Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 03:10 am BST

PDB ID	:	2XAH
Title	:	Crystal structure of LSD1-CoREST in complex with (+)-trans-2- phenylcycl opropyl-1-amine
Authors	:	Binda, C.; Valente, S.; Romanenghi, M.; Pilotto, S.; Cirilli, R.; Karytinos, 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

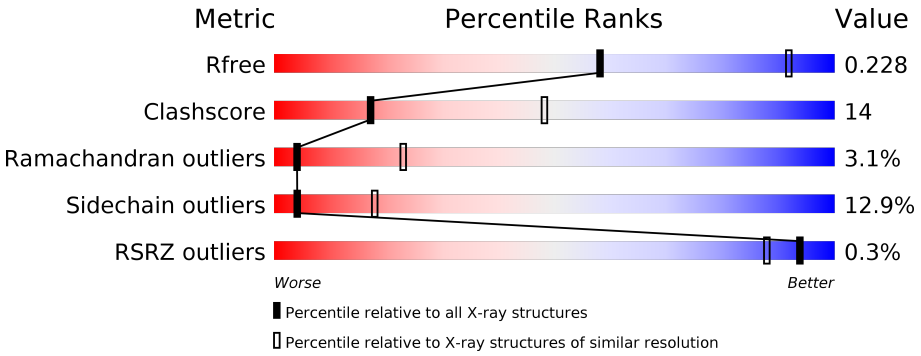
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 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 <=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	50% 24% . 22%
2	B	482	18% 8% . 72%

2 Entry composition

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.

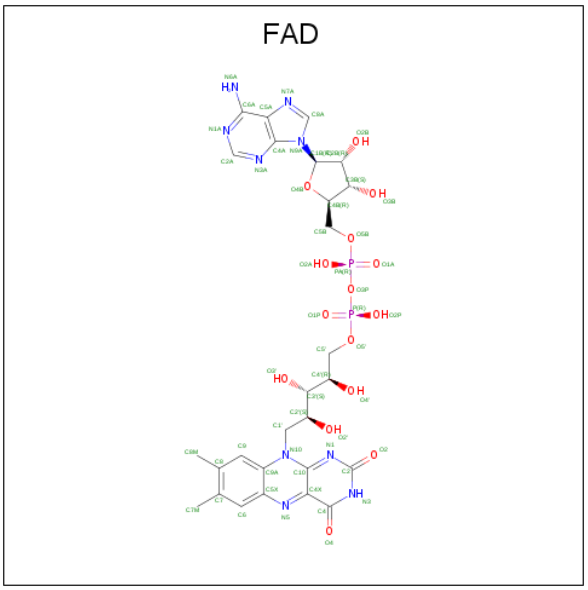
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

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.

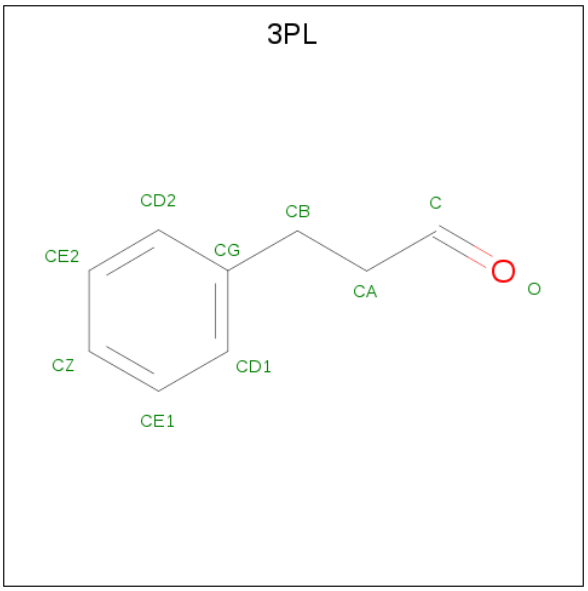
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: 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 (three-letter code: 3PL) (formula: $C_9H_{10}O$).



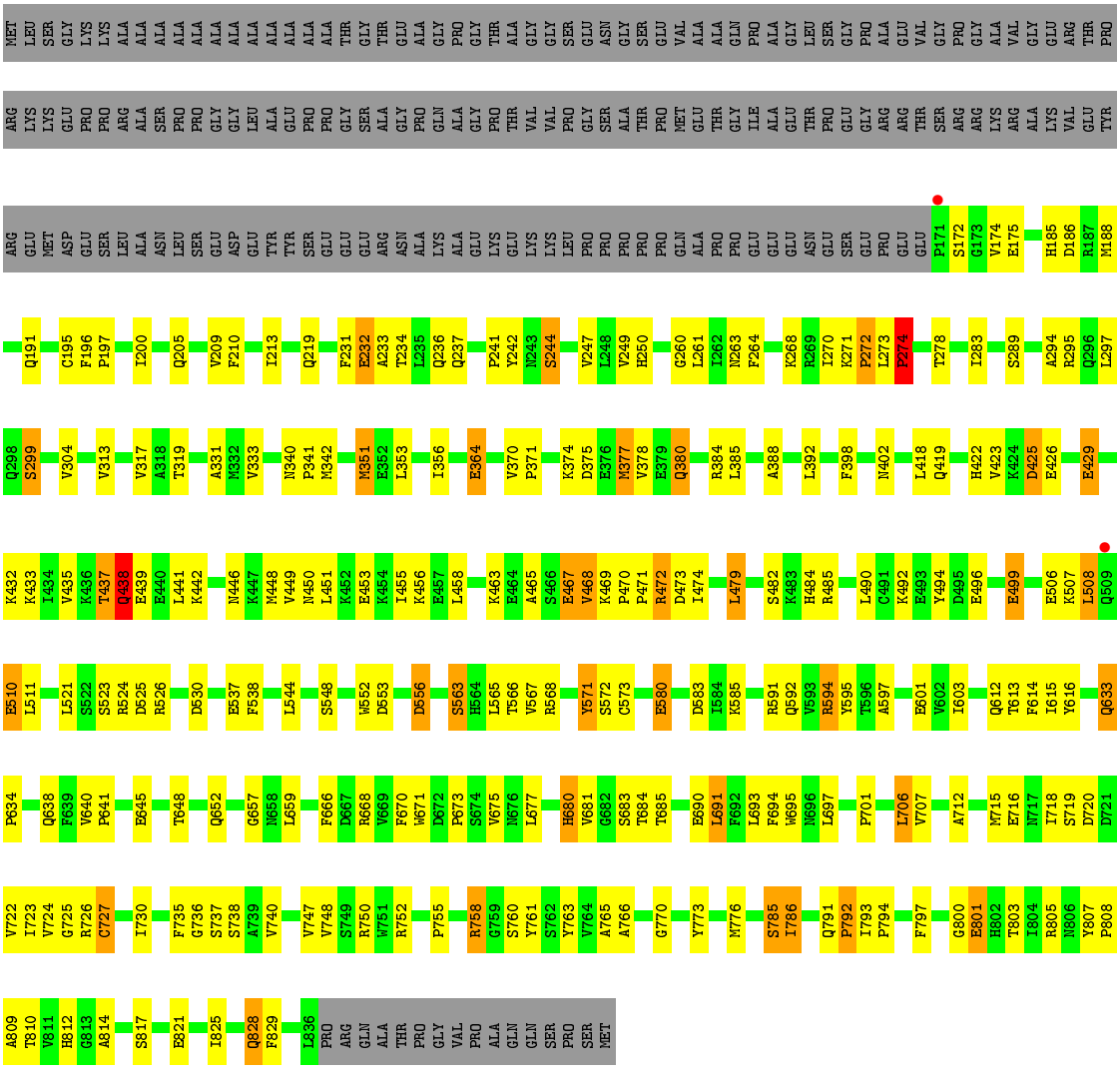
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 9 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

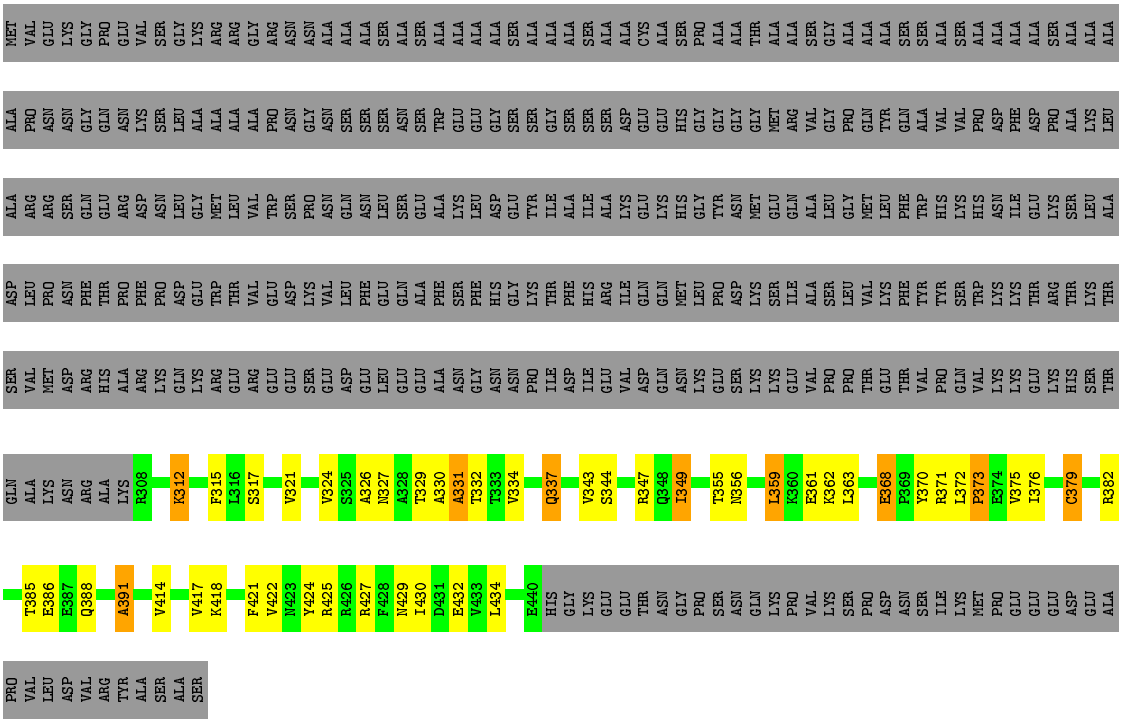
- Molecule 1: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1

Chain A:



- Molecule 2: REST COREPRESSOR 1

Chain B:


MET VAL GLU LYS GLY PRO GLU VAL SER GLY LYS ARG ARG GLY ARG ASN ASN ALA ALA ALA SER ALA SER ALA ALA ALA ALA SER ALA ALA ALA ALA ALA SER SER ALA ALA CYS ALA SER PRO ALA ALA THR ALA ALA SER GLY ALA ALA ALA SER SER ALA SER ALA ALA ALA ALA SER ALA ALA
ALA PRO ASN ASN GLY GLN ASN LYS SER LEU ALA ALA ALA ALA PRO ASN GLY ASN SER SER SER ASN SER TRP GLU GLU GLY SER SER SER SER ASP GLU GLU HIS GLY GLY GLY GLY MET ARG VAL GLY PRO GLN TYR GLN ALA VAL VAL PRO ASP PHE ASP PRO ALA LYS LEU
ALA ARG ARG SER GLN GLU ARG ASP ASN LEU GLY MET LEU VAL TRP SER PRO ASN GLN ASN LEU SER GLU ALA LYS LEU ASP GLU TYR ILE ALA ILE ALA LYS GLU LYS HIS GLY TYR ASN MET GLU GLN ALA LEU GLY MET LEU PHE TRP HIS LYS HIS ASN ILE GLU LYS SER LEU ALA
ASP LEU PRO ASN PHE THR PRO PHE PRO ASP GLU TRP THR VAL GLU ASP LYS VAL LEU PHE GLU GLN ALA PHE SER PHE HIS GLY LYS THR PHE HIS ARG ILE GLN GLN MET LEU PRO ASP LYS SER ILE ALA SER LEU VAL LYS PHE TYR TYR SER TRP LYS LYS THR ARG THR LYS THR
SER VAL MET ASP ARG HIS ALA ARG LYS GLN LYS ARG GLU ARG GLU GLU SER GLU ASP GLU LEU GLU GLU ALA ASN GLY ASN ASN PRO ILE ASP ILE GLU GLU VAL ASP GLN ASN LYS GLU SER LYS LYS GLU VAL PRO PRO THR GLU THR VAL PRO GLN VAL LYS LYS GLU LYS HIS SER THR
GLN ALA LYS ASN ARG ALA LYS R308 K312 F315 L316 S317 V321 V324 S325 A326 N327 A328 T329 A330 A331 T332 T333 V334 Q337 V343 S344 R347 Q348 I349 T355 N356 L359 K360 E361 K362 L363 E368 P369 Y370 R371 L372 P373 E374 V375 I376 C379 R382
T385 E386 E387 Q388 A391 V414 V417 K418 F421 V422 N423 Y424 R425 R426 R427 F428 N429 I430 D431 E432 V433 L434 E440 HIS GLY LYS GLU GLU THR ASN GLY PRO SER ASN GLN LYS PRO VAL LYS SER PRO ASP ASN SER ILE LYS MET PRO GLU GLU GLU ASP GLU ALA
PRO VAL LEU ASP VAL ARG TYR ALA SER ALA SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.96Å 181.50Å 234.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.75 – 3.10 71.84 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (90.75-3.10) 99.9 (71.84-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.32 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	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.*

[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: 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	0.68	0/5331	0.77	0/7232
2	B	0.58	0/1091	0.69	1/1471 (0.1%)
All	All	0.67	0/6422	0.76	1/8703 (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	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	359	LEU	CA-CB-CG	5.95	128.98	115.30

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

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	160	0
2	B	1076	0	1091	31	0
3	A	53	0	31	3	0
4	A	10	0	9	2	0
All	All	6356	0	6383	177	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 14.

All (177) 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
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.20	0.99
1:A:758:ARG:HH11	1:A:758:ARG:HG2	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:OE1	1:A:453:GLU:HA	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:HG2	1:A:758:ARG:NH1	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:760:SER:HB2	3:A:900:FAD:HM83	1.81	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:506:GLU:C	1:A:508:LEU:H	2.04	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
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:715:MET:HE3	1:A:723:ILE:HG12	1.87	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:377:MET:HE2	1:A:378:VAL:HG22	1.90	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HD2	1:A:494:TYR:O	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
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: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
2:B:337:GLN:HE21	2:B:337:GLN:CA	2.27	0.48
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:H1'1	3:A:900:FAD:H9	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:437:THR:C	1:A:439:GLU:H	2.19	0.46
1:A:758:ARG:CG	1:A:758:ARG:NH1	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.27	0.45
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:670:PHE:HD1	1:A:670:PHE:O	2.00	0.44
1:A:657:GLY:HA2	1:A:752:ARG:HH22	1.83	0.44
1:A:670:PHE:CD1	1:A:670:PHE:C	2.91	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:356:ILE:HD11	1:A:566:THR:CG2	2.47	0.44
1:A:374:LYS:O	1:A:375:ASP:C	2.55	0.44
1:A:506:GLU:C	1:A:508:LEU:N	2.68	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:449:VAL:HA	2:B:363:LEU:HD21	2.00	0.43
1:A:319:THR:HB	1:A:572:SER:HB3	2.01	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:340:ASN:O	1:A:341:PRO:C	2.55	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:828:GLN:HG3	1:A:828:GLN:O	2.18	0.42
2:B:329:THR:C	2:B:331:ALA:N	2.73	0.42
1:A:333:VAL:HG21	4:A:901:3PL:CZ	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	2:B:337:GLN:HE21	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
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
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:380:GLN:O	1:A:384:ARG:HD3	2.20	0.41
1:A:786:ILE:HD12	1:A:786:ILE:H	1.85	0.41
1:A:370:VAL:HA	1:A:371:PRO:HD3	1.85	0.41
1:A:474:ILE:HA	1:A:474:ILE:HD12	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:HA	2:B:434:LEU:HD23	2.00	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:392:LEU:HD21	1:A:398:PHE:CD2	2.55	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%)	4 24
2	B	131/482 (27%)	112 (86%)	13 (10%)	6 (5%)	2 15
All	All	795/1334 (60%)	694 (87%)	76 (10%)	25 (3%)	4 23

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 (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%)	498 (88%)	68 (12%)	5 20
2	B	117/395 (30%)	97 (83%)	20 (17%)	2 9
All	All	683/1094 (62%)	595 (87%)	88 (13%)	4 18

All (88) 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	236	GLN
1	A	237	GLN
1	A	247	VAL
1	A	263	ASN
1	A	268	LYS
1	A	271	LYS
1	A	278	THR
1	A	299	SER
1	A	313	VAL
1	A	351	MET
1	A	377	MET
1	A	380	GLN
1	A	402	ASN
1	A	423	VAL
1	A	426	GLU
1	A	429	GLU
1	A	433	LYS
1	A	437	THR
1	A	438	GLN
1	A	458	LEU
1	A	467	GLU
1	A	469	LYS
1	A	472	ARG
1	A	473	ASP
1	A	479	LEU
1	A	482	SER
1	A	485	ARG
1	A	492	LYS
1	A	508	LEU
1	A	523	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	571	TYR
1	A	580	GLU
1	A	591	ARG
1	A	594	ARG
1	A	612	GLN
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	691	LEU
1	A	706	LEU
1	A	719	SER
1	A	727	CYS
1	A	758	ARG
1	A	785	SER
1	A	786	ILE
1	A	793	ILE
1	A	821	GLU
1	A	828	GLN
2	B	312	LYS
2	B	332	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	361	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	362	LYS
2	B	368	GLU
2	B	375	VAL
2	B	376	ILE
2	B	379	CYS
2	B	382	ARG
2	B	385	THR
2	B	386	GLU
2	B	414	VAL
2	B	422	VAL
2	B	432	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	259	HIS
1	A	419	GLN
1	A	484	HIS
1	A	778	GLN
1	A	828	GLN
2	B	337	GLN
2	B	419	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 (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	51,58,58	2.06	6 (11%)	60,89,89	2.21	18 (30%)
4	3PL	A	901	3	10,10,10	0.92	0	11,11,11	1.66	3 (27%)

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	3PL	A	901	3	-	0/3/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	900	FAD	C4X-C10	10.23	1.49	1.38
3	A	900	FAD	C4X-N5	5.36	1.41	1.33
3	A	900	FAD	C9A-N10	4.63	1.44	1.38
3	A	900	FAD	C5X-N5	3.26	1.40	1.35
3	A	900	FAD	C5'-C4'	3.03	1.56	1.51
3	A	900	FAD	C10-N1	2.52	1.36	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	FAD	C4-N3-C2	8.03	121.92	115.14
3	A	900	FAD	C9A-N10-C10	-6.35	113.60	121.91
3	A	900	FAD	C1'-N10-C9A	-5.07	114.30	118.29
3	A	900	FAD	N3A-C2A-N1A	-4.69	121.35	128.68
3	A	900	FAD	C5X-C9A-N10	4.43	120.93	117.72
3	A	900	FAD	C4X-N5-C5X	-3.46	113.31	116.77
3	A	900	FAD	P-O3P-PA	-3.26	121.65	132.83
3	A	900	FAD	O4B-C1B-C2B	-2.82	102.81	106.93
3	A	900	FAD	C4X-C4-N3	-2.66	119.79	123.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	FAD	O2A-PA-O1A	2.55	124.86	112.24
4	A	901	3PL	CB-CA-C	-2.54	103.55	111.89
4	A	901	3PL	CE1-CD1-CG	-2.51	116.79	120.63
4	A	901	3PL	CA-CB-CG	-2.50	106.81	113.18
3	A	900	FAD	O5'-P-O1P	-2.47	99.41	109.07
3	A	900	FAD	C5'-C4'-C3'	-2.47	107.44	112.20
3	A	900	FAD	C6-C5X-N5	-2.43	116.38	119.05
3	A	900	FAD	O4'-C4'-C5'	2.33	115.15	109.92
3	A	900	FAD	O4'-C4'-C3'	2.24	114.56	109.10
3	A	900	FAD	C4X-C10-N10	-2.19	118.06	120.30
3	A	900	FAD	N6A-C6A-N1A	2.15	123.04	118.57
3	A	900	FAD	C6-C5X-C9A	2.05	121.74	119.05

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
3	A	900	FAD	PA-O3P-P-O5'
3	A	900	FAD	O4B-C4B-C5B-O5B
3	A	900	FAD	P-O3P-PA-O2A

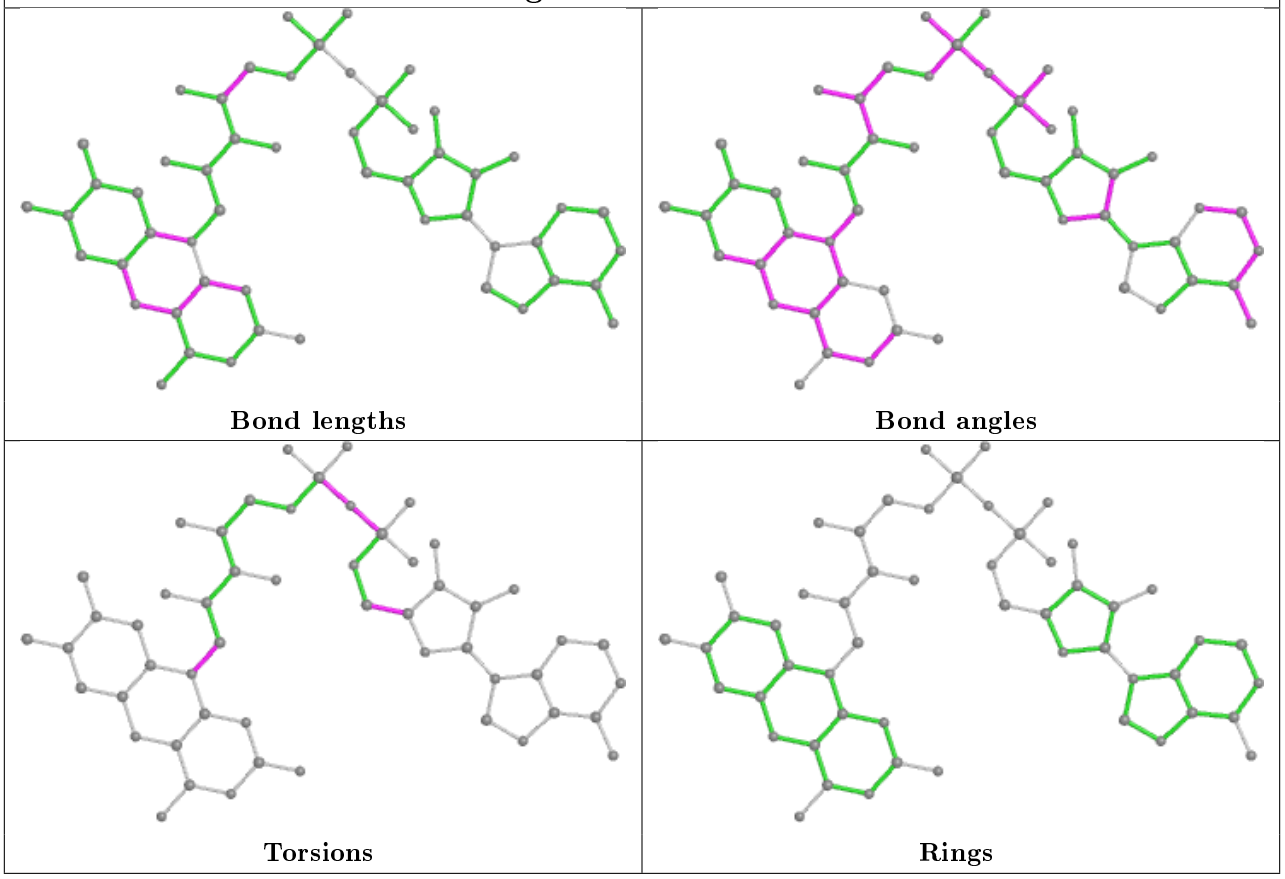
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	900	FAD	3	0
4	A	901	3PL	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 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	666/852 (78%)	-0.23	2 (0%) 94 88	26, 56, 85, 101	0
2	B	133/482 (27%)	-0.04	0 100 100	58, 87, 99, 109	0
All	All	799/1334 (59%)	-0.20	2 (0%) 94 88	26, 61, 94, 109	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	GLN	2.2
1	A	171	PRO	2.2

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 carbohydrates in this entry.

6.4 Ligands

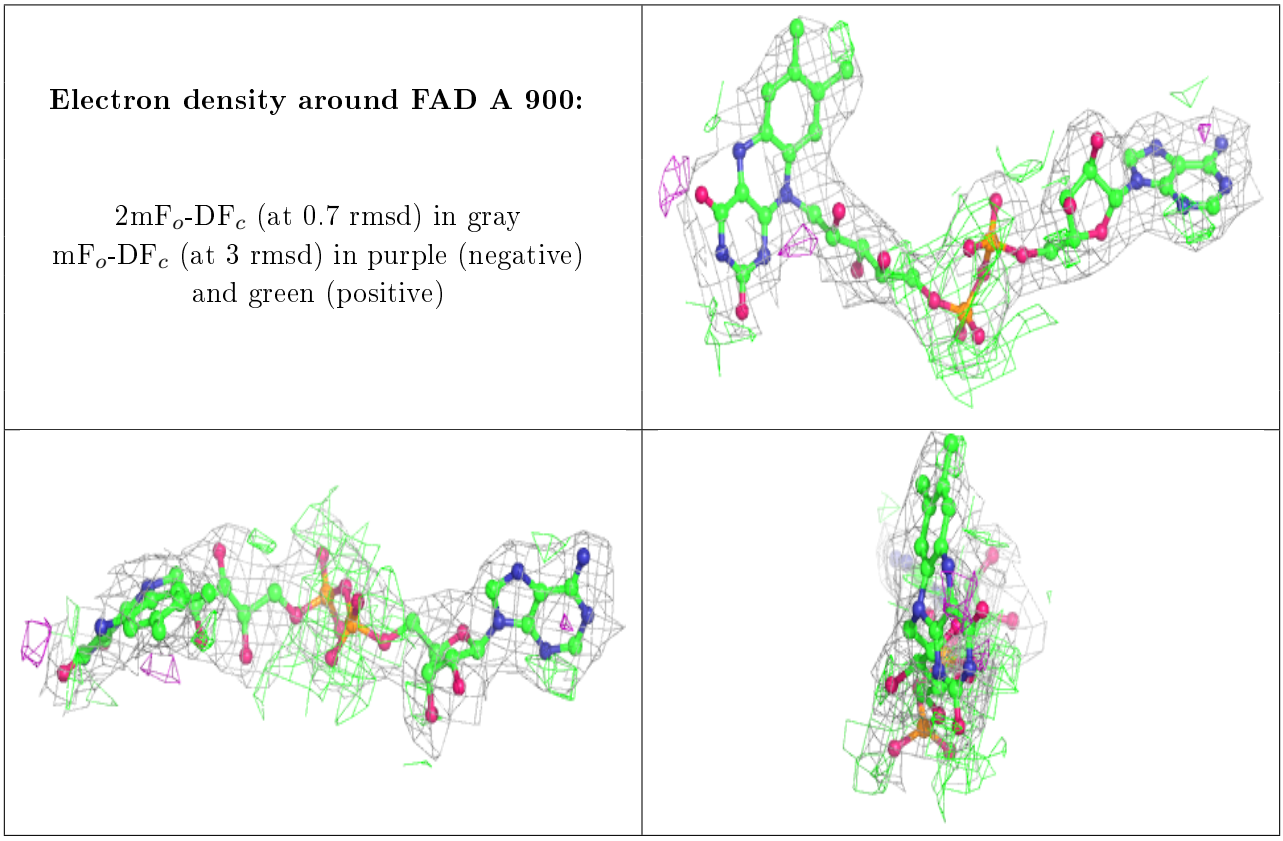
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	3PL	A	901	10/10	0.94	0.26	54,57,58,59	0
3	FAD	A	900	53/53	0.98	0.18	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.

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

There are no such residues in this entry.