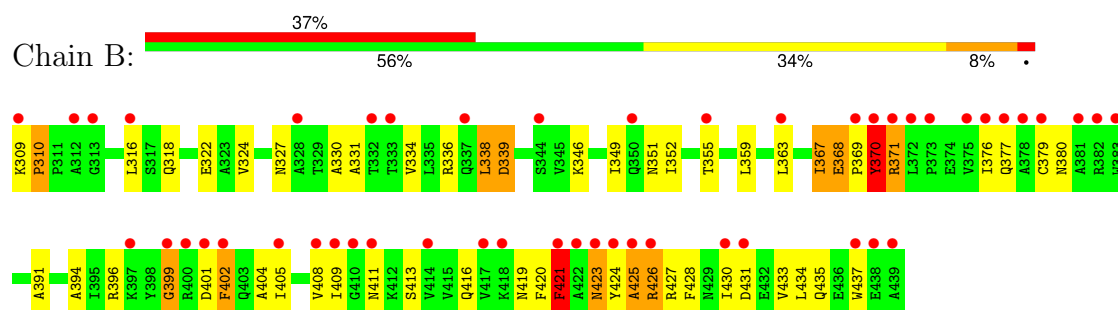
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Lysine-specific histone demethylase 1A



- Molecule 2: REST corepressor 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.49Å 179.41Å 235.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.46 – 2.66 36.46 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.1 (36.46-2.66) 99.4 (36.46-2.66)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.20	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.239 , 0.250 0.242 , 0.253	Depositor DCC
$R_{free}$ test set	1996 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	72.6	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 56.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, A1A5U, 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	0.63	14/5260 (0.3%)	0.85	37/7141 (0.5%)
2	B	0.97	7/1055 (0.7%)	1.28	17/1427 (1.2%)
All	All	0.70	21/6315 (0.3%)	0.94	54/8568 (0.6%)

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	5
2	B	0	4
All	All	0	9

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	373	GLU	CD-OE2	14.91	1.53	1.25
1	A	655	GLY	CA-C	12.04	1.60	1.52
2	B	368	GLU	CD-OE2	9.80	1.44	1.25
1	A	439	GLU	CD-OE2	9.28	1.43	1.25
1	A	467	GLU	CD-OE2	9.25	1.43	1.25
1	A	740	VAL	CA-C	-8.94	1.46	1.53
1	A	427	GLN	CD-NE2	8.53	1.51	1.33
2	B	368	GLU	CD-OE1	7.73	1.40	1.25
2	B	339	ASP	CG-OD2	7.62	1.39	1.25
2	B	370	TYR	CA-CB	7.62	1.64	1.53
1	A	740	VAL	N-CA	7.47	1.52	1.46
1	A	740	VAL	C-N	7.42	1.42	1.33
2	B	421	PHE	CG-CD1	-6.53	1.25	1.38
1	A	467	GLU	CD-OE1	6.45	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	352	GLU	CD-OE2	5.99	1.36	1.25
1	A	439	GLU	CD-OE1	5.84	1.36	1.25
2	B	421	PHE	CA-CB	5.75	1.61	1.53
1	A	372	LYS	C-N	5.37	1.41	1.33
1	A	373	GLU	CD-OE1	5.17	1.35	1.25
1	A	453	GLU	CD-OE2	5.13	1.35	1.25
2	B	370	TYR	CE1-CZ	5.08	1.50	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	421	PHE	CB-CA-C	17.62	138.38	111.06
1	A	740	VAL	CA-C-O	16.64	128.97	119.15
1	A	453	GLU	CG-CD-OE1	-11.03	93.04	118.40
1	A	373	GLU	CG-CD-OE1	-10.95	93.21	118.40
2	B	421	PHE	N-CA-CB	-9.38	96.10	110.91
2	B	370	TYR	N-CA-C	-9.35	102.06	112.72
1	A	373	GLU	CA-CB-CG	8.25	130.61	114.10
1	A	352	GLU	CG-CD-OE1	-8.01	99.98	118.40
2	B	346	LYS	CD-CE-NZ	-7.98	86.36	111.90
1	A	448	MET	CB-CG-SD	-7.78	89.36	112.70
1	A	467	GLU	OE1-CD-OE2	7.50	140.89	122.90
1	A	379	GLU	CA-C-N	-7.39	110.37	120.28
1	A	379	GLU	C-N-CA	-7.39	110.37	120.28
2	B	336	ARG	CG-CD-NE	7.38	128.22	112.00
2	B	368	GLU	N-CA-CB	7.30	121.75	110.43
1	A	427	GLN	N-CA-C	-7.14	103.43	111.14
1	A	373	GLU	OE1-CD-OE2	7.10	139.93	122.90
2	B	402	PHE	CA-CB-CG	7.00	120.80	113.80
1	A	439	GLU	OE1-CD-OE2	6.94	139.55	122.90
1	A	467	GLU	CG-CD-OE1	-6.91	102.51	118.40
1	A	439	GLU	CG-CD-OE1	-6.80	102.77	118.40
1	A	404	LYS	CD-CE-NZ	-6.66	90.59	111.90
2	B	336	ARG	NE-CZ-NH2	6.55	125.10	119.20
1	A	380	GLN	N-CA-C	6.47	118.34	111.28
2	B	368	GLU	OE1-CD-OE2	6.43	138.32	122.90
1	A	739	ALA	CA-C-N	-6.41	117.97	122.59
1	A	739	ALA	C-N-CA	-6.41	117.97	122.59
1	A	404	LYS	CA-CB-CG	6.38	126.87	114.10
1	A	427	GLN	CG-CD-NE2	6.33	125.89	116.40
2	B	339	ASP	OD1-CG-OD2	6.25	137.89	122.90
1	A	472	ARG	CA-CB-CG	-6.12	101.85	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	GLU	CG-CD-OE1	-6.12	104.33	118.40
2	B	367	ILE	CA-C-N	-6.11	112.45	120.09
2	B	367	ILE	C-N-CA	-6.11	112.45	120.09
1	A	427	GLN	CG-CD-OE1	-6.09	108.62	120.80
1	A	351	MET	CA-C-N	-6.01	113.71	122.19
1	A	351	MET	C-N-CA	-6.01	113.71	122.19
1	A	740	VAL	O-C-N	-5.99	116.36	121.57
1	A	503	LYS	CB-CG-CD	-5.88	97.77	111.30
1	A	439	GLU	CA-CB-CG	5.86	125.82	114.10
1	A	699	LYS	CG-CD-CE	-5.79	97.98	111.30
2	B	370	TYR	CE1-CZ-OH	5.71	137.03	119.90
2	B	370	TYR	CB-CG-CD1	5.70	129.35	120.80
1	A	352	GLU	CA-CB-CG	5.66	125.42	114.10
2	B	339	ASP	CB-CG-OD1	-5.61	105.50	118.40
1	A	373	GLU	N-CA-CB	5.49	118.29	110.16
1	A	380	GLN	CA-CB-CG	5.48	125.06	114.10
2	B	371	ARG	NE-CZ-NH1	-5.24	116.26	121.50
2	B	368	GLU	CG-CD-OE2	-5.20	106.43	118.40
1	A	699	LYS	CD-CE-NZ	5.13	128.33	111.90
1	A	427	GLN	CA-CB-CG	-5.13	103.84	114.10
1	A	453	GLU	OE1-CD-OE2	5.11	135.17	122.90
1	A	404	LYS	CG-CD-CE	5.05	122.91	111.30
1	A	425	ASP	OD1-CG-OD2	5.04	134.99	122.90

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	352	GLU	Sidechain
1	A	373	GLU	Sidechain,Mainchain
1	A	440	GLU	Sidechain
1	A	453	GLU	Sidechain
2	B	310	PRO	Mainchain
2	B	338	LEU	Peptide
2	B	370	TYR	Sidechain
2	B	421	PHE	Peptide

## 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	5148	5155	5159	135	1
2	B	1040	1032	1044	95	1
3	A	53	31	31	15	0
4	A	12	16	16	0	0
5	A	28	23	0	1	0
6	A	1	0	0	0	0
All	All	6282	6257	6250	203	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 16.

All (203) 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:459:HIS:CG	2:B:370:TYR:HB3	1.76	1.21
2:B:421:PHE:CD1	2:B:430:ILE:HG21	1.84	1.12
1:A:760:SER:HB2	3:A:901:FAD:HM82	1.15	1.08
2:B:421:PHE:CE1	2:B:430:ILE:HG21	1.87	1.08
2:B:428:PHE:HB2	2:B:430:ILE:HD11	1.40	1.03
1:A:645:GLU:OE2	1:A:649:SER:OG	1.75	1.03
1:A:456:LYS:HA	2:B:370:TYR:CD1	1.97	0.99
1:A:760:SER:HB2	3:A:901:FAD:C8M	1.95	0.96
1:A:459:HIS:CB	2:B:370:TYR:HB3	1.99	0.93
1:A:760:SER:CB	3:A:901:FAD:HM82	2.00	0.91
2:B:421:PHE:CE1	2:B:430:ILE:CG2	2.54	0.91
2:B:370:TYR:CD2	2:B:370:TYR:N	2.36	0.90
1:A:659:LEU:HD11	3:A:901:FAD:HM73	1.53	0.89
1:A:761:TYR:HD2	3:A:901:FAD:C9	1.87	0.87
2:B:430:ILE:O	2:B:433:VAL:HG22	1.74	0.86
1:A:360:CYS:O	1:A:362:LEU:HD12	1.77	0.85
2:B:413:SER:N	2:B:416:GLN:OE1	2.10	0.84
2:B:370:TYR:N	2:B:370:TYR:HD2	1.73	0.84
2:B:428:PHE:HB2	2:B:430:ILE:CD1	2.07	0.84
1:A:456:LYS:HA	2:B:370:TYR:HD1	1.40	0.83
2:B:421:PHE:CZ	2:B:434:LEU:HD11	2.15	0.82
2:B:368:GLU:HA	2:B:368:GLU:OE1	1.77	0.81
1:A:691:LEU:HD12	1:A:705:ALA:HB1	1.63	0.80
1:A:425:ASP:OD1	2:B:338:LEU:HD13	1.83	0.79
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLU:O	1:A:499:GLU:HG2	1.83	0.78
1:A:332:MET:HG3	1:A:333:VAL:HG23	1.66	0.77
1:A:583:ASP:OD1	1:A:585:LYS:NZ	2.19	0.76
1:A:470:PRO:O	1:A:472:ARG:HG2	1.87	0.74
2:B:402:PHE:HA	2:B:405:ILE:HD12	1.69	0.74
1:A:456:LYS:HG3	2:B:370:TYR:CE1	2.26	0.71
1:A:459:HIS:CD2	2:B:370:TYR:HB3	2.25	0.70
2:B:421:PHE:HZ	2:B:434:LEU:HD11	1.53	0.70
1:A:761:TYR:CD2	3:A:901:FAD:C9	2.74	0.70
1:A:245:ASP:OD1	1:A:247:VAL:HG12	1.92	0.69
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.23	0.69
1:A:456:LYS:CG	2:B:370:TYR:CE1	2.77	0.67
2:B:380:ASN:HB2	2:B:411:ASN:OD1	1.94	0.67
1:A:435:VAL:HG12	2:B:349:ILE:HG12	1.77	0.66
1:A:760:SER:OG	1:A:761:TYR:N	2.24	0.65
1:A:456:LYS:CG	2:B:370:TYR:HE1	2.10	0.64
1:A:761:TYR:HD2	3:A:901:FAD:H9	1.63	0.64
2:B:368:GLU:OE1	2:B:371:ARG:NH2	2.31	0.64
1:A:720:ASP:OD1	1:A:750:ARG:NH2	2.28	0.63
1:A:693:LEU:HD23	1:A:694:PHE:C	2.23	0.62
1:A:439:GLU:O	1:A:442:LYS:HB3	2.01	0.61
1:A:459:HIS:HB2	2:B:370:TYR:HB3	1.82	0.60
1:A:697:LEU:HD23	1:A:697:LEU:N	2.16	0.60
1:A:229:LEU:CD2	1:A:234:THR:OG1	2.49	0.60
1:A:360:CYS:O	1:A:362:LEU:CD1	2.49	0.60
1:A:425:ASP:OD1	2:B:338:LEU:CD1	2.49	0.60
1:A:351:MET:HA	1:A:569:ASN:HD21	1.66	0.59
1:A:659:LEU:HD11	3:A:901:FAD:C7M	2.29	0.59
1:A:449:VAL:HA	2:B:363:LEU:HD21	1.85	0.58
1:A:205:GLN:O	1:A:209:VAL:HG23	2.02	0.58
2:B:369:PRO:C	2:B:370:TYR:HD2	2.11	0.58
1:A:193:ALA:HB2	1:A:200:ILE:HD13	1.85	0.58
1:A:542:THR:HG1	1:A:546:THR:HG1	1.52	0.58
1:A:538:PHE:HD1	1:A:708:ALA:HB2	1.68	0.58
1:A:388:ALA:HB1	2:B:316:LEU:HD11	1.85	0.57
1:A:760:SER:CB	3:A:901:FAD:C8M	2.73	0.57
1:A:432:LYS:HA	1:A:435:VAL:HG22	1.85	0.57
2:B:351:ASN:O	2:B:355:THR:HG23	2.05	0.57
1:A:503:LYS:HA	1:A:506:GLU:HG2	1.87	0.57
2:B:405:ILE:HA	2:B:408:VAL:HG22	1.86	0.56
1:A:470:PRO:C	1:A:472:ARG:HG2	2.29	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:LEU:HD23	1:A:694:PHE:O	2.05	0.56
2:B:430:ILE:C	2:B:433:VAL:HG22	2.30	0.56
1:A:658:ASN:HA	1:A:760:SER:HB3	1.87	0.56
1:A:470:PRO:O	1:A:472:ARG:CG	2.54	0.56
2:B:377:GLN:CG	2:B:411:ASN:HD22	2.19	0.56
1:A:331:ALA:HA	3:A:901:FAD:N5	2.21	0.56
1:A:809:ALA:HB3	5:A:904:A1A5U:C24	2.36	0.55
1:A:661:LYS:H	1:A:749:SER:HB3	1.72	0.54
1:A:456:LYS:CD	2:B:370:TYR:HE1	2.21	0.54
1:A:456:LYS:CD	2:B:370:TYR:CE1	2.90	0.54
1:A:526:ARG:NH1	1:A:530:ASP:OD1	2.41	0.53
1:A:172:SER:N	1:A:175:GLU:OE1	2.41	0.53
2:B:421:PHE:HE1	2:B:430:ILE:CG2	2.20	0.53
1:A:470:PRO:N	1:A:471:PRO:HD2	2.24	0.53
1:A:355:LYS:HG2	1:A:565:LEU:CD2	2.39	0.52
1:A:459:HIS:HB2	2:B:370:TYR:CB	2.39	0.52
2:B:421:PHE:CE1	2:B:430:ILE:HG22	2.43	0.52
1:A:459:HIS:CG	2:B:370:TYR:CB	2.69	0.52
2:B:391:ALA:HB2	2:B:409:ILE:HD11	1.91	0.52
2:B:396:ARG:HH11	2:B:396:ARG:HG3	1.75	0.52
1:A:333:VAL:HG13	1:A:565:LEU:O	2.09	0.52
2:B:419:ASN:HB3	2:B:423:ASN:OD1	2.08	0.52
2:B:421:PHE:CE1	2:B:434:LEU:HD11	2.44	0.52
1:A:229:LEU:HD21	1:A:234:THR:OG1	2.10	0.52
2:B:425:ALA:O	2:B:426:ARG:C	2.53	0.51
1:A:332:MET:HE3	1:A:661:LYS:HZ3	1.75	0.51
1:A:209:VAL:O	1:A:213:ILE:HG13	2.11	0.51
1:A:648:THR:O	1:A:652:GLN:HG2	2.11	0.51
1:A:427:GLN:NE2	1:A:518:ASP:HA	2.27	0.50
1:A:380:GLN:O	1:A:381:GLU:C	2.54	0.50
1:A:332:MET:HE3	1:A:661:LYS:NZ	2.27	0.49
1:A:376:GLU:O	1:A:377:MET:C	2.50	0.49
1:A:432:LYS:O	1:A:435:VAL:HG22	2.12	0.49
1:A:815:LEU:C	1:A:815:LEU:HD23	2.37	0.49
2:B:309:LYS:N	2:B:310:PRO:CD	2.75	0.49
1:A:349:VAL:O	1:A:349:VAL:HG12	2.11	0.49
2:B:318:GLN:O	2:B:322:GLU:HG3	2.12	0.49
1:A:435:VAL:HG12	2:B:349:ILE:CG1	2.43	0.49
1:A:815:LEU:O	1:A:819:LEU:HG	2.12	0.49
1:A:213:ILE:HD13	1:A:249:VAL:HG22	1.93	0.49
2:B:430:ILE:O	2:B:430:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:HIS:CB	2:B:370:TYR:CB	2.81	0.49
1:A:671:TRP:O	1:A:673:PRO:HD3	2.13	0.49
1:A:355:LYS:HE2	1:A:563:SER:OG	2.13	0.49
1:A:730:ILE:O	1:A:734:ILE:HG12	2.13	0.48
1:A:768:SER:OG	1:A:772:ASP:OD2	2.20	0.48
1:A:810:THR:HA	3:A:901:FAD:N1	2.28	0.48
2:B:327:ASN:HB3	2:B:330:ALA:HB2	1.94	0.48
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.48	0.48
2:B:424:TYR:O	2:B:427:ARG:N	2.47	0.48
2:B:430:ILE:H	2:B:430:ILE:HD12	1.79	0.48
1:A:361:PRO:HB2	1:A:363:TYR:CE1	2.49	0.47
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.95	0.47
1:A:691:LEU:HD12	1:A:705:ALA:CB	2.41	0.47
1:A:659:LEU:HG	3:A:901:FAD:HM71	1.97	0.47
1:A:196:PHE:HB3	1:A:199:ILE:HD12	1.96	0.47
1:A:728:LEU:HD21	1:A:743:PRO:HD3	1.96	0.47
2:B:324:VAL:HG13	2:B:331:ALA:HB2	1.97	0.47
1:A:487:LEU:HD21	2:B:370:TYR:O	2.15	0.47
1:A:676:ASN:HA	1:A:696:ASN:OD1	2.15	0.47
2:B:369:PRO:HB2	2:B:370:TYR:HE2	1.79	0.47
1:A:273:LEU:HB2	1:A:274:PRO:HD2	1.97	0.46
2:B:430:ILE:HA	2:B:433:VAL:HG22	1.98	0.46
2:B:368:GLU:N	2:B:369:PRO:CD	2.79	0.46
1:A:538:PHE:CZ	1:A:706:LEU:HD23	2.51	0.46
2:B:420:PHE:HA	2:B:423:ASN:HB2	1.96	0.46
1:A:456:LYS:CB	2:B:370:TYR:HE1	2.29	0.46
1:A:210:PHE:C	1:A:210:PHE:CD1	2.94	0.46
2:B:318:GLN:HG3	2:B:322:GLU:OE2	2.15	0.45
2:B:424:TYR:O	2:B:425:ALA:C	2.58	0.45
2:B:368:GLU:OE1	2:B:371:ARG:CZ	2.64	0.45
1:A:453:GLU:HA	1:A:453:GLU:OE1	2.17	0.45
1:A:760:SER:CA	3:A:901:FAD:C8M	2.94	0.45
1:A:538:PHE:CE1	1:A:659:LEU:HD13	2.52	0.45
1:A:693:LEU:HD23	1:A:694:PHE:N	2.31	0.45
2:B:399:GLY:HA3	2:B:437:TRP:CE2	2.51	0.45
2:B:428:PHE:C	2:B:430:ILE:HD12	2.42	0.45
1:A:667:ASP:OD1	1:A:744:LYS:HE2	2.17	0.45
2:B:369:PRO:HB2	2:B:370:TYR:CE2	2.52	0.45
1:A:407:SER:OG	1:A:410:GLN:HG3	2.17	0.44
2:B:368:GLU:OE1	2:B:371:ARG:NE	2.51	0.44
1:A:435:VAL:CG1	2:B:349:ILE:HG12	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:ILE:O	1:A:804:ILE:HG23	2.16	0.44
2:B:394:ALA:HB2	2:B:408:VAL:HG21	2.00	0.44
1:A:603:ILE:HG13	1:A:615:ILE:HD13	2.00	0.44
1:A:628:GLY:HA3	1:A:758:ARG:HB2	2.00	0.44
2:B:355:THR:O	2:B:359:LEU:CD1	2.66	0.43
2:B:376:ILE:HG13	2:B:377:GLN:N	2.32	0.43
2:B:419:ASN:O	2:B:420:PHE:C	2.60	0.43
1:A:523:SER:O	1:A:527:GLN:HG3	2.18	0.43
1:A:541:ALA:O	1:A:657:GLY:HA3	2.18	0.43
1:A:691:LEU:CD1	1:A:727:CYS:SG	3.07	0.43
1:A:233:ALA:O	1:A:236:GLN:HB3	2.17	0.43
1:A:333:VAL:HG12	1:A:334:VAL:N	2.33	0.43
1:A:410:GLN:O	1:A:413:GLU:HG2	2.19	0.43
3:A:901:FAD:N1	3:A:901:FAD:H2'	2.32	0.43
2:B:396:ARG:HG3	2:B:396:ARG:NH1	2.33	0.43
2:B:419:ASN:C	2:B:423:ASN:OD1	2.62	0.43
1:A:373:GLU:OE1	1:A:373:GLU:C	2.62	0.43
2:B:394:ALA:CB	2:B:408:VAL:HG21	2.48	0.43
1:A:245:ASP:OD1	1:A:247:VAL:CG1	2.64	0.43
1:A:425:ASP:C	1:A:427:GLN:N	2.75	0.43
1:A:694:PHE:CD1	1:A:731:LEU:HD21	2.54	0.42
1:A:283:ILE:HD12	1:A:294:ALA:HB2	2.01	0.42
1:A:341:PRO:HD2	1:A:812:HIS:HB2	2.01	0.42
1:A:594:ARG:HA	1:A:640:VAL:O	2.20	0.42
1:A:781:THR:HA	1:A:794:PRO:HA	2.02	0.42
1:A:694:PHE:N	1:A:694:PHE:CD2	2.87	0.42
2:B:401:ASP:O	2:B:404:ALA:N	2.52	0.42
1:A:371:PRO:O	1:A:372:LYS:C	2.60	0.42
1:A:804:ILE:O	1:A:804:ILE:CG2	2.68	0.42
2:B:379:CYS:SG	2:B:416:GLN:OE1	2.78	0.41
1:A:439:GLU:HG2	2:B:352:ILE:HD13	2.02	0.41
2:B:324:VAL:HG12	2:B:324:VAL:O	2.19	0.41
2:B:367:ILE:O	2:B:368:GLU:C	2.60	0.41
2:B:368:GLU:N	2:B:369:PRO:HD3	2.35	0.41
2:B:401:ASP:O	2:B:404:ALA:HB3	2.21	0.41
2:B:430:ILE:CA	2:B:433:VAL:HG22	2.50	0.41
1:A:415:VAL:HG13	2:B:316:LEU:HD21	2.03	0.41
1:A:440:GLU:HG2	1:A:504:LEU:HD13	2.02	0.41
2:B:309:LYS:O	2:B:309:LYS:HD3	2.21	0.41
1:A:363:TYR:CB	1:A:734:ILE:HD12	2.51	0.41
1:A:537:GLU:CG	1:A:544:LEU:HG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:424:TYR:O	2:B:425:ALA:O	2.39	0.41
1:A:538:PHE:CD1	1:A:708:ALA:HB2	2.53	0.41
2:B:428:PHE:CB	2:B:430:ILE:CD1	2.90	0.41
2:B:431:ASP:O	2:B:435:GLN:HG3	2.19	0.41
1:A:485:ARG:HD2	2:B:404:ALA:HB1	2.02	0.41
1:A:659:LEU:CD1	3:A:901:FAD:C7M	2.98	0.41
1:A:435:VAL:CG1	2:B:349:ILE:CG1	2.99	0.41
1:A:240:ALA:HB1	1:A:241:PRO:HA	2.03	0.40
1:A:659:LEU:C	1:A:659:LEU:HD12	2.45	0.40
2:B:430:ILE:O	2:B:433:VAL:CG2	2.58	0.40
1:A:333:VAL:CG1	1:A:334:VAL:N	2.84	0.40
2:B:405:ILE:O	2:B:408:VAL:HG22	2.22	0.40
2:B:309:LYS:O	2:B:309:LYS:CG	2.69	0.40
2:B:330:ALA:O	2:B:334:VAL:HG23	2.21	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:324:ASN:OD1	2:B:351:ASN:HD21[8_544]	1.54	0.06

## 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	658/660 (100%)	634 (96%)	21 (3%)	3 (0%)	25	40
2	B	129/131 (98%)	114 (88%)	10 (8%)	5 (4%)	2	4
All	All	787/791 (100%)	748 (95%)	31 (4%)	8 (1%)	13	21

All (8) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	B	425	ALA
1	A	236	GLN
1	A	237	GLN
2	B	339	ASP
2	B	426	ARG
2	B	423	ASN
1	A	273	LEU
2	B	399	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	556/559 (100%)	555 (100%)	1 (0%)	92	97
2	B	111/111 (100%)	109 (98%)	2 (2%)	54	73
All	All	667/670 (100%)	664 (100%)	3 (0%)	89	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	GLN
2	B	370	TYR
2	B	421	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	460	GLN
1	A	540	ASN
1	A	587	ASN
1	A	606	ASN
1	A	676	ASN
1	A	806	ASN
2	B	350	GLN
2	B	380	ASN

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Mol	Chain	Res	Type
2	B	411	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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$
3	FAD	A	901	-	54,58,58	0.91	1 (1%)	71,89,89	1.02	5 (7%)
4	GOL	A	902	-	5,5,5	1.00	1 (20%)	5,5,5	1.17	1 (20%)
4	GOL	A	903	-	5,5,5	0.88	0	5,5,5	1.07	0
5	A1A5U	A	904	-	30,31,31	3.33	9 (30%)	39,42,42	1.27	6 (15%)

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	-	-	15/30/50/50	0/6/6/6
4	GOL	A	902	-	-	0/4/4/4	-
4	GOL	A	903	-	-	0/4/4/4	-
5	A1A5U	A	904	-	-	1/15/22/22	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	904	A1A5U	C22-C23	-13.91	1.32	1.53
5	A	904	A1A5U	C03-C04	6.99	1.56	1.49
5	A	904	A1A5U	C05-C06	5.09	1.58	1.49
3	A	901	FAD	C1'-C2'	4.33	1.58	1.52
5	A	904	A1A5U	C24-N03	-3.97	1.34	1.46
5	A	904	A1A5U	C15-C16	3.37	1.44	1.39
5	A	904	A1A5U	C23-N03	2.85	1.61	1.47
5	A	904	A1A5U	O01-C16	2.57	1.43	1.37
5	A	904	A1A5U	C09-C10	2.43	1.49	1.44
5	A	904	A1A5U	C08-C07	2.18	1.42	1.38
4	A	902	GOL	O2-C2	-2.01	1.37	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	FAD	C4'-C3'-C2'	4.41	120.91	113.57
3	A	901	FAD	O3'-C3'-C4'	-3.18	101.71	108.93
5	A	904	A1A5U	C05-C04-C03	-3.15	120.01	123.62
3	A	901	FAD	O2'-C2'-C3'	-3.06	102.08	109.25
3	A	901	FAD	C5'-C4'-C3'	2.82	117.53	112.22
5	A	904	A1A5U	C06-C05-C04	-2.59	120.94	123.94
5	A	904	A1A5U	C22-C21-C24	-2.54	98.73	102.25
5	A	904	A1A5U	C03-C04-N01	2.42	118.98	115.40
5	A	904	A1A5U	C19-N01-C04	2.25	121.89	118.01
5	A	904	A1A5U	C22-C23-N03	-2.24	100.58	105.68
3	A	901	FAD	C5A-C6A-N6A	2.04	123.42	120.31
4	A	902	GOL	C3-C2-C1	-2.04	104.33	111.80

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	FAD	C5B-O5B-PA-O1A
3	A	901	FAD	C5B-O5B-PA-O3P

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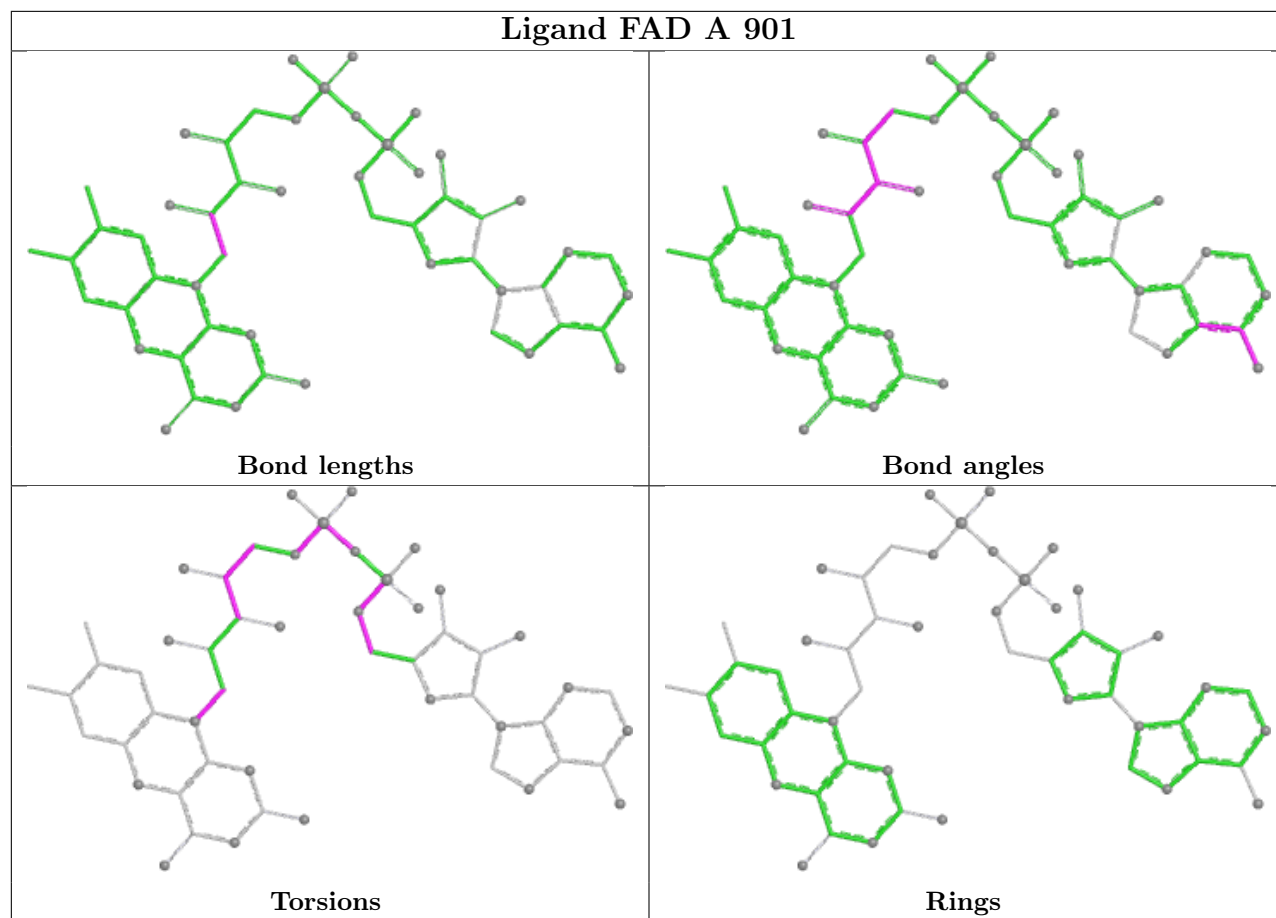
Mol	Chain	Res	Type	Atoms
3	A	901	FAD	C3'-C4'-C5'-O5'
3	A	901	FAD	O4'-C4'-C5'-O5'
3	A	901	FAD	C2'-C3'-C4'-O4'
3	A	901	FAD	O3'-C3'-C4'-O4'
3	A	901	FAD	O3'-C3'-C4'-C5'
5	A	904	A1A5U	C21-C17-O01-C16
3	A	901	FAD	C2'-C3'-C4'-C5'
3	A	901	FAD	C5B-O5B-PA-O2A
3	A	901	FAD	C2'-C1'-N10-C10
3	A	901	FAD	C5'-O5'-P-O1P
3	A	901	FAD	C5'-O5'-P-O2P
3	A	901	FAD	C5'-O5'-P-O3P
3	A	901	FAD	C4B-C5B-O5B-PA
3	A	901	FAD	PA-O3P-P-O2P

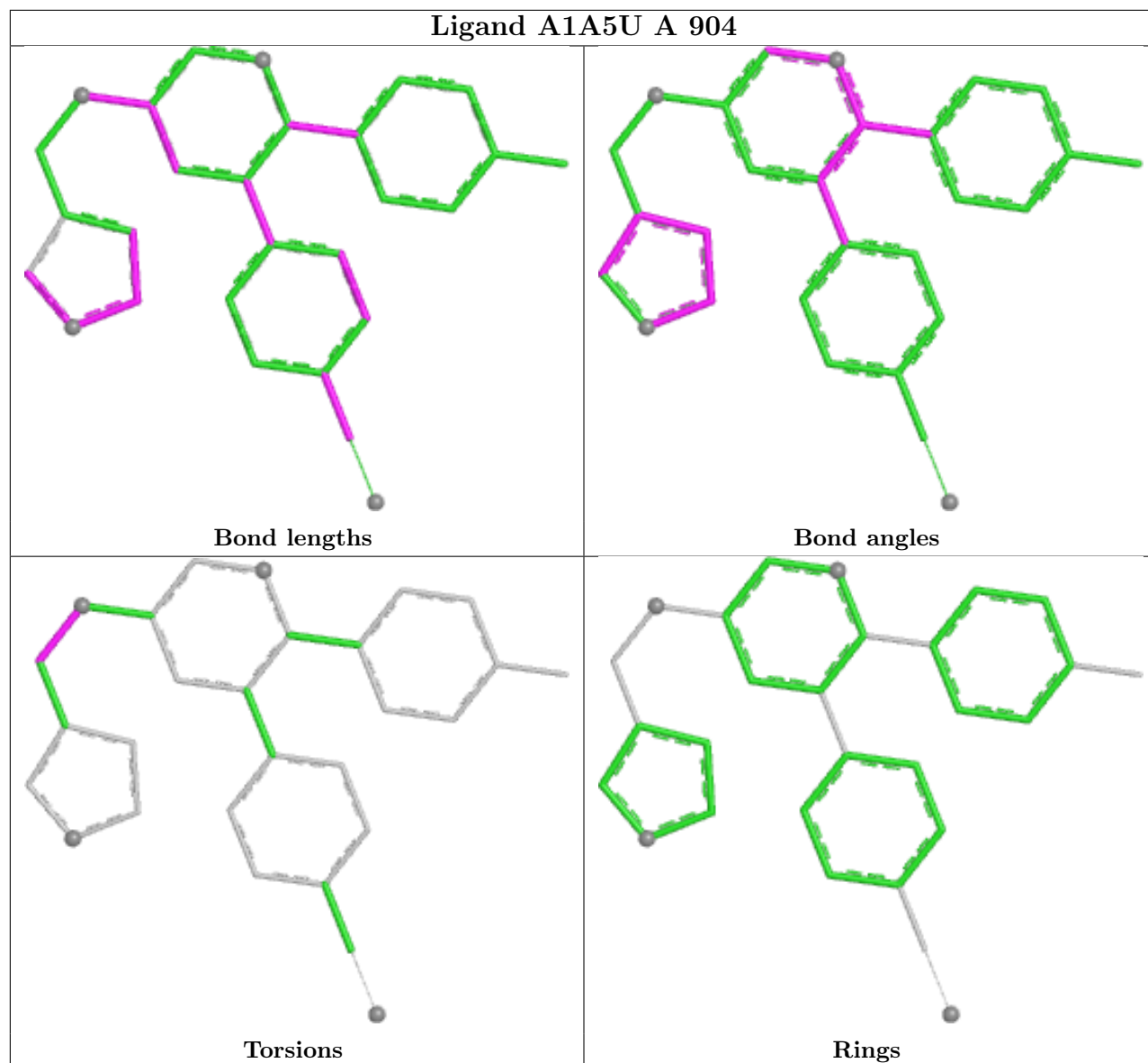
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	FAD	15	0
5	A	904	A1A5U	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, 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	660/660 (100%)	0.87	77 (11%)	10 10	51, 89, 129, 159	0
2	B	131/131 (100%)	1.95	49 (37%)	1 0	89, 127, 153, 186	0
All	All	791/791 (100%)	1.05	126 (15%)	6 5	51, 97, 139, 186	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	421	PHE	9.8
2	B	370	TYR	8.6
2	B	425	ALA	7.9
1	A	469	ALA	7.2
2	B	439	ALA	7.1
1	A	269	ALA	7.1
1	A	470	PRO	5.9
1	A	471	PRO	5.5
1	A	273	LEU	5.4
2	B	422	ALA	5.1
2	B	376	ILE	5.1
2	B	371	ARG	5.0
2	B	402	PHE	4.8
1	A	667	ASP	4.8
1	A	571	TYR	4.7
1	A	600	CYS	4.5
1	A	472	ARG	4.3
2	B	312	ALA	4.2
1	A	668	ARG	3.9
2	B	309	LYS	3.9
1	A	272	PRO	3.8
1	A	276	LYS	3.7
1	A	373	GLU	3.6
2	B	379	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	369	PRO	3.5
1	A	275	THR	3.5
1	A	787	PRO	3.5
2	B	430	ILE	3.5
1	A	359	LYS	3.4
1	A	511	LEU	3.4
2	B	378	ALA	3.3
2	B	372	LEU	3.3
1	A	506	GLU	3.3
1	A	508	LEU	3.3
2	B	400	ARG	3.3
1	A	466	SER	3.2
2	B	411	ASN	3.2
2	B	337	GLN	3.1
2	B	383	TRP	3.1
1	A	358	GLN	3.1
2	B	438	GLU	3.1
1	A	680	HIS	3.1
2	B	363	LEU	3.1
1	A	569	ASN	3.0
2	B	426	ARG	3.0
1	A	733	GLY	3.0
1	A	172	SER	3.0
2	B	382	ARG	3.0
1	A	239	GLU	2.9
1	A	241	PRO	2.9
1	A	785	SER	2.9
2	B	377	GLN	2.8
1	A	831	GLY	2.8
1	A	503	LYS	2.8
1	A	333	VAL	2.8
2	B	375	VAL	2.8
2	B	316	LEU	2.7
1	A	567	VAL	2.7
1	A	618	CYS	2.7
1	A	561	THR	2.7
2	B	414	VAL	2.6
1	A	502	GLY	2.6
1	A	357	LYS	2.6
1	A	739	ALA	2.6
1	A	737	SER	2.6
2	B	418	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	435	VAL	2.6
1	A	467	GLU	2.5
1	A	741	PRO	2.5
2	B	417	VAL	2.4
1	A	446	ASN	2.4
1	A	728	LEU	2.4
2	B	408	VAL	2.4
1	A	750	ARG	2.4
2	B	405	ILE	2.4
1	A	243	ASN	2.4
2	B	313	GLY	2.4
2	B	423	ASN	2.4
1	A	244	SER	2.4
1	A	242	TYR	2.4
1	A	573	CYS	2.4
1	A	331	ALA	2.3
2	B	381	ALA	2.3
1	A	324	ASN	2.3
2	B	401	ASP	2.3
1	A	271	LYS	2.3
2	B	373	PRO	2.3
1	A	377	MET	2.3
2	B	355	THR	2.3
2	B	397	LYS	2.3
1	A	361	PRO	2.3
1	A	519	VAL	2.3
1	A	504	LEU	2.3
2	B	424	TYR	2.3
1	A	237	GLN	2.3
2	B	332	THR	2.2
1	A	740	VAL	2.2
2	B	344	SER	2.2
1	A	351	MET	2.2
1	A	699	LYS	2.2
1	A	760	SER	2.2
2	B	399	GLY	2.2
2	B	410	GLY	2.2
1	A	453	GLU	2.2
1	A	730	ILE	2.2
2	B	350	GLN	2.2
1	A	570	GLY	2.2
1	A	430	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	459	HIS	2.1
1	A	507	LYS	2.1
1	A	352	GLU	2.1
1	A	738	SER	2.1
2	B	333	THR	2.1
1	A	402	ASN	2.1
2	B	409	ILE	2.1
1	A	717	ASN	2.1
1	A	439	GLU	2.1
1	A	514	ASN	2.1
2	B	431	ASP	2.1
1	A	173	GLY	2.1
1	A	431	TRP	2.0
1	A	205	GLN	2.0
1	A	231	PHE	2.0
2	B	437	TRP	2.0
1	A	683	SER	2.0
2	B	328	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](#)

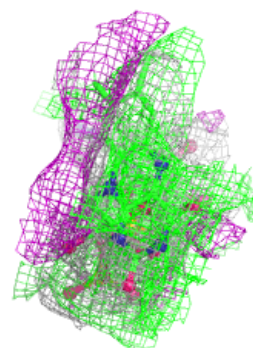
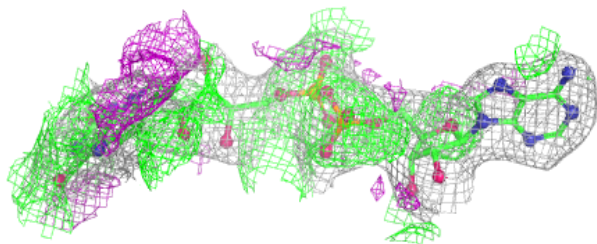
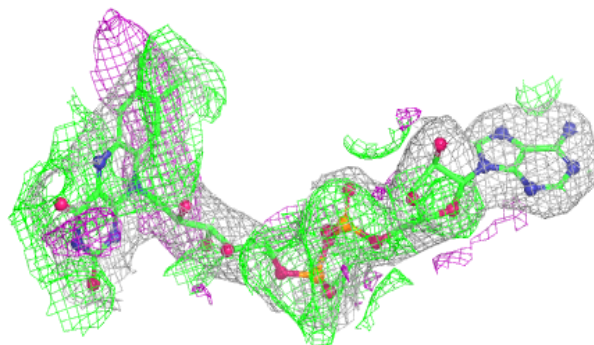
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	903	6/6	0.88	0.23	67,83,110,110	0
3	FAD	A	901	53/53	0.89	0.22	45,74,126,168	0
4	GOL	A	902	6/6	0.93	0.17	74,102,119,123	0
5	A1A5U	A	904	28/28	0.94	0.16	57,71,94,97	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.

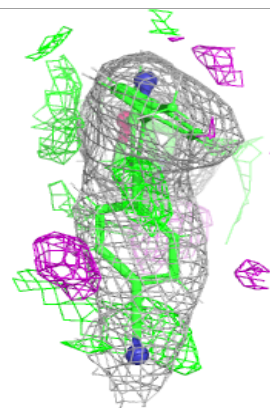
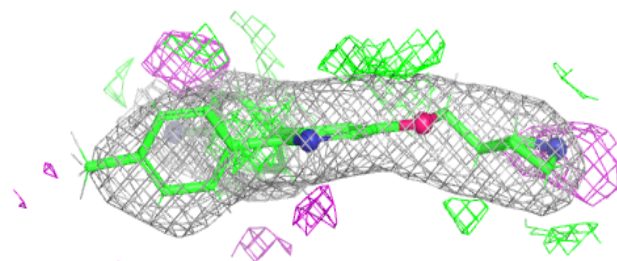
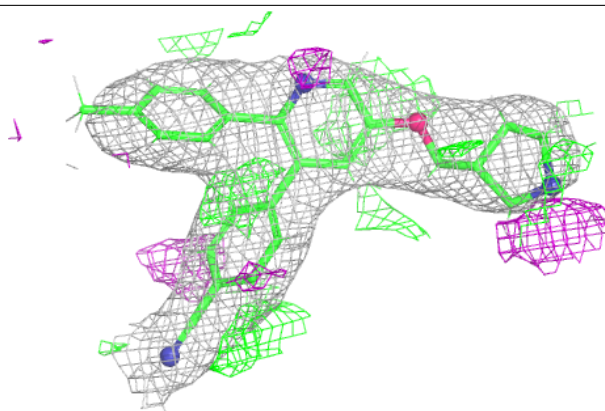
**Electron density around FAD A 901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around A1A5U A 904:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers ⓘ

There are no such residues in this entry.