Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:11 PM GMT

PDB ID	:	4KUM
Title	:	Structure of LSD1-CoREST-Tetrahydrofolate complex
Authors	:	Luka, Z.; Pakhomova, S.; Loukachevitch, L.V.; Calcutt, M.W.; Newcomer, M.E.; Wagner, C.
Deposited on	:	2013-05-22
Resolution	:	3.05 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:

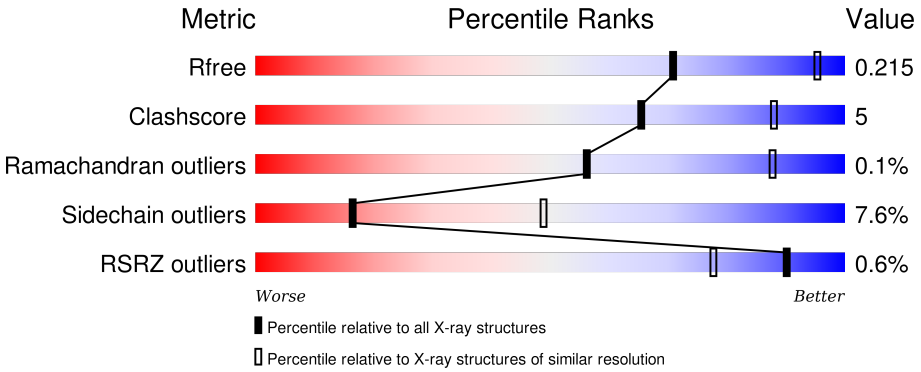
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

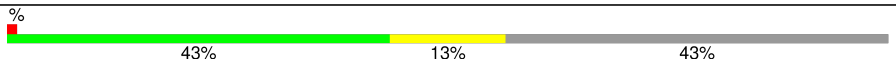
The reported resolution of this entry is 3.05 Å.

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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	666	
2	B	235	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6409 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	2	0
			5228	3330	910	968	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
			1070	673	191	203	3			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	248	MET	-	EXPRESSION TAG	UNP J3KN32
B	249	GLY	-	EXPRESSION TAG	UNP J3KN32
B	250	SER	-	EXPRESSION TAG	UNP J3KN32
B	251	SER	-	EXPRESSION TAG	UNP J3KN32
B	252	HIS	-	EXPRESSION TAG	UNP J3KN32
B	253	HIS	-	EXPRESSION TAG	UNP J3KN32
B	254	HIS	-	EXPRESSION TAG	UNP J3KN32
B	255	HIS	-	EXPRESSION TAG	UNP J3KN32
B	256	HIS	-	EXPRESSION TAG	UNP J3KN32
B	257	HIS	-	EXPRESSION TAG	UNP J3KN32
B	258	SER	-	EXPRESSION TAG	UNP J3KN32
B	259	SER	-	EXPRESSION TAG	UNP J3KN32
B	260	GLY	-	EXPRESSION TAG	UNP J3KN32
B	261	LEU	-	EXPRESSION TAG	UNP J3KN32
B	262	VAL	-	EXPRESSION TAG	UNP J3KN32
B	263	PRO	-	EXPRESSION TAG	UNP J3KN32
B	264	ARG	-	EXPRESSION TAG	UNP J3KN32
B	265	GLY	-	EXPRESSION TAG	UNP J3KN32
B	266	SER	-	EXPRESSION TAG	UNP J3KN32
B	267	HIS	-	EXPRESSION TAG	UNP J3KN32

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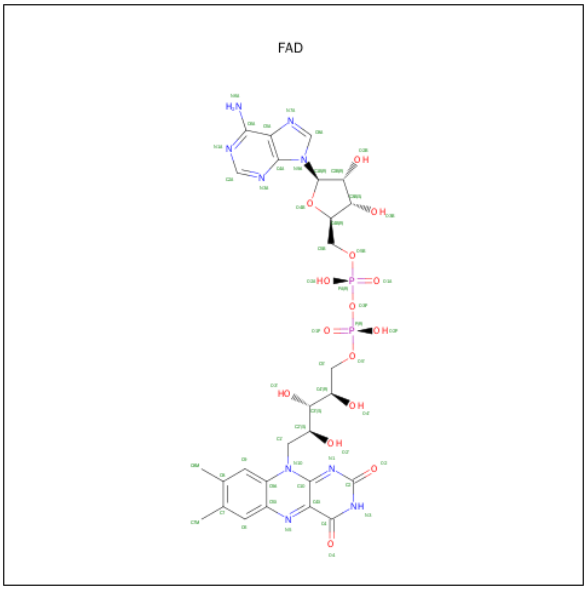
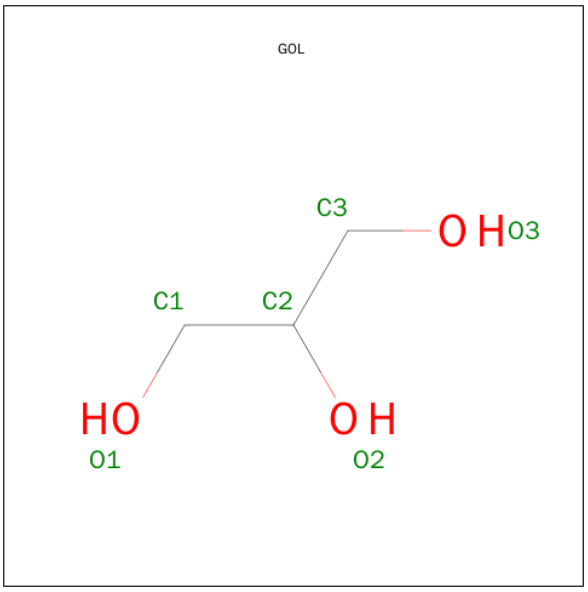
Chain	Residue	Modelled	Actual	Comment	Reference
B	268	MET	-	EXPRESSION TAG	UNP J3KN32
B	269	ALA	-	EXPRESSION TAG	UNP J3KN32
B	270	SER	-	EXPRESSION TAG	UNP J3KN32
B	271	MET	-	EXPRESSION TAG	UNP J3KN32
B	272	THR	-	EXPRESSION TAG	UNP J3KN32
B	273	GLY	-	EXPRESSION TAG	UNP J3KN32
B	274	GLY	-	EXPRESSION TAG	UNP J3KN32
B	275	GLN	-	EXPRESSION TAG	UNP J3KN32
B	276	GLN	-	EXPRESSION TAG	UNP J3KN32
B	277	MET	-	EXPRESSION TAG	UNP J3KN32
B	278	GLY	-	EXPRESSION TAG	UNP J3KN32
B	279	ARG	-	EXPRESSION TAG	UNP J3KN32
B	280	GLY	-	EXPRESSION TAG	UNP J3KN32
B	281	SER	-	EXPRESSION TAG	UNP J3KN32
B	282	GLU	-	EXPRESSION TAG	UNP J3KN32
B	283	PHE	-	EXPRESSION TAG	UNP J3KN32
B	284	GLY	-	EXPRESSION TAG	UNP J3KN32
B	285	ARG	-	EXPRESSION TAG	UNP J3KN32

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



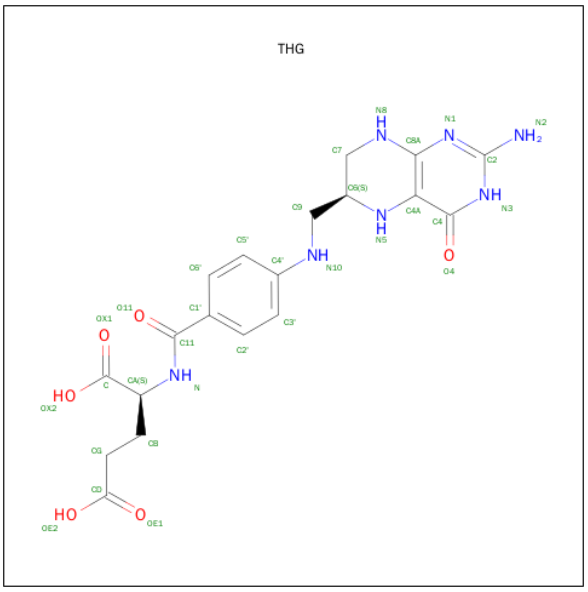
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0

- Molecule 5 is (6S)-5,6,7,8-TETRAHYDROFOLATE (three-letter code: THG) (formula: $C_{19}H_{23}N_7O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	A	1	32	19	7	6	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Cl 1 1	0	0

- Molecule 7 is water.

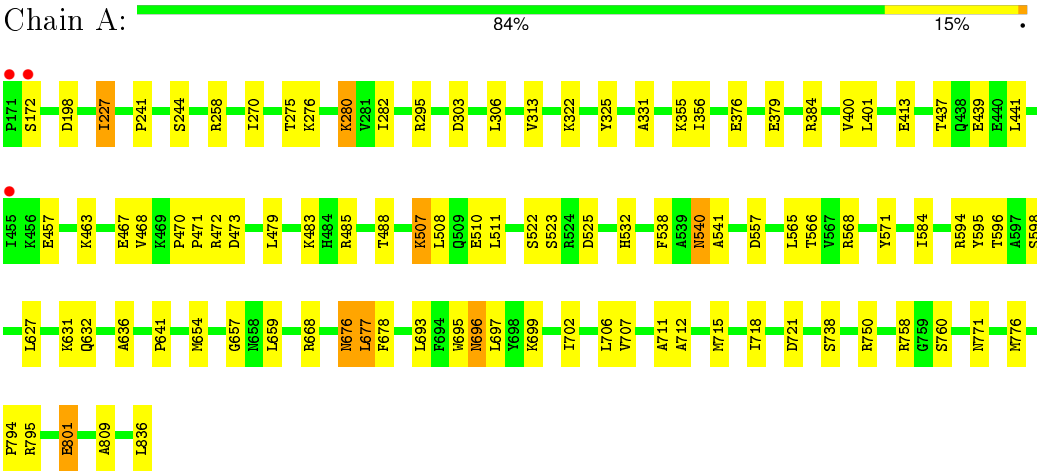
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	19	Total O 19 19	0	0

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.

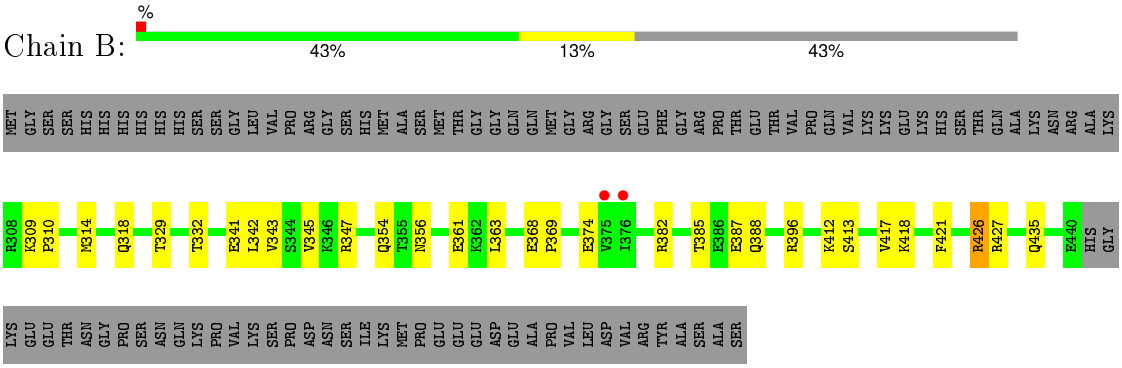
- Molecule 1: Lysine-specific histone demethylase 1A

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	123.86Å 179.37Å 235.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.05 46.90 – 3.03	Depositor EDS
% Data completeness (in resolution range)	92.8 (40.00-3.05) 91.7 (46.90-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.34 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.196 , 0.217 0.196 , 0.215	Depositor DCC
R_{free} test set	2355 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	64.4	Xtriage
Anisotropy	1.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 59.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 46885 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6409	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: THG, GOL, FAD, CL

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	0.57	0/5342	0.79	0/7246
2	B	0.45	0/1085	0.68	0/1464
All	All	0.55	0/6427	0.77	0/8710

There are no bond length outliers.

There are no bond angle outliers.

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	5228	0	5264	57	0
2	B	1070	0	1080	12	0
3	A	53	0	31	4	0
4	A	6	0	8	2	0
5	A	32	0	21	0	0
6	A	1	0	0	0	0
7	A	19	0	0	2	0
All	All	6409	0	6404	64	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 5.

All (64) 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:760:SER:HB2	3:A:901:FAD:HM83	1.75	0.69
1:A:538:PHE:CE1	1:A:706:LEU:HD13	2.28	0.69
1:A:325:TYR:HB3	1:A:702:ILE:HD11	1.74	0.69
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.29	0.67
1:A:468:VAL:O	1:A:472:ARG:NH1	2.28	0.66
1:A:463:LYS:O	1:A:467:GLU:HG3	1.95	0.66
1:A:760:SER:CB	3:A:901:FAD:HM83	2.28	0.64
1:A:781:THR:HB	1:A:794:PRO:HA	1.80	0.64
1:A:793:ILE:N	1:A:793:ILE:HD12	2.15	0.61
1:A:331:ALA:HA	3:A:901:FAD:N5	2.15	0.61
1:A:718:ILE:O	1:A:750:ARG:NH2	2.33	0.61
1:A:449:VAL:HA	2:B:363:LEU:HD21	1.83	0.61
1:A:632:GLN:NE2	1:A:636:ALA:HB2	2.17	0.60
1:A:632:GLN:OE1	1:A:758[A]:ARG:NE	2.34	0.60
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.83	0.60
1:A:379:GLU:HG2	1:A:532:HIS:CE1	2.37	0.60
1:A:540:ASN:N	1:A:540:ASN:HD22	2.02	0.58
1:A:619:ASP:O	1:A:795:ARG:NH1	2.37	0.58
1:A:507:LYS:O	1:A:510:GLU:HG2	2.04	0.57
1:A:470:PRO:HA	1:A:471:PRO:C	2.26	0.56
1:A:241:PRO:O	1:A:244:SER:HB2	2.07	0.53
1:A:801:GLU:HG2	1:A:809:ALA:H	1.73	0.53
1:A:793:ILE:H	1:A:793:ILE:HD12	1.72	0.53
1:A:331:ALA:HA	3:A:901:FAD:C4X	2.40	0.51
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.46	0.51
1:A:384:ARG:HB3	2:B:314:MET:CE	2.41	0.50
1:A:280:LYS:HD2	1:A:303:ASP:HB3	1.93	0.50
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.94	0.50
1:A:510:GLU:HG3	1:A:511:LEU:N	2.27	0.49
1:A:355:LYS:HA	1:A:565:LEU:HD23	1.95	0.48
1:A:198:ASP:OD1	1:A:198:ASP:N	2.47	0.48
1:A:711:ALA:O	1:A:715:MET:HG2	2.14	0.48
2:B:387:GLU:OE1	2:B:412:LYS:NZ	2.46	0.48
1:A:488:THR:HG21	2:B:374:GLU:OE1	2.13	0.47
2:B:385:THR:HA	2:B:388:GLN:HE21	1.78	0.47
2:B:413:SER:O	2:B:417:VAL:HG23	2.14	0.47
1:A:479:LEU:HD11	1:A:483:LYS:HE2	1.95	0.47
2:B:309:LYS:HG3	2:B:310:PRO:HD2	1.96	0.47
2:B:368:GLU:N	2:B:369:PRO:CD	2.79	0.46
1:A:441:LEU:HD23	2:B:356:ASN:ND2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:TRP:HE1	1:A:706:LEU:HD11	1.82	0.45
1:A:678:PHE:O	1:A:693:LEU:HD12	2.15	0.45
1:A:627:LEU:O	1:A:631:LYS:HG3	2.17	0.44
1:A:413:GLU:HG3	4:A:902:GOL:C3	2.48	0.44
1:A:306:LEU:HD13	1:A:584:ILE:HG12	2.01	0.43
1:A:541:ALA:O	1:A:657:GLY:HA3	2.19	0.43
1:A:707:VAL:HG12	1:A:712:ALA:HA	2.01	0.43
1:A:413:GLU:HG3	4:A:902:GOL:H32	2.00	0.42
1:A:771:ASN:HB2	7:A:1010:HOH:O	2.18	0.42
1:A:654:MET:HE1	1:A:776:MET:HG2	2.02	0.42
2:B:426:ARG:HG3	2:B:427:ARG:H	1.84	0.42
1:A:379:GLU:CG	1:A:532:HIS:CE1	3.02	0.42
1:A:522:SER:O	1:A:525:ASP:HB2	2.20	0.42
2:B:418:LYS:O	2:B:421:PHE:HB2	2.19	0.42
1:A:696:ASN:CG	1:A:696:ASN:O	2.55	0.42
1:A:676:ASN:HB3	1:A:677:LEU:HD22	2.01	0.42
1:A:538:PHE:CZ	1:A:706:LEU:HD13	2.55	0.41
1:A:781:THR:HB	1:A:794:PRO:CA	2.49	0.41
1:A:632:GLN:CD	1:A:758[B]:ARG:HD2	2.41	0.41
1:A:227:ILE:HD11	1:A:270:ILE:HD11	2.02	0.41
1:A:313:VAL:HG22	7:A:1009:HOH:O	2.20	0.41
1:A:437:THR:CG2	1:A:508:LEU:HD21	2.51	0.41
1:A:282:ILE:HD13	1:A:282:ILE:HA	1.93	0.41
1:A:793:ILE:N	1:A:793:ILE:CD1	2.81	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	665/666 (100%)	644 (97%)	20 (3%)	1 (0%)	52 84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	131/235 (56%)	125 (95%)	6 (5%)	0	100 100
All	All	796/901 (88%)	769 (97%)	26 (3%)	1 (0%)	56 88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	792	PRO

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	567/566 (100%)	529 (93%)	38 (7%)	20 53
2	B	116/203 (57%)	102 (88%)	14 (12%)	6 23
All	All	683/769 (89%)	631 (92%)	52 (8%)	16 49

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	SER
1	A	227	ILE
1	A	258	ARG
1	A	275	THR
1	A	276	LYS
1	A	280	LYS
1	A	295	ARG
1	A	322	LYS
1	A	376	GLU
1	A	400	VAL
1	A	401	LEU
1	A	439	GLU
1	A	453	GLU
1	A	454	LYS
1	A	457	GLU

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Mol	Chain	Res	Type
1	A	473	ASP
1	A	485	ARG
1	A	507	LYS
1	A	523	SER
1	A	540	ASN
1	A	557	ASP
1	A	568	ARG
1	A	571	TYR
1	A	594	ARG
1	A	596	THR
1	A	598	SER
1	A	611	SER
1	A	659	LEU
1	A	668	ARG
1	A	676	ASN
1	A	677	LEU
1	A	696	ASN
1	A	699	LYS
1	A	721	ASP
1	A	738	SER
1	A	781	THR
1	A	801	GLU
1	A	836	LEU
2	B	318	GLN
2	B	329	THR
2	B	332	THR
2	B	341	GLU
2	B	342	LEU
2	B	343	VAL
2	B	345	VAL
2	B	347	ARG
2	B	354	GLN
2	B	361	GLU
2	B	382	ARG
2	B	396	ARG
2	B	426	ARG
2	B	435	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	GLN

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Mol	Chain	Res	Type
1	A	410	GLN
1	A	450	ASN
1	A	532	HIS
1	A	540	ASN
1	A	633	GLN
1	A	652	GLN
2	B	318	GLN
2	B	348	GLN
2	B	354	GLN
2	B	388	GLN
2	B	435	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	-	48,58,58	1.20	4 (8%)	54,89,89	2.56	13 (24%)
4	GOL	A	902	-	5,5,5	0.42	0	5,5,5	0.66	0
5	THG	A	903	-	26,34,34	0.96	1 (3%)	28,47,47	1.66	6 (21%)

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	GOL	A	902	-	-	0/4/4/4	0/0/0/0
5	THG	A	903	-	-	0/16/31/31	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	FAD	C6-C5X	-3.05	1.37	1.41
3	A	901	FAD	C8-C7	2.55	1.47	1.41
3	A	901	FAD	C9A-C5X	2.77	1.48	1.42
3	A	901	FAD	C4X-C10	3.11	1.46	1.41
5	A	903	THG	C4A-C8A	3.61	1.49	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	FAD	N3A-C2A-N1A	-8.88	122.09	128.89
3	A	901	FAD	C4X-C10-N10	-5.48	117.29	120.52
3	A	901	FAD	C4-C4X-C10	-4.96	116.77	119.94
3	A	901	FAD	C4X-C4-N3	-3.88	118.29	123.59
5	A	903	THG	C1'-C11-N	-3.38	110.91	116.93
3	A	901	FAD	C4A-C5A-N7A	-2.50	107.18	109.48
3	A	901	FAD	P-O3P-PA	-2.30	126.28	132.73
3	A	901	FAD	O2B-C2B-C3B	2.05	118.51	111.83
3	A	901	FAD	C2B-C1B-N9A	2.12	117.53	114.29
3	A	901	FAD	C4X-N5-C5X	2.39	119.52	116.76
5	A	903	THG	O11-C11-N	2.41	126.80	122.44
3	A	901	FAD	O2A-PA-O3P	2.47	116.29	105.09
5	A	903	THG	C4-C4A-C8A	2.58	116.90	114.56
5	A	903	THG	C2-N1-C8A	2.81	120.86	114.54
3	A	901	FAD	C5X-C9A-N10	3.10	119.97	117.62
5	A	903	THG	CG-CB-CA	3.16	119.42	112.99
3	A	901	FAD	C1'-N10-C9A	3.40	122.68	118.86
5	A	903	THG	C4-N3-C2	4.63	122.37	115.94
3	A	901	FAD	C4-N3-C2	10.09	123.97	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	FAD	4	0
4	A	902	GOL	2	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	666/666 (100%)	-0.09	3 (0%)	91	81	45, 83, 129, 156	0
2	B	133/235 (56%)	0.24	2 (1%)	76	55	79, 115, 140, 163	0
All	All	799/901 (88%)	-0.04	5 (0%)	90	78	45, 89, 133, 163	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	SER	3.0
2	B	375	VAL	2.5
1	A	171	PRO	2.5
2	B	376	ILE	2.4
1	A	455	ILE	2.1

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
5	THG	A	903	32/32	0.85	0.29	1.37	102,119,136,142	0
3	FAD	A	901	53/53	0.98	0.21	-0.18	37,54,78,86	0
4	GOL	A	902	6/6	0.94	0.18	-1.06	65,70,73,75	0
6	CL	A	904	1/1	0.95	0.28	-	71,71,71,71	0

6.5 Other polymers (i)

There are no such residues in this entry.