Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 07:48 pm GMT

PDB ID	:	2Y48
Title	:	Crystal structure of LSD1-CoREST in complex with a N-terminal SNAIL peptide
Authors	:	Baron, R.; Binda, C.; Tortorici, M.; McCammon, J.A.; Mattevi, A.
Deposited on	:	2011-01-05
Resolution	:	3.00 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:

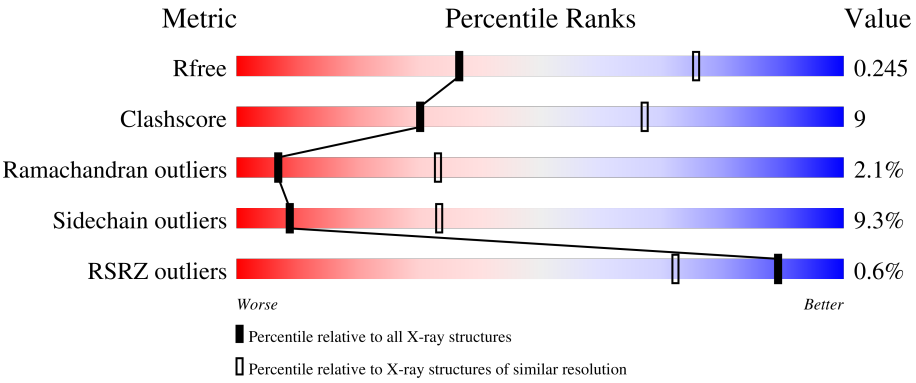
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	65% 23% · 9%
2	B	178	2% 53% 20% · 25%
3	C	20	30% 15% 55%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6416 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 DEMETHYLASE 1A.

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

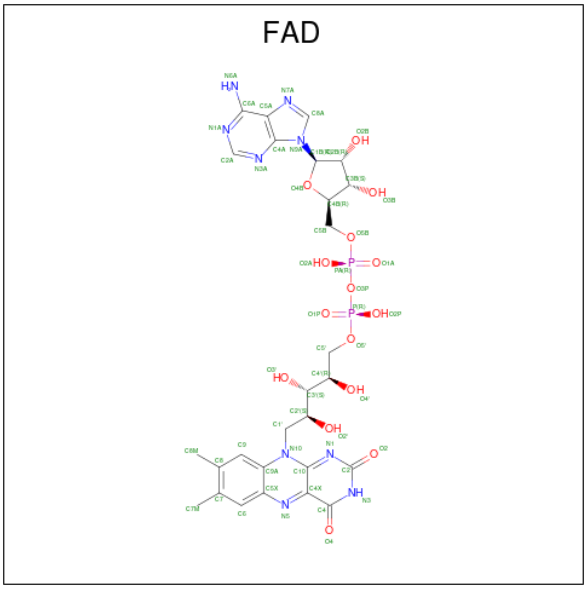
- Molecule 2 is a protein called REST COREPRESSOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	133	1076	676	194	203	3	0	0	0

- Molecule 3 is a protein called ZINC FINGER PROTEIN SNAI1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	9	77	51	16	10	0	0	0

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



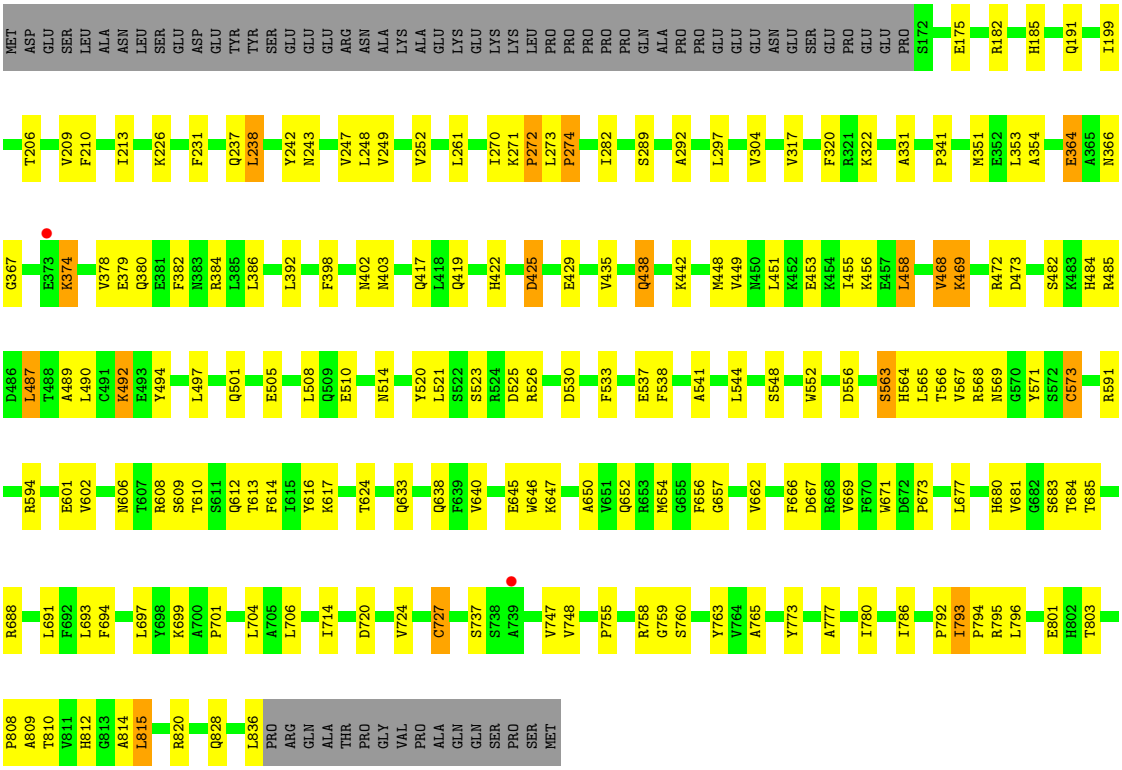
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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.

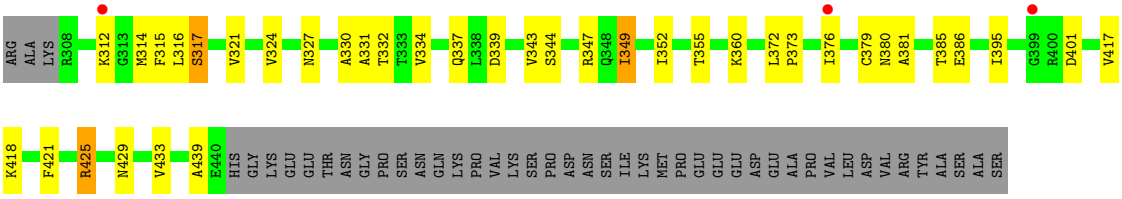
• Molecule 1: LYSINE-SPECIFIC DEMETHYLASE 1A

Chain A:



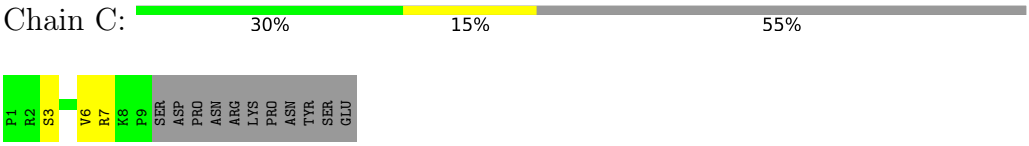
• Molecule 2: REST COREPRESSOR 1

Chain B:



• Molecule 3: ZINC FINGER PROTEIN SNAI1

Chain C:


30%
15%
55%
P1
R2
S3
V6
R7
K8
P9
SER
ASP
PRO
ASN
ARG
LYS
PRO
ASN
TYR
SER
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.17Å 181.46Å 234.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.77 – 3.00 71.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (71.77-3.00) 99.5 (71.77-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.246 0.207 , 0.245	Depositor DCC
R_{free} test set	992 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å^2)	77.5	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6416	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.68	1/5323 (0.0%)	0.74	2/7221 (0.0%)
2	B	0.52	0/1091	0.61	0/1471
3	C	0.80	0/79	0.77	0/104
All	All	0.65	1/6493 (0.0%)	0.72	2/8796 (0.0%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	727	CYS	CB-SG	-5.74	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	795	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	820	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	792	PRO	Peptide

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	5210	0	5244	110	0
2	B	1076	0	1091	19	0
3	C	77	0	89	3	0
4	A	53	0	31	5	0
All	All	6416	0	6455	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (120) 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:760:SER:HB2	4:A:900:FAD:HM83	1.43	1.00
1:A:794:PRO:HD2	1:A:828:GLN:NE2	1.81	0.96
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.53	0.88
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.54	0.87
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.91	0.83
1:A:270:ILE:O	1:A:272:PRO:HD3	1.77	0.83
1:A:494:TYR:CD1	1:A:494:TYR:O	2.36	0.78
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.48	0.76
1:A:453:GLU:HA	1:A:453:GLU:OE1	1.87	0.74
1:A:384:ARG:HB3	2:B:314:MET:CE	2.16	0.74
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.69	0.73
1:A:331:ALA:HA	4:A:900:FAD:N5	2.04	0.72
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.25	0.71
1:A:384:ARG:NH1	2:B:312:LYS:O	2.22	0.70
1:A:693:LEU:HD12	1:A:694:PHE:H	1.56	0.70
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.72	0.70
1:A:458:LEU:HB3	1:A:487:LEU:HD12	1.74	0.69
1:A:606:ASN:HD22	1:A:609:SER:H	1.40	0.69
1:A:801:GLU:HG2	1:A:809:ALA:H	1.58	0.68
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.75	0.66
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.29	0.66
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.36	0.65
1:A:537:GLU:HG2	1:A:544:LEU:HD21	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:PHE:CE2	1:A:759:GLY:HA3	2.32	0.64
1:A:331:ALA:HA	4:A:900:FAD:C4X	2.28	0.64
1:A:392:LEU:HD23	1:A:398:PHE:HD2	1.63	0.64
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.30	0.61
1:A:209:VAL:O	1:A:213:ILE:HG13	2.00	0.61
1:A:537:GLU:HG2	1:A:544:LEU:CD2	2.33	0.58
1:A:666:PHE:O	1:A:701:PRO:HG2	2.04	0.58
1:A:601:GLU:HA	1:A:616:TYR:O	2.04	0.58
1:A:693:LEU:HD12	1:A:694:PHE:N	2.18	0.57
1:A:438:GLN:HG2	2:B:352:ILE:HG22	1.87	0.56
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.88	0.56
1:A:402:ASN:O	1:A:403:ASN:HB2	2.07	0.55
1:A:671:TRP:O	1:A:673:PRO:HD3	2.06	0.55
1:A:794:PRO:CD	1:A:828:GLN:NE2	2.64	0.54
1:A:468:VAL:O	1:A:472:ARG:NH1	2.41	0.54
1:A:808:PRO:O	1:A:810:THR:HG23	2.09	0.53
1:A:379:GLU:OE1	3:C:7:ARG:NH1	2.43	0.52
1:A:289:SER:HB3	1:A:814:ALA:HB1	1.91	0.52
1:A:435:VAL:HG12	2:B:349:ILE:HG13	1.91	0.52
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.93	0.51
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.92	0.51
1:A:548:SER:O	1:A:552:TRP:HB3	2.11	0.50
1:A:646:TRP:CZ3	1:A:647:LYS:HE2	2.46	0.50
1:A:801:GLU:HG2	1:A:809:ALA:N	2.25	0.50
1:A:501:GLN:O	1:A:505:GLU:HB2	2.12	0.50
1:A:182:ARG:NH1	1:A:341:PRO:HD3	2.28	0.49
1:A:650:ALA:O	1:A:654:MET:HG3	2.12	0.49
2:B:324:VAL:HG12	2:B:324:VAL:O	2.12	0.49
2:B:324:VAL:HG13	2:B:331:ALA:HA	1.95	0.49
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.42	0.49
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.42	0.49
1:A:419:GLN:HE22	2:B:315:PHE:H	1.59	0.49
1:A:693:LEU:HD21	3:C:6:VAL:HG21	1.95	0.49
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.75	0.49
1:A:351:MET:HB3	1:A:567:VAL:HG13	1.95	0.48
1:A:297:LEU:HB2	1:A:304:VAL:HG21	1.96	0.47
1:A:455:ILE:HD11	1:A:490:LEU:O	2.14	0.47
1:A:435:VAL:HG13	2:B:349:ILE:HG13	1.96	0.47
1:A:606:ASN:HD21	1:A:608:ARG:HB2	1.80	0.47
2:B:317:SER:O	2:B:321:VAL:HG23	2.12	0.47
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ALA:O	1:A:492:LYS:HB3	2.15	0.47
1:A:533:PHE:O	1:A:537:GLU:HG3	2.15	0.47
2:B:417:VAL:O	2:B:421:PHE:HD1	1.98	0.47
1:A:366:ASN:OD1	1:A:367:GLY:N	2.48	0.47
1:A:448:MET:HG3	1:A:497:LEU:HD23	1.97	0.47
1:A:351:MET:HA	1:A:569:ASN:HD21	1.78	0.46
1:A:760:SER:CB	4:A:900:FAD:HM83	2.29	0.46
1:A:777:ALA:HB2	1:A:803:THR:HB	1.97	0.46
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.80	0.46
1:A:568:ARG:NH1	1:A:699:LYS:HG2	2.30	0.46
1:A:175:GLU:HG2	1:A:185:HIS:CG	2.51	0.45
1:A:273:LEU:HA	1:A:274:PRO:HD2	1.68	0.45
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.97	0.45
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.52	0.45
1:A:563:SER:O	1:A:565:LEU:HD12	2.16	0.45
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.99	0.45
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.66	0.44
1:A:210:PHE:CE1	1:A:252:VAL:HG22	2.53	0.44
2:B:421:PHE:O	2:B:425:ARG:HB2	2.18	0.44
1:A:374:LYS:O	1:A:378:VAL:HG23	2.18	0.44
1:A:685:THR:O	1:A:688:ARG:HG2	2.18	0.44
1:A:317:VAL:HG12	1:A:317:VAL:O	2.17	0.44
1:A:520:TYR:CE2	1:A:521:LEU:HD12	2.53	0.43
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.33	0.43
1:A:473:ASP:OD1	1:A:473:ASP:C	2.57	0.43
1:A:541:ALA:O	1:A:657:GLY:HA3	2.19	0.43
1:A:331:ALA:HA	4:A:900:FAD:C5X	2.49	0.43
1:A:720:ASP:O	1:A:724:VAL:HG23	2.19	0.43
1:A:669:VAL:HG11	1:A:673:PRO:HG3	1.99	0.43
1:A:320:PHE:CD1	1:A:747:VAL:HG21	2.53	0.43
1:A:613:THR:HG22	1:A:614:PHE:N	2.33	0.43
1:A:801:GLU:CG	1:A:809:ALA:HA	2.49	0.43
2:B:418:LYS:O	2:B:421:PHE:HB2	2.19	0.43
1:A:292:ALA:HB2	1:A:815:LEU:HD22	2.01	0.42
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.18	0.42
1:A:780:ILE:HB	1:A:796:LEU:HB3	2.01	0.42
1:A:379:GLU:O	1:A:382:PHE:HB3	2.18	0.42
1:A:469:LYS:HE3	1:A:469:LYS:HA	2.01	0.42
1:A:521:LEU:HD22	1:A:525:ASP:HB3	2.01	0.42
1:A:763:TYR:CE1	1:A:765:ALA:HB2	2.54	0.42
1:A:341:PRO:HG2	1:A:812:HIS:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:HA	1:A:681:VAL:HB	2.01	0.42
1:A:422:HIS:HA	1:A:425:ASP:HB2	2.01	0.42
3:C:6:VAL:O	3:C:7:ARG:HB2	2.19	0.42
1:A:354:ALA:HB2	1:A:568:ARG:HD2	2.01	0.42
1:A:594:ARG:HA	1:A:640:VAL:O	2.20	0.42
2:B:380:ASN:OD1	2:B:381:ALA:N	2.53	0.42
1:A:656:PHE:CE2	1:A:759:GLY:CA	3.01	0.41
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.55	0.41
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.94	0.41
1:A:451:LEU:C	1:A:453:GLU:N	2.74	0.41
1:A:606:ASN:ND2	1:A:609:SER:H	2.14	0.41
2:B:395:ILE:HG22	2:B:433:VAL:HG12	2.03	0.41
1:A:815:LEU:C	1:A:815:LEU:HD13	2.42	0.40
1:A:601:GLU:OE2	1:A:617:LYS:HE2	2.21	0.40
1:A:530:ASP:OD2	1:A:685:THR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	663/730 (91%)	594 (90%)	58 (9%)	11 (2%)	9 39
2	B	131/178 (74%)	111 (85%)	15 (12%)	5 (4%)	3 18
3	C	7/20 (35%)	6 (86%)	0	1 (14%)	0 1
All	All	801/928 (86%)	711 (89%)	73 (9%)	17 (2%)	7 33

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	VAL
1	A	737	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	429	ASN
1	A	364	GLU
1	A	274	PRO
2	B	425	ARG
2	B	439	ALA
3	C	3	SER
1	A	425	ASP
1	A	510	GLU
1	A	793	ILE
2	B	401	ASP
1	A	271	LYS
1	A	322	LYS
1	A	573	CYS
2	B	373	PRO
1	A	272	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	565/623 (91%)	516 (91%)	49 (9%)	10 37
2	B	117/156 (75%)	102 (87%)	15 (13%)	4 19
3	C	9/20 (45%)	9 (100%)	0	100 100
All	All	691/799 (86%)	627 (91%)	64 (9%)	9 33

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	206	THR
1	A	226	LYS
1	A	237	GLN
1	A	238	LEU
1	A	247	VAL
1	A	374	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	380	GLN
1	A	417	GLN
1	A	429	GLU
1	A	438	GLN
1	A	449	VAL
1	A	456	LYS
1	A	458	LEU
1	A	469	LYS
1	A	482	SER
1	A	485	ARG
1	A	487	LEU
1	A	492	LYS
1	A	508	LEU
1	A	514	ASN
1	A	523	SER
1	A	526	ARG
1	A	538	PHE
1	A	556	ASP
1	A	563	SER
1	A	564	HIS
1	A	571	TYR
1	A	573	CYS
1	A	591	ARG
1	A	610	THR
1	A	612	GLN
1	A	624	THR
1	A	633	GLN
1	A	638	GLN
1	A	645	GLU
1	A	652	GLN
1	A	667	ASP
1	A	677	LEU
1	A	680	HIS
1	A	683	SER
1	A	684	THR
1	A	704	LEU
1	A	706	LEU
1	A	714	ILE
1	A	786	ILE
1	A	793	ILE
1	A	815	LEU
1	A	836	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	316	LEU
2	B	317	SER
2	B	332	THR
2	B	334	VAL
2	B	337	GLN
2	B	339	ASP
2	B	343	VAL
2	B	344	SER
2	B	347	ARG
2	B	349	ILE
2	B	360	LYS
2	B	376	ILE
2	B	379	CYS
2	B	385	THR
2	B	386	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	358	GLN
1	A	419	GLN
1	A	438	GLN
1	A	606	ASN
1	A	742	GLN
1	A	778	GLN
1	A	828	GLN
2	B	337	GLN
2	B	350	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 (i)

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	900	-	53,58,58	1.16	4 (7%)	68,89,89	1.62	15 (22%)

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	900	-	-	1/30/50/50	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	FAD	C4X-N5	3.84	1.38	1.30
4	A	900	FAD	C2A-N3A	2.88	1.36	1.32
4	A	900	FAD	C10-N1	2.74	1.38	1.33
4	A	900	FAD	C2A-N1A	2.70	1.38	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	900	FAD	N3A-C2A-N1A	-6.45	118.60	128.68
4	A	900	FAD	C4-N3-C2	-3.32	119.50	125.64
4	A	900	FAD	O4B-C1B-C2B	-3.12	102.37	106.93
4	A	900	FAD	C5'-C4'-C3'	-2.98	106.44	112.20
4	A	900	FAD	O4-C4-C4X	-2.94	118.81	126.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	900	FAD	C4X-C4-N3	2.56	119.69	113.19
4	A	900	FAD	C5X-C9A-N10	2.49	120.52	117.95
4	A	900	FAD	C4-C4X-C10	2.46	120.92	116.79
4	A	900	FAD	O2'-C2'-C1'	-2.43	103.92	109.80
4	A	900	FAD	C4X-C10-N1	-2.43	119.10	124.73
4	A	900	FAD	O3'-C3'-C2'	2.41	114.62	108.81
4	A	900	FAD	C1B-N9A-C4A	-2.35	122.51	126.64
4	A	900	FAD	O3B-C3B-C4B	-2.23	104.61	111.05
4	A	900	FAD	P-O3P-PA	-2.18	125.33	132.83
4	A	900	FAD	C9A-C5X-N5	-2.15	120.10	122.43

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	900	FAD	O4B-C4B-C5B-O5B

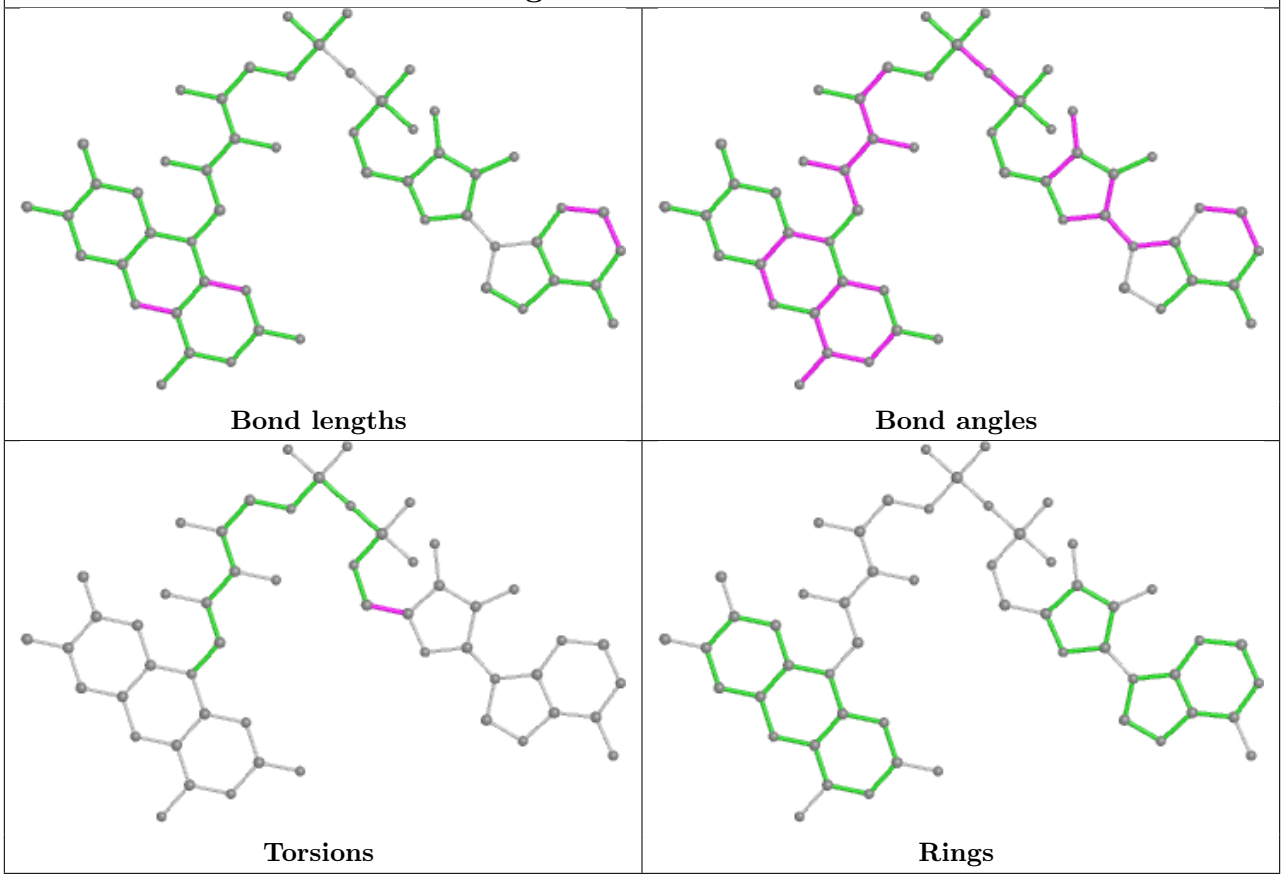
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	900	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 then 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.

Ligand FAD A 900



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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	665/730 (91%)	-0.00	2 (0%) 94 84	41, 69, 100, 115	0
2	B	133/178 (74%)	0.16	3 (2%) 60 31	72, 104, 119, 127	0
3	C	9/20 (45%)	0.01	0 100 100	63, 66, 91, 91	0
All	All	807/928 (86%)	0.02	5 (0%) 89 72	41, 76, 111, 127	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	739	ALA	2.6
2	B	312	LYS	2.2
2	B	399	GLY	2.1
1	A	373	GLU	2.1
2	B	376	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

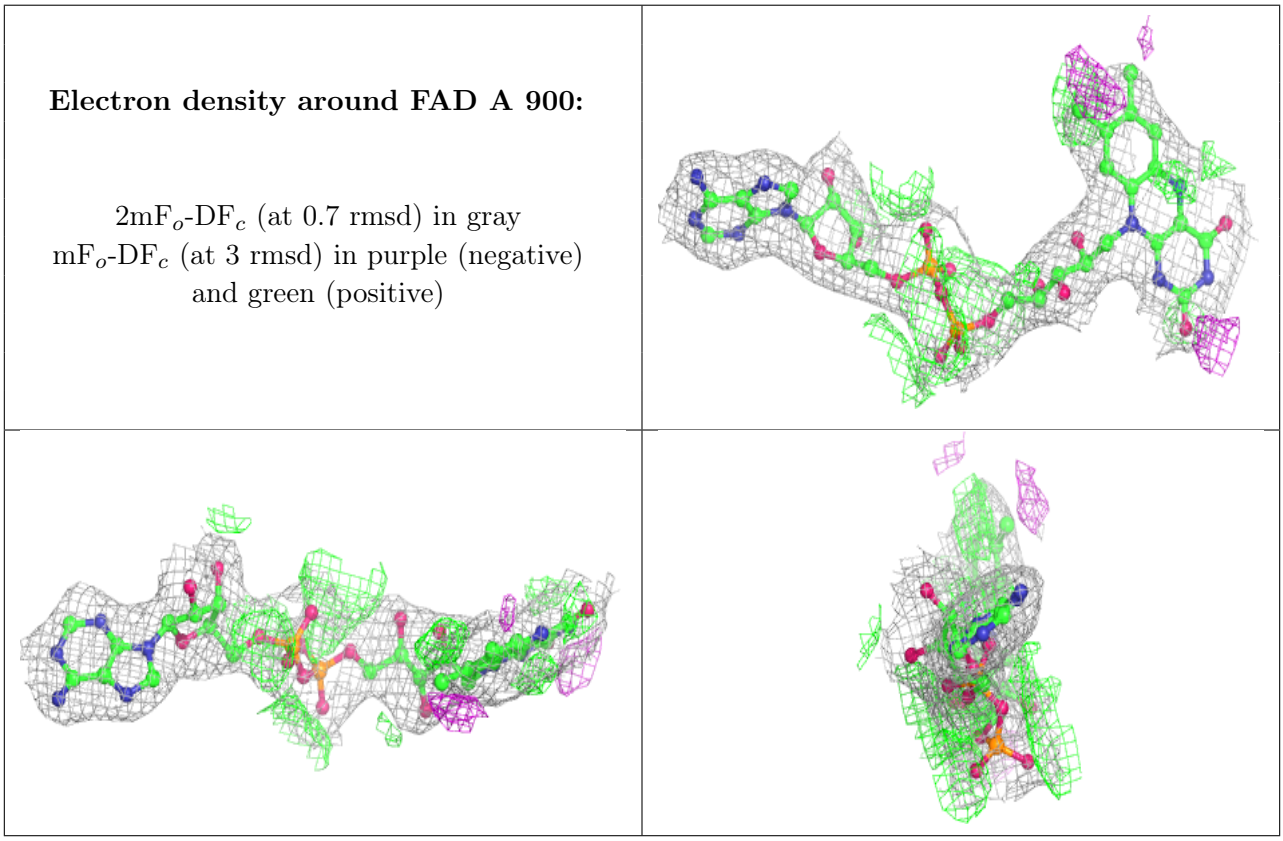
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FAD	A	900	53/53	0.98	0.22	38,42,59,60	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 900:

$2mF_o$-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 (i)

There are no such residues in this entry.