W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:29 PM GMT

PDB ID	:	3ZN1
Title	:	LSD1-CoREST in complex with PRLYLV peptide
Authors	:	Tortorici, M.; Borrello, M.T.; Tardugno, M.; Chiarelli, L.R.; Pilotto, S.; Ciossani, G.; Vellore, N.A.; Cowan, J.; O'Connell, M.; Mai, A.; Baron, R.; Ganesan, A.; Mattevi, A.
Deposited on	:	2013-02-13
Resolution	:	3.10 Å(reported)

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

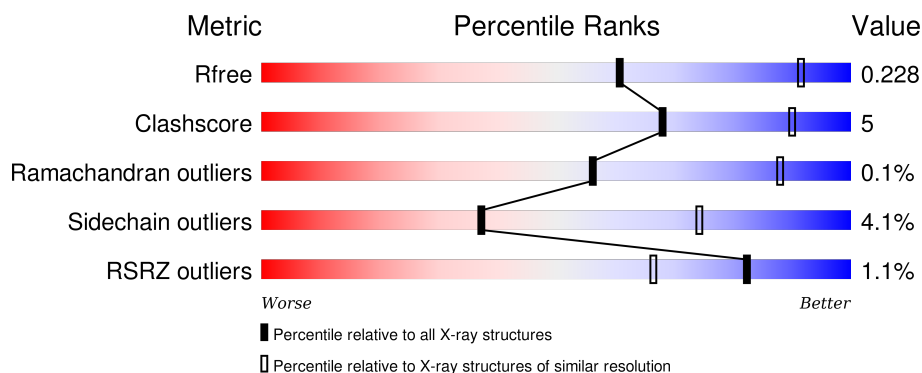|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.228
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		4.1%
RSRZ outliers		1.1%

Worse   *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	872	64% 12% 24%
2	B	482	% 24% • 72%
3	C	6	83% 17%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6399 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			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	PRO	ALA	CONFLICT	UNP O60341
A	.	-	ASP	DELETION	UNP O60341
A	.	-	THR	DELETION	UNP O60341
A	.	-	VAL	DELETION	UNP O60341
A	.	-	LYS	DELETION	UNP O60341

- 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 PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	0	0	0
			53	37	9	7			

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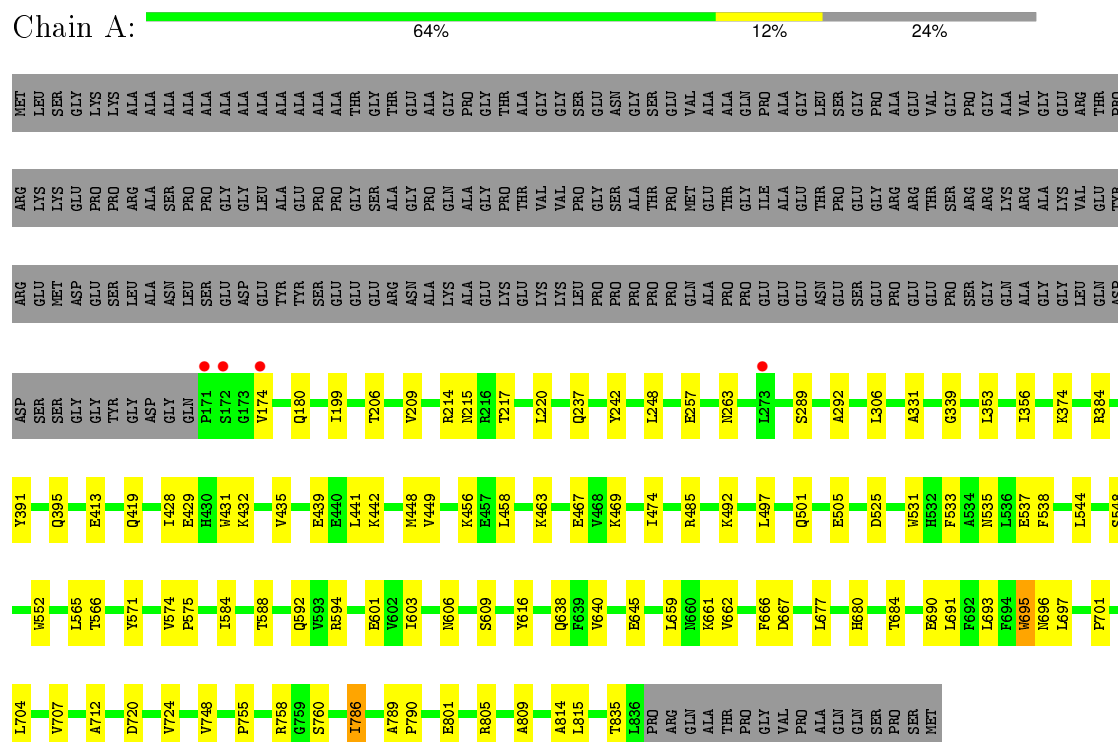
FAD

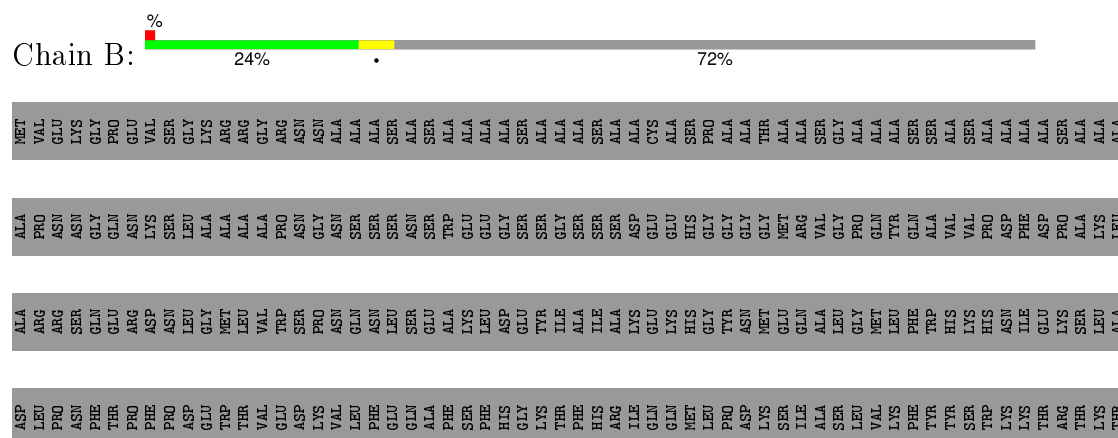| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	53	27	9	15	2	0	0

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:

SER VAL MET ASP HIS ALA ARG LYS GLN LYS ARG GLU ARG GLU GLU SER GLU ASP GLU LEU GLU GLU ALA ASN GLY ASN ASN PRO ILE ASP ILE GLU VAL ASP GLN ASN LYS GLU SER LYS GLU VAL PRO PRO THR GLU THR VAL PRO GLN VAL LYS LYS GLU LYS LYS HIS SER THR

GLN ALA LYS ASN ARG ALA LYS R308 K312 G313 M314 F315 T332 Q337 I349 T355 N356 E361 D364 Y370 R371 L372 P373 E374 V375 I376 T385 Q393 F402 D407 V414 M419 F420 F421 R425 E440 HIS GLY LYS GLU GLU THR ASN GLY

PRO SER ASN GLN LYS PRO VAL LYS SER PRO ASP ASN SER ILE LYS MET PRO GLU GLU GLU ASP GLU ALA PRO VAL LEU ASP VAL ARG TYR ALA SER ALA SER

● Molecule 3: PEPTIDE

Chain C:

83%   17%

P1 V6

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	120.23Å 181.06Å 232.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.94 – 3.10 53.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (53.94-3.10) 99.7 (53.94-3.10)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.210 , 0.230 0.212 , 0.228	Depositor DCC
R_{free} test set	893 reflections (1.97%)	DCC
Wilson B-factor (Å^2)	84.3	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Outliers	0 of 46303 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6399	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.42	3/5331 (0.1%)	0.49	0/7232
2	B	0.39	0/1091	0.46	0/1471
3	C	0.29	0/54	0.68	0/72
All	All	0.42	3/6476 (0.0%)	0.49	0/8775

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	695	TRP	CD2-CE2	5.09	1.47	1.41
1	A	531	TRP	CD2-CE2	5.07	1.47	1.41
1	A	431	TRP	CD2-CE2	5.01	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	57	0
2	B	1076	0	1091	15	0
3	C	53	0	62	1	0
4	A	53	0	31	4	0
All	All	6399	0	6436	60	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 (60) 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	4:A:900:FAD:HM83	1.56	0.85
1:A:384:ARG:HB3	2:B:314:MET:HE1	1.62	0.80
1:A:384:ARG:HH22	2:B:313:GLY:HA3	1.51	0.74
1:A:384:ARG:HB3	2:B:314:MET:CE	2.24	0.67
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.76	0.67
1:A:199:ILE:HD11	1:A:248:LEU:HD11	1.75	0.67
1:A:801:GLU:HG2	1:A:809:ALA:H	1.63	0.63
1:A:356:ILE:HD11	1:A:566:THR:HG23	1.81	0.63
1:A:419:GLN:HE22	2:B:315:PHE:H	1.47	0.63
1:A:693:LEU:HD21	3:C:6:VAL:HG21	1.81	0.62
1:A:257:GLU:HG3	1:A:263:ASN:HD22	1.66	0.61
1:A:548:SER:O	1:A:552:TRP:HB3	2.02	0.60
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.32	0.59
1:A:331:ALA:HA	4:A:900:FAD:N5	2.21	0.56
1:A:501:GLN:O	1:A:505:GLU:HB2	2.06	0.55
1:A:760:SER:CB	4:A:900:FAD:HM83	2.31	0.54
1:A:485:ARG:HG3	2:B:407:ASP:HB2	1.89	0.53
1:A:353:LEU:HB3	1:A:565:LEU:HD22	1.90	0.53
1:A:331:ALA:HA	4:A:900:FAD:C4X	2.40	0.52
1:A:435:VAL:O	1:A:439:GLU:HB2	2.09	0.52
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.92	0.52
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.93	0.51
1:A:755:PRO:HA	1:A:758:ARG:NH1	2.26	0.50
1:A:789:ALA:HB1	1:A:790:PRO:HD2	1.92	0.50
1:A:292:ALA:HB2	1:A:815:LEU:HD22	1.95	0.49
1:A:306:LEU:HD13	1:A:584:ILE:HG12	1.93	0.49
1:A:601:GLU:HA	1:A:616:TYR:O	2.13	0.48
1:A:537:GLU:HG2	1:A:544:LEU:HG	1.96	0.48
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.95	0.47
1:A:435:VAL:HG13	2:B:349:ILE:HG13	1.97	0.47
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.79	0.47
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.97	0.47
2:B:421:PHE:O	2:B:425:ARG:HB2	2.14	0.47
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.95	0.47
1:A:384:ARG:NH2	2:B:313:GLY:HA3	2.24	0.47
1:A:594:ARG:HG2	1:A:640:VAL:HB	1.96	0.47
1:A:533:PHE:O	1:A:537:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ILE:H	1:A:786:ILE:HD12	1.80	0.46
1:A:690:GLU:HG2	1:A:691:LEU:HD12	1.98	0.45
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.52	0.45
1:A:695:TRP:HB2	1:A:704:LEU:HB3	2.00	0.44
1:A:666:PHE:O	1:A:701:PRO:HG2	2.18	0.44
1:A:456:LYS:HG2	2:B:370:TYR:CE2	2.51	0.44
1:A:428:ILE:O	1:A:432:LYS:HB2	2.18	0.43
1:A:217:THR:HA	1:A:220:LEU:HD12	2.01	0.43
1:A:801:GLU:HG2	1:A:809:ALA:N	2.32	0.43
1:A:606:ASN:ND2	1:A:609:SER:H	2.17	0.43
1:A:180:GLN:HA	1:A:339:GLY:HA2	2.01	0.42
1:A:574:VAL:HB	1:A:575:PRO:CD	2.50	0.42
1:A:374:LYS:HE3	1:A:525:ASP:OD1	2.20	0.42
1:A:214:ARG:HD2	1:A:215:ASN:OD1	2.20	0.42
1:A:289:SER:HB3	1:A:814:ALA:HB1	2.02	0.42
1:A:391:TYR:CD1	1:A:395:GLN:HG3	2.54	0.41
1:A:463:LYS:O	1:A:467:GLU:HG2	2.20	0.41
1:A:448:MET:HG3	1:A:497:LEU:HD23	2.03	0.41
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.86	0.40
1:A:474:ILE:HG23	2:B:393:GLN:HE22	1.85	0.40
1:A:720:ASP:O	1:A:724:VAL:HG23	2.21	0.40
2:B:372:LEU:HA	2:B:373:PRO:HD2	1.77	0.40
2:B:361:GLU:O	2:B:364:ASP:HB2	2.22	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	664/872 (76%)	637 (96%)	26 (4%)	1 (0%)	52	84
2	B	131/482 (27%)	121 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	4/6 (67%)	4 (100%)	0	0	100	100
All	All	799/1360 (59%)	762 (95%)	36 (4%)	1 (0%)	56	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	805	ARG

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	566/711 (80%)	543 (96%)	23 (4%)	37	74
2	B	117/395 (30%)	112 (96%)	5 (4%)	35	72
3	C	6/6 (100%)	6 (100%)	0	100	100
All	All	689/1112 (62%)	661 (96%)	28 (4%)	37	74

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	174	VAL
1	A	206	THR
1	A	237	GLN
1	A	413	GLU
1	A	429	GLU
1	A	449	VAL
1	A	458	LEU
1	A	469	LYS
1	A	492	LYS
1	A	535	ASN
1	A	538	PHE
1	A	571	TYR
1	A	588	THR
1	A	638	GLN

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Mol	Chain	Res	Type
1	A	645	GLU
1	A	659	LEU
1	A	667	ASP
1	A	677	LEU
1	A	680	HIS
1	A	684	THR
1	A	696	ASN
1	A	786	ILE
1	A	835	THR
2	B	332	THR
2	B	337	GLN
2	B	349	ILE
2	B	385	THR
2	B	419	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	419	GLN
1	A	438	GLN
1	A	460	GLN
1	A	535	ASN
1	A	606	ASN
1	A	742	GLN
2	B	318	GLN
2	B	348	GLN
2	B	419	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	900	-	48,58,58	1.40	7 (14%)	54,89,89	2.13	11 (20%)

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	900	-	-	0/30/50/50	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	900	FAD	C10-N10	2.45	1.42	1.39
4	A	900	FAD	C9A-N10	2.80	1.42	1.38
4	A	900	FAD	C8-C7	3.21	1.49	1.41
4	A	900	FAD	C4-C4X	3.29	1.47	1.41
4	A	900	FAD	C5A-C4A	3.30	1.47	1.40
4	A	900	FAD	C9A-C5X	3.65	1.50	1.42
4	A	900	FAD	C4X-C10	4.10	1.48	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	900	FAD	N3A-C2A-N1A	-7.87	122.87	128.89
4	A	900	FAD	C4-C4X-C10	-4.21	117.24	119.94
4	A	900	FAD	C4X-C4-N3	-3.72	118.50	123.59
4	A	900	FAD	P-O3P-PA	-3.13	123.93	132.73
4	A	900	FAD	C4X-C10-N10	-2.95	118.78	120.52
4	A	900	FAD	C1B-N9A-C4A	-2.37	123.37	126.94
4	A	900	FAD	C4A-C5A-N7A	-2.26	107.40	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	900	FAD	C1'-N10-C9A	2.14	121.26	118.86
4	A	900	FAD	C5X-C9A-N10	2.68	119.66	117.62
4	A	900	FAD	C4X-N5-C5X	3.51	120.80	116.76
4	A	900	FAD	C4-N3-C2	8.27	122.40	115.25

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
4	A	900	FAD	4	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	666/872 (76%)	0.07	4 (0%)	90	80	48, 85, 122, 153	0
2	B	133/482 (27%)	0.44	5 (3%)	44	21	80, 114, 137, 156	0
3	C	6/6 (100%)	-0.02	0	100	100	79, 86, 89, 97	0
All	All	805/1360 (59%)	0.13	9 (1%)	82	66	48, 90, 128, 156	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	374	GLU	3.4
2	B	376	ILE	3.0
1	A	171	PRO	2.4
2	B	414	VAL	2.4
2	B	402	PHE	2.3
1	A	174	VAL	2.3
1	A	273	LEU	2.3
2	B	312	LYS	2.2
1	A	172	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. 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, 95th 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
4	FAD	A	900	53/53	0.98	0.23	-0.16	54,64,79,80	0

6.5 Other polymers (i)

There are no such residues in this entry.