



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:09 AM UTC

PDB ID : 2XAH / pdb_00002xah
Title : Crystal structure of LSD1-CoREST in complex with (+)-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)
Xtriage (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

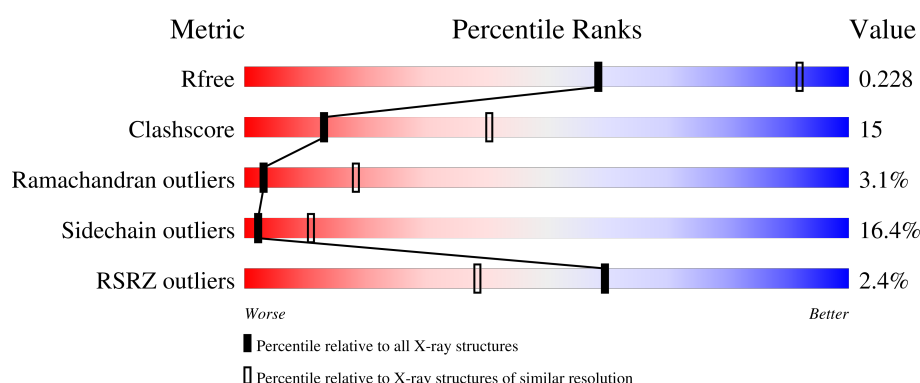
1 Overall quality at a glance

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	47% 25% 6% 22%
2	B	482	2% 17% 9% • 72%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6356 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.

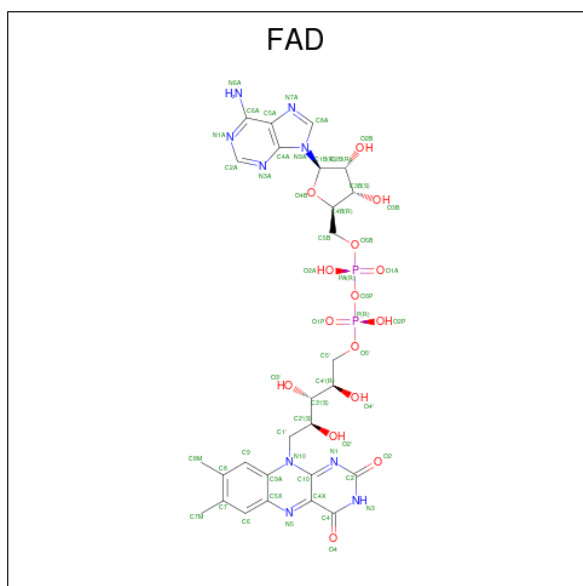
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

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.

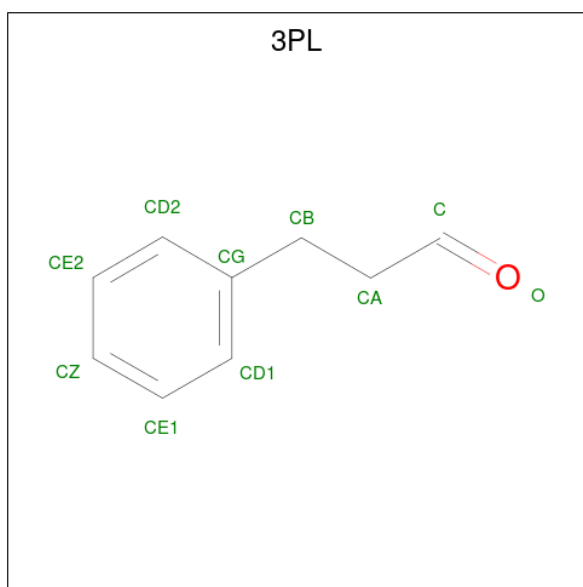
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

- 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-PHENYLPROPANAL (CCD ID: 3PL) (formula: $C_9H_{10}O$).

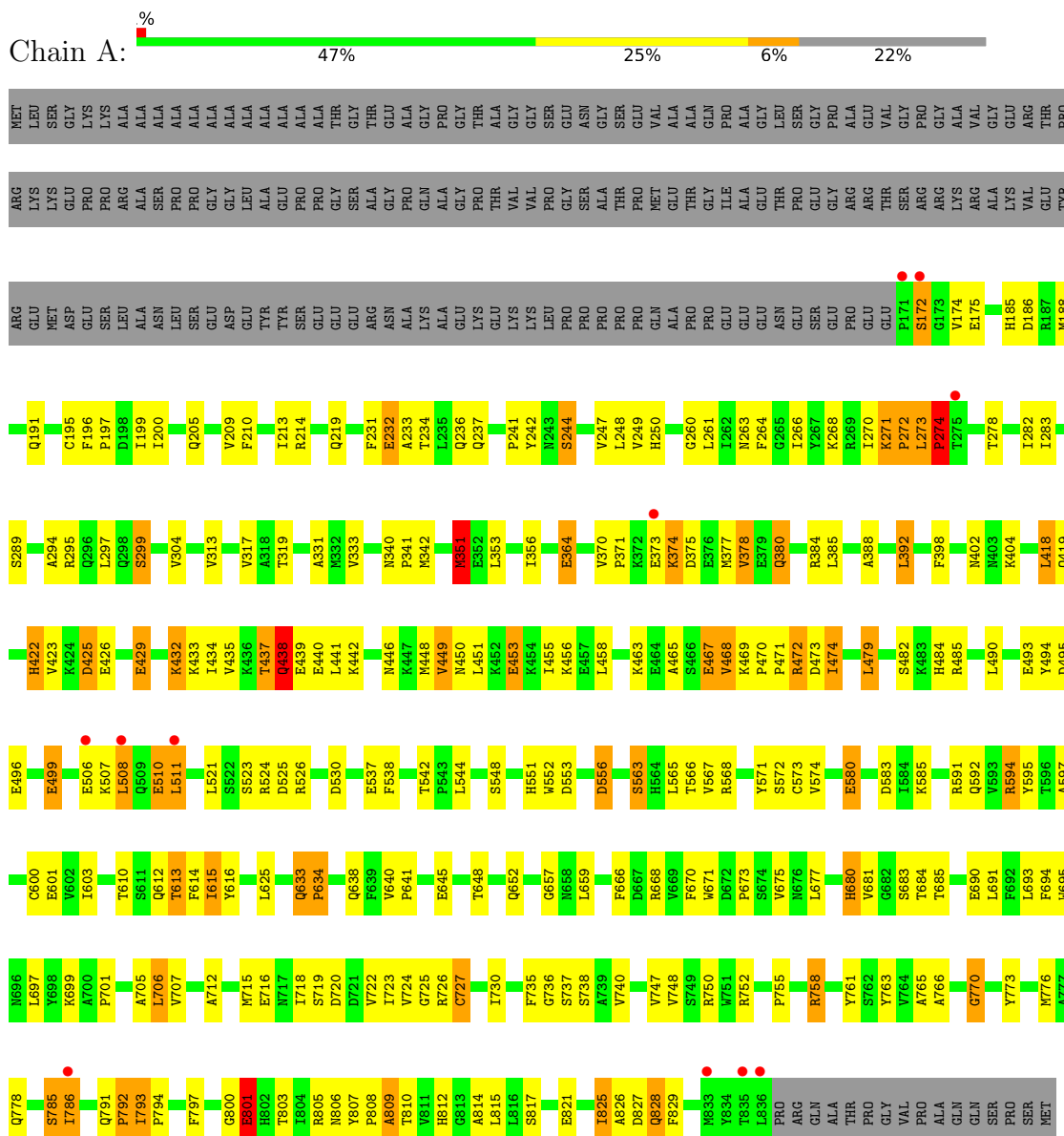


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	10	9	1	0	0

3 Residue-property plots

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 1



• 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, α , β , γ	119.96Å 181.50Å 234.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.75 – 3.10 90.75 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (90.75-3.10) 99.9 (90.75-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.208 , 0.228 0.206 , 0.228	Depositor DCC
R_{free} test set	900 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6356	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: 3PL, 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	0.84	0/5331	1.11	17/7232 (0.2%)
2	B	0.69	0/1091	0.96	4/1471 (0.3%)
All	All	0.82	0/6422	1.09	21/8703 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	634	PRO	CA-C-N	8.81	128.88	119.90
1	A	634	PRO	C-N-CA	8.81	128.88	119.90
1	A	793	ILE	CA-C-N	8.35	128.11	119.76
1	A	793	ILE	C-N-CA	8.35	128.11	119.76
1	A	172	SER	N-CA-C	7.69	118.76	108.38
1	A	770	GLY	N-CA-C	-7.35	105.54	114.66
1	A	440	GLU	N-CA-C	-6.93	103.81	111.36
1	A	613	THR	N-CA-C	6.36	120.42	110.32
1	A	625	LEU	CA-C-N	6.08	126.10	119.89
1	A	625	LEU	C-N-CA	6.08	126.10	119.89
2	B	377	GLN	N-CA-C	5.85	119.01	109.24
1	A	351	MET	N-CA-C	-5.76	101.17	110.32
1	A	705	ALA	N-CA-C	5.43	117.27	108.41
1	A	199	ILE	N-CA-C	5.24	115.45	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	542	THR	CA-C-N	5.21	126.36	119.84
1	A	542	THR	C-N-CA	5.21	126.36	119.84
2	B	372	LEU	CA-C-N	5.17	126.30	119.84
2	B	372	LEU	C-N-CA	5.17	126.30	119.84
1	A	474	ILE	N-CA-C	5.14	117.47	111.05
1	A	809	ALA	N-CA-C	5.06	118.58	111.90
2	B	314	MET	N-CA-C	-5.06	101.16	109.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	PRO	Peptide
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	173	0
2	B	1076	0	1091	31	0
3	A	53	0	31	2	0
4	A	10	0	9	2	0
All	All	6356	0	6383	190	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 15.

All (190) 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:794:PRO:HD2	1:A:828:GLN:HE22	1.11	1.10
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.15	1.07
1:A:755:PRO:HA	1:A:758:ARG:NH1	1.69	1.07
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.39	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.20	0.99
1:A:758:ARG:HG2	1:A:758:ARG:HH11	1.25	0.97
1:A:794:PRO:HD2	1:A:828:GLN:NE2	1.80	0.95
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.07	0.90
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.11	0.86
1:A:494:TYR:CD2	1:A:494:TYR:O	2.31	0.84
1:A:671:TRP:O	1:A:673:PRO:HD3	1.80	0.81
1:A:716:GLU:HG2	1:A:750:ARG:HG2	1.62	0.81
1:A:437:THR:HG22	1:A:508:LEU:HD12	1.62	0.80
1:A:209:VAL:O	1:A:213:ILE:HG13	1.81	0.79
1:A:453:GLU:HA	1:A:453:GLU:OE1	1.83	0.78
1:A:392:LEU:HD23	1:A:398:PHE:HB3	1.64	0.78
2:B:317:SER:O	2:B:321:VAL:HG23	1.83	0.76
1:A:758:ARG:NH1	1:A:758:ARG:HG2	1.95	0.74
1:A:384:ARG:NH2	2:B:312:LYS:O	2.20	0.74
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.70	0.71
1:A:690:GLU:HG2	1:A:691:LEU:HD12	1.73	0.69
1:A:260:GLY:O	1:A:264:PHE:CD2	2.47	0.68
1:A:188:MET:HE3	1:A:210:PHE:CE2	2.29	0.67
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.75	0.67
1:A:755:PRO:CA	1:A:758:ARG:HH12	2.01	0.66
1:A:506:GLU:C	1:A:508:LEU:H	2.04	0.66
1:A:794:PRO:CD	1:A:828:GLN:HE22	2.00	0.65
1:A:761:TYR:CE2	4:A:901:3PL:HA2	2.31	0.64
1:A:437:THR:CG2	1:A:508:LEU:HD12	2.28	0.64
1:A:463:LYS:O	1:A:467:GLU:HG2	1.98	0.64
1:A:435:VAL:HG12	2:B:349:ILE:HG13	1.80	0.64
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.80	0.63
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.34	0.63
1:A:241:PRO:O	1:A:244:SER:HB3	1.99	0.63
1:A:392:LEU:CD2	1:A:398:PHE:HB3	2.29	0.63
1:A:666:PHE:O	1:A:701:PRO:HG2	2.00	0.62
1:A:438:GLN:O	1:A:438:GLN:HG3	1.99	0.62
1:A:374:LYS:O	1:A:378:VAL:HG23	2.00	0.61
2:B:424:TYR:CD1	2:B:427:ARG:NH2	2.68	0.61
1:A:260:GLY:O	1:A:264:PHE:HD2	1.83	0.61
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.00	0.60
1:A:548:SER:O	1:A:552:TRP:HB3	2.01	0.60
1:A:437:THR:HG22	1:A:508:LEU:CD1	2.32	0.60
2:B:417:VAL:O	2:B:421:PHE:HD1	1.85	0.59
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.84	0.59
1:A:693:LEU:HD12	1:A:694:PHE:N	2.18	0.58
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.86	0.57
1:A:807:TYR:N	1:A:808:PRO:HD3	2.19	0.57
1:A:828:GLN:HG2	1:A:829:PHE:CE2	2.39	0.56
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.63	0.56
1:A:377:MET:HE2	1:A:378:VAL:HG22	1.88	0.56
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.35	0.56
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.88	0.55
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.42	0.55
1:A:736:GLY:O	1:A:738:SER:N	2.40	0.55
1:A:429:GLU:HA	1:A:432:LYS:HB2	1.89	0.54
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.43	0.54
1:A:715:MET:CE	1:A:723:ILE:HG12	2.38	0.54
1:A:553:ASP:O	1:A:556:ASP:HB2	2.07	0.54
1:A:470:PRO:HB2	1:A:471:PRO:HA	1.89	0.54
1:A:801:GLU:HG2	1:A:809:ALA:H	1.73	0.54
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.73	0.54
1:A:295:ARG:O	1:A:299:SER:HB3	2.09	0.53
1:A:351:MET:HB3	1:A:567:VAL:HG13	1.90	0.53
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.39	0.53
1:A:419:GLN:HE22	2:B:315:PHE:H	1.56	0.52
1:A:351:MET:HE3	1:A:574:VAL:HG21	1.92	0.52
1:A:720:ASP:O	1:A:724:VAL:HG23	2.10	0.52
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.92	0.51
1:A:603:ILE:HG12	1:A:615:ILE:HD13	1.92	0.51
1:A:437:THR:C	1:A:439:GLU:H	2.19	0.51
1:A:715:MET:HE1	1:A:723:ILE:HG12	1.92	0.51
1:A:563:SER:O	1:A:565:LEU:HD12	2.11	0.51
1:A:530:ASP:OD2	1:A:685:THR:HA	2.11	0.51
1:A:392:LEU:CD2	1:A:398:PHE:CD2	2.94	0.50
1:A:750:ARG:HG3	1:A:750:ARG:NH1	2.25	0.50
1:A:801:GLU:HG2	1:A:809:ALA:N	2.25	0.50
1:A:494:TYR:O	1:A:494:TYR:HD2	1.89	0.50
1:A:594:ARG:HA	1:A:640:VAL:O	2.11	0.50
1:A:446:ASN:OD1	2:B:359:LEU:HD11	2.12	0.49
1:A:695:TRP:HE1	1:A:706:LEU:HD22	1.77	0.49
1:A:468:VAL:O	1:A:472:ARG:NH1	2.44	0.49
1:A:601:GLU:HA	1:A:616:TYR:O	2.12	0.49
1:A:455:ILE:HD11	1:A:490:LEU:O	2.13	0.49
1:A:537:GLU:HG2	1:A:544:LEU:HD21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:O	1:A:388:ALA:HB3	2.12	0.49
1:A:716:GLU:CG	1:A:750:ARG:HG2	2.39	0.49
1:A:196:PHE:N	1:A:197:PRO:CD	2.76	0.48
1:A:449:VAL:HG12	1:A:450:ASN:N	2.27	0.48
1:A:670:PHE:C	1:A:670:PHE:CD1	2.91	0.48
1:A:465:ALA:CB	1:A:479:LEU:HD23	2.43	0.48
1:A:693:LEU:HD12	1:A:694:PHE:H	1.79	0.48
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.49	0.48
2:B:327:ASN:ND2	2:B:330:ALA:HB2	2.29	0.48
1:A:289:SER:HB3	1:A:814:ALA:HB1	1.96	0.48
1:A:374:LYS:O	1:A:375:ASP:C	2.55	0.48
2:B:337:GLN:HE21	2:B:337:GLN:CA	2.27	0.48
1:A:340:ASN:O	1:A:341:PRO:C	2.55	0.47
1:A:763:TYR:CE1	1:A:765:ALA:HB2	2.50	0.47
1:A:691:LEU:HD22	1:A:727:CYS:SG	2.53	0.47
2:B:388:GLN:O	2:B:391:ALA:HB3	2.14	0.47
3:A:900:FAD:H9	3:A:900:FAD:H1'1	1.72	0.47
1:A:232:GLU:O	1:A:234:THR:N	2.48	0.47
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.96	0.47
1:A:770:GLY:O	1:A:773:TYR:HB2	2.14	0.47
1:A:175:GLU:HG2	1:A:185:HIS:CG	2.50	0.47
1:A:510:GLU:HG3	1:A:511:LEU:HD23	1.97	0.47
1:A:283:ILE:HD12	1:A:294:ALA:HB2	1.96	0.46
1:A:758:ARG:NH1	1:A:758:ARG:CG	2.70	0.46
1:A:342:MET:HG2	1:A:812:HIS:HB3	1.97	0.46
1:A:776:MET:HB3	1:A:803:THR:HG22	1.97	0.46
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.79	0.46
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.81	0.46
1:A:422:HIS:HA	1:A:425:ASP:HB2	1.98	0.46
1:A:496:GLU:O	1:A:499:GLU:HB3	2.15	0.46
1:A:364:GLU:HA	1:A:681:VAL:HB	1.98	0.45
1:A:640:VAL:HA	1:A:641:PRO:HA	1.80	0.45
1:A:736:GLY:C	1:A:738:SER:H	2.24	0.45
1:A:806:ASN:C	1:A:807:TYR:CD2	2.95	0.45
2:B:312:LYS:HE3	2:B:312:LYS:HA	1.98	0.45
1:A:273:LEU:HA	1:A:274:PRO:HD2	1.76	0.45
1:A:392:LEU:HD23	1:A:398:PHE:CB	2.42	0.45
1:A:690:GLU:CG	1:A:691:LEU:HD12	2.44	0.45
2:B:324:VAL:HG12	2:B:324:VAL:O	2.17	0.45
2:B:329:THR:C	2:B:331:ALA:N	2.73	0.45
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.27	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:VAL:HG11	1:A:571:TYR:HA	1.99	0.45
1:A:791:GLN:HA	1:A:792:PRO:HD3	1.88	0.45
1:A:670:PHE:CZ	1:A:740:VAL:HG22	2.53	0.44
1:A:657:GLY:HA2	1:A:752:ARG:HH22	1.83	0.44
1:A:670:PHE:HD1	1:A:670:PHE:O	2.00	0.44
1:A:493:GLU:C	1:A:495:ASP:H	2.25	0.44
1:A:814:ALA:O	1:A:817:SER:N	2.50	0.44
2:B:424:TYR:CE1	2:B:427:ARG:NH2	2.85	0.44
1:A:271:LYS:O	1:A:272:PRO:C	2.60	0.44
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.47	0.44
1:A:473:ASP:OD1	1:A:473:ASP:C	2.60	0.44
1:A:294:ALA:O	1:A:295:ARG:C	2.61	0.43
1:A:493:GLU:C	1:A:495:ASP:N	2.76	0.43
1:A:297:LEU:HB2	1:A:304:VAL:HG21	2.01	0.43
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.18	0.43
1:A:319:THR:HB	1:A:572:SER:HB3	2.01	0.43
1:A:449:VAL:HA	2:B:363:LEU:HD21	2.00	0.43
1:A:331:ALA:HA	3:A:900:FAD:C4X	2.48	0.43
1:A:456:LYS:HA	2:B:370:TYR:CD1	2.50	0.43
1:A:594:ARG:HB3	1:A:640:VAL:HB	2.00	0.43
1:A:801:GLU:CG	1:A:809:ALA:HA	2.49	0.43
1:A:707:VAL:CG1	1:A:712:ALA:HA	2.49	0.43
2:B:368:GLU:OE2	2:B:371:ARG:NH1	2.52	0.43
1:A:800:GLY:O	1:A:803:THR:N	2.45	0.43
1:A:484:HIS:CD2	2:B:372:LEU:CD1	3.02	0.42
1:A:583:ASP:OD1	1:A:585:LYS:NZ	2.52	0.42
1:A:613:THR:HG22	1:A:614:PHE:N	2.32	0.42
1:A:548:SER:HB2	1:A:766:ALA:HA	2.00	0.42
1:A:333:VAL:HG21	4:A:901:3PL:CZ	2.49	0.42
1:A:353:LEU:HB3	1:A:565:LEU:HD23	2.01	0.42
1:A:295:ARG:NH2	1:A:580:GLU:O	2.53	0.42
1:A:317:VAL:HG13	1:A:571:TYR:HB3	2.01	0.42
1:A:613:THR:CG2	1:A:614:PHE:N	2.82	0.42
1:A:270:ILE:O	1:A:272:PRO:HD3	2.20	0.41
2:B:337:GLN:HE21	2:B:337:GLN:HA	1.84	0.41
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.54	0.41
1:A:231:PHE:CZ	1:A:250:HIS:HB2	2.56	0.41
1:A:506:GLU:C	1:A:508:LEU:N	2.68	0.41
2:B:372:LEU:HA	2:B:373:PRO:HD2	1.73	0.41
1:A:392:LEU:HD22	1:A:398:PHE:HD2	1.86	0.41
1:A:209:VAL:HG12	1:A:213:ILE:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.86	0.41
1:A:506:GLU:O	1:A:508:LEU:N	2.54	0.41
1:A:351:MET:HE3	1:A:574:VAL:CG2	2.51	0.41
1:A:826:ALA:O	1:A:827:ASP:C	2.63	0.41
1:A:380:GLN:O	1:A:384:ARG:HD3	2.20	0.41
1:A:451:LEU:C	1:A:453:GLU:N	2.77	0.41
1:A:786:ILE:H	1:A:786:ILE:HD12	1.85	0.41
1:A:370:VAL:HA	1:A:371:PRO:HD3	1.85	0.41
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.95	0.40
1:A:808:PRO:O	1:A:810:THR:HG23	2.22	0.40
2:B:425:ARG:HA	2:B:430:ILE:HG13	2.02	0.40
2:B:434:LEU:HD23	2:B:434:LEU:HA	2.00	0.40
1:A:232:GLU:H	1:A:232:GLU:CD	2.29	0.40
1:A:633:GLN:HA	1:A:634:PRO:HA	1.51	0.40
1:A:747:VAL:HG12	1:A:748:VAL:N	2.36	0.40
2:B:418:LYS:O	2:B:421:PHE:HB2	2.22	0.40
1:A:797:PHE:CG	1:A:825:ILE:HD11	2.56	0.40
1:A:248:LEU:O	1:A:249:VAL:C	2.65	0.40
1:A:392:LEU:HD21	1:A:398:PHE:CD2	2.55	0.40
1:A:551:HIS:O	1:A:552:TRP:C	2.65	0.40
1:A:680:HIS:CD2	1:A:730:ILE:HG23	2.57	0.40
1:A:722:VAL:O	1:A:726:ARG:HG3	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	664/852 (78%)	582 (88%)	63 (10%)	19 (3%)	3	19
2	B	131/482 (27%)	112 (86%)	13 (10%)	6 (5%)	2	12
All	All	795/1334 (60%)	694 (87%)	76 (10%)	25 (3%)	3	18

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	510	GLU
1	A	737	SER
1	A	233	ALA
1	A	425	ASP
1	A	438	GLN
1	A	468	VAL
1	A	507	LYS
1	A	801	GLU
2	B	326	ALA
1	A	232	GLU
1	A	244	SER
1	A	274	PRO
1	A	364	GLU
2	B	373	PRO
2	B	429	ASN
1	A	573	CYS
1	A	805	ARG
2	B	331	ALA
2	B	379	CYS
1	A	272	PRO
1	A	499	GLU
1	A	597	ALA
1	A	725	GLY
2	B	391	ALA
1	A	785	SER

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%)	478 (84%)	88 (16%)	2 12
2	B	117/395 (30%)	93 (80%)	24 (20%)	1 5
All	All	683/1094 (62%)	571 (84%)	112 (16%)	2 11

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	SER
1	A	191	GLN
1	A	195	CYS
1	A	200	ILE
1	A	205	GLN
1	A	214	ARG
1	A	236	GLN
1	A	237	GLN
1	A	247	VAL
1	A	263	ASN
1	A	266	ILE
1	A	268	LYS
1	A	271	LYS
1	A	273	LEU
1	A	274	PRO
1	A	278	THR
1	A	282	ILE
1	A	299	SER
1	A	313	VAL
1	A	351	MET
1	A	373	GLU
1	A	374	LYS
1	A	378	VAL
1	A	380	GLN
1	A	392	LEU
1	A	402	ASN
1	A	404	LYS
1	A	418	LEU
1	A	422	HIS
1	A	423	VAL
1	A	426	GLU
1	A	429	GLU
1	A	432	LYS
1	A	433	LYS
1	A	434	ILE
1	A	437	THR
1	A	438	GLN
1	A	449	VAL
1	A	453	GLU
1	A	458	LEU
1	A	467	GLU
1	A	469	LYS
1	A	472	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	479	LEU
1	A	482	SER
1	A	485	ARG
1	A	508	LEU
1	A	511	LEU
1	A	523	SER
1	A	524	ARG
1	A	526	ARG
1	A	538	PHE
1	A	556	ASP
1	A	563	SER
1	A	568	ARG
1	A	580	GLU
1	A	591	ARG
1	A	594	ARG
1	A	600	CYS
1	A	610	THR
1	A	612	GLN
1	A	615	ILE
1	A	633	GLN
1	A	638	GLN
1	A	645	GLU
1	A	648	THR
1	A	652	GLN
1	A	659	LEU
1	A	668	ARG
1	A	675	VAL
1	A	677	LEU
1	A	680	HIS
1	A	683	SER
1	A	684	THR
1	A	699	LYS
1	A	706	LEU
1	A	719	SER
1	A	727	CYS
1	A	758	ARG
1	A	778	GLN
1	A	785	SER
1	A	786	ILE
1	A	793	ILE
1	A	801	GLU
1	A	815	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	821	GLU
1	A	825	ILE
1	A	828	GLN
2	B	312	LYS
2	B	314	MET
2	B	332	THR
2	B	333	THR
2	B	334	VAL
2	B	337	GLN
2	B	343	VAL
2	B	344	SER
2	B	347	ARG
2	B	349	ILE
2	B	359	LEU
2	B	361	GLU
2	B	362	LYS
2	B	368	GLU
2	B	375	VAL
2	B	376	ILE
2	B	385	THR
2	B	386	GLU
2	B	392	VAL
2	B	414	VAL
2	B	422	VAL
2	B	430	ILE
2	B	432	GLU
2	B	435	GLN

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	237	GLN
1	A	259	HIS
1	A	298	GLN
1	A	419	GLN
1	A	484	HIS
1	A	742	GLN
1	A	778	GLN
1	A	828	GLN
2	B	337	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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
4	3PL	A	901	3	9,10,10	1.02	0	11,11,11	1.70	3 (27%)
3	FAD	A	900	4	58,58,58	1.29	6 (10%)	85,89,89	1.82	24 (28%)

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	3PL	A	901	3	-	1/4/4/4	0/1/1/1
3	FAD	A	900	4	-	3/34/50/50	0/5/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C4X-N5	4.74	1.41	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C5'-C4'	3.15	1.56	1.51
3	A	900	FAD	C10-N10	2.59	1.42	1.37
3	A	900	FAD	C8A-N7A	2.35	1.36	1.31
3	A	900	FAD	C4-N3	-2.10	1.34	1.38
3	A	900	FAD	C9A-N10	2.09	1.44	1.41

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	900	FAD	N3A-C2A-N1A	-4.78	121.35	128.58
3	A	900	FAD	C9A-N10-C10	-4.69	113.60	120.75
3	A	900	FAD	C5A-C4A-N3A	-4.33	120.75	126.72
3	A	900	FAD	C4A-N9A-C8A	4.23	110.18	105.74
3	A	900	FAD	N9A-C8A-N7A	-3.84	108.48	113.94
3	A	900	FAD	N3A-C4A-N9A	3.59	133.27	127.17
3	A	900	FAD	C5X-C9A-N10	3.27	120.93	117.97
3	A	900	FAD	C1'-N10-C9A	-3.26	114.30	120.63
3	A	900	FAD	C2A-N3A-C4A	3.05	119.29	111.83
3	A	900	FAD	C5X-N5-C4X	-2.95	113.31	118.09
3	A	900	FAD	C4X-C10-N1	-2.89	117.51	124.59
4	A	901	3PL	CE1-CD1-CG	-2.72	116.79	120.61
3	A	900	FAD	O2A-PA-O1A	2.67	124.86	112.44
4	A	901	3PL	CA-CB-CG	-2.65	106.81	113.21
3	A	900	FAD	C4X-C4-N3	2.57	119.79	113.25
3	A	900	FAD	C5'-C4'-C3'	-2.53	107.44	112.22
3	A	900	FAD	O5'-P-O1P	-2.40	99.41	108.94
3	A	900	FAD	O4'-C4'-C5'	2.34	115.15	109.99
3	A	900	FAD	C5A-N7A-C8A	2.34	107.13	103.45
4	A	901	3PL	CZ-CE2-CD2	-2.30	117.40	120.24
3	A	900	FAD	O4'-C4'-C3'	2.27	114.56	109.25
3	A	900	FAD	C2'-C1'-N10	2.22	120.68	110.20
3	A	900	FAD	O4-C4-C4X	-2.11	120.96	126.53
3	A	900	FAD	C4-N3-C2	-2.10	121.92	125.64
3	A	900	FAD	N6A-C6A-N1A	2.09	123.04	118.38
3	A	900	FAD	C4A-C5A-N7A	-2.06	108.22	110.58
3	A	900	FAD	N10-C10-N1	2.01	124.42	118.51

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	FAD	C2'-C1'-N10-C10

Continued on next page...

Continued from previous page...

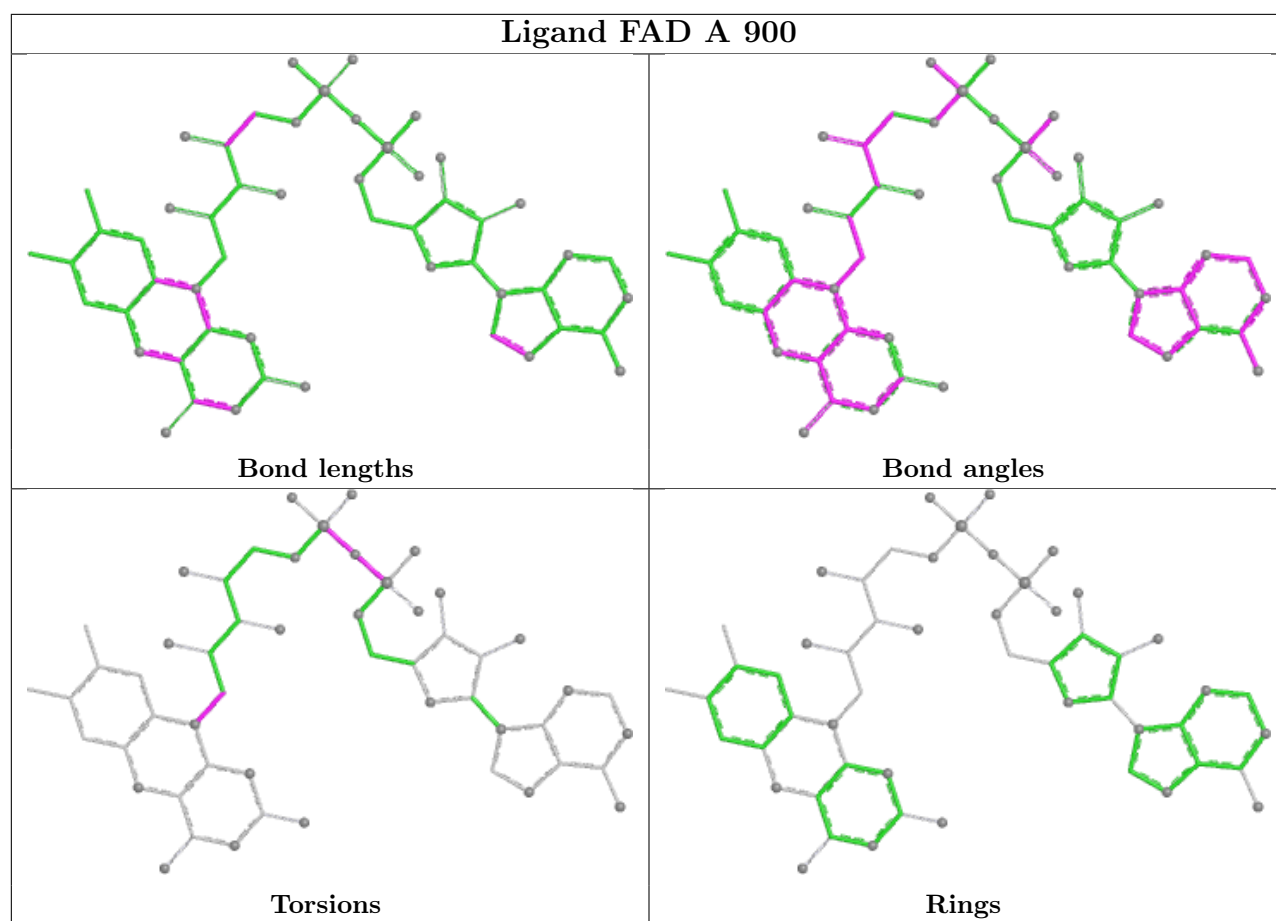
Mol	Chain	Res	Type	Atoms
4	A	901	3PL	O-C-CA-CB
3	A	900	FAD	PA-O3P-P-O5'
3	A	900	FAD	P-O3P-PA-O2A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	3PL	2	0
3	A	900	FAD	2	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%)	-0.13	11 (1%) 69 48	26, 56, 85, 101	0
2	B	133/482 (27%)	0.56	8 (6%) 27 15	58, 87, 99, 109	0
All	All	799/1334 (59%)	-0.02	19 (2%) 59 38	26, 61, 94, 109	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	9.0
1	A	171	PRO	4.5
2	B	376	ILE	3.8
2	B	375	VAL	3.7
2	B	374	GLU	3.5
1	A	833	MET	3.2
1	A	275	THR	3.2
2	B	337	GLN	3.0
2	B	440	GLU	2.8
1	A	373	GLU	2.7
1	A	172	SER	2.6
2	B	340	MET	2.5
1	A	508	LEU	2.4
2	B	426	ARG	2.3
1	A	506	GLU	2.2
1	A	511	LEU	2.2
1	A	835	THR	2.2
2	B	414	VAL	2.1
1	A	786	ILE	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](#)

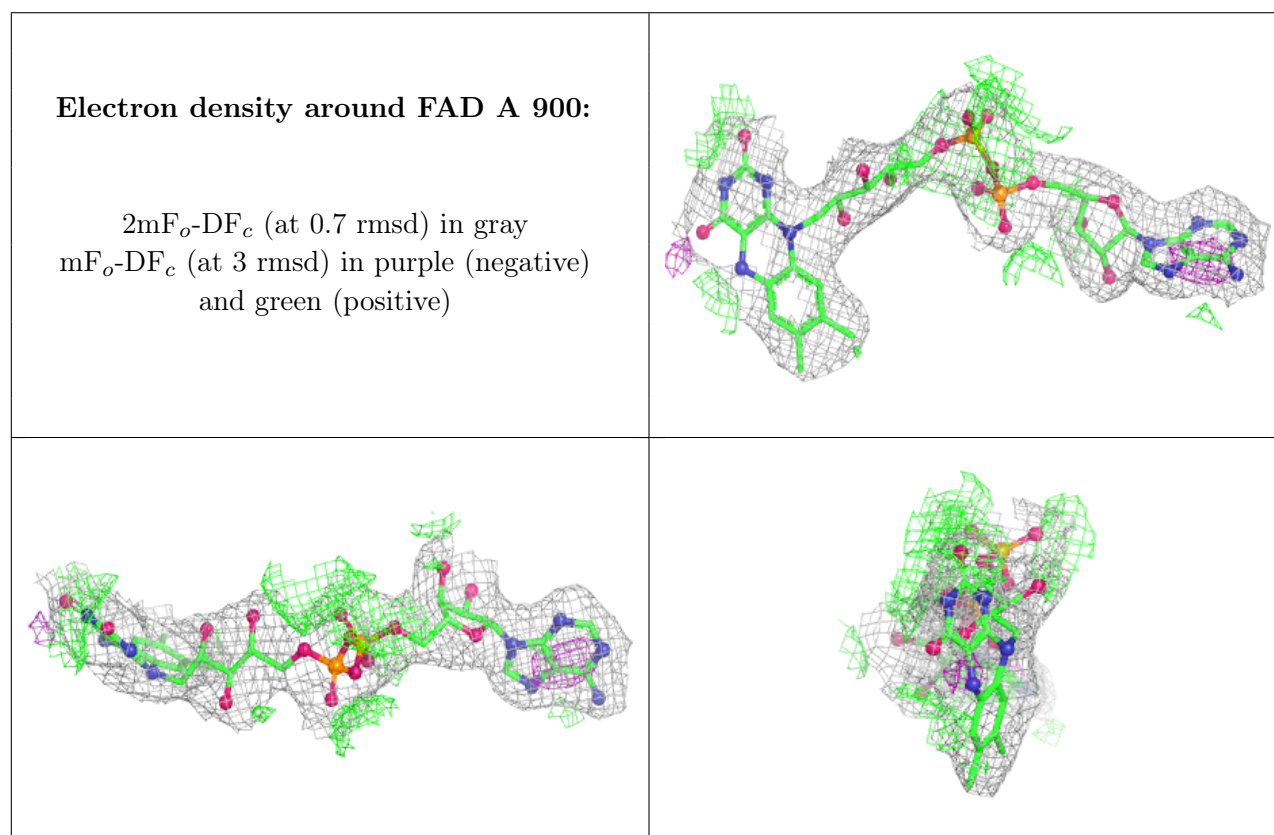
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
4	3PL	A	901	10/10	0.94	0.16	54,57,58,59	0
3	FAD	A	900	53/53	0.98	0.07	23,31,48,51	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.