



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 01:19 pm BST

PDB ID : 2XAF
Title : Crystal structure of LSD1-CoREST in complex with para-bromo-(+)-cis-2-phenylcyclopropyl-1-amine
Authors : Binda, C.; Valente, S.; Romanenghi, M.; Pilotto, S.; Cirilli, R.; Karytinis, A.; Ciossani, G.; Botrugno, O.A.; Forneris, F.; Tardugno, M.; Edmondson, D.E.; Minucci, S.; Mattevi, A.; Mai, A.
Deposited on : 2010-03-31
Resolution : 3.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

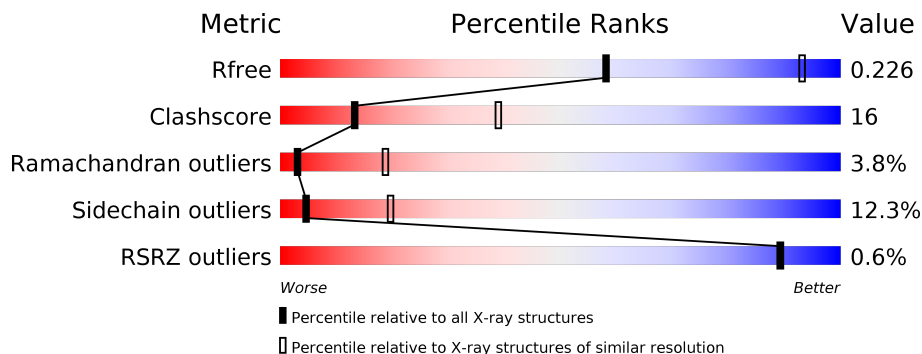
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	852	 48% 27% 22%
2	B	482	 13% 11% 72%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6357 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.

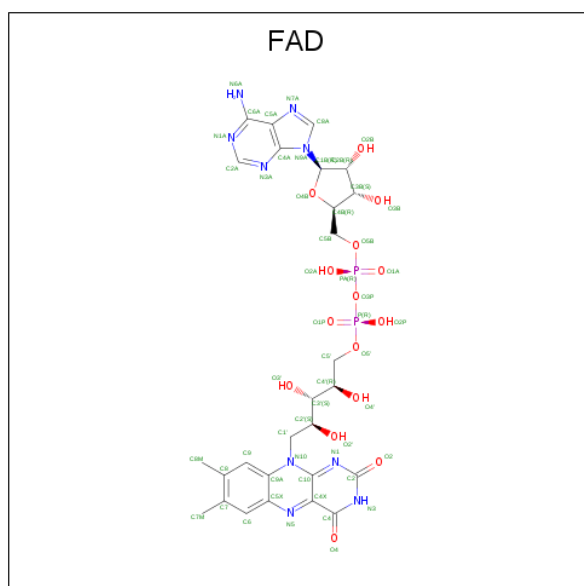
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	666	5217	3324	906	967	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

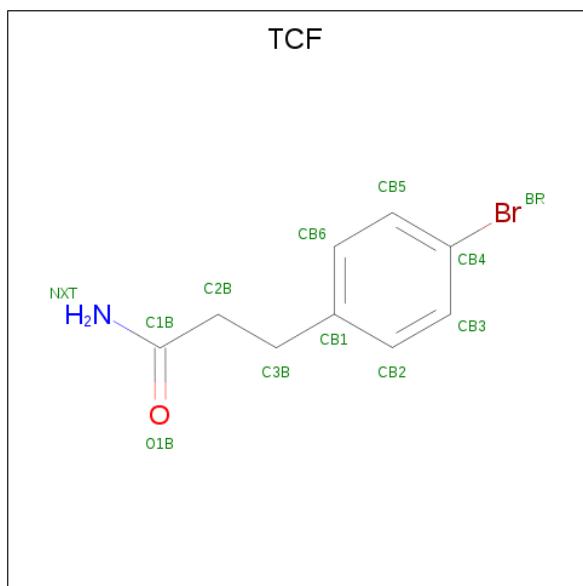
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is 3-(4-BROMOPHENYL)PROPANAMIDE (three-letter code: TCF) (formula:

C₉H₁₀BrNO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	Br	C	O		
4	A	1	11	1	9	1	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.56Å 179.48Å 235.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.51 – 3.25 30.51 – 3.25	Depositor EDS
% Data completeness (in resolution range)	94.6 (30.51-3.25) 94.6 (30.51-3.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 3.24Å)	Xtrriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.202 , 0.229 0.202 , 0.226	Depositor DCC
R_{free} test set	735 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å ²)	73.6	Xtrriage
Anisotropy	0.031	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6357	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TCF, 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	0.72	1/5331 (0.0%)	0.81	3/7232 (0.0%)
2	B	0.61	0/1091	0.73	1/1471 (0.1%)
All	All	0.70	1/6422 (0.0%)	0.80	4/8703 (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	-5.10	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	815	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	258	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	B	359	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	281	VAL	CB-CA-C	-5.14	101.64	111.40

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	5217	0	5252	166	0
2	B	1076	0	1091	55	0
3	A	53	0	31	3	0
4	A	11	0	8	3	0
All	All	6357	0	6382	206	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 16.

All (206) 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:755:PRO:HA	1:A:758:ARG:NH1	1.62	1.13
3:A:900:FAD:C4X	4:A:901:TCF:H3B1	1.78	1.11
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.16	1.11
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.56	1.01
1:A:671:TRP:O	1:A:673:PRO:HD3	1.62	0.99
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.27	0.98
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.03	0.93
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.47	0.92
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.53	0.89
1:A:209:VAL:O	1:A:213:ILE:HG13	1.76	0.85
2:B:424:TYR:CD1	2:B:427:ARG:NH2	2.47	0.83
1:A:658:ASN:ND2	1:A:752:ARG:HB2	1.94	0.82
1:A:801:GLU:CG	1:A:809:ALA:HA	2.10	0.81
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.16	0.81
1:A:755:PRO:CA	1:A:758:ARG:HH12	1.93	0.80
3:A:900:FAD:C4X	4:A:901:TCF:C3B	2.61	0.77
1:A:484:HIS:HD2	2:B:372:LEU:HD13	1.51	0.76
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.70	0.74
1:A:720:ASP:O	1:A:724:VAL:HG23	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:GLN:O	2:B:341:GLU:HB2	1.87	0.73
1:A:451:LEU:C	1:A:453:GLU:H	1.90	0.73
1:A:453:GLU:OE1	1:A:453:GLU:CA	2.36	0.73
1:A:452:LYS:HE3	2:B:366:GLY:O	1.91	0.70
1:A:506:GLU:C	1:A:508:LEU:H	1.94	0.70
1:A:693:LEU:HD12	1:A:694:PHE:H	1.57	0.68
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.24	0.68
3:A:900:FAD:C10	4:A:901:TCF:H3B1	2.23	0.68
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.76	0.67
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.26	0.66
2:B:429:ASN:HB3	2:B:432:GLU:OE2	1.95	0.66
1:A:534:ALA:HA	1:A:537:GLU:HG3	1.77	0.65
1:A:451:LEU:C	1:A:453:GLU:N	2.48	0.65
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.77	0.65
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.79	0.65
1:A:379:GLU:O	1:A:382:PHE:HB3	1.97	0.65
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.78	0.64
1:A:693:LEU:HD12	1:A:694:PHE:N	2.12	0.64
1:A:808:PRO:O	1:A:810:THR:HG23	1.97	0.64
1:A:343:ALA:O	1:A:346:SER:OG	2.15	0.64
1:A:506:GLU:O	1:A:508:LEU:N	2.27	0.64
1:A:437:THR:HG22	1:A:508:LEU:HD21	1.80	0.63
1:A:726:ARG:O	1:A:730:ILE:HG13	1.99	0.63
1:A:418:LEU:HD11	2:B:324:VAL:HG21	1.79	0.63
2:B:418:LYS:O	2:B:421:PHE:HB2	1.98	0.63
2:B:424:TYR:CE1	2:B:427:ARG:NH2	2.67	0.63
1:A:520:TYR:CD2	1:A:521:LEU:HG	2.33	0.63
2:B:426:ARG:HB3	2:B:427:ARG:HG3	1.79	0.62
1:A:391:TYR:CD2	1:A:395:GLN:HG3	2.35	0.62
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.65	0.61
1:A:665:CYS:HB2	1:A:745:GLU:O	2.00	0.61
1:A:270:ILE:O	1:A:272:PRO:HD3	2.00	0.60
1:A:659:LEU:HD12	1:A:660:ASN:N	2.16	0.60
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.83	0.60
1:A:807:TYR:N	1:A:808:PRO:HD3	2.17	0.60
1:A:533:PHE:O	1:A:537:GLU:HG2	2.01	0.60
1:A:385:LEU:O	1:A:388:ALA:HB3	2.01	0.59
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.03	0.58
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.38	0.58
1:A:456:LYS:HG2	2:B:370:TYR:CE1	2.38	0.58
1:A:551:HIS:O	1:A:553:ASP:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASN:OD1	1:A:368:GLN:N	2.38	0.56
1:A:694:PHE:HA	1:A:704:LEU:O	2.05	0.56
1:A:541:ALA:O	1:A:542:THR:HB	2.05	0.56
1:A:346:SER:HA	1:A:351:MET:SD	2.45	0.56
1:A:402:ASN:O	1:A:403:ASN:HB2	2.06	0.56
2:B:388:GLN:O	2:B:391:ALA:HB3	2.05	0.56
1:A:363:TYR:CD2	1:A:734:ILE:HG13	2.42	0.55
1:A:295:ARG:NH2	1:A:580:GLU:O	2.40	0.55
1:A:710:GLU:OE1	1:A:710:GLU:HA	2.06	0.55
1:A:506:GLU:C	1:A:508:LEU:N	2.60	0.54
2:B:399:GLY:O	2:B:434:LEU:HD21	2.08	0.54
1:A:548:SER:HB2	1:A:766:ALA:HA	1.89	0.54
1:A:548:SER:O	1:A:552:TRP:HB3	2.08	0.54
2:B:350:GLN:H	2:B:350:GLN:HE21	1.54	0.54
2:B:337:GLN:HA	2:B:337:GLN:HE21	1.71	0.54
2:B:369:PRO:HB2	2:B:370:TYR:CD2	2.43	0.54
2:B:370:TYR:CD2	2:B:370:TYR:N	2.75	0.54
2:B:400:ARG:O	2:B:402:PHE:N	2.41	0.54
1:A:377:MET:HE2	1:A:378:VAL:HG22	1.89	0.53
1:A:361:PRO:HB2	1:A:363:TYR:HE1	1.74	0.53
1:A:456:LYS:HG2	2:B:370:TYR:HE1	1.73	0.53
1:A:473:ASP:OD1	1:A:473:ASP:C	2.47	0.52
2:B:421:PHE:O	2:B:425:ARG:HB2	2.09	0.52
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.91	0.52
1:A:340:ASN:HA	1:A:560:PHE:CZ	2.45	0.52
1:A:177:ALA:HB1	1:A:218:LEU:HB3	1.92	0.52
2:B:413:SER:O	2:B:415:VAL:N	2.42	0.51
1:A:690:GLU:HG2	1:A:691:LEU:HD12	1.92	0.51
2:B:369:PRO:HB2	2:B:370:TYR:CE2	2.45	0.51
1:A:724:VAL:O	1:A:728:LEU:HG	2.10	0.51
1:A:761:TYR:HB2	1:A:809:ALA:HB1	1.92	0.51
1:A:340:ASN:HB2	1:A:560:PHE:CD2	2.46	0.51
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.74	0.51
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.40	0.51
1:A:362:LEU:C	1:A:363:TYR:CD1	2.85	0.50
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.94	0.50
1:A:374:LYS:O	1:A:375:ASP:C	2.50	0.50
1:A:800:GLY:O	1:A:803:THR:N	2.37	0.50
1:A:761:TYR:HB2	1:A:809:ALA:CB	2.42	0.49
1:A:510:GLU:HG3	1:A:511:LEU:HD23	1.95	0.49
1:A:214:ARG:HD2	1:A:215:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.31	0.48
1:A:384:ARG:NH2	2:B:312:LYS:O	2.46	0.48
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.78	0.48
1:A:771:ASN:HA	1:A:805:ARG:NH1	2.28	0.48
1:A:377:MET:O	1:A:377:MET:HG2	2.12	0.48
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.54	0.48
1:A:419:GLN:NE2	2:B:315:PHE:O	2.44	0.48
1:A:241:PRO:O	1:A:244:SER:HB3	2.14	0.48
2:B:413:SER:C	2:B:415:VAL:H	2.16	0.48
1:A:337:LEU:O	1:A:339:GLY:N	2.46	0.47
2:B:417:VAL:O	2:B:420:PHE:HB3	2.14	0.47
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.96	0.47
2:B:317:SER:O	2:B:321:VAL:HG23	2.14	0.47
1:A:260:GLY:O	1:A:264:PHE:CD2	2.67	0.47
1:A:384:ARG:NH1	2:B:312:LYS:O	2.45	0.47
1:A:374:LYS:O	1:A:378:VAL:HG23	2.15	0.47
1:A:666:PHE:O	1:A:701:PRO:HG2	2.13	0.47
1:A:448:MET:CB	2:B:363:LEU:HD11	2.43	0.47
1:A:650:ALA:O	1:A:654:MET:HG3	2.15	0.47
2:B:425:ARG:HA	2:B:430:ILE:HG13	1.97	0.47
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.50	0.47
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.50	0.47
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.76	0.46
1:A:192:GLU:HG3	1:A:255:TYR:OH	2.15	0.46
1:A:468:VAL:O	1:A:472:ARG:NH1	2.45	0.46
1:A:485:ARG:O	1:A:487:LEU:N	2.49	0.46
2:B:368:GLU:HB2	2:B:369:PRO:HD3	1.98	0.46
2:B:370:TYR:N	2:B:370:TYR:HD2	2.14	0.46
1:A:457:GLU:O	1:A:457:GLU:HG2	2.15	0.46
2:B:352:ILE:CG2	2:B:352:ILE:O	2.63	0.46
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.98	0.46
1:A:680:HIS:CD2	1:A:730:ILE:HG23	2.51	0.46
1:A:566:THR:HG21	1:A:697:LEU:HD21	1.98	0.45
1:A:594:ARG:HA	1:A:640:VAL:O	2.16	0.45
1:A:520:TYR:CE2	1:A:521:LEU:HG	2.51	0.45
1:A:437:THR:HG22	1:A:438:GLN:N	2.30	0.45
1:A:450:ASN:HA	1:A:453:GLU:HB2	1.96	0.45
1:A:286:SER:HB2	1:A:291:LEU:HD21	1.99	0.45
1:A:310:ARG:NH2	1:A:756:TRP:HB2	2.31	0.45
1:A:380:GLN:HE21	1:A:380:GLN:HB3	1.52	0.45
1:A:424:LYS:O	1:A:426:GLU:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:ILE:H	2:B:376:ILE:HG13	1.52	0.45
1:A:273:LEU:HA	1:A:274:PRO:HD2	1.81	0.45
1:A:340:ASN:OD1	1:A:342:MET:N	2.45	0.45
1:A:662:VAL:HB	1:A:705:ALA:HB3	1.99	0.45
1:A:209:VAL:HG13	1:A:242:TYR:CD1	2.49	0.44
1:A:317:VAL:HG12	1:A:317:VAL:O	2.17	0.44
1:A:451:LEU:O	1:A:453:GLU:N	2.50	0.44
1:A:366:ASN:OD1	1:A:367:GLY:N	2.51	0.44
1:A:568:ARG:NH2	1:A:699:LYS:HA	2.32	0.44
1:A:361:PRO:HB2	1:A:363:TYR:CE1	2.52	0.44
2:B:394:ALA:O	2:B:398:TYR:HB2	2.17	0.44
1:A:535:ASN:HD22	1:A:535:ASN:HA	1.51	0.44
1:A:572:SER:O	1:A:576:VAL:HG23	2.18	0.44
1:A:474:ILE:HA	1:A:474:ILE:HD12	1.74	0.43
2:B:347:ARG:HG3	2:B:348:GLN:N	2.33	0.43
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.52	0.43
1:A:807:TYR:N	1:A:808:PRO:CD	2.81	0.43
1:A:447:LYS:HD3	1:A:497:LEU:HD21	2.00	0.43
1:A:606:ASN:ND2	1:A:609:SER:H	2.15	0.43
1:A:647:LYS:HE3	1:A:798:PHE:CE1	2.54	0.43
1:A:245:ASP:O	1:A:249:VAL:HG23	2.19	0.43
1:A:291:LEU:HG	1:A:291:LEU:H	1.69	0.43
1:A:297:LEU:HD23	1:A:297:LEU:HA	1.72	0.43
2:B:425:ARG:NH1	2:B:431:ASP:OD1	2.51	0.43
1:A:231:PHE:CZ	1:A:250:HIS:HB2	2.53	0.43
1:A:643:LEU:HA	1:A:643:LEU:HD23	1.76	0.43
1:A:181:SER:OG	1:A:218:LEU:HD22	2.19	0.43
1:A:319:THR:HA	1:A:328:ASP:HA	2.01	0.43
1:A:419:GLN:HB3	1:A:520:TYR:CE1	2.53	0.43
1:A:603:ILE:HG12	1:A:615:ILE:HD13	2.00	0.43
2:B:349:ILE:O	2:B:350:GLN:C	2.57	0.43
1:A:801:GLU:HG2	1:A:809:ALA:HA	1.96	0.43
1:A:196:PHE:N	1:A:197:PRO:CD	2.83	0.42
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.55	0.42
1:A:564:HIS:CD2	1:A:564:HIS:N	2.87	0.42
1:A:565:LEU:HD12	1:A:565:LEU:N	2.35	0.42
1:A:248:LEU:O	1:A:249:VAL:C	2.57	0.42
1:A:364:GLU:OE1	1:A:524:ARG:NE	2.53	0.42
1:A:284:ILE:HD13	1:A:590:VAL:HG11	2.02	0.42
1:A:640:VAL:HA	1:A:641:PRO:HA	1.87	0.42
2:B:372:LEU:HA	2:B:373:PRO:HD2	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LYS:HG2	2:B:370:TYR:OH	2.19	0.42
1:A:606:ASN:HD22	1:A:609:SER:H	1.68	0.42
1:A:319:THR:HG21	1:A:321:ARG:NH2	2.35	0.42
1:A:319:THR:OG1	1:A:572:SER:HB3	2.20	0.41
1:A:747:VAL:HG12	1:A:748:VAL:N	2.35	0.41
1:A:669:VAL:HG11	1:A:673:PRO:HG3	2.02	0.41
1:A:758:ARG:HH11	1:A:758:ARG:HG2	1.86	0.41
1:A:374:LYS:O	1:A:377:MET:N	2.53	0.41
1:A:533:PHE:O	1:A:537:GLU:CG	2.69	0.41
1:A:536:LEU:HD12	1:A:536:LEU:HA	1.90	0.41
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.35	0.41
2:B:424:TYR:O	2:B:425:ARG:C	2.59	0.41
1:A:377:MET:CE	1:A:378:VAL:HG22	2.51	0.41
1:A:311:ASP:N	1:A:311:ASP:OD1	2.53	0.41
1:A:750:ARG:O	1:A:753:ALA:HB3	2.21	0.41
2:B:320:ASP:O	2:B:323:ALA:HB3	2.21	0.40
1:A:814:ALA:O	1:A:815:LEU:C	2.59	0.40
2:B:383:TRP:CE3	2:B:412:LYS:HE2	2.56	0.40
1:A:494:TYR:CD2	1:A:494:TYR:O	2.74	0.40
1:A:568:ARG:NH1	1:A:699:LYS:HE3	2.36	0.40
1:A:448:MET:HG3	1:A:497:LEU:HD23	2.04	0.40
2:B:349:ILE:HG22	2:B:350:GLN:N	2.37	0.40
2:B:405:ILE:O	2:B:409:ILE:HG13	2.22	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	664/852 (78%)	575 (87%)	65 (10%)	24 (4%)	3 20
2	B	131/482 (27%)	99 (76%)	26 (20%)	6 (5%)	2 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	795/1334 (60%)	674 (85%)	91 (11%)	30 (4%)	3 19

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	274	PRO
1	A	507	LYS
2	B	341	GLU
2	B	373	PRO
1	A	275	THR
1	A	425	ASP
1	A	438	GLN
1	A	452	LYS
1	A	482	SER
1	A	486	ASP
1	A	499	GLU
1	A	552	TRP
1	A	579	ALA
1	A	785	SER
1	A	793	ILE
1	A	801	GLU
2	B	414	VAL
2	B	426	ARG
1	A	243	ASN
1	A	373	GLU
1	A	428	ILE
1	A	737	SER
1	A	809	ALA
2	B	331	ALA
1	A	338	GLY
1	A	364	GLU
2	B	401	ASP
1	A	316	ARG
1	A	332	MET
1	A	468	VAL

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	566/699 (81%)	505 (89%)	61 (11%)	6	24
2	B	117/395 (30%)	94 (80%)	23 (20%)	1	5
All	All	683/1094 (62%)	599 (88%)	84 (12%)	4	20

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	VAL
1	A	183	LEU
1	A	191	GLN
1	A	205	GLN
1	A	237	GLN
1	A	238	LEU
1	A	247	VAL
1	A	263	ASN
1	A	271	LYS
1	A	274	PRO
1	A	276	LYS
1	A	281	VAL
1	A	296	GLN
1	A	313	VAL
1	A	329	LEU
1	A	351	MET
1	A	359	LYS
1	A	377	MET
1	A	380	GLN
1	A	404	LYS
1	A	413	GLU
1	A	429	GLU
1	A	433	LYS
1	A	437	THR
1	A	438	GLN
1	A	449	VAL
1	A	453	GLU
1	A	458	LEU
1	A	466	SER
1	A	469	LYS
1	A	479	LEU
1	A	485	ARG
1	A	487	LEU

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Mol	Chain	Res	Type
1	A	512	GLU
1	A	514	ASN
1	A	519	VAL
1	A	523	SER
1	A	524	ARG
1	A	526	ARG
1	A	535	ASN
1	A	537	GLU
1	A	556	ASP
1	A	571	TYR
1	A	591	ARG
1	A	600	CYS
1	A	607	THR
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	659	LEU
1	A	663	VAL
1	A	684	THR
1	A	699	LYS
1	A	727	CYS
1	A	786	ILE
1	A	793	ILE
1	A	815	LEU
1	A	835	THR
2	B	308	ARG
2	B	316	LEU
2	B	317	SER
2	B	332	THR
2	B	337	GLN
2	B	342	LEU
2	B	344	SER
2	B	347	ARG
2	B	348	GLN
2	B	349	ILE
2	B	350	GLN
2	B	351	ASN
2	B	352	ILE
2	B	370	TYR

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Mol	Chain	Res	Type
2	B	375	VAL
2	B	376	ILE
2	B	382	ARG
2	B	385	THR
2	B	390	LEU
2	B	414	VAL
2	B	420	PHE
2	B	422	VAL
2	B	432	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	380	GLN
1	A	402	ASN
1	A	422	HIS
1	A	438	GLN
1	A	460	GLN
1	A	484	HIS
1	A	509	GLN
1	A	535	ASN
1	A	564	HIS
2	B	337	GLN
2	B	348	GLN
2	B	350	GLN
2	B	423	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 carbohydrates in this entry.

5.6 Ligand geometry

2 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	900	4	51,58,58	2.85	11 (21%)	60,89,89	2.47	18 (30%)
4	TCF	A	901	3	11,11,12	0.83	0	13,13,15	2.11	4 (30%)

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	900	4	-	4/30/50/50	0/6/6/6
4	TCF	A	901	3	-	1/3/4/5	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C4X-N5	9.35	1.46	1.33
3	A	900	FAD	C2A-N3A	9.10	1.46	1.32
3	A	900	FAD	C4X-C10	8.79	1.47	1.38
3	A	900	FAD	C2A-N1A	8.24	1.49	1.33
3	A	900	FAD	C9A-N10	4.85	1.45	1.38
3	A	900	FAD	O4-C4	4.27	1.35	1.24
3	A	900	FAD	C5X-N5	3.61	1.41	1.35
3	A	900	FAD	C4-C4X	2.79	1.46	1.41
3	A	900	FAD	C10-N1	2.62	1.36	1.33
3	A	900	FAD	C2B-C1B	-2.18	1.50	1.53
3	A	900	FAD	C5'-C4'	2.05	1.54	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAD	N3A-C2A-N1A	-9.14	114.40	128.68
3	A	900	FAD	C4-N3-C2	7.84	121.77	115.14
3	A	900	FAD	C9A-N10-C10	-5.91	114.17	121.91
3	A	900	FAD	C4-C4X-C10	-5.34	116.42	119.95
3	A	900	FAD	C5X-C9A-N10	5.20	121.48	117.72
4	A	901	TCF	BR-CB4-CB3	4.56	125.93	119.30
3	A	900	FAD	C4X-C10-N10	-3.92	116.27	120.30
3	A	900	FAD	C4X-C4-N3	-3.23	119.02	123.43
3	A	900	FAD	C1'-N10-C10	-3.02	115.70	118.41
3	A	900	FAD	C6-C5X-N5	-3.00	115.74	119.05
3	A	900	FAD	P-O3P-PA	-2.97	122.65	132.83
4	A	901	TCF	C3B-CB1-CB6	-2.92	113.84	121.23
3	A	900	FAD	O4B-C1B-C2B	-2.82	102.80	106.93
3	A	900	FAD	C1B-N9A-C4A	-2.77	121.77	126.64
4	A	901	TCF	BR-CB4-CB5	-2.66	115.43	119.30
3	A	900	FAD	C4X-N5-C5X	-2.60	114.17	116.77
3	A	900	FAD	O5'-C5'-C4'	2.42	115.83	109.36
4	A	901	TCF	C3B-CB1-CB2	2.41	127.32	121.23
3	A	900	FAD	C4-C4X-N5	-2.37	115.89	118.60
3	A	900	FAD	O2A-PA-O1A	2.23	123.25	112.24
3	A	900	FAD	C2A-N1A-C6A	2.18	122.48	118.75
3	A	900	FAD	C9-C9A-C5X	-2.17	116.17	119.88

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	FAD	C2'-C1'-N10-C10
3	A	900	FAD	PA-O3P-P-O5'
4	A	901	TCF	C1B-C2B-C3B-CB1
3	A	900	FAD	O4B-C4B-C5B-O5B
3	A	900	FAD	P-O3P-PA-O2A

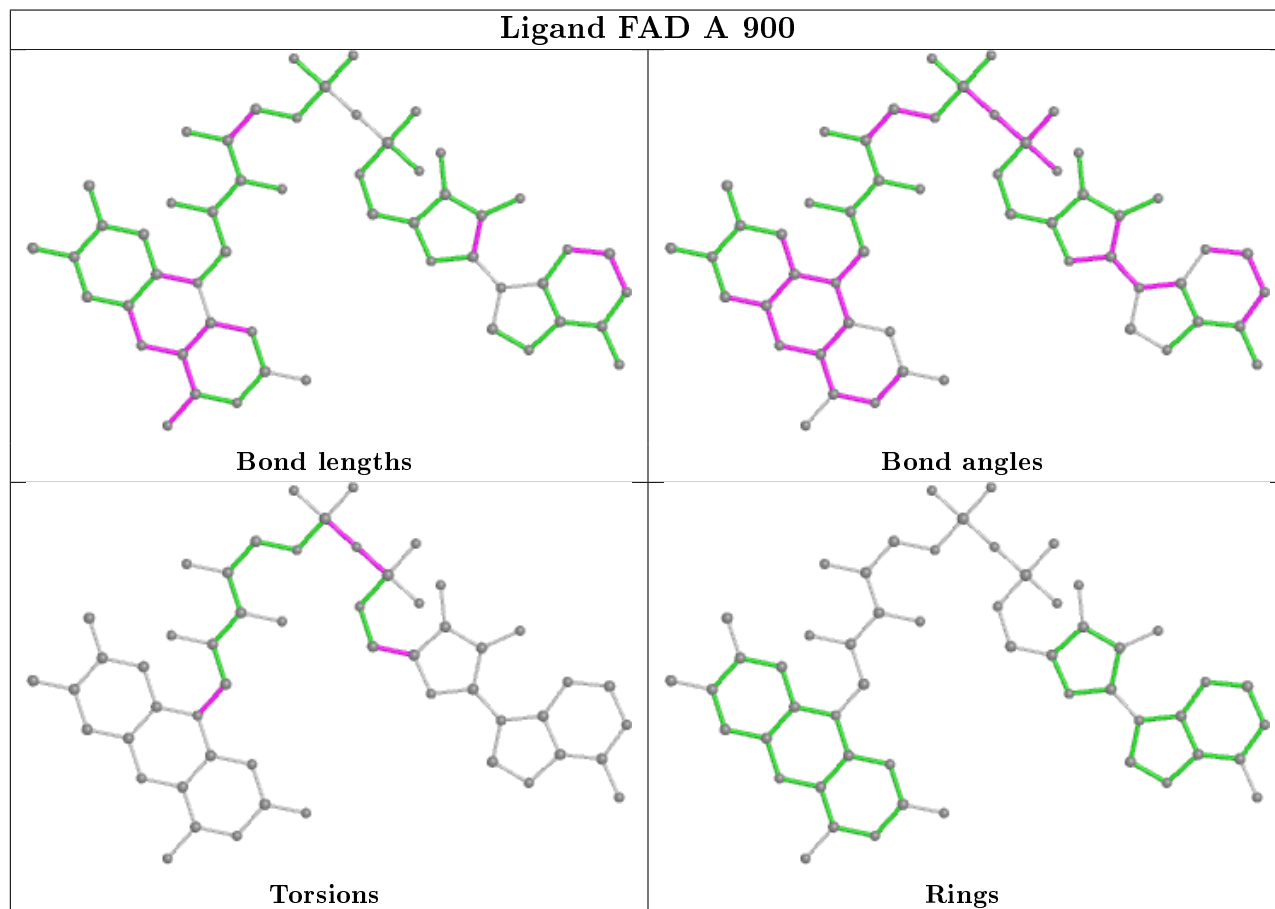
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAD	3	0
4	A	901	TCF	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	666/852 (78%)	-0.40	1 (0%) 95 95	28, 62, 91, 105	0
2	B	133/482 (27%)	-0.12	4 (3%) 50 48	64, 93, 108, 115	0
All	All	799/1334 (59%)	-0.35	5 (0%) 89 89	28, 67, 98, 115	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	3.4
2	B	376	ILE	3.2
2	B	374	GLU	2.8
2	B	308	ARG	2.5
2	B	378	LYS	2.4

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](#)

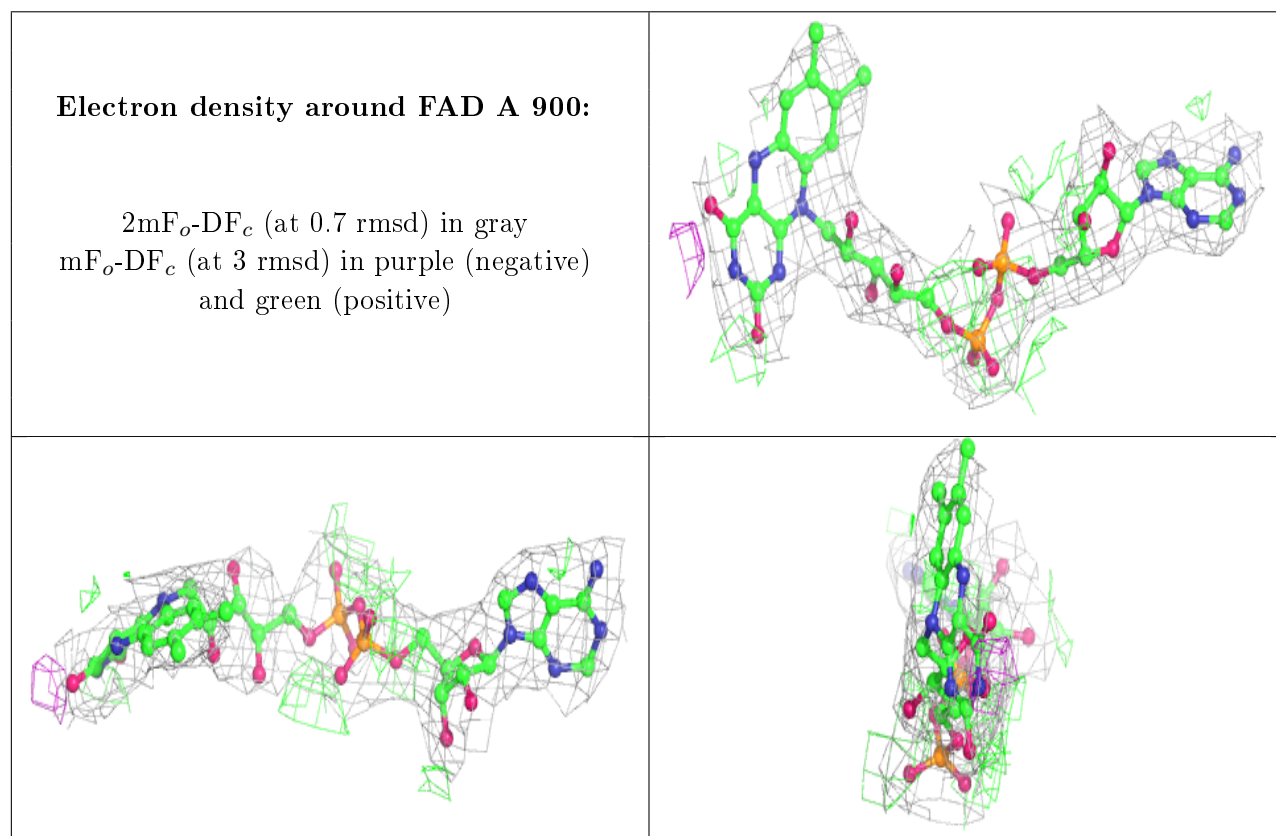
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	TCF	A	901	11/12	0.95	0.17	57,64,72,80	0
3	FAD	A	900	53/53	0.98	0.20	28,41,58,59	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.