Full wwPDB X-ray Structure Validation Report (i)

May 27, 2020 – 10:27 pm BST

PDB ID	:	2XAJ
Title	:	Crystal structure of LSD1-CoREST in complex with (-)-trans-2- phenylcyclo propyl-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	:	3.30 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:

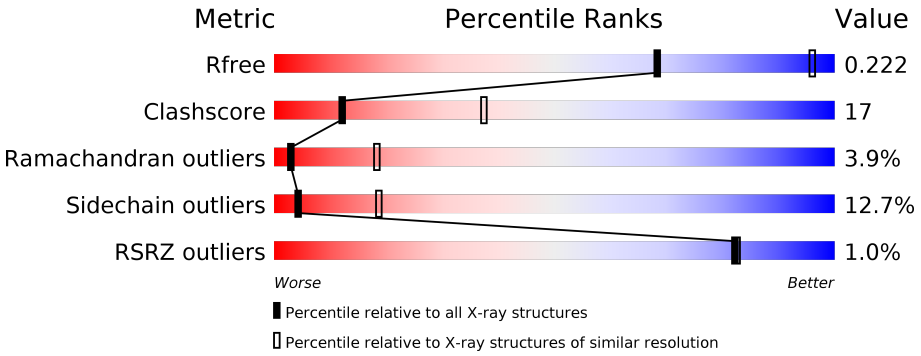
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

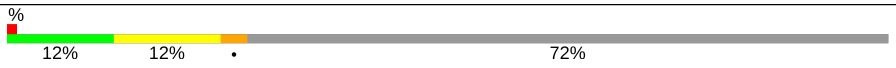
The reported resolution of this entry is 3.30 Å.

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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	
2	B	482	

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.

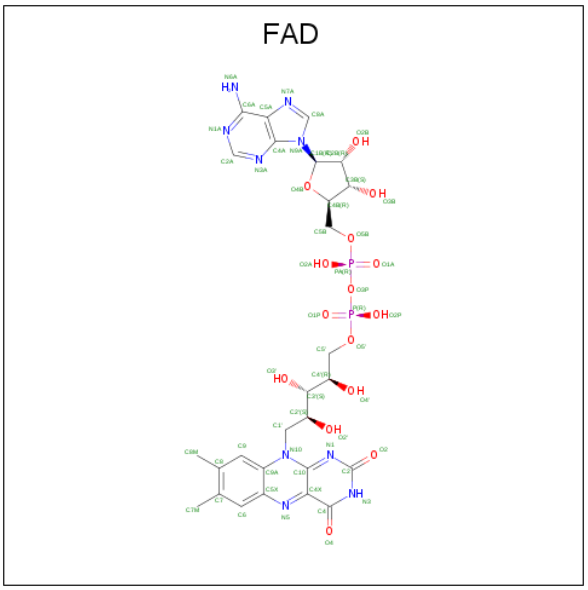
- Molecule 1 is a protein called LYSINE-SPECIFIC HISTONE DEMETHYLASE 1.

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			

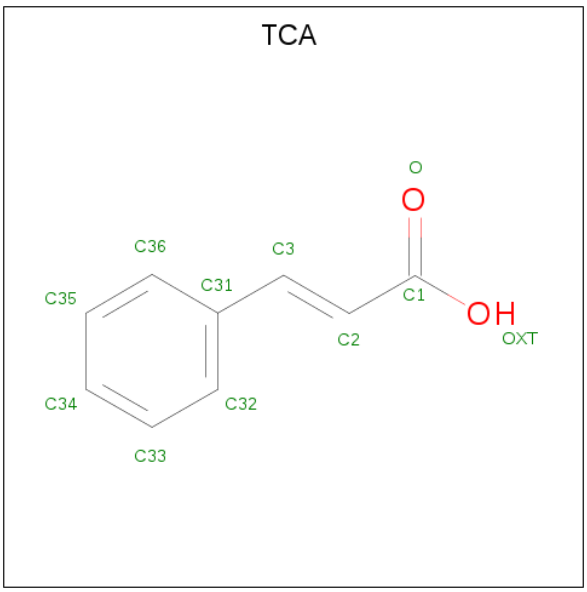
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is PHENYLETHYLENECARBOXYLIC ACID (three-letter code: TCA)

(formula: $C_9H_8O_2$).



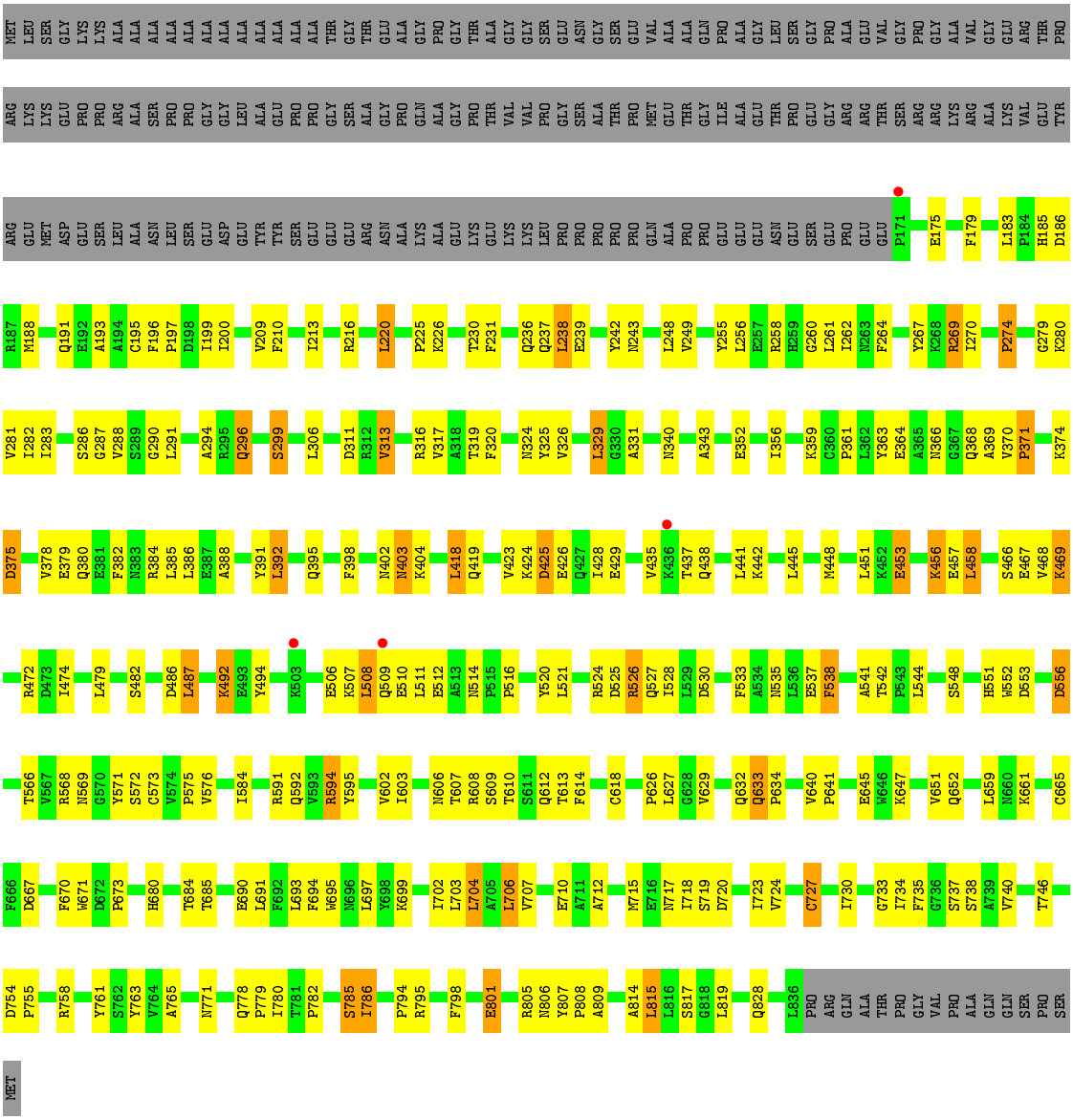
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 9 1	0	0

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.

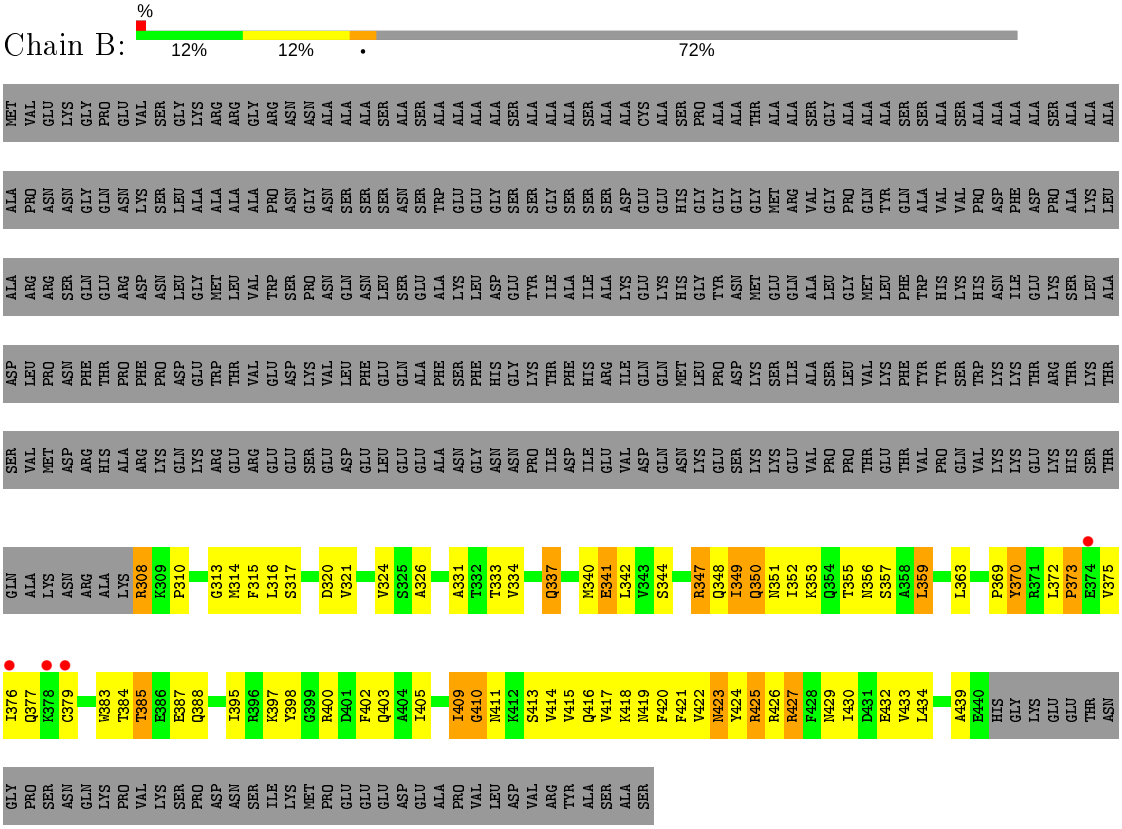
- Molecule 1: LYSINE-SPECIFIC HISTONE DEMETHYLASE 1

Chain A:



- Molecule 2: REST COREPRESSOR 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.08Å 179.78Å 235.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.45 – 3.30 68.63 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (71.45-3.30) 99.8 (68.63-3.30)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0090	Depositor
R, R_{free}	0.199 , 0.227 0.199 , 0.222	Depositor DCC
R_{free} test set	747 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å^2)	78.2	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	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)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/5331	0.82	3/7232 (0.0%)
2	B	0.63	0/1091	0.74	1/1471 (0.1%)
All	All	0.70	0/6422	0.81	4/8703 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	815	LEU	CA-CB-CG	6.28	129.75	115.30
1	A	258	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	258	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	B	359	LEU	CA-CB-CG	5.34	127.58	115.30

There are no chirality outliers.

There are no planarity outliers.

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	167	0
2	B	1076	0	1091	68	0
3	A	53	0	31	4	0
4	A	10	0	7	3	0
All	All	6356	0	6381	218	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 17.

All (218) 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	1.61	1.14
1:A:286:SER:O	1:A:291:LEU:HD11	1.56	1.03
1:A:794:PRO:HD2	1:A:828:GLN:HE22	1.25	0.98
1:A:453:GLU:OE1	1:A:453:GLU:HA	1.68	0.92
1:A:755:PRO:HA	1:A:758:ARG:HH12	1.30	0.91
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.58	0.86
2:B:308:ARG:HH11	2:B:308:ARG:HA	1.41	0.85
1:A:794:PRO:HD2	1:A:828:GLN:NE2	1.91	0.84
1:A:384:ARG:HH22	2:B:313:GLY:HA3	1.44	0.83
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.46	0.81
1:A:510:GLU:HG3	1:A:511:LEU:HD23	1.62	0.80
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.45	0.79
1:A:671:TRP:O	1:A:673:PRO:HD3	1.83	0.78
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.66	0.77
1:A:755:PRO:CA	1:A:758:ARG:HH12	1.98	0.77
1:A:548:SER:O	1:A:552:TRP:HB3	1.85	0.76
1:A:384:ARG:NH2	2:B:313:GLY:HA3	1.99	0.76
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.20	0.75
2:B:317:SER:O	2:B:321:VAL:HG23	1.88	0.73
1:A:286:SER:O	1:A:291:LEU:CD1	2.35	0.73
1:A:566:THR:HG21	1:A:697:LEU:CD2	2.20	0.72
1:A:188:MET:HG2	1:A:210:PHE:CE2	2.25	0.72
1:A:419:GLN:HB3	1:A:520:TYR:CE1	2.25	0.71
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.22	0.70
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.73	0.69
1:A:720:ASP:O	1:A:724:VAL:HG23	1.91	0.69
2:B:308:ARG:NH1	2:B:308:ARG:HA	2.09	0.67
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.78	0.65
1:A:195:CYS:C	1:A:197:PRO:HD3	2.17	0.65
1:A:209:VAL:O	1:A:213:ILE:HG13	1.97	0.65
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.78	0.65
1:A:807:TYR:N	1:A:808:PRO:HD3	2.12	0.64
1:A:391:TYR:CD2	1:A:395:GLN:HG3	2.32	0.64
1:A:537:GLU:HG2	1:A:544:LEU:HD21	1.80	0.63
1:A:469:LYS:HA	1:A:469:LYS:HE3	1.81	0.62
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.16	0.62
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HB3	2:B:356:ASN:HD21	1.65	0.62
2:B:337:GLN:O	2:B:341:GLU:HB2	1.98	0.61
1:A:453:GLU:OE1	1:A:453:GLU:CA	2.46	0.61
1:A:695:TRP:HE1	1:A:706:LEU:HD22	1.63	0.61
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.82	0.60
1:A:594:ARG:HA	1:A:640:VAL:O	2.01	0.59
1:A:755:PRO:CA	1:A:758:ARG:NH1	2.50	0.59
1:A:419:GLN:HE22	2:B:315:PHE:H	1.52	0.58
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.67	0.58
1:A:287:GLY:HA3	3:A:900:FAD:O5B	2.03	0.58
2:B:397:LYS:O	2:B:397:LYS:HG2	2.03	0.58
1:A:441:LEU:O	1:A:445:LEU:HG	2.04	0.58
1:A:456:LYS:HG2	2:B:370:TYR:HE1	1.67	0.58
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.86	0.57
1:A:671:TRP:HA	1:A:735:PHE:CE1	2.40	0.57
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.40	0.56
1:A:283:ILE:HD12	1:A:294:ALA:HB2	1.86	0.56
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.86	0.56
2:B:424:TYR:CD1	2:B:427:ARG:NH2	2.74	0.55
1:A:506:GLU:O	1:A:508:LEU:N	2.38	0.55
2:B:350:GLN:CA	2:B:350:GLN:HE21	2.19	0.55
2:B:370:TYR:N	2:B:370:TYR:HD2	2.04	0.55
1:A:801:GLU:CG	1:A:809:ALA:HA	2.37	0.55
1:A:761:TYR:CE2	4:A:901:TCA:H3	2.42	0.55
1:A:456:LYS:HG2	2:B:370:TYR:CE1	2.41	0.55
2:B:370:TYR:CD2	2:B:370:TYR:N	2.73	0.55
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.72	0.55
1:A:695:TRP:HE1	1:A:706:LEU:CD2	2.20	0.55
1:A:458:LEU:HD12	1:A:487:LEU:HD12	1.89	0.54
1:A:385:LEU:O	1:A:388:ALA:HB3	2.08	0.54
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.89	0.54
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.38	0.54
1:A:216:ARG:O	1:A:220:LEU:HD12	2.08	0.53
1:A:468:VAL:O	1:A:472:ARG:NH1	2.42	0.53
2:B:333:THR:HG22	2:B:334:VAL:N	2.23	0.53
2:B:337:GLN:HA	2:B:337:GLN:HE21	1.73	0.53
2:B:377:GLN:NE2	2:B:410:GLY:HA3	2.24	0.53
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.09	0.52
1:A:690:GLU:HG2	1:A:691:LEU:HD12	1.92	0.52
1:A:196:PHE:N	1:A:197:PRO:HD3	2.25	0.52
1:A:525:ASP:O	1:A:528:ILE:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:LEU:HD23	2:B:356:ASN:ND2	2.24	0.52
1:A:445:LEU:HB2	2:B:359:LEU:HD12	1.91	0.52
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.92	0.51
2:B:383:TRP:HB3	2:B:388:GLN:HE21	1.75	0.51
2:B:418:LYS:O	2:B:421:PHE:HB2	2.09	0.51
1:A:319:THR:HB	1:A:572:SER:HB3	1.93	0.51
1:A:374:LYS:NZ	1:A:525:ASP:OD1	2.40	0.51
1:A:647:LYS:HE3	1:A:798:PHE:CE1	2.45	0.51
1:A:782:PRO:HG3	1:A:795:ARG:HG3	1.91	0.51
2:B:417:VAL:O	2:B:420:PHE:HB3	2.10	0.51
1:A:255:TYR:CD2	1:A:256:LEU:HD23	2.45	0.51
3:A:900:FAD:C4X	4:A:901:TCA:C3	2.88	0.51
2:B:369:PRO:C	2:B:370:TYR:HD2	2.14	0.50
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.47	0.50
1:A:269:ARG:HH12	1:A:299:SER:HB2	1.77	0.50
1:A:374:LYS:O	1:A:375:ASP:C	2.50	0.50
1:A:551:HIS:O	1:A:553:ASP:N	2.45	0.50
1:A:193:ALA:HB2	1:A:200:ILE:HD13	1.94	0.50
2:B:421:PHE:O	2:B:425:ARG:HB2	2.11	0.49
1:A:260:GLY:O	1:A:264:PHE:CD2	2.65	0.49
1:A:379:GLU:O	1:A:382:PHE:HB3	2.13	0.49
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.93	0.49
1:A:456:LYS:CG	2:B:370:TYR:HE1	2.25	0.49
2:B:347:ARG:HG3	2:B:348:GLN:N	2.28	0.49
1:A:693:LEU:HD12	1:A:694:PHE:N	2.27	0.48
1:A:724:VAL:O	1:A:727:CYS:HB2	2.13	0.48
1:A:256:LEU:HB3	1:A:262:ILE:HG12	1.94	0.48
1:A:230:THR:HG23	1:A:270:ILE:HD12	1.95	0.48
1:A:458:LEU:CD1	1:A:487:LEU:HD12	2.43	0.48
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.95	0.48
2:B:415:VAL:HG22	2:B:419:ASN:HD21	1.77	0.48
1:A:740:VAL:O	1:A:740:VAL:HG12	2.13	0.48
1:A:541:ALA:O	1:A:542:THR:HB	2.14	0.48
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.95	0.48
1:A:680:HIS:CD2	1:A:730:ILE:HG23	2.49	0.48
1:A:331:ALA:HA	3:A:900:FAD:N5	2.29	0.48
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.49	0.48
1:A:606:ASN:HD22	1:A:609:SER:H	1.61	0.48
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.54	0.47
1:A:238:LEU:HD22	1:A:239:GLU:H	1.79	0.47
2:B:383:TRP:CZ2	2:B:420:PHE:HD1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASP:O	2:B:324:VAL:HG23	2.14	0.47
2:B:350:GLN:CA	2:B:350:GLN:NE2	2.77	0.47
2:B:405:ILE:O	2:B:409:ILE:HG13	2.15	0.47
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.97	0.47
1:A:370:VAL:HA	1:A:371:PRO:HD2	1.65	0.47
1:A:364:GLU:OE2	1:A:370:VAL:HG22	2.15	0.47
1:A:626:PRO:HB2	1:A:629:VAL:HG23	1.97	0.47
1:A:533:PHE:O	1:A:537:GLU:HG3	2.15	0.46
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.45	0.46
1:A:525:ASP:O	1:A:527:GLN:N	2.48	0.46
1:A:647:LYS:O	1:A:651:VAL:HG23	2.16	0.46
1:A:807:TYR:N	1:A:808:PRO:CD	2.79	0.46
1:A:418:LEU:HD13	2:B:324:VAL:HG21	1.98	0.46
1:A:786:ILE:HD12	1:A:786:ILE:H	1.80	0.46
1:A:806:ASN:C	1:A:807:TYR:CD2	2.89	0.46
2:B:372:LEU:HA	2:B:373:PRO:HD2	1.62	0.46
1:A:627:LEU:CD1	1:A:651:VAL:HG13	2.46	0.46
1:A:311:ASP:N	1:A:311:ASP:OD1	2.49	0.45
2:B:400:ARG:O	2:B:402:PHE:N	2.47	0.45
1:A:670:PHE:CD1	1:A:670:PHE:C	2.90	0.45
1:A:575:PRO:O	1:A:576:VAL:C	2.55	0.45
2:B:377:GLN:OE1	2:B:411:ASN:HB3	2.17	0.45
1:A:755:PRO:HA	1:A:758:ARG:CZ	2.39	0.45
1:A:763:TYR:HE1	1:A:765:ALA:HA	1.81	0.45
1:A:320:PHE:O	1:A:326:VAL:HA	2.16	0.45
1:A:530:ASP:OD2	1:A:685:THR:HA	2.17	0.45
2:B:385:THR:HA	2:B:388:GLN:HG3	1.97	0.45
1:A:319:THR:CB	1:A:572:SER:HB3	2.47	0.44
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.47	0.44
1:A:448:MET:HB3	2:B:363:LEU:HD11	1.98	0.44
2:B:416:GLN:O	2:B:419:ASN:HB2	2.17	0.44
1:A:492:LYS:HA	1:A:492:LYS:HE3	1.99	0.44
1:A:325:TYR:CE2	1:A:665:CYS:HB3	2.52	0.44
1:A:280:LYS:O	1:A:618:CYS:HB2	2.18	0.44
2:B:369:PRO:HB2	2:B:370:TYR:CE2	2.53	0.44
2:B:403:GLN:OE1	2:B:403:GLN:HA	2.18	0.44
1:A:366:ASN:OD1	1:A:368:GLN:HG3	2.18	0.44
1:A:633:GLN:HA	1:A:634:PRO:HA	1.52	0.44
2:B:429:ASN:O	2:B:432:GLU:N	2.51	0.43
1:A:402:ASN:O	1:A:403:ASN:HB2	2.18	0.43
1:A:424:LYS:O	1:A:426:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.82	0.43
2:B:415:VAL:O	2:B:419:ASN:ND2	2.50	0.43
1:A:255:TYR:HD2	1:A:256:LEU:HD23	1.84	0.42
1:A:363:TYR:CE2	1:A:734:ILE:HG23	2.54	0.42
1:A:474:ILE:HA	1:A:474:ILE:HD12	1.79	0.42
1:A:352:GLU:OE1	1:A:569:ASN:HB3	2.19	0.42
1:A:361:PRO:HB2	1:A:363:TYR:CE1	2.54	0.42
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.85	0.42
1:A:329:LEU:HA	1:A:661:LYS:HD2	2.02	0.42
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.83	0.42
1:A:340:ASN:O	1:A:343:ALA:HB3	2.19	0.42
2:B:413:SER:OG	2:B:415:VAL:HG12	2.20	0.42
2:B:421:PHE:HE2	2:B:434:LEU:HD11	1.84	0.42
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.77	0.42
1:A:374:LYS:O	1:A:378:VAL:HG23	2.18	0.42
1:A:418:LEU:HA	1:A:418:LEU:HD12	1.77	0.42
2:B:420:PHE:HA	2:B:423:ASN:HD22	1.85	0.42
1:A:424:LYS:O	1:A:425:ASP:C	2.58	0.42
1:A:553:ASP:O	1:A:556:ASP:HB2	2.19	0.42
1:A:606:ASN:HD21	1:A:608:ARG:HB2	1.84	0.42
1:A:754:ASP:HA	1:A:755:PRO:HD2	1.63	0.42
2:B:340:MET:O	2:B:342:LEU:N	2.52	0.42
2:B:415:VAL:HG22	2:B:419:ASN:ND2	2.35	0.42
1:A:595:TYR:CE2	1:A:641:PRO:HD2	2.55	0.42
2:B:409:ILE:O	2:B:411:ASN:N	2.50	0.41
1:A:325:TYR:HA	1:A:702:ILE:HD11	2.03	0.41
2:B:369:PRO:C	2:B:370:TYR:CD2	2.92	0.41
1:A:691:LEU:CD2	1:A:727:CYS:SG	3.08	0.41
1:A:710:GLU:OE1	1:A:710:GLU:HA	2.20	0.41
1:A:317:VAL:HG12	1:A:317:VAL:O	2.20	0.41
1:A:366:ASN:OD1	1:A:368:GLN:N	2.53	0.41
1:A:296:GLN:HG2	1:A:819:LEU:HD22	2.01	0.41
1:A:814:ALA:O	1:A:817:SER:N	2.53	0.41
3:A:900:FAD:C4	4:A:901:TCA:H36	2.51	0.41
2:B:384:THR:O	2:B:387:GLU:N	2.54	0.41
2:B:425:ARG:HA	2:B:430:ILE:HG13	2.02	0.41
2:B:419:ASN:HD22	2:B:419:ASN:N	2.19	0.41
1:A:361:PRO:HB2	1:A:363:TYR:HE1	1.86	0.41
1:A:419:GLN:HB3	1:A:520:TYR:CD1	2.54	0.41
1:A:239:GLU:OE1	1:A:239:GLU:HA	2.20	0.41
1:A:724:VAL:HG11	1:A:746:THR:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLU:HG2	1:A:185:HIS:CG	2.56	0.41
1:A:506:GLU:C	1:A:508:LEU:N	2.75	0.41
2:B:349:ILE:O	2:B:353:LYS:HB2	2.20	0.41
2:B:432:GLU:O	2:B:433:VAL:C	2.59	0.41
1:A:538:PHE:O	1:A:538:PHE:CG	2.72	0.40
2:B:369:PRO:HB2	2:B:370:TYR:CD2	2.56	0.40
2:B:350:GLN:NE2	2:B:350:GLN:HA	2.37	0.40
1:A:442:LYS:HE3	2:B:355:THR:HG21	2.03	0.40
1:A:306:LEU:HD13	1:A:584:ILE:HG12	2.03	0.40
1:A:613:THR:CG2	1:A:614:PHE:N	2.84	0.40
1:A:703:LEU:HD23	1:A:703:LEU:HA	1.98	0.40
1:A:715:MET:CE	1:A:723:ILE:HG12	2.52	0.40
1:A:778:GLN:HA	1:A:779:PRO:HD2	1.87	0.40
1:A:287:GLY:O	1:A:290:GLY:N	2.55	0.40
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.74	0.40
2:B:310:PRO:HB3	2:B:316:LEU:HD12	2.04	0.40
1:A:771:ASN:HA	1:A:805:ARG:NH1	2.36	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%)	566 (85%)	75 (11%)	23 (4%)	3 21
2	B	131/482 (27%)	102 (78%)	21 (16%)	8 (6%)	1 10
All	All	795/1334 (60%)	668 (84%)	96 (12%)	31 (4%)	3 18

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	425	ASP

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Mol	Chain	Res	Type
1	A	737	SER
1	A	801	GLU
2	B	326	ALA
2	B	341	GLU
1	A	279	GLY
1	A	288	VAL
1	A	507	LYS
1	A	526	ARG
1	A	573	CYS
1	A	738	SER
2	B	331	ALA
2	B	373	PRO
2	B	410	GLY
2	B	426	ARG
1	A	274	PRO
1	A	316	ARG
1	A	508	LEU
1	A	785	SER
1	A	236	GLN
1	A	313	VAL
1	A	375	ASP
1	A	403	ASN
1	A	516	PRO
1	A	225	PRO
1	A	369	ALA
2	B	425	ARG
2	B	439	ALA
1	A	371	PRO
1	A	428	ILE
1	A	733	GLY

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	117/395 (30%)	98 (84%)	19 (16%)	2 10
All	All	683/1094 (62%)	596 (87%)	87 (13%)	4 19

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	PHE
1	A	183	LEU
1	A	191	GLN
1	A	220	LEU
1	A	226	LYS
1	A	237	GLN
1	A	238	LEU
1	A	267	TYR
1	A	269	ARG
1	A	274	PRO
1	A	281	VAL
1	A	296	GLN
1	A	299	SER
1	A	313	VAL
1	A	324	ASN
1	A	329	LEU
1	A	359	LYS
1	A	380	GLN
1	A	392	LEU
1	A	404	LYS
1	A	418	LEU
1	A	423	VAL
1	A	429	GLU
1	A	437	THR
1	A	438	GLN
1	A	453	GLU
1	A	456	LYS
1	A	457	GLU
1	A	458	LEU
1	A	466	SER
1	A	467	GLU
1	A	469	LYS
1	A	479	LEU
1	A	482	SER
1	A	487	LEU
1	A	492	LYS

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Mol	Chain	Res	Type
1	A	509	GLN
1	A	512	GLU
1	A	514	ASN
1	A	524	ARG
1	A	526	ARG
1	A	535	ASN
1	A	538	PHE
1	A	556	ASP
1	A	568	ARG
1	A	571	TYR
1	A	591	ARG
1	A	594	ARG
1	A	607	THR
1	A	610	THR
1	A	612	GLN
1	A	632	GLN
1	A	633	GLN
1	A	645	GLU
1	A	652	GLN
1	A	659	LEU
1	A	667	ASP
1	A	684	THR
1	A	699	LYS
1	A	704	LEU
1	A	706	LEU
1	A	717	ASN
1	A	719	SER
1	A	727	CYS
1	A	780	ILE
1	A	785	SER
1	A	786	ILE
1	A	815	LEU
2	B	308	ARG
2	B	337	GLN
2	B	344	SER
2	B	347	ARG
2	B	349	ILE
2	B	350	GLN
2	B	351	ASN
2	B	352	ILE
2	B	357	SER
2	B	370	TYR

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Mol	Chain	Res	Type
2	B	375	VAL
2	B	376	ILE
2	B	379	CYS
2	B	385	THR
2	B	409	ILE
2	B	414	VAL
2	B	422	VAL
2	B	423	ASN
2	B	427	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	410	GLN
1	A	419	GLN
1	A	422	HIS
1	A	438	GLN
1	A	484	HIS
1	A	535	ASN
1	A	564	HIS
1	A	828	GLN
2	B	337	GLN
2	B	348	GLN
2	B	350	GLN
2	B	388	GLN
2	B	419	ASN
2	B	423	ASN

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 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	$\#\|Z\| > 2$
4	TCA	A	901	3	10,10,11	3.54	2 (20%)	11,11,13	3.54	2 (18%)
3	FAD	A	900	4	51,58,58	2.84	12 (23%)	60,89,89	2.53	16 (26%)

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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	TCA	C2-C3	10.40	1.52	1.34
3	A	900	FAD	C4X-N5	9.16	1.46	1.33
3	A	900	FAD	C2A-N3A	8.90	1.46	1.32
3	A	900	FAD	C4X-C10	8.58	1.47	1.38
3	A	900	FAD	C2A-N1A	7.93	1.48	1.33
3	A	900	FAD	C9A-N10	4.89	1.45	1.38
3	A	900	FAD	O4-C4	4.83	1.36	1.24
3	A	900	FAD	C5X-N5	3.95	1.41	1.35
3	A	900	FAD	C4-C4X	2.84	1.46	1.41
4	A	901	TCA	C2-C1	2.84	1.53	1.44
3	A	900	FAD	C1'-N10	2.48	1.50	1.48
3	A	900	FAD	C10-N1	2.46	1.36	1.33
3	A	900	FAD	C5'-C4'	2.16	1.54	1.51
3	A	900	FAD	C2B-C1B	-2.09	1.50	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	TCA	C31-C3-C2	-11.00	109.78	127.21
3	A	900	FAD	N3A-C2A-N1A	-9.35	114.07	128.68
3	A	900	FAD	C4-N3-C2	8.76	122.54	115.14
3	A	900	FAD	C9A-N10-C10	-6.07	113.96	121.91
3	A	900	FAD	C5X-C9A-N10	5.37	121.60	117.72
3	A	900	FAD	C4-C4X-C10	-5.06	116.60	119.95
3	A	900	FAD	C4-C4X-N5	-3.61	114.47	118.60
3	A	900	FAD	C4X-C4-N3	-3.58	118.54	123.43
3	A	900	FAD	C4X-C10-N10	-3.34	116.87	120.30
3	A	900	FAD	C6-C5X-N5	-3.13	115.60	119.05
3	A	900	FAD	C4X-N5-C5X	-3.03	113.75	116.77
4	A	901	TCA	O-C1-C2	-2.91	115.73	125.67
3	A	900	FAD	C1B-N9A-C4A	-2.82	121.69	126.64
3	A	900	FAD	P-O3P-PA	-2.61	123.88	132.83
3	A	900	FAD	O4B-C1B-C2B	-2.38	103.45	106.93
3	A	900	FAD	C2A-N1A-C6A	2.28	122.66	118.75
3	A	900	FAD	O5'-C5'-C4'	2.24	115.33	109.36
3	A	900	FAD	O2A-PA-O1A	2.03	122.29	112.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	TCA	C1-C2-C3-C31
3	A	900	FAD	C2'-C1'-N10-C10
3	A	900	FAD	PA-O3P-P-O5'
4	A	901	TCA	C2-C3-C31-C36
4	A	901	TCA	C2-C3-C31-C32
3	A	900	FAD	O4B-C4B-C5B-O5B

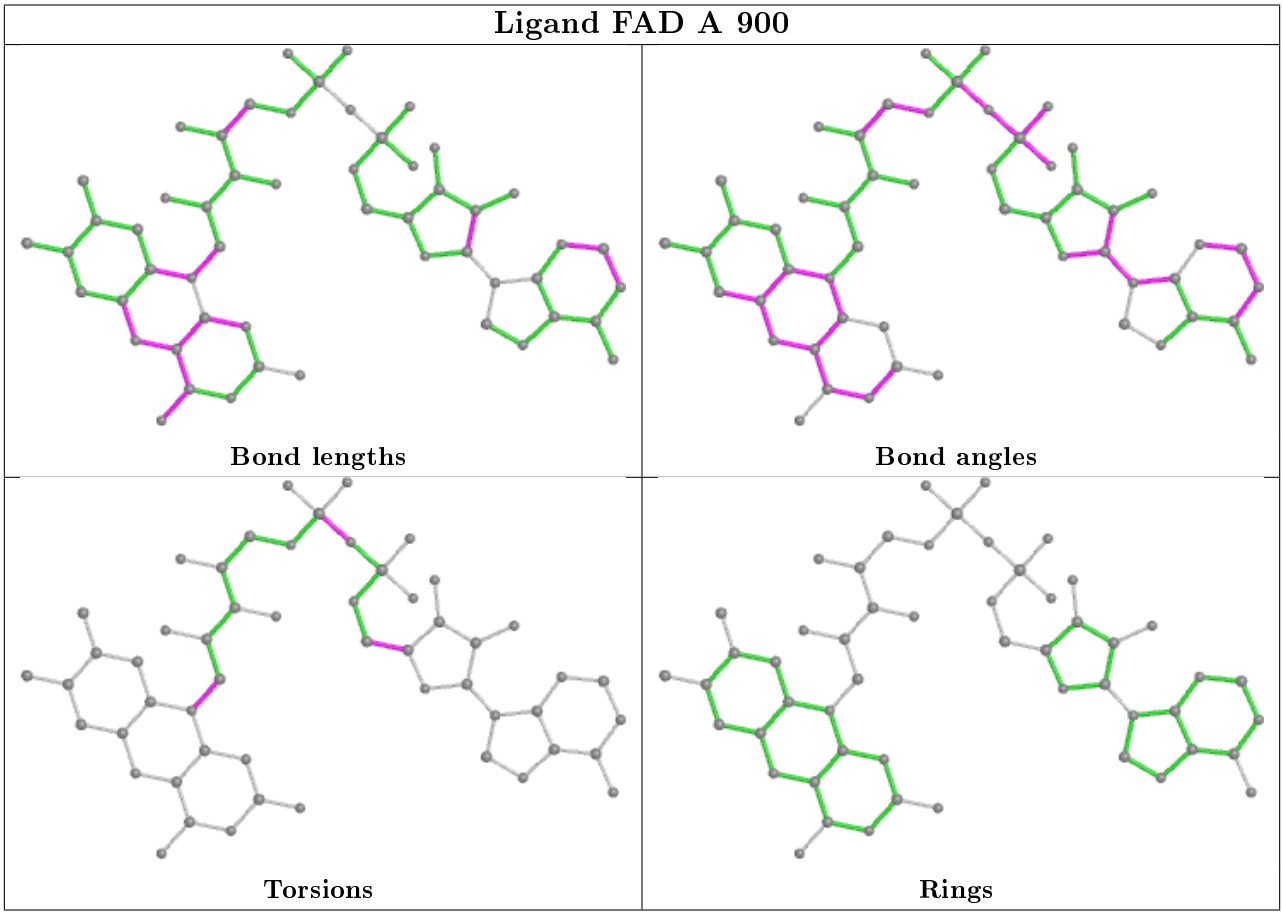
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	TCA	3	0
3	A	900	FAD	4	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.



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%)	0.15	4 (0%)	89	90	34, 65, 93, 107	0
2	B	133/482 (27%)	0.45	4 (3%)	50	49	66, 94, 110, 118	0
All	All	799/1334 (59%)	0.20	8 (1%)	82	82	34, 70, 101, 118	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	2.6
2	B	376	ILE	2.4
1	A	509	GLN	2.3
2	B	374	GLU	2.3
2	B	378	LYS	2.3
1	A	436	LYS	2.2
1	A	503	LYS	2.1
2	B	379	CYS	2.0

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,

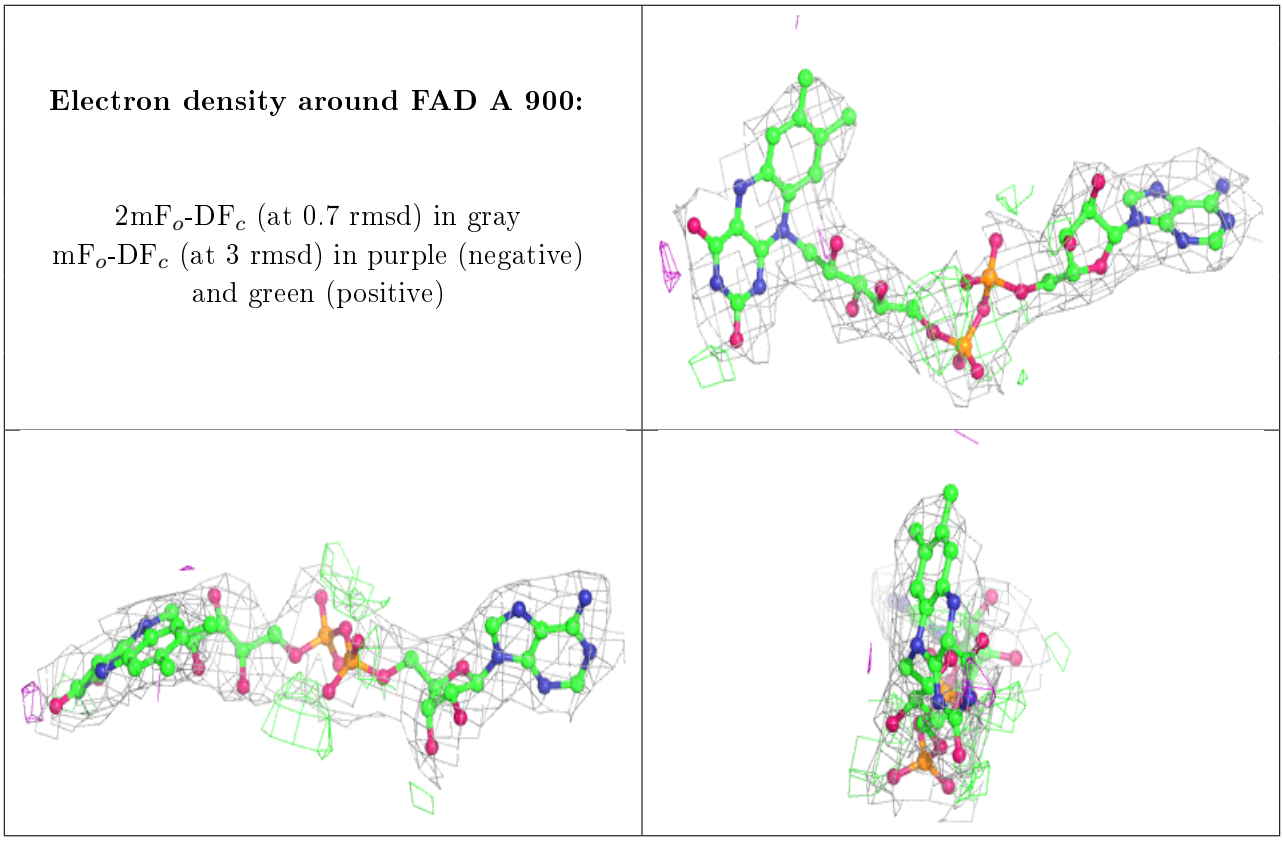
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TCA	A	901	10/11	0.96	0.38	59,69,71,71	0
3	FAD	A	900	53/53	0.99	0.23	37,43,59,61	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.