



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:12 PM UTC

PDB ID : 2XAG / pdb_00002xag
Title : Crystal structure of LSD1-CoREST in complex with para-bromo-(-)-trans- 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 : 3.10 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

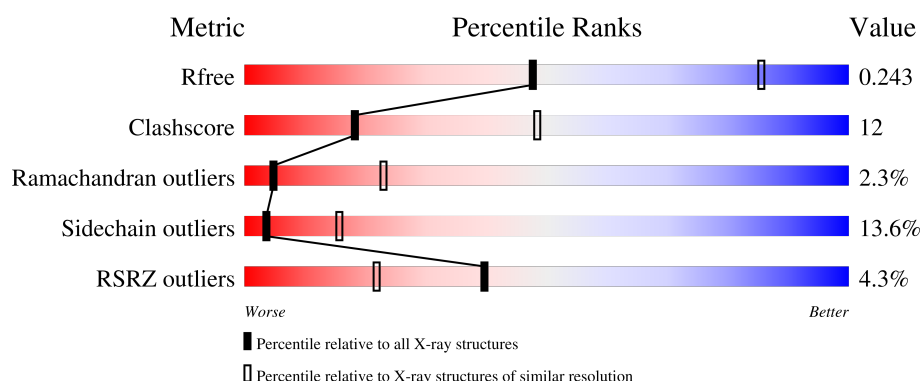
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

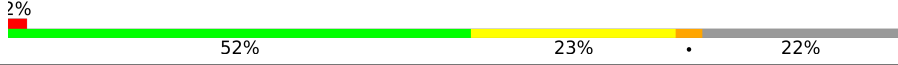
The reported resolution of this entry is 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	852	
2	B	482	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TCF	A	901	-	-	X	-

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.

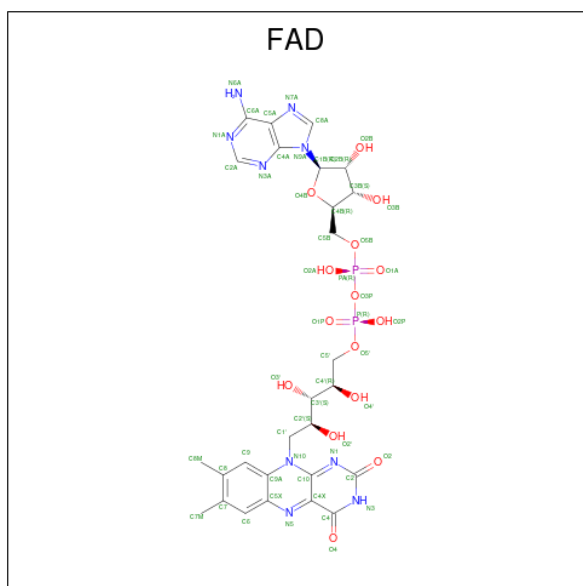
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5217	3324	906	967	20			

- Molecule 2 is a protein called REST COREPRESSOR 1.

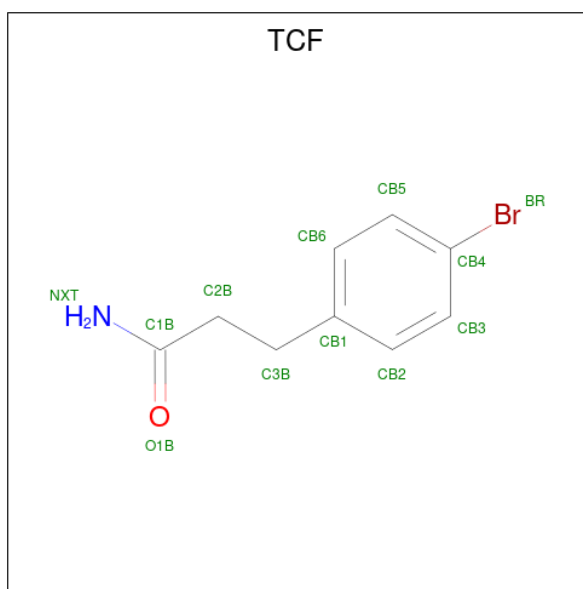
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

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



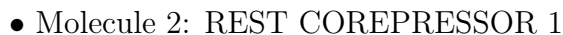
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 3-(4-BROMOPHENYL)PROPANAMIDE (CCD ID: TCF) (formula: $C_9H_{10}BrNO$).



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

- Molecule 1: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	116.47Å 178.03Å 236.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.96 – 3.10 71.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (71.96-3.10) 95.0 (71.96-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.209 , 0.245 0.209 , 0.243	Depositor DCC
R_{free} test set	808 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å ²)	77.2	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6357	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, TCF

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	0.83	0/5331	1.06	11/7232 (0.2%)
2	B	0.71	0/1091	0.92	2/1471 (0.1%)
All	All	0.81	0/6422	1.04	13/8703 (0.1%)

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	791	GLN	CA-C-N	-8.67	111.71	120.98
1	A	791	GLN	C-N-CA	-8.67	111.71	120.98
1	A	542	THR	N-CA-C	8.45	115.73	108.13
1	A	700	ALA	CA-C-N	6.65	128.15	119.84
1	A	700	ALA	C-N-CA	6.65	128.15	119.84
1	A	770	GLY	N-CA-C	-6.19	107.86	114.67
1	A	834	TYR	N-CA-C	5.83	119.86	112.87
2	B	372	LEU	CA-C-N	5.72	126.99	119.84
2	B	372	LEU	C-N-CA	5.72	126.99	119.84
1	A	634	PRO	CA-C-N	5.37	125.38	119.90
1	A	634	PRO	C-N-CA	5.37	125.38	119.90
1	A	172	SER	N-CA-C	5.15	116.64	108.96
1	A	556	ASP	N-CA-C	5.06	116.61	111.14

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 ⓘ

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	133	0
2	B	1076	0	1091	30	0
3	A	53	0	31	5	0
4	A	11	0	8	7	0
All	All	6357	0	6382	154	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 12.

All (154) 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:566:THR:HG21	1:A:697:LEU:HD22	1.32	1.07
3:A:900:FAD:C4X	4:A:901:TCF:H3B1	1.85	1.06
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.99	0.78
1:A:693:LEU:HD12	1:A:694:PHE:N	2.00	0.77
3:A:900:FAD:C10	4:A:901:TCF:H3B1	2.15	0.76
1:A:448:MET:HE2	2:B:363:LEU:HD13	1.68	0.75
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.68	0.74
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.70	0.73
3:A:900:FAD:C4X	4:A:901:TCF:C3B	2.64	0.72
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.15	0.72
2:B:421:PHE:O	2:B:425:ARG:HB2	1.88	0.72
1:A:435:VAL:HG13	2:B:349:ILE:HG13	1.73	0.70
1:A:677:LEU:HD23	1:A:677:LEU:N	2.08	0.68
1:A:227:ILE:HG22	1:A:268:LYS:HB3	1.79	0.65
1:A:374:LYS:HE3	1:A:525:ASP:OD1	1.97	0.64
1:A:437:THR:CG2	1:A:508:LEU:HD21	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.28	0.63
1:A:263:ASN:C	1:A:267:TYR:HE1	2.07	0.62
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.36	0.61
1:A:548:SER:HB2	1:A:766:ALA:HA	1.82	0.61
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.31	0.61
1:A:693:LEU:HD12	1:A:694:PHE:H	1.66	0.60
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.32	0.60
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.82	0.60
1:A:448:MET:HE2	2:B:363:LEU:CD1	2.32	0.60
1:A:263:ASN:C	1:A:267:TYR:CE1	2.81	0.58
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.85	0.58
1:A:553:ASP:O	1:A:556:ASP:HB2	2.02	0.58
1:A:384:ARG:HB3	2:B:314:MET:HE3	1.86	0.57
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.05	0.57
1:A:588:THR:HG22	1:A:604:ALA:HB1	1.86	0.57
1:A:437:THR:HG22	1:A:508:LEU:HD21	1.86	0.57
1:A:379:GLU:O	1:A:382:PHE:HB3	2.05	0.56
2:B:425:ARG:HA	2:B:430:ILE:HG13	1.87	0.56
1:A:478:PHE:O	1:A:482:SER:HB3	2.04	0.56
1:A:188:MET:SD	1:A:200:ILE:HG13	2.46	0.56
1:A:671:TRP:O	1:A:673:PRO:HD3	2.06	0.55
1:A:188:MET:HE3	1:A:210:PHE:CE2	2.41	0.55
1:A:707:VAL:CG1	1:A:712:ALA:HA	2.36	0.54
1:A:548:SER:O	1:A:552:TRP:HB3	2.07	0.54
2:B:317:SER:O	2:B:321:VAL:HG23	2.07	0.54
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.43	0.54
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.90	0.53
1:A:385:LEU:O	1:A:388:ALA:HB3	2.08	0.53
1:A:773:TYR:CE1	1:A:808:PRO:HB3	2.43	0.53
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.09	0.53
1:A:172:SER:HA	1:A:176:GLY:HA3	1.91	0.52
1:A:588:THR:HG22	1:A:604:ALA:CB	2.39	0.52
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.91	0.52
1:A:374:LYS:O	1:A:378:VAL:HG23	2.10	0.52
2:B:384:THR:O	2:B:388:GLN:HG3	2.10	0.51
1:A:473:ASP:OD1	1:A:473:ASP:C	2.54	0.51
2:B:347:ARG:HG3	2:B:348:GLN:N	2.26	0.51
1:A:677:LEU:N	1:A:677:LEU:CD2	2.73	0.51
2:B:361:GLU:O	2:B:364:ASP:HB2	2.12	0.51
2:B:377:GLN:OE1	2:B:411:ASN:HB3	2.11	0.51
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLU:HA	1:A:453:GLU:OE1	2.11	0.50
1:A:203:PRO:C	1:A:205:GLN:N	2.70	0.50
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.47	0.49
1:A:677:LEU:HD23	1:A:677:LEU:H	1.76	0.49
1:A:563:SER:O	1:A:565:LEU:HD12	2.12	0.49
1:A:335:THR:HG21	4:A:901:TCF:HB3	1.95	0.49
1:A:797:PHE:CG	1:A:825:ILE:HD11	2.48	0.49
2:B:362:LYS:C	2:B:364:ASP:H	2.20	0.49
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.95	0.49
1:A:465:ALA:CB	1:A:479:LEU:HD23	2.43	0.49
1:A:280:LYS:O	1:A:618:CYS:HB2	2.13	0.49
1:A:664:LEU:HD23	1:A:746:THR:HG22	1.95	0.48
2:B:380:ASN:O	2:B:416:GLN:NE2	2.46	0.48
1:A:707:VAL:HG12	1:A:712:ALA:CA	2.41	0.48
1:A:485:ARG:O	1:A:487:LEU:N	2.46	0.48
1:A:541:ALA:O	1:A:657:GLY:HA3	2.14	0.48
1:A:543:PRO:C	1:A:545:SER:H	2.22	0.48
1:A:695:TRP:HE1	1:A:706:LEU:HD22	1.79	0.48
1:A:542:THR:OG1	1:A:543:PRO:HD2	2.13	0.47
1:A:485:ARG:O	1:A:486:ASP:C	2.57	0.47
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.80	0.47
1:A:776:MET:HE2	1:A:802:HIS:HD2	1.79	0.47
1:A:807:TYR:N	1:A:808:PRO:CD	2.78	0.47
2:B:350:GLN:HE21	2:B:350:GLN:HB3	1.51	0.47
1:A:203:PRO:C	1:A:205:GLN:H	2.22	0.46
1:A:594:ARG:CZ	1:A:640:VAL:HG11	2.45	0.46
1:A:306:LEU:HD13	1:A:584:ILE:HG12	1.98	0.46
1:A:572:SER:O	1:A:573:CYS:C	2.58	0.46
2:B:310:PRO:O	2:B:311:PRO:C	2.59	0.46
1:A:554:GLN:C	1:A:556:ASP:H	2.24	0.46
1:A:179:PHE:C	1:A:181:SER:H	2.23	0.46
1:A:521:LEU:HB3	1:A:525:ASP:HB2	1.98	0.46
2:B:417:VAL:O	2:B:420:PHE:HB3	2.16	0.46
1:A:656:PHE:CE2	1:A:759:GLY:HA3	2.51	0.45
1:A:366:ASN:OD1	1:A:368:GLN:N	2.48	0.45
1:A:451:LEU:HD12	1:A:451:LEU:HA	1.64	0.45
1:A:667:ASP:OD1	1:A:667:ASP:N	2.44	0.45
1:A:725:GLY:C	1:A:727:CYS:N	2.75	0.45
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.81	0.44
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.75	0.44
1:A:384:ARG:NH2	2:B:312:LYS:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LEU:HB2	1:A:693:LEU:HD11	1.99	0.44
1:A:801:GLU:HG3	3:A:900:FAD:O3'	2.18	0.44
1:A:374:LYS:CE	1:A:525:ASP:OD1	2.65	0.44
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.99	0.44
1:A:266:ILE:O	1:A:266:ILE:HG22	2.17	0.44
1:A:601:GLU:OE1	1:A:617:LYS:HE3	2.18	0.44
1:A:773:TYR:HE1	1:A:808:PRO:HB3	1.82	0.43
1:A:533:PHE:O	1:A:537:GLU:CG	2.66	0.43
2:B:418:LYS:O	2:B:421:PHE:HB2	2.18	0.43
1:A:568:ARG:HH11	1:A:568:ARG:HG2	1.84	0.43
1:A:728:LEU:HD21	1:A:743:PRO:HG3	1.99	0.43
1:A:801:GLU:CG	1:A:809:ALA:HA	2.48	0.43
1:A:693:LEU:HD12	1:A:693:LEU:C	2.43	0.43
1:A:230:THR:OG1	1:A:232:GLU:HB2	2.18	0.43
1:A:340:ASN:OD1	1:A:342:MET:HG2	2.18	0.43
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.91	0.43
2:B:394:ALA:O	2:B:398:TYR:N	2.51	0.43
2:B:414:VAL:O	2:B:418:LYS:HG3	2.19	0.43
1:A:235:LEU:O	1:A:236:GLN:C	2.61	0.43
1:A:465:ALA:HB1	1:A:479:LEU:HD23	2.01	0.42
1:A:410:GLN:HE21	1:A:410:GLN:HB3	1.72	0.42
1:A:282:ILE:HG21	1:A:602:VAL:HG21	2.02	0.42
1:A:374:LYS:O	1:A:375:ASP:C	2.61	0.42
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.34	0.42
1:A:537:GLU:OE2	1:A:544:LEU:N	2.50	0.42
1:A:297:LEU:HD21	1:A:822:ALA:HA	2.00	0.42
2:B:428:PHE:O	2:B:429:ASN:C	2.63	0.42
1:A:434:ILE:O	1:A:435:VAL:C	2.61	0.42
1:A:537:GLU:OE2	1:A:543:PRO:HA	2.19	0.42
1:A:761:TYR:CZ	4:A:901:TCF:H3B2	2.54	0.42
1:A:386:LEU:O	1:A:389:THR:OG1	2.29	0.42
1:A:469:LYS:HA	1:A:470:PRO:HD3	1.90	0.42
1:A:647:LYS:HB2	1:A:647:LYS:HE2	1.87	0.42
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.55	0.42
1:A:640:VAL:O	1:A:640:VAL:HG12	2.19	0.42
1:A:543:PRO:C	1:A:545:SER:N	2.76	0.41
1:A:172:SER:HA	1:A:176:GLY:CA	2.50	0.41
1:A:317:VAL:HG13	1:A:571:TYR:HB3	2.02	0.41
1:A:182:ARG:NH1	1:A:341:PRO:HD3	2.36	0.41
1:A:826:ALA:O	1:A:827:ASP:C	2.60	0.41
1:A:761:TYR:CE2	4:A:901:TCF:H3B2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:LEU:O	1:A:512:GLU:HB2	2.21	0.41
1:A:495:ASP:OD1	2:B:371:ARG:NH2	2.54	0.41
1:A:276:LYS:HB2	1:A:276:LYS:HE3	1.86	0.41
1:A:331:ALA:HA	3:A:900:FAD:N5	2.36	0.41
1:A:725:GLY:O	1:A:726:ARG:C	2.64	0.41
1:A:188:MET:HE3	1:A:210:PHE:CD2	2.56	0.40
1:A:280:LYS:N	1:A:619:ASP:OD2	2.51	0.40
1:A:335:THR:CG2	4:A:901:TCF:HB3	2.50	0.40
1:A:533:PHE:O	1:A:537:GLU:HG2	2.21	0.40
1:A:613:THR:HG22	1:A:614:PHE:N	2.36	0.40
1:A:665:CYS:HB2	1:A:745:GLU:HB2	2.03	0.40
1:A:707:VAL:O	1:A:712:ALA:HB2	2.20	0.40
1:A:245:ASP:OD1	1:A:247:VAL:HG23	2.21	0.40
1:A:456:LYS:HA	2:B:370:TYR:CD1	2.57	0.40
2:B:340:MET:C	2:B:342:LEU:N	2.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	664/852 (78%)	573 (86%)	77 (12%)	14 (2%)	5	25
2	B	131/482 (27%)	104 (79%)	23 (18%)	4 (3%)	3	18
All	All	795/1334 (60%)	677 (85%)	100 (13%)	18 (2%)	5	23

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	VAL
1	A	486	ASP
1	A	428	ILE

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Mol	Chain	Res	Type
1	A	287	GLY
1	A	402	ASN
1	A	555	ASP
1	A	608	ARG
2	B	314	MET
2	B	373	PRO
2	B	425	ARG
1	A	204	GLN
1	A	274	PRO
1	A	429	GLU
1	A	232	GLU
1	A	552	TRP
1	A	801	GLU
2	B	312	LYS
1	A	507	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/699 (81%)	494 (87%)	72 (13%)	4	18
2	B	117/395 (30%)	96 (82%)	21 (18%)	2	9
All	All	683/1094 (62%)	590 (86%)	93 (14%)	3	16

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	SER
1	A	191	GLN
1	A	205	GLN
1	A	206	THR
1	A	226	LYS
1	A	238	LEU
1	A	247	VAL
1	A	268	LYS

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Mol	Chain	Res	Type
1	A	277	LYS
1	A	278	THR
1	A	281	VAL
1	A	288	VAL
1	A	304	VAL
1	A	329	LEU
1	A	355	LYS
1	A	372	LYS
1	A	402	ASN
1	A	413	GLU
1	A	417	GLN
1	A	429	GLU
1	A	432	LYS
1	A	433	LYS
1	A	436	LYS
1	A	438	GLN
1	A	439	GLU
1	A	449	VAL
1	A	453	GLU
1	A	454	LYS
1	A	457	GLU
1	A	466	SER
1	A	469	LYS
1	A	472	ARG
1	A	479	LEU
1	A	482	SER
1	A	487	LEU
1	A	492	LYS
1	A	499	GLU
1	A	506	GLU
1	A	512	GLU
1	A	514	ASN
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	568	ARG
1	A	580	GLU
1	A	594	ARG
1	A	607	THR

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Mol	Chain	Res	Type
1	A	609	SER
1	A	632	GLN
1	A	633	GLN
1	A	638	GLN
1	A	640	VAL
1	A	645	GLU
1	A	652	GLN
1	A	669	VAL
1	A	675	VAL
1	A	677	LEU
1	A	684	THR
1	A	699	LYS
1	A	706	LEU
1	A	714	ILE
1	A	727	CYS
1	A	737	SER
1	A	791	GLN
1	A	815	LEU
1	A	821	GLU
1	A	825	ILE
1	A	833	MET
1	A	836	LEU
2	B	308	ARG
2	B	316	LEU
2	B	319	GLU
2	B	333	THR
2	B	337	GLN
2	B	345	VAL
2	B	349	ILE
2	B	350	GLN
2	B	375	VAL
2	B	376	ILE
2	B	379	CYS
2	B	382	ARG
2	B	385	THR
2	B	392	VAL
2	B	414	VAL
2	B	415	VAL
2	B	422	VAL
2	B	423	ASN
2	B	425	ARG
2	B	426	ARG

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Mol	Chain	Res	Type
2	B	432	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	GLN
1	A	395	GLN
1	A	410	GLN
1	A	427	GLN
1	A	430	HIS
1	A	438	GLN
1	A	540	ASN
1	A	632	GLN
2	B	318	GLN
2	B	348	GLN
2	B	350	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	58,58,58	2.37	12 (20%)	85,89,89	1.96	21 (24%)
4	TCF	A	901	3	10,11,12	0.75	0	13,13,15	1.19	1 (7%)

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	-	3/34/50/50	0/5/6/6
4	TCF	A	901	3	-	2/4/4/5	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C2A-N1A	8.06	1.48	1.33
3	A	900	FAD	C4X-N5	7.82	1.47	1.30
3	A	900	FAD	O4-C4	6.87	1.36	1.23
3	A	900	FAD	C2A-N3A	6.61	1.45	1.33
3	A	900	FAD	O2-C2	6.01	1.36	1.24
3	A	900	FAD	C5'-C4'	2.86	1.55	1.51
3	A	900	FAD	C9A-N10	2.66	1.45	1.41
3	A	900	FAD	C5A-N7A	-2.46	1.34	1.39
3	A	900	FAD	C10-N10	2.33	1.42	1.37
3	A	900	FAD	C8A-N7A	2.23	1.36	1.31
3	A	900	FAD	PA-O3P	2.09	1.61	1.59
3	A	900	FAD	P-O3P	2.08	1.61	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAD	N3A-C2A-N1A	-9.75	113.82	128.58
3	A	900	FAD	C9A-N10-C10	-4.30	114.19	120.75
3	A	900	FAD	C2A-N3A-C4A	3.71	120.90	111.83
3	A	900	FAD	C5X-C9A-N10	3.59	121.21	117.97
3	A	900	FAD	N9A-C8A-N7A	-3.42	109.09	113.94
3	A	900	FAD	C5A-C4A-N3A	-3.41	122.02	126.72
3	A	900	FAD	C1'-N10-C9A	-2.64	115.50	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAD	O4-C4-C4X	-2.63	119.60	126.53
3	A	900	FAD	C4A-N9A-C8A	2.59	108.45	105.74
3	A	900	FAD	C4X-C10-N1	-2.55	118.35	124.59
3	A	900	FAD	O2A-PA-O1A	2.49	124.03	112.44
3	A	900	FAD	O3P-P-O1P	-2.44	103.37	110.70
3	A	900	FAD	N3A-C4A-N9A	2.43	131.30	127.17
3	A	900	FAD	C6A-C5A-C4A	2.29	120.31	117.18
3	A	900	FAD	C2A-N1A-C6A	2.28	122.47	118.73
3	A	900	FAD	C2'-C1'-N10	2.27	120.93	110.20
3	A	900	FAD	C5X-N5-C4X	-2.24	114.46	118.09
3	A	900	FAD	C5A-C6A-N6A	-2.22	117.78	123.29
3	A	900	FAD	C5A-N7A-C8A	2.11	106.77	103.45
4	A	901	TCF	C3B-CB1-CB6	-2.05	115.95	121.18
3	A	900	FAD	C5'-C4'-C3'	-2.01	108.42	112.22
3	A	900	FAD	O4B-C1B-C2B	-2.01	102.31	106.62

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	TCF	C1B-C2B-C3B-CB1
3	A	900	FAD	C2'-C1'-N10-C10
4	A	901	TCF	C2B-C3B-CB1-CB6
3	A	900	FAD	P-O3P-PA-O2A
3	A	900	FAD	O4B-C4B-C5B-O5B

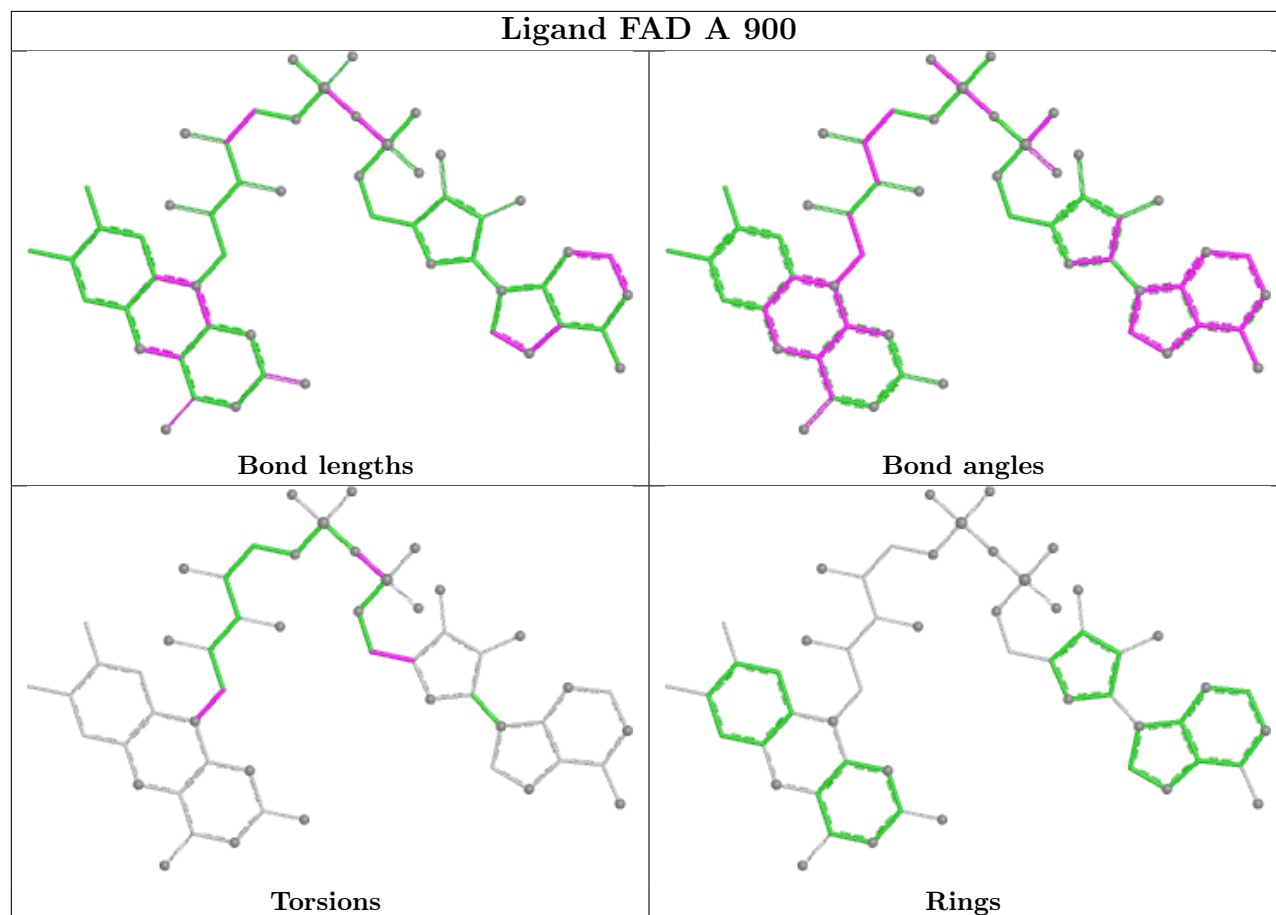
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAD	5	0
4	A	901	TCF	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	666/852 (78%)	-0.02	18 (2%) 56 35	34, 63, 92, 104	0
2	B	133/482 (27%)	0.74	16 (12%) 9 5	66, 93, 107, 113	0
All	All	799/1334 (59%)	0.11	34 (4%) 40 22	34, 67, 99, 113	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	MET	6.2
1	A	836	LEU	5.6
1	A	373	GLU	5.1
2	B	376	ILE	4.2
1	A	509	GLN	4.0
2	B	375	VAL	3.5
2	B	308	ARG	3.4
1	A	833	MET	3.3
2	B	374	GLU	3.3
2	B	348	GLN	3.1
1	A	275	THR	3.0
1	A	355	LYS	2.7
1	A	369	ALA	2.7
1	A	239	GLU	2.7
2	B	379	CYS	2.6
1	A	171	PRO	2.6
1	A	403	ASN	2.6
2	B	337	GLN	2.6
1	A	205	GLN	2.5
1	A	652	GLN	2.4
1	A	236	GLN	2.4
1	A	380	GLN	2.4
2	B	332	THR	2.4
2	B	414	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	453	GLU	2.3
1	A	492	LYS	2.3
2	B	426	ARG	2.3
2	B	315	PHE	2.2
2	B	328	ALA	2.2
2	B	329	THR	2.1
2	B	361	GLU	2.1
2	B	362	LYS	2.1
2	B	331	ALA	2.1
1	A	791	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

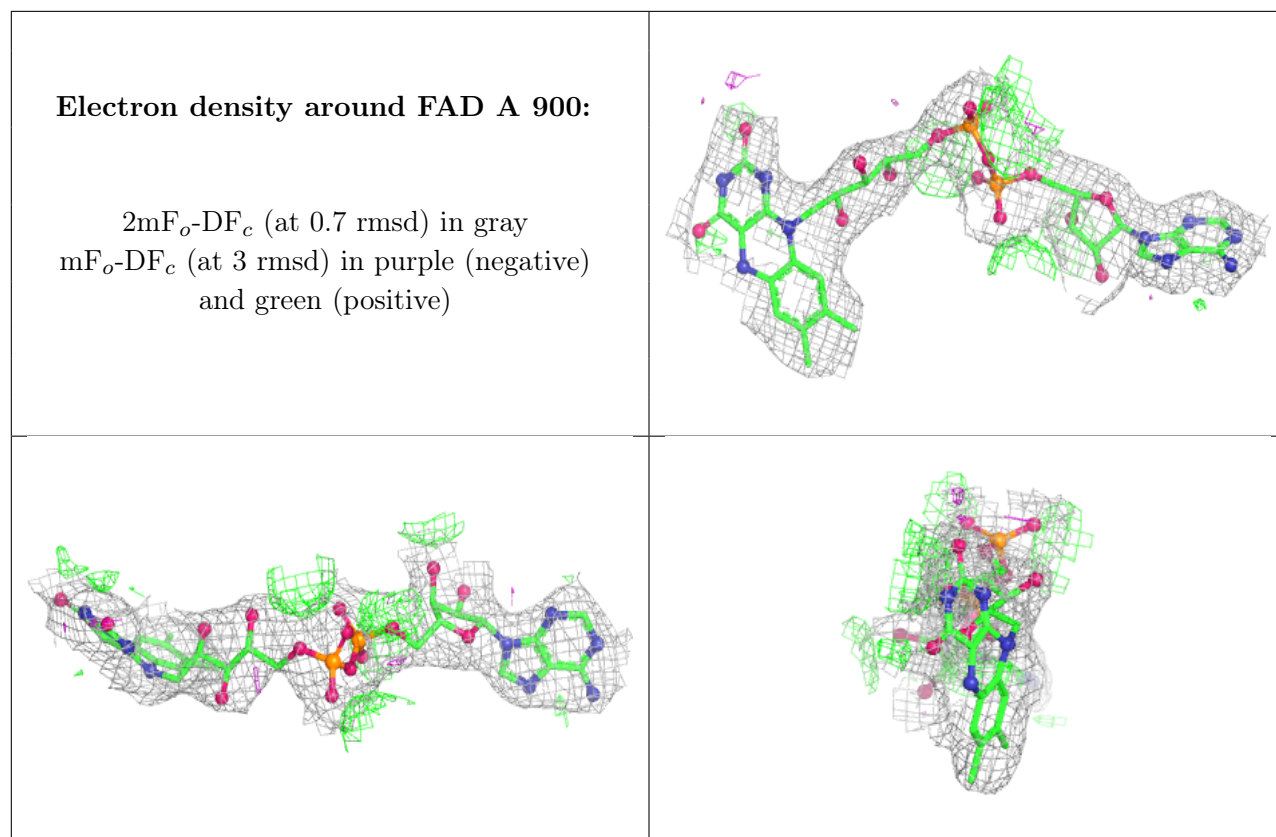
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	TCF	A	901	11/12	0.94	0.15	64,75,82,90	0
3	FAD	A	900	53/53	0.98	0.07	32,40,62,63	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.