Full wwPDB X-ray Structure Validation Report (i)

May 13, 2024 – 03:07 pm BST

PDB ID	:	8Q1G
Title	:	LSD1-CoREST bound to Acetylated K14 of Histone H3
Authors	:	Barone, M.; Mattevi, A.
Deposited on	:	2023-07-31
Resolution	:	2.60 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

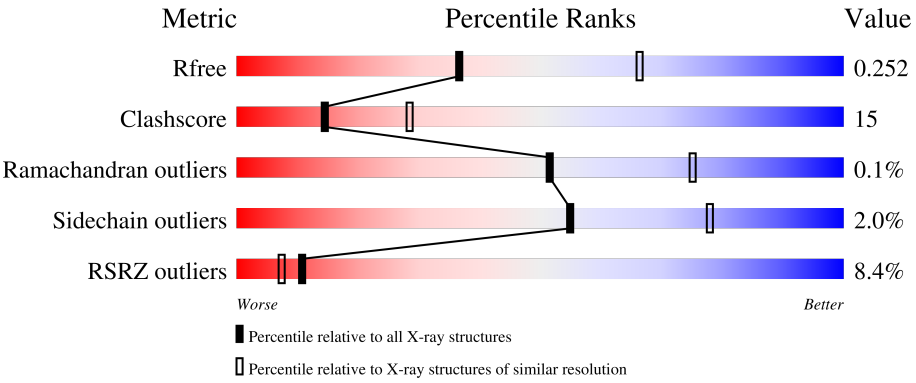
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	730	5% 65% 25% · 9%
2	B	178	15% 37% 34% · 25%
3	C	21	14% 38% 38% 24%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6471 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 1A.

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			

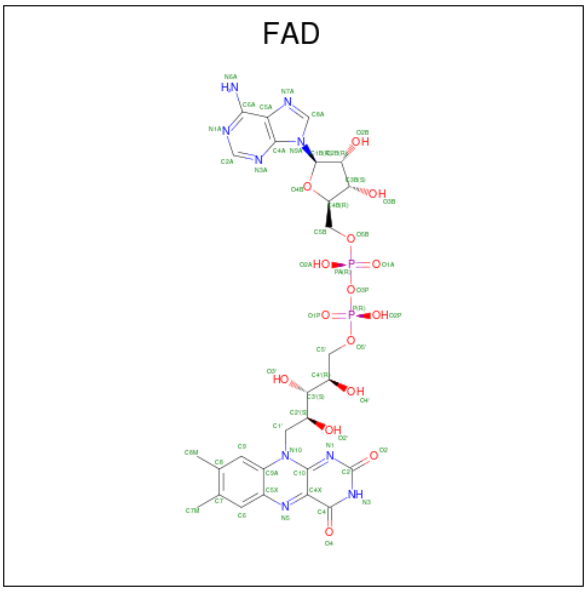
- Molecule 3 is a protein called Histone H3.3C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	S	0	0	0
			117	69	25	22	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	LYS	conflict	UNP Q6NXT2

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 5 is water.

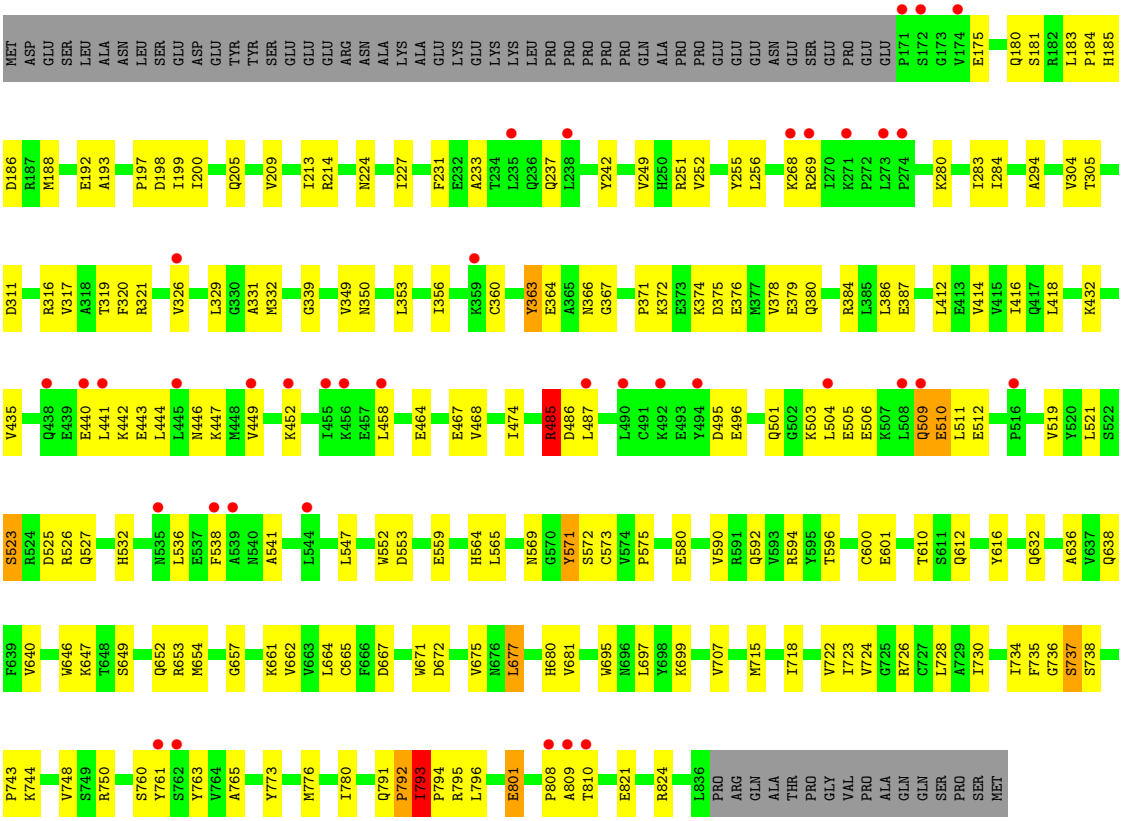
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		

3 Residue-property plots (i)

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.

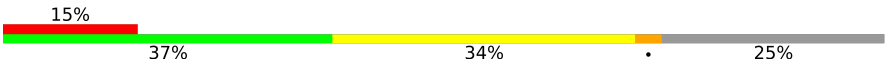
• Molecule 1: Lysine-specific histone demethylase 1A

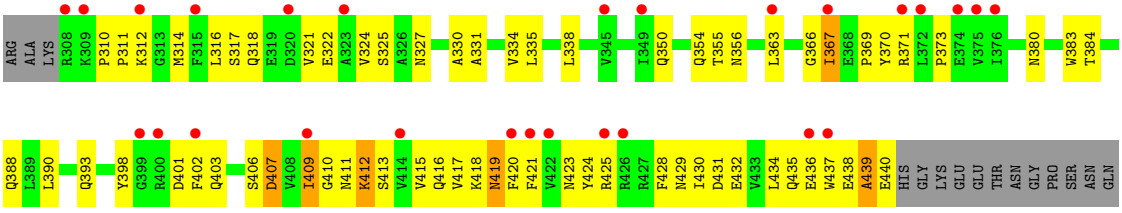
Chain A:

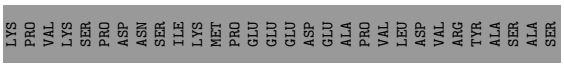


• Molecule 2: REST corepressor 1

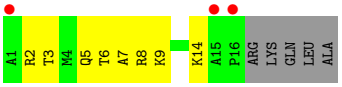
Chain B:







• Molecule 3: Histone H3.3C



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.51Å 179.69Å 232.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.73 – 2.60 48.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (48.73-2.60) 95.0 (48.73-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158)	Depositor
R, R_{free}	0.222 , 0.255 0.223 , 0.252	Depositor DCC
R_{free} test set	1949 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å^2)	81.2	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 72.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6471	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: ALY, 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	0.49	0/5331	0.77	12/7232 (0.2%)
2	B	0.46	0/1091	0.94	11/1471 (0.7%)
3	C	0.40	0/104	0.71	0/136
All	All	0.48	0/6526	0.80	23/8839 (0.3%)

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	4
2	B	0	1
All	All	0	5

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	409	ILE	N-CA-C	-11.65	79.54	111.00
1	A	652	GLN	CB-CA-C	-9.48	91.43	110.40
2	B	419	ASN	CB-CA-C	-8.34	93.71	110.40
2	B	439	ALA	N-CA-C	-8.27	88.69	111.00
1	A	737	SER	CB-CA-C	7.99	125.29	110.10
2	B	367	ILE	CB-CA-C	7.45	126.51	111.60
1	A	699	LYS	CB-CA-C	-7.39	95.62	110.40
2	B	373	PRO	CB-CA-C	-7.22	93.94	112.00
1	A	510	GLU	CB-CA-C	-6.75	96.89	110.40
2	B	410	GLY	N-CA-C	6.75	129.98	113.10
1	A	468	VAL	CB-CA-C	6.75	124.22	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	468	VAL	N-CA-C	-6.43	93.63	111.00
2	B	409	ILE	CB-CA-C	-6.35	98.89	111.60
1	A	738	SER	N-CA-CB	-6.19	101.22	110.50
1	A	485	ARG	CB-CA-C	-6.03	98.33	110.40
1	A	610	THR	CB-CA-C	5.81	127.30	111.60
2	B	439	ALA	CB-CA-C	5.68	118.62	110.10
2	B	412	LYS	CA-CB-CG	-5.63	101.02	113.40
2	B	412	LYS	CB-CG-CD	5.32	125.42	111.60
1	A	652	GLN	N-CA-C	5.27	125.24	111.00
1	A	612	GLN	CB-CA-C	5.20	120.81	110.40
1	A	738	SER	N-CA-C	5.14	124.88	111.00
2	B	419	ASN	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ARG	Sidechain
1	A	509	GLN	Peptide
1	A	526	ARG	Sidechain
1	A	792	PRO	Peptide
2	B	367	ILE	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	149	0
2	B	1076	0	1091	60	0
3	C	117	0	126	10	0
4	A	53	0	31	4	0
5	A	8	0	0	2	0
All	All	6471	0	6500	200	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 (200) 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)
2:B:419:ASN:O	2:B:423:ASN:OD1	1.61	1.15
1:A:374:LYS:NZ	1:A:525:ASP:OD1	2.07	0.86
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.63	0.81
1:A:760:SER:HB2	4:A:901:FAD:HM83	1.64	0.80
1:A:209:VAL:O	1:A:213:ILE:HD12	1.86	0.75
1:A:379:GLU:HG3	1:A:532:HIS:CE1	2.24	0.72
1:A:331:ALA:HA	4:A:901:FAD:C4X	2.19	0.71
1:A:485:ARG:O	1:A:485:ARG:HD2	1.90	0.70
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.75	0.69
1:A:495:ASP:OD1	2:B:371:ARG:NH2	2.25	0.69
1:A:671:TRP:HA	1:A:735:PHE:CE2	2.28	0.69
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.56	0.68
2:B:406:SER:O	2:B:409:ILE:O	2.11	0.68
1:A:198:ASP:OD1	1:A:199:ILE:HG13	1.94	0.68
2:B:406:SER:OG	2:B:412:LYS:O	2.08	0.67
2:B:432:GLU:HA	2:B:435:GLN:HG2	1.76	0.67
1:A:485:ARG:HG2	2:B:407:ASP:HB2	1.77	0.67
1:A:536:LEU:HD23	3:C:5:GLN:HE22	1.57	0.67
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.30	0.67
1:A:671:TRP:HA	1:A:735:PHE:HE2	1.59	0.66
2:B:318:GLN:NE2	2:B:322:GLU:OE2	2.29	0.66
1:A:592:GLN:HG3	1:A:638:GLN:HB3	1.77	0.66
1:A:728:LEU:HD11	1:A:743:PRO:HD3	1.78	0.65
1:A:184:PRO:O	1:A:214:ARG:NH2	2.30	0.65
1:A:734:ILE:HG22	1:A:735:PHE:CD1	2.31	0.65
2:B:419:ASN:O	2:B:423:ASN:CG	2.35	0.64
1:A:672:ASP:HB3	1:A:675:VAL:HG22	1.80	0.64
1:A:193:ALA:HB2	1:A:200:ILE:HD13	1.80	0.63
1:A:821:GLU:OE2	1:A:824:ARG:NH1	2.32	0.63
2:B:334:VAL:HG13	2:B:335:LEU:HD23	1.81	0.63
1:A:331:ALA:HA	4:A:901:FAD:N5	2.14	0.62
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.82	0.62
1:A:501:GLN:O	1:A:505:GLU:HB2	2.00	0.62
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.82	0.61
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.14	0.61
1:A:233:ALA:O	1:A:237:GLN:HG3	2.01	0.61
2:B:425:ARG:HA	2:B:430:ILE:HD13	1.83	0.60
1:A:198:ASP:OD1	1:A:199:ILE:N	2.34	0.60
1:A:280:LYS:HE3	1:A:305:THR:HG23	1.83	0.60
1:A:677:LEU:HD12	3:C:7:ALA:HB2	1.83	0.60
2:B:434:LEU:O	2:B:438:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HG22	1:A:268:LYS:HB2	1.83	0.60
1:A:553:ASP:OD2	5:A:1001:HOH:O	2.17	0.59
2:B:388:GLN:HB3	2:B:428:PHE:HE2	1.67	0.59
2:B:439:ALA:O	2:B:440:GLU:CB	2.50	0.59
1:A:722:VAL:O	1:A:726:ARG:HG3	2.01	0.59
1:A:175:GLU:HG2	1:A:185:HIS:CG	2.37	0.59
1:A:188:MET:HE3	1:A:200:ILE:HB	1.85	0.58
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.86	0.58
2:B:415:VAL:O	2:B:418:LYS:N	2.38	0.57
1:A:412:LEU:O	1:A:416:ILE:HG13	2.04	0.57
1:A:320:PHE:HB2	1:A:329:LEU:HD11	1.87	0.56
1:A:353:LEU:HD13	1:A:565:LEU:HD22	1.87	0.56
1:A:750:ARG:HG3	1:A:750:ARG:NH1	2.20	0.56
1:A:760:SER:CB	4:A:901:FAD:HM83	2.35	0.56
1:A:360:CYS:O	3:C:8:ARG:NH2	2.38	0.56
1:A:332:MET:HE3	1:A:661:LYS:HZ2	1.69	0.55
2:B:437:TRP:HE3	2:B:438:GLU:HG2	1.72	0.55
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.71	0.55
1:A:364:GLU:HA	1:A:681:VAL:HB	1.89	0.55
1:A:506:GLU:HA	1:A:509:GLN:OE1	2.07	0.55
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.71	0.54
1:A:284:ILE:HG12	1:A:590:VAL:HG21	1.88	0.54
1:A:594:ARG:HA	1:A:640:VAL:O	2.07	0.54
1:A:510:GLU:HB3	1:A:511:LEU:HD23	1.90	0.54
1:A:255:TYR:CD2	1:A:256:LEU:HD23	2.41	0.54
1:A:332:MET:CE	1:A:661:LYS:NZ	2.70	0.54
1:A:384:ARG:NH1	2:B:312:LYS:O	2.37	0.54
2:B:425:ARG:HA	2:B:430:ILE:CD1	2.38	0.53
1:A:205:GLN:O	1:A:209:VAL:HG23	2.09	0.53
1:A:442:LYS:CE	2:B:355:THR:HG21	2.39	0.53
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.90	0.53
1:A:366:ASN:OD1	1:A:367:GLY:N	2.41	0.53
1:A:379:GLU:OE1	3:C:8:ARG:HD2	2.09	0.52
2:B:425:ARG:NH1	2:B:431:ASP:OD1	2.42	0.52
2:B:437:TRP:CE3	2:B:438:GLU:HG2	2.45	0.52
1:A:374:LYS:O	1:A:378:VAL:HG23	2.10	0.52
1:A:801:GLU:HG3	1:A:809:ALA:CA	2.39	0.52
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.44	0.52
1:A:601:GLU:HA	1:A:616:TYR:O	2.10	0.51
2:B:324:VAL:HG13	2:B:331:ALA:HB2	1.91	0.51
1:A:349:VAL:HG12	1:A:350:ASN:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:SER:OG	2:B:415:VAL:HG12	2.11	0.51
1:A:594:ARG:HG2	1:A:640:VAL:HB	1.92	0.50
1:A:649:SER:HB3	1:A:653:ARG:NH1	2.25	0.50
2:B:432:GLU:O	2:B:436:GLU:HB2	2.10	0.50
1:A:188:MET:HE3	1:A:200:ILE:CB	2.42	0.50
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.94	0.50
1:A:198:ASP:OD2	1:A:251:ARG:NH2	2.44	0.50
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.46	0.50
1:A:380:GLN:O	1:A:384:ARG:HG3	2.12	0.49
2:B:430:ILE:H	2:B:430:ILE:HD12	1.76	0.49
1:A:387:GLU:HB2	2:B:311:PRO:HG3	1.94	0.49
1:A:780:ILE:HB	1:A:796:LEU:HB3	1.94	0.49
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.94	0.49
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.94	0.49
1:A:646:TRP:CZ3	1:A:647:LYS:HE2	2.47	0.49
2:B:432:GLU:HA	2:B:435:GLN:CG	2.41	0.49
1:A:432:LYS:HA	1:A:435:VAL:HG22	1.95	0.49
2:B:310:PRO:HB3	2:B:316:LEU:HD12	1.93	0.49
2:B:417:VAL:HG12	2:B:421:PHE:HE1	1.77	0.48
1:A:379:GLU:OE1	3:C:8:ARG:NH1	2.46	0.48
2:B:388:GLN:HB3	2:B:428:PHE:CE2	2.48	0.48
1:A:464:GLU:HA	1:A:467:GLU:HG2	1.95	0.48
1:A:371:PRO:O	1:A:372:LYS:C	2.51	0.48
1:A:726:ARG:O	1:A:730:ILE:HG12	2.13	0.48
1:A:474:ILE:HG23	2:B:393:GLN:HE22	1.78	0.48
1:A:572:SER:O	1:A:575:PRO:HD2	2.13	0.48
1:A:750:ARG:HG3	1:A:750:ARG:HH11	1.78	0.48
1:A:384:ARG:NH2	2:B:312:LYS:O	2.47	0.47
1:A:680:HIS:CD2	1:A:730:ILE:HD12	2.49	0.47
1:A:213:ILE:HG22	1:A:252:VAL:HG11	1.96	0.47
1:A:319:THR:HB	1:A:572:SER:HB3	1.96	0.47
1:A:374:LYS:O	1:A:375:ASP:C	2.52	0.47
1:A:632:GLN:NE2	1:A:636:ALA:HB2	2.29	0.47
1:A:776:MET:HE2	1:A:776:MET:HB3	1.70	0.47
2:B:411:ASN:O	2:B:412:LYS:HG2	2.15	0.47
1:A:356:ILE:HD13	1:A:695:TRP:HZ3	1.80	0.47
1:A:649:SER:HB3	1:A:653:ARG:HH12	1.78	0.47
2:B:402:PHE:CD2	2:B:418:LYS:HG2	2.49	0.47
1:A:569:ASN:OD1	1:A:569:ASN:N	2.42	0.47
1:A:736:GLY:O	1:A:737:SER:C	2.53	0.47
2:B:322:GLU:HA	2:B:325:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ARG:HG2	1:A:326:VAL:HG12	1.97	0.47
2:B:369:PRO:C	2:B:370:TYR:HD1	2.17	0.47
2:B:380:ASN:O	2:B:416:GLN:NE2	2.48	0.47
1:A:509:GLN:HA	1:A:512:GLU:HB3	1.96	0.46
2:B:439:ALA:O	2:B:440:GLU:HB3	2.14	0.46
1:A:443:GLU:O	1:A:447:LYS:NZ	2.48	0.46
1:A:452:LYS:HE3	2:B:366:GLY:O	2.16	0.46
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.51	0.46
1:A:571:TYR:O	1:A:572:SER:C	2.53	0.46
1:A:181:SER:O	1:A:183:LEU:HD13	2.15	0.46
2:B:401:ASP:O	2:B:403:GLN:N	2.49	0.46
1:A:596:THR:HA	5:A:1002:HOH:O	2.15	0.46
2:B:327:ASN:OD1	2:B:330:ALA:N	2.48	0.46
1:A:372:LYS:O	1:A:376:GLU:HG3	2.15	0.45
1:A:707:VAL:HG11	1:A:715:MET:HG3	1.98	0.45
1:A:559:GLU:HB2	3:C:3:THR:HG22	1.99	0.45
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.51	0.45
1:A:808:PRO:O	1:A:810:THR:HG23	2.16	0.45
2:B:363:LEU:HD23	2:B:363:LEU:N	2.31	0.45
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.99	0.45
1:A:763:TYR:HE1	1:A:765:ALA:HA	1.82	0.45
1:A:197:PRO:HA	1:A:200:ILE:HG22	1.99	0.45
2:B:318:GLN:O	2:B:321:VAL:HG22	2.17	0.45
1:A:665:CYS:O	1:A:744:LYS:N	2.46	0.44
2:B:420:PHE:CD2	2:B:424:TYR:CD2	3.05	0.44
1:A:734:ILE:HG22	1:A:735:PHE:CE1	2.53	0.44
1:A:332:MET:CE	1:A:661:LYS:HZ3	2.30	0.44
1:A:485:ARG:HD2	1:A:485:ARG:C	2.38	0.44
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.63	0.44
1:A:185:HIS:CE1	1:A:186:ASP:HB3	2.53	0.43
1:A:283:ILE:HD12	1:A:294:ALA:HB2	1.99	0.43
2:B:403:GLN:O	2:B:406:SER:N	2.50	0.43
1:A:440:GLU:HB3	1:A:504:LEU:CD1	2.48	0.43
1:A:224:ASN:ND2	1:A:227:ILE:HD11	2.34	0.43
2:B:383:TRP:CD2	2:B:412:LYS:NZ	2.62	0.43
1:A:791:GLN:HA	1:A:792:PRO:HD3	1.91	0.43
2:B:383:TRP:CE3	2:B:412:LYS:NZ	2.82	0.43
3:C:14:ALY:HE2	3:C:14:ALY:HH31	1.72	0.43
1:A:564:HIS:ND1	3:C:6:THR:OG1	2.32	0.43
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.46	0.43
2:B:317:SER:O	2:B:321:VAL:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:HIS:ND1	1:A:186:ASP:HB3	2.34	0.42
2:B:350:GLN:O	2:B:354:GLN:HG3	2.20	0.42
2:B:429:ASN:HB3	2:B:432:GLU:CG	2.49	0.42
1:A:183:LEU:HD23	1:A:214:ARG:HD3	2.02	0.42
1:A:458:LEU:HB3	1:A:487:LEU:HD12	2.01	0.42
1:A:677:LEU:CD1	3:C:7:ALA:HB2	2.47	0.42
1:A:521:LEU:HB3	1:A:525:ASP:HB2	2.01	0.42
1:A:446:ASN:O	1:A:449:VAL:HG12	2.20	0.41
1:A:485:ARG:C	1:A:485:ARG:CD	2.88	0.41
1:A:793:ILE:HA	1:A:794:PRO:HD3	1.75	0.41
1:A:367:GLY:HA2	1:A:734:ILE:CD1	2.51	0.41
1:A:367:GLY:HA2	1:A:734:ILE:HD12	2.02	0.41
1:A:458:LEU:HD21	1:A:486:ASP:HB3	2.02	0.41
1:A:503:LYS:HB2	1:A:503:LYS:HE2	1.49	0.41
1:A:192:GLU:OE1	1:A:214:ARG:NH1	2.48	0.41
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.92	0.41
1:A:523:SER:O	1:A:527:GLN:HG3	2.20	0.41
2:B:334:VAL:O	2:B:338:LEU:HG	2.20	0.41
2:B:401:ASP:O	2:B:402:PHE:C	2.58	0.41
2:B:430:ILE:HG22	2:B:434:LEU:HD12	2.01	0.41
3:C:2:ARG:O	3:C:9:LYS:HE3	2.21	0.41
2:B:429:ASN:HB3	2:B:432:GLU:CD	2.40	0.41
1:A:316:ARG:NH1	1:A:801:GLU:OE1	2.53	0.41
1:A:667:ASP:OD1	1:A:667:ASP:N	2.45	0.41
1:A:600:CYS:SG	1:A:795:ARG:HB3	2.60	0.41
2:B:384:THR:O	2:B:388:GLN:HG3	2.21	0.41
1:A:317:VAL:HG22	1:A:331:ALA:HB3	2.03	0.41
1:A:443:GLU:HG3	1:A:444:LEU:N	2.36	0.41
1:A:680:HIS:NE2	1:A:730:ILE:HD12	2.36	0.41
1:A:414:VAL:O	1:A:418:LEU:HG	2.22	0.40
1:A:541:ALA:O	1:A:657:GLY:HA3	2.21	0.40
1:A:571:TYR:O	1:A:573:CYS:N	2.54	0.40
1:A:664:LEU:HD21	1:A:724:VAL:HG13	2.01	0.40
1:A:763:TYR:CE1	1:A:765:ALA:HA	2.57	0.40
2:B:370:TYR:CD1	2:B:370:TYR:N	2.90	0.40
1:A:311:ASP:OD1	1:A:311:ASP:N	2.40	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	664/730 (91%)	633 (95%)	30 (4%)	1 (0%)	47 71
2	B	131/178 (74%)	123 (94%)	8 (6%)	0	100 100
3	C	13/21 (62%)	11 (85%)	2 (15%)	0	100 100
All	All	808/929 (87%)	767 (95%)	40 (5%)	1 (0%)	51 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	793	ILE

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	566/623 (91%)	553 (98%)	13 (2%)	50 75
2	B	117/156 (75%)	116 (99%)	1 (1%)	78 91
3	C	10/14 (71%)	10 (100%)	0	100 100
All	All	693/793 (87%)	679 (98%)	14 (2%)	55 78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	304	VAL
1	A	363	TYR

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Mol	Chain	Res	Type
1	A	485	ARG
1	A	496	GLU
1	A	519	VAL
1	A	523	SER
1	A	538	PHE
1	A	571	TYR
1	A	580	GLU
1	A	654	MET
1	A	677	LEU
1	A	793	ILE
1	A	801	GLU
2	B	407	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	A	532	HIS
1	A	812	HIS
2	B	429	ASN
3	C	5	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)

1 non-standard protein/DNA/RNA residue is 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	ALY	C	14	3	10,11,12	1.07	0	7,12,14	0.84	0

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	ALY	C	14	3	-	2/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	14	ALY	OH-CH-NZ-CE
3	C	14	ALY	CH3-CH-NZ-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	14	ALY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	FAD	A	901	-	53,58,58	0.54	1 (1%)	68,89,89	0.73	2 (2%)

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	FAD	A	901	-	-	6/30/50/50	0/6/6/6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	FAD	C8A-N7A	-2.02	1.31	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	FAD	O2A-PA-O1A	2.59	125.04	112.24
4	A	901	FAD	C5A-C6A-N6A	2.53	124.20	120.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	FAD	PA-O3P-P-O5'
4	A	901	FAD	C2'-C3'-C4'-O4'
4	A	901	FAD	C2'-C3'-C4'-C5'
4	A	901	FAD	O4B-C4B-C5B-O5B
4	A	901	FAD	P-O3P-PA-O2A
4	A	901	FAD	O3'-C3'-C4'-C5'

There are no ring outliers.

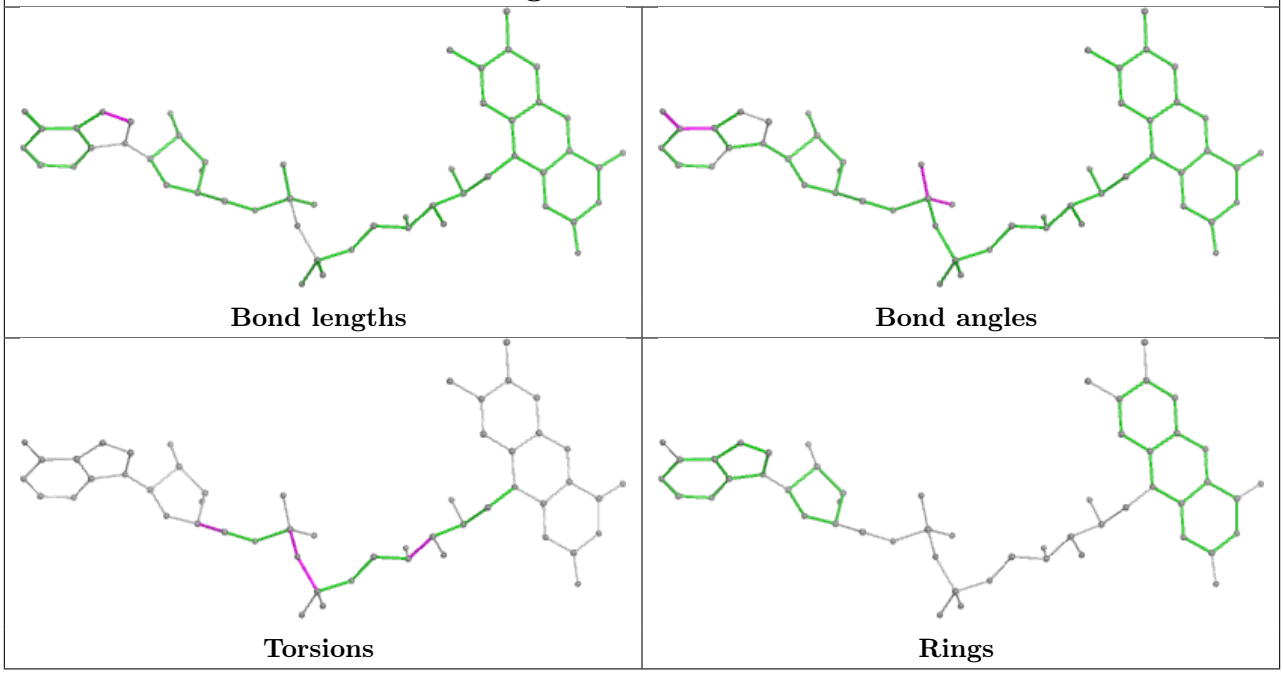
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	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.

Ligand FAD A 901



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	666/730 (91%)	0.66	38 (5%) 23 18	61, 89, 122, 140	0
2	B	133/178 (74%)	1.02	27 (20%) 1 0	91, 122, 141, 156	0
3	C	15/21 (71%)	1.03	3 (20%) 1 0	74, 83, 118, 137	0
All	All	814/929 (87%)	0.72	68 (8%) 11 7	61, 94, 132, 156	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	6.6
2	B	375	VAL	6.2
3	C	16	PRO	5.7
2	B	414	VAL	5.5
2	B	367	ILE	4.8
2	B	372	LEU	4.3
1	A	274	PRO	3.8
1	A	273	LEU	3.7
1	A	508	LEU	3.7
1	A	172	SER	3.4
2	B	436	GLU	3.3
1	A	238	LEU	3.3
2	B	308	ARG	3.3
2	B	422	VAL	3.1
1	A	458	LEU	3.1
1	A	441	LEU	3.1
2	B	399	GLY	3.1
2	B	323	ALA	3.0
1	A	516	PRO	3.0
2	B	426	ARG	3.0
2	B	312	LYS	2.9
1	A	455	ILE	2.8
2	B	309	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	449	VAL	2.8
1	A	504	LEU	2.7
2	B	402	PHE	2.7
1	A	269	ARG	2.6
1	A	494	TYR	2.6
2	B	376	ILE	2.6
2	B	349	ILE	2.6
1	A	539	ALA	2.6
1	A	174	VAL	2.6
1	A	359	LYS	2.5
2	B	374	GLU	2.5
2	B	420	PHE	2.5
2	B	400	ARG	2.5
1	A	809	ALA	2.4
1	A	492	LYS	2.4
1	A	762	SER	2.3
1	A	440	GLU	2.3
1	A	490	LEU	2.3
2	B	320	ASP	2.3
2	B	409	ILE	2.3
1	A	271	LYS	2.3
1	A	235	LEU	2.3
1	A	808	PRO	2.2
1	A	452	LYS	2.2
1	A	509	GLN	2.2
3	C	1	ALA	2.2
2	B	363	LEU	2.2
2	B	437	TRP	2.2
1	A	326	VAL	2.2
1	A	544	LEU	2.1
1	A	268	LYS	2.1
2	B	315	PHE	2.1
1	A	445	LEU	2.1
1	A	761	TYR	2.1
1	A	438	GLN	2.1
2	B	421	PHE	2.1
2	B	345	VAL	2.1
1	A	810	THR	2.1
1	A	538	PHE	2.1
3	C	15	ALA	2.1
2	B	425	ARG	2.1
1	A	456	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	371	ARG	2.0
1	A	535	ASN	2.0
1	A	487	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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
3	ALY	C	14	12/13	0.93	0.20	81,101,118,120	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

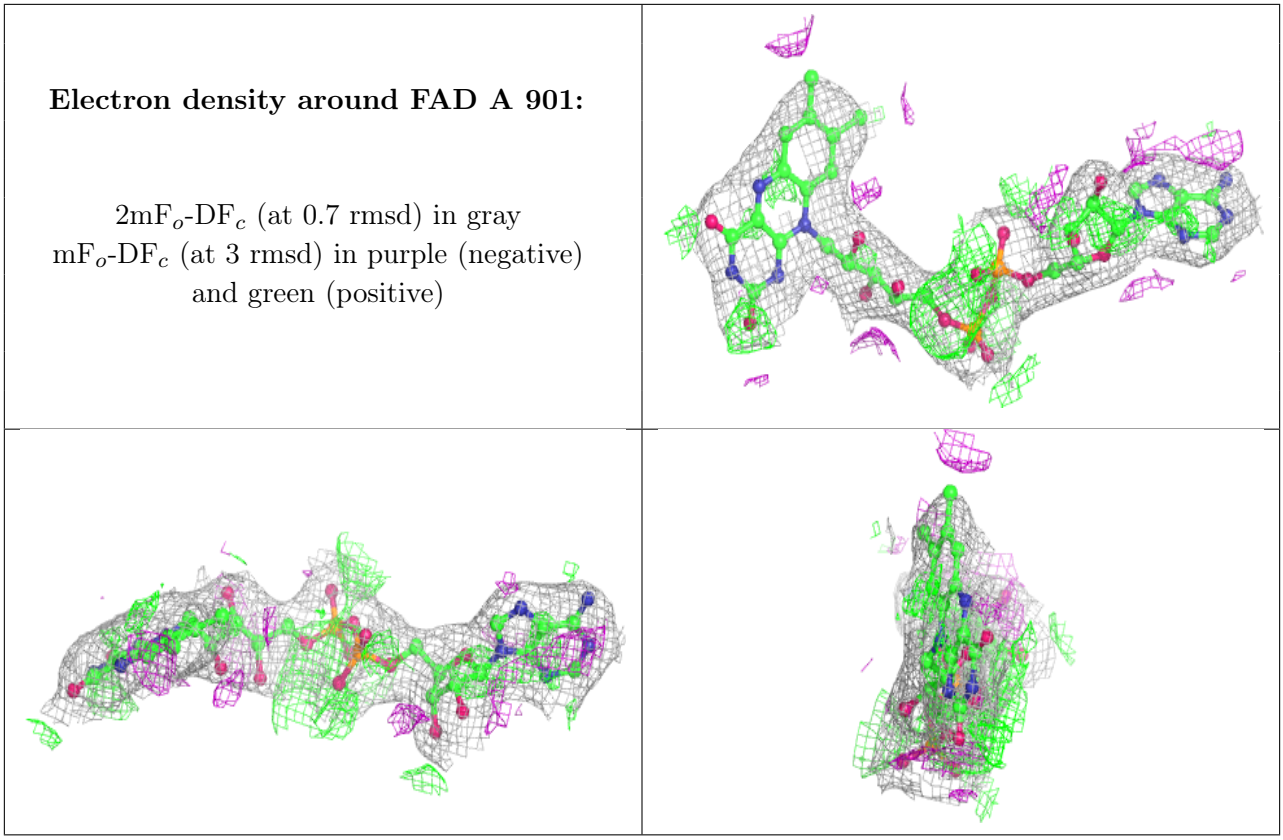
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	FAD	A	901	53/53	0.96	0.26	59,70,78,81	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 901:

$2mF_o$-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.