Full wwPDB X-ray Structure Validation Report (i)

Feb 13, 2017 – 04:07 PM EST

PDB ID	:	5LGT
Title	:	Thieno[3,2-b]pyrrole-5-carboxamides as Novel Reversible Inhibitors of Histone Lysine Demethylase KDM1A/LSD1: Compound 15
Authors	:	Mattevi, A.; Ciossani, G.
Deposited on	:	2016-07-08
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/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:

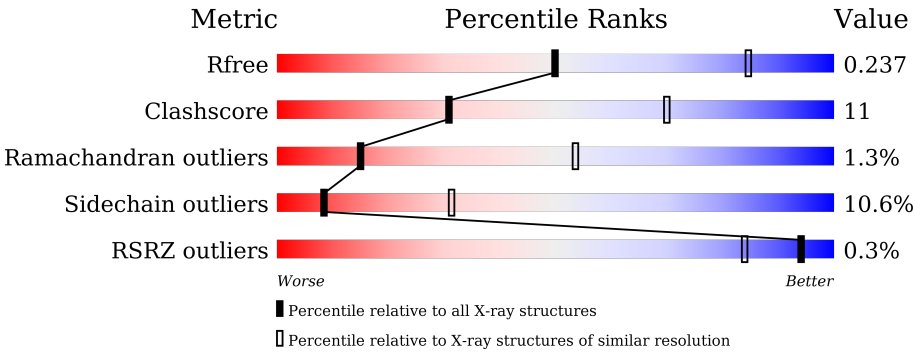
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	67% 22% · 9%
2	B	178	% 46% 24% 5% 25%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6377 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.

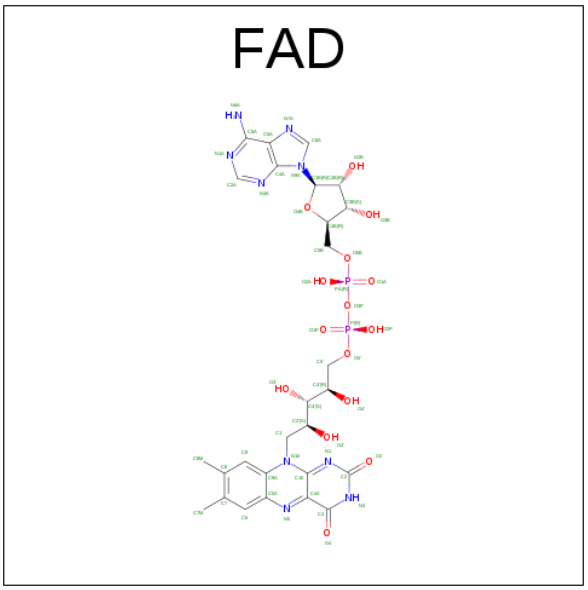
- Molecule 1 is a protein called Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5214	3323	905	966	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			

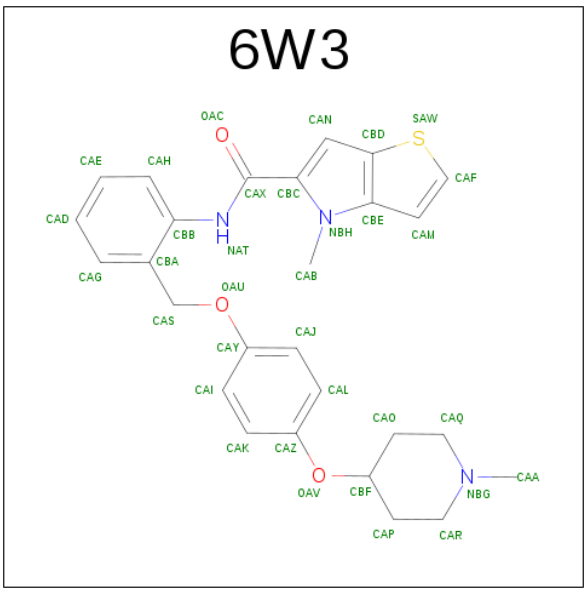
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is 4-methyl- {N}-[2-[[4-(1-methylpiperidin-4-yl)oxyphenoxy]methyl]phenyl]thien

o[3,2-b]pyrrole-5-carboxamide (three-letter code: 6W3) (formula: $C_{27}H_{29}N_3O_3S$).



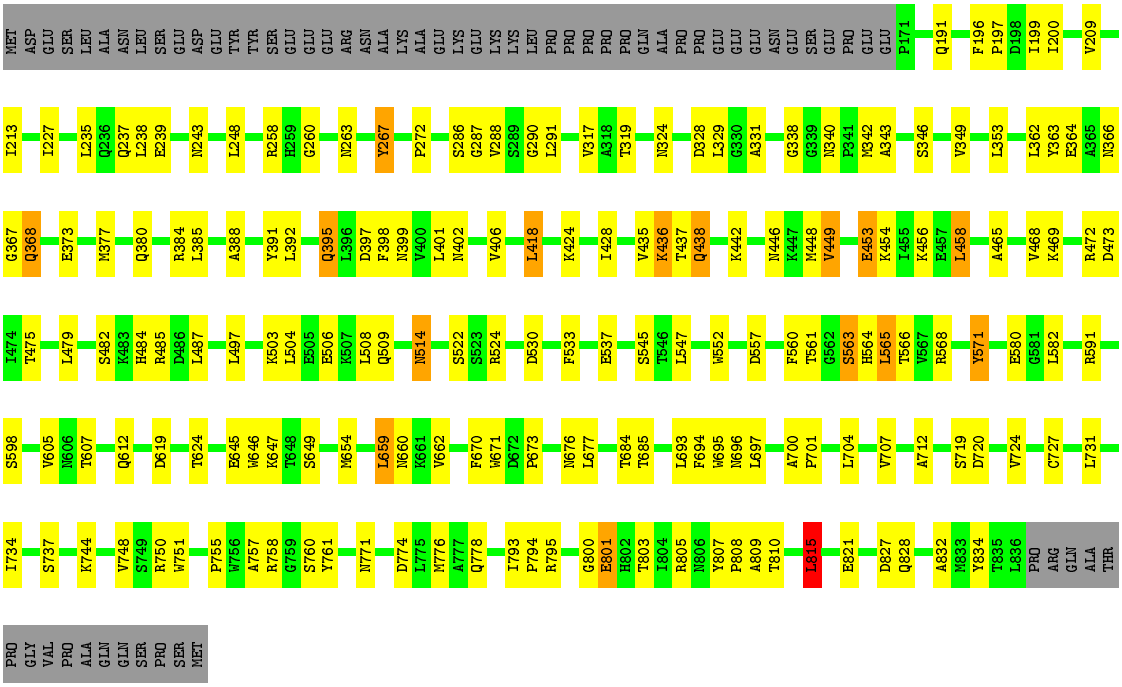
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	34	27	3	3	1	0	0

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 errors 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.

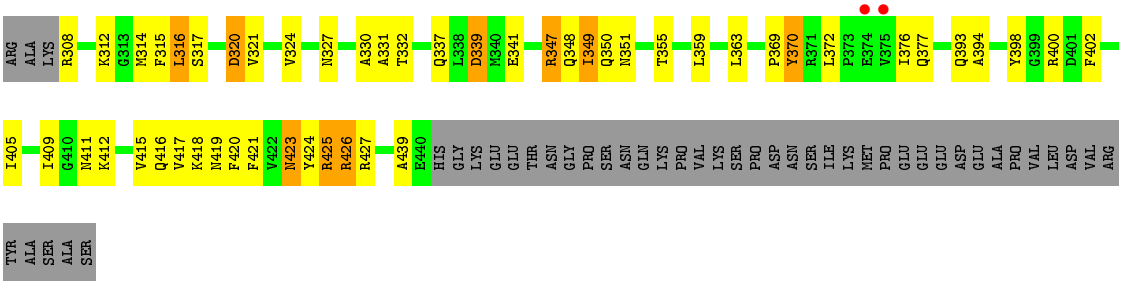
- Molecule 1: Lysine-specific histone demethylase 1A

Chain A:



- Molecule 2: REST corepressor 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	120.07Å 178.69Å 235.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.70 – 3.00 55.32 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (57.70-3.00) 97.3 (55.32-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.212 , 0.230 0.219 , 0.237	Depositor DCC
R_{free} test set	967 reflections (1.99%)	DCC
Wilson B-factor (Å^2)	83.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 56.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6377	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, 6W3

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	0.46	0/5328	0.67	1/7228 (0.0%)
2	B	0.42	0/1091	0.65	0/1471
All	All	0.45	0/6419	0.67	1/8699 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	815	LEU	CA-CB-CG	5.23	127.33	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	5214	0	5248	112	0
2	B	1076	0	1091	47	0
3	A	53	0	31	4	0
4	A	34	0	0	0	0
All	All	6377	0	6370	139	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 11.

All (139) 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:327:ASN:HB3	2:B:330:ALA:HB2	1.52	0.91
2:B:421:PHE:O	2:B:425:ARG:HB2	1.79	0.82
1:A:760:SER:HB2	3:A:901:FAD:HM83	1.64	0.80
1:A:286:SER:O	1:A:291:LEU:HD11	1.85	0.77
1:A:619:ASP:O	1:A:795:ARG:NH1	2.19	0.76
2:B:377:GLN:HB3	2:B:411:ASN:HB3	1.73	0.69
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.76	0.68
1:A:671:TRP:O	1:A:673:PRO:HD3	1.93	0.68
1:A:727:CYS:O	1:A:731:LEU:HD12	1.94	0.68
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.75	0.67
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.76	0.67
1:A:340:ASN:OD1	1:A:342:MET:N	2.27	0.67
1:A:384:ARG:NH2	2:B:312:LYS:O	2.27	0.67
1:A:435:VAL:HG12	2:B:349:ILE:HD12	1.77	0.67
1:A:435:VAL:CG1	2:B:349:ILE:HD12	2.25	0.66
2:B:423:ASN:O	2:B:426:ARG:HD2	1.96	0.66
1:A:435:VAL:HG23	1:A:436:LYS:N	2.11	0.66
1:A:437:THR:HG22	1:A:508:LEU:HD21	1.79	0.65
1:A:418:LEU:CD1	2:B:324:VAL:HG21	2.26	0.65
1:A:564:HIS:C	1:A:565:LEU:HD12	2.16	0.64
1:A:468:VAL:O	1:A:472:ARG:NH1	2.30	0.64
2:B:317:SER:O	2:B:321:VAL:HG23	1.97	0.64
2:B:377:GLN:CB	2:B:411:ASN:HB3	2.29	0.62
1:A:438:GLN:HE22	1:A:508:LEU:HD13	1.64	0.62
1:A:807:TYR:N	1:A:808:PRO:HD3	2.14	0.62
1:A:343:ALA:O	1:A:346:SER:OG	2.15	0.61
1:A:514:ASN:O	1:A:514:ASN:ND2	2.33	0.61
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.83	0.60
2:B:370:TYR:N	2:B:370:TYR:CD1	2.66	0.60
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.83	0.60
1:A:801:GLU:CG	1:A:809:ALA:HA	2.32	0.59
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.38	0.58
1:A:832:ALA:HB1	1:A:834:TYR:CE2	2.39	0.58
1:A:392:LEU:HD11	2:B:316:LEU:HD22	1.85	0.57
2:B:415:VAL:HG22	2:B:419:ASN:HD21	1.71	0.56
1:A:196:PHE:N	1:A:197:PRO:CD	2.69	0.55
1:A:815:LEU:C	1:A:815:LEU:HD12	2.27	0.55
1:A:563:SER:O	1:A:565:LEU:CD1	2.54	0.55
1:A:287:GLY:O	1:A:290:GLY:N	2.41	0.54
1:A:720:ASP:O	1:A:724:VAL:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:GLU:HG2	1:A:809:ALA:H	1.73	0.53
1:A:565:LEU:HD12	1:A:565:LEU:N	2.23	0.53
1:A:475:THR:HA	2:B:393:GLN:OE1	2.09	0.53
1:A:424:LYS:HE3	2:B:339:ASP:OD1	2.09	0.53
2:B:370:TYR:N	2:B:370:TYR:HD1	2.06	0.53
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.44	0.53
1:A:800:GLY:O	1:A:803:THR:OG1	2.25	0.52
2:B:416:GLN:HA	2:B:419:ASN:HD22	1.75	0.52
1:A:821:GLU:OE2	1:A:821:GLU:HA	2.10	0.52
1:A:437:THR:CG2	1:A:508:LEU:HD21	2.39	0.51
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.46	0.51
1:A:794:PRO:HD2	1:A:828:GLN:NE2	2.26	0.51
1:A:435:VAL:CG2	1:A:436:LYS:N	2.72	0.51
1:A:199:ILE:HD11	1:A:248:LEU:CD1	2.40	0.51
1:A:676:ASN:HB2	1:A:677:LEU:HD23	1.92	0.50
1:A:366:ASN:OD1	1:A:368:GLN:N	2.44	0.50
1:A:199:ILE:CD1	1:A:248:LEU:HD11	2.42	0.50
1:A:591:ARG:NH1	1:A:605:VAL:HG21	2.26	0.50
2:B:347:ARG:HG3	2:B:348:GLN:N	2.25	0.50
1:A:456:LYS:CG	2:B:370:TYR:HE2	2.25	0.50
1:A:331:ALA:HA	3:A:901:FAD:N5	2.27	0.49
1:A:456:LYS:HG3	2:B:370:TYR:HE2	1.77	0.49
2:B:417:VAL:O	2:B:420:PHE:HB3	2.13	0.49
1:A:366:ASN:OD1	1:A:367:GLY:N	2.45	0.49
1:A:808:PRO:O	1:A:810:THR:HG23	2.12	0.49
1:A:693:LEU:HD12	1:A:694:PHE:H	1.79	0.48
1:A:384:ARG:NH1	2:B:312:LYS:O	2.46	0.48
1:A:807:TYR:N	1:A:808:PRO:CD	2.77	0.48
1:A:287:GLY:HA3	3:A:901:FAD:O5B	2.14	0.48
1:A:435:VAL:CG1	2:B:349:ILE:CD1	2.92	0.48
1:A:503:LYS:O	1:A:506:GLU:HG2	2.13	0.48
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.95	0.48
1:A:399:ASN:C	1:A:406:VAL:HG23	2.34	0.48
1:A:385:LEU:O	1:A:388:ALA:HB3	2.13	0.47
1:A:449:VAL:HA	2:B:363:LEU:HD21	1.95	0.47
1:A:530:ASP:OD2	1:A:685:THR:HA	2.15	0.47
1:A:196:PHE:N	1:A:197:PRO:HD3	2.29	0.47
1:A:338:GLY:HA3	1:A:561:THR:OG1	2.15	0.47
1:A:340:ASN:HB2	1:A:560:PHE:CD2	2.50	0.47
1:A:453:GLU:OE1	1:A:453:GLU:HA	2.15	0.46
2:B:369:PRO:C	2:B:370:TYR:HD1	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:HIS:CD2	2:B:372:LEU:CD1	2.98	0.46
1:A:435:VAL:HG13	2:B:349:ILE:CD1	2.44	0.46
1:A:677:LEU:N	1:A:677:LEU:HD23	2.31	0.46
1:A:258:ARG:NH1	1:A:827:ASP:OD1	2.48	0.46
1:A:670:PHE:O	1:A:670:PHE:CD1	2.70	0.45
2:B:402:PHE:CE2	2:B:418:LYS:HG2	2.51	0.45
2:B:421:PHE:O	2:B:425:ARG:CB	2.60	0.45
1:A:659:LEU:O	1:A:659:LEU:HG	2.17	0.45
1:A:755:PRO:HA	1:A:758:ARG:NH1	2.31	0.44
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.52	0.44
1:A:368:GLN:HE21	1:A:368:GLN:HA	1.81	0.44
1:A:465:ALA:HB1	1:A:479:LEU:HD23	1.99	0.44
1:A:646:TRP:CZ3	1:A:647:LYS:HE2	2.52	0.44
1:A:446:ASN:OD1	2:B:359:LEU:HD11	2.17	0.44
2:B:405:ILE:O	2:B:409:ILE:HG13	2.18	0.44
1:A:287:GLY:C	1:A:291:LEU:HD12	2.39	0.44
1:A:319:THR:HA	1:A:328:ASP:HA	2.00	0.44
1:A:346:SER:O	1:A:349:VAL:O	2.36	0.44
1:A:442:LYS:HE3	2:B:355:THR:HG21	2.00	0.44
1:A:504:LEU:O	1:A:508:LEU:HG	2.17	0.44
1:A:469:LYS:HA	1:A:469:LYS:HE2	1.99	0.43
1:A:238:LEU:O	1:A:243:ASN:ND2	2.52	0.43
1:A:456:LYS:HG2	2:B:370:TYR:CE2	2.53	0.43
1:A:487:LEU:HD23	2:B:372:LEU:HG	2.00	0.43
1:A:565:LEU:N	1:A:565:LEU:CD1	2.81	0.43
2:B:315:PHE:C	2:B:316:LEU:HG	2.39	0.43
2:B:320:ASP:O	2:B:324:VAL:HG23	2.18	0.43
1:A:676:ASN:HB2	1:A:677:LEU:CD2	2.49	0.43
2:B:400:ARG:O	2:B:402:PHE:CD1	2.72	0.43
2:B:424:TYR:O	2:B:427:ARG:N	2.46	0.43
1:A:566:THR:HG21	1:A:697:LEU:HD22	2.01	0.43
1:A:362:LEU:C	1:A:363:TYR:CD1	2.92	0.42
1:A:448:MET:SD	1:A:497:LEU:HB3	2.59	0.42
1:A:465:ALA:CB	1:A:479:LEU:HD23	2.50	0.42
1:A:533:PHE:O	1:A:537:GLU:HG3	2.20	0.42
2:B:369:PRO:HB2	2:B:370:TYR:CE1	2.55	0.42
1:A:340:ASN:OD1	1:A:342:MET:HB2	2.19	0.42
1:A:456:LYS:CG	2:B:370:TYR:CE2	3.02	0.42
1:A:331:ALA:HA	3:A:901:FAD:C4X	2.50	0.42
2:B:369:PRO:HB2	2:B:370:TYR:CD1	2.54	0.42
2:B:347:ARG:O	2:B:350:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:TRP:HB3	1:A:697:LEU:HD12	2.02	0.41
1:A:391:TYR:CD1	1:A:395:GLN:HG3	2.55	0.41
2:B:347:ARG:CG	2:B:348:GLN:N	2.82	0.41
1:A:209:VAL:O	1:A:213:ILE:HG13	2.20	0.41
1:A:694:PHE:HA	1:A:704:LEU:O	2.20	0.41
2:B:424:TYR:O	2:B:425:ARG:C	2.59	0.41
1:A:258:ARG:HA	1:A:258:ARG:HD3	1.83	0.41
1:A:317:VAL:HG13	1:A:571:TYR:HB3	2.01	0.41
1:A:707:VAL:HG12	1:A:712:ALA:HA	2.02	0.41
1:A:774:ASP:OD2	1:A:805:ARG:NH1	2.52	0.41
2:B:324:VAL:HG13	2:B:331:ALA:HA	2.03	0.41
1:A:267:TYR:CD1	1:A:267:TYR:N	2.89	0.41
1:A:815:LEU:C	1:A:815:LEU:CD1	2.90	0.41
1:A:660:ASN:HD21	1:A:751:TRP:H	1.69	0.40
1:A:454:LYS:O	1:A:458:LEU:HB2	2.21	0.40
1:A:263:ASN:C	1:A:267:TYR:CE2	2.95	0.40
2:B:394:ALA:O	2:B:398:TYR:N	2.49	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%)	612 (92%)	44 (7%)	8 (1%)	16	56
2	B	131/178 (74%)	112 (86%)	17 (13%)	2 (2%)	13	50
All	All	795/908 (88%)	724 (91%)	61 (8%)	10 (1%)	15	53

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	288	VAL

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Mol	Chain	Res	Type
1	A	364	GLU
1	A	737	SER
1	A	260	GLY
1	A	612	GLN
2	B	439	ALA
2	B	425	ARG
1	A	272	PRO
1	A	757	ALA
1	A	428	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	565/623 (91%)	509 (90%)	56 (10%)	10 35
2	B	117/156 (75%)	101 (86%)	16 (14%)	4 20
All	All	682/779 (88%)	610 (89%)	72 (11%)	8 31

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	200	ILE
1	A	227	ILE
1	A	235	LEU
1	A	237	GLN
1	A	239	GLU
1	A	267	TYR
1	A	324	ASN
1	A	329	LEU
1	A	368	GLN
1	A	373	GLU
1	A	377	MET
1	A	380	GLN
1	A	395	GLN

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Mol	Chain	Res	Type
1	A	397	ASP
1	A	401	LEU
1	A	402	ASN
1	A	418	LEU
1	A	436	LYS
1	A	438	GLN
1	A	449	VAL
1	A	453	GLU
1	A	458	LEU
1	A	473	ASP
1	A	482	SER
1	A	485	ARG
1	A	509	GLN
1	A	514	ASN
1	A	522	SER
1	A	524	ARG
1	A	545	SER
1	A	557	ASP
1	A	563	SER
1	A	565	LEU
1	A	568	ARG
1	A	571	TYR
1	A	580	GLU
1	A	582	LEU
1	A	598	SER
1	A	607	THR
1	A	624	THR
1	A	645	GLU
1	A	649	SER
1	A	654	MET
1	A	659	LEU
1	A	684	THR
1	A	696	ASN
1	A	719	SER
1	A	744	LYS
1	A	750	ARG
1	A	771	ASN
1	A	776	MET
1	A	778	GLN
1	A	793	ILE
1	A	801	GLU
1	A	815	LEU

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Mol	Chain	Res	Type
2	B	308	ARG
2	B	314	MET
2	B	316	LEU
2	B	320	ASP
2	B	332	THR
2	B	337	GLN
2	B	339	ASP
2	B	341	GLU
2	B	347	ARG
2	B	349	ILE
2	B	351	ASN
2	B	370	TYR
2	B	376	ILE
2	B	412	LYS
2	B	423	ASN
2	B	426	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	GLN
1	A	368	GLN
1	A	380	GLN
1	A	395	GLN
1	A	438	GLN
1	A	509	GLN
1	A	633	GLN
1	A	660	ASN
1	A	696	ASN
1	A	778	GLN
1	A	828	GLN
2	B	337	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 (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	901	-	52,58,58	1.23	6 (11%)	52,89,89	2.74	19 (36%)
4	6W3	A	902	-	34,38,38	1.60	6 (17%)	41,53,53	2.08	8 (19%)

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	901	-	-	0/30/50/50	0/6/6/6
4	6W3	A	902	-	-	0/14/27/27	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	6W3	CAN-CBC	-5.63	1.33	1.38
4	A	902	6W3	CAS-CBA	-3.84	1.41	1.51
4	A	902	6W3	CBB-NAT	-3.05	1.36	1.41
3	A	901	FAD	C6-C5X	-2.75	1.37	1.41
4	A	902	6W3	CBC-CAX	-2.70	1.33	1.50
4	A	902	6W3	CAN-CBD	-2.25	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	6W3	CAF-SAW	-2.02	1.61	1.71
3	A	901	FAD	C8-C7	2.31	1.47	1.41
3	A	901	FAD	C9A-N10	2.91	1.42	1.38
3	A	901	FAD	C5A-C4A	2.95	1.47	1.40
3	A	901	FAD	C9A-C5X	3.01	1.48	1.42
3	A	901	FAD	C4X-C10	3.29	1.46	1.40

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	FAD	N3A-C2A-N1A	-7.92	122.65	128.87
4	A	902	6W3	CAQ-CAO-CBF	-6.21	103.84	110.23
3	A	901	FAD	C1B-N9A-C4A	-5.84	120.29	126.81
3	A	901	FAD	C4X-C10-N10	-5.52	116.51	120.52
4	A	902	6W3	CAO-CAQ-NBG	-5.21	104.06	111.33
3	A	901	FAD	C4X-C4-N3	-4.25	117.96	123.52
4	A	902	6W3	CAP-CAR-NBG	-4.19	105.49	111.33
3	A	901	FAD	N3-C2-N1	-3.64	121.56	127.69
3	A	901	FAD	C4B-O4B-C1B	-2.96	106.50	109.64
3	A	901	FAD	C6-C5X-N5	-2.79	115.43	118.92
3	A	901	FAD	C4-C4X-N5	-2.73	115.37	118.70
3	A	901	FAD	O5'-P-O1P	-2.08	100.69	109.21
3	A	901	FAD	C4-C4X-C10	-2.06	118.62	119.94
4	A	902	6W3	CAN-CBC-CAX	-2.01	124.55	129.81
4	A	902	6W3	OAC-CAX-NAT	2.15	128.50	123.68
3	A	901	FAD	C2A-N1A-C6A	2.25	122.78	118.77
3	A	901	FAD	O2A-PA-O1A	2.29	124.47	112.56
3	A	901	FAD	O4B-C1B-N9A	2.56	112.94	108.11
3	A	901	FAD	C5X-C9A-N10	2.66	119.57	117.58
3	A	901	FAD	N6A-C6A-N1A	2.76	123.14	118.52
3	A	901	FAD	O4'-C4'-C3'	2.84	116.26	108.96
4	A	902	6W3	CAN-CBD-CBE	3.14	108.98	106.24
3	A	901	FAD	C6-C5X-C9A	3.88	123.39	119.11
4	A	902	6W3	CAB-NBH-CBC	4.81	130.85	124.51
3	A	901	FAD	C1'-N10-C9A	5.16	124.81	118.83
4	A	902	6W3	CAF-SAW-CBD	5.16	97.33	91.56
3	A	901	FAD	C4-N3-C2	9.51	123.09	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.14	0 100 100	45, 79, 114, 151	0
2	B	133/178 (74%)	0.10	2 (1%) 76 49	72, 107, 127, 151	0
All	All	799/908 (87%)	-0.10	2 (0%) 94 84	45, 84, 121, 151	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	374	GLU	2.8
2	B	375	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	FAD	A	901	53/53	0.97	0.22	-0.06	46,54,65,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	6W3	A	902	34/34	0.96	0.22	-0.65	68,78,88,94	0

6.5 Other polymers (i)

There are no such residues in this entry.