Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2016 – 03:51 PM EDT

PDB ID	:	5L3E
Title	:	LSD1-CoREST1 in complex with quinazoline-derivative reversible inhibitor
Authors	:	Speranzini, V.; Rotili, D.; Ciossani, G.; Pilotto, S.; Forgione, M.; Lucidi, A.; Forneris, F.; Velankar, S.; Mai, A.; Mattevi, A.
Deposited on	:	2016-04-10
Resolution	:	2.80 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 ⓘ symbol.

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

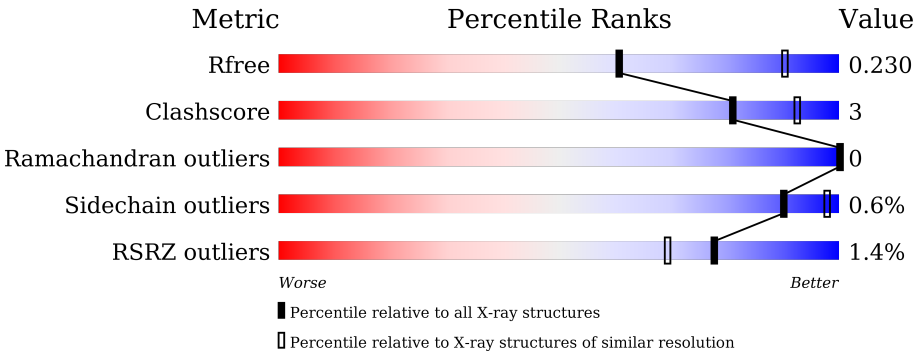
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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

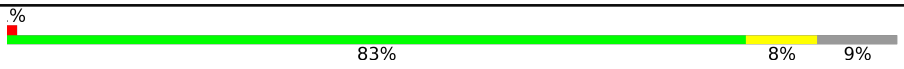
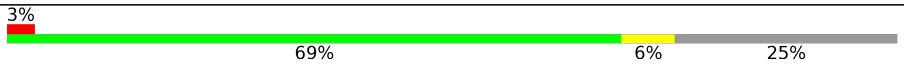
The reported resolution of this entry is 2.80 Å.

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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	
2	B	178	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	E11	A	903	-	-	-	X
4	E11	A	904	-	-	-	X
5	NA	A	907	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6522 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.

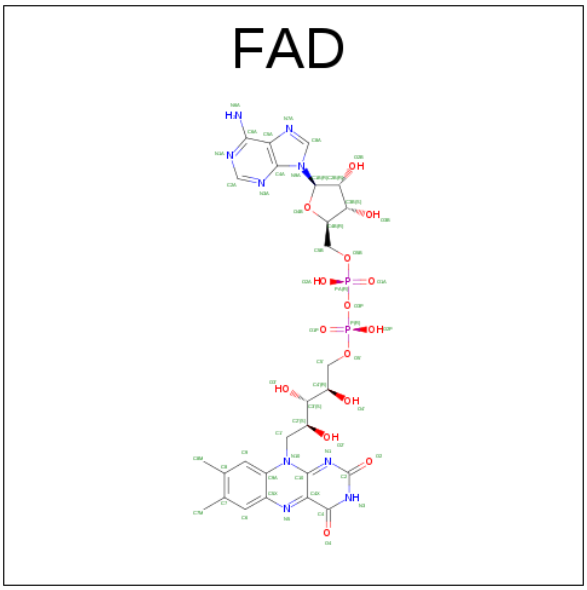
- Molecule 1 is a protein called Lysine-specific histone demethylase 1A.

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			

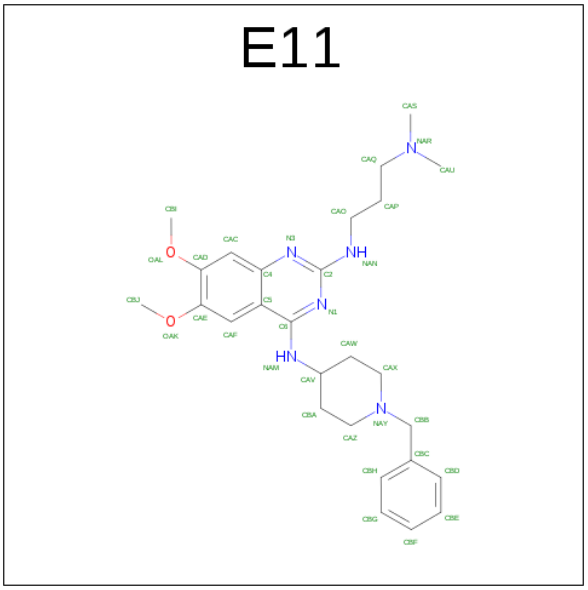
- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 4 is N 4 -(1-benzylpiperidin-4-yl)-N 2 -[3-(dimethylamino)propyl]-6,7-dimethoxyq

uinazoline-2,4-diamine (three-letter code: E11) (formula: $C_{27}H_{38}N_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 35 27 6 2	0	0
4	A	1	Total C N O 35 27 6 2	0	0
4	A	1	Total C N O 35 27 6 2	0	0
4	A	1	Total C N O 35 27 6 2	0	0
4	A	1	Total C N O 35 27 6 2	0	0

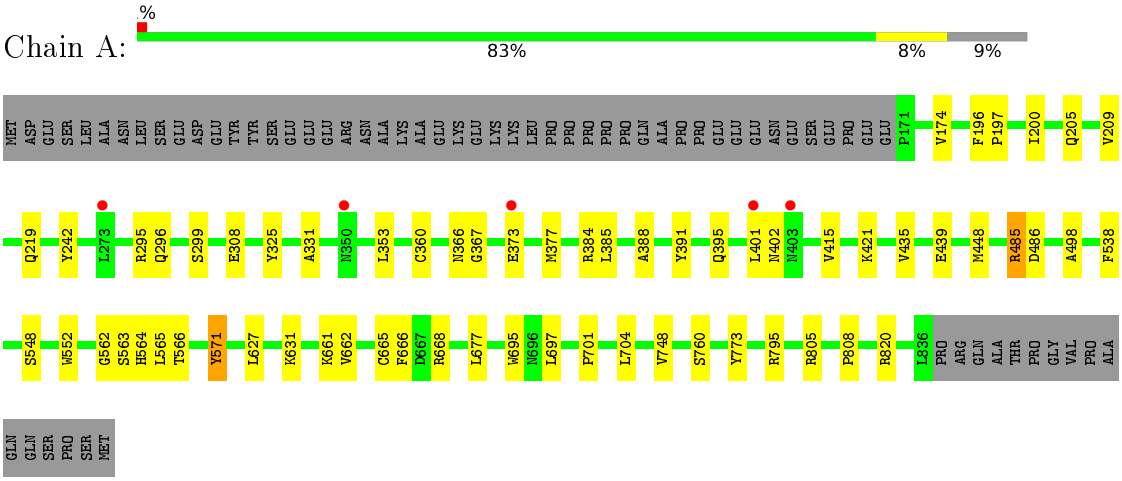
- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

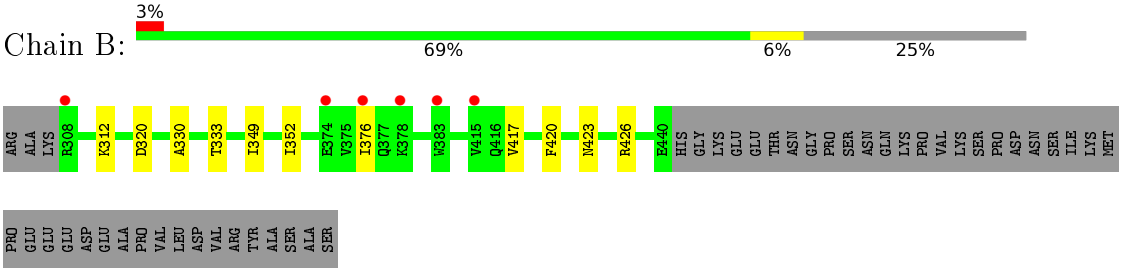
3 Residue-property plots (i)

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



- Molecule 2: REST corepressor 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	116.57Å 178.40Å 233.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.57 – 2.80 97.58 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (98.57-2.80) 99.7 (97.58-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.200 , 0.224 0.210 , 0.230	Depositor DCC
R_{free} test set	1165 reflections (1.98%)	DCC
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.8	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	0.94	EDS
Total number of atoms	6522	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: E11, NA, 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	0.68	0/5331	0.87	8/7232 (0.1%)
2	B	0.58	0/1091	0.78	0/1471
All	All	0.66	0/6422	0.86	8/8703 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	820	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	795	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	795	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	571	TYR	CB-CG-CD1	5.61	124.36	121.00
1	A	820	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	295	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	A	805	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	295	ARG	NE-CZ-NH1	-5.26	117.67	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5217	0	5252	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1076	0	1091	8	0
3	A	53	0	31	5	0
4	A	175	0	190	2	0
5	A	1	0	0	0	0
All	All	6522	0	6564	43	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 3.

All (43) 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:353:LEU:HB3	1:A:565:LEU:HD23	1.67	0.77
1:A:760:SER:HB2	3:A:901:FAD:HM83	1.75	0.69
1:A:760:SER:CB	3:A:901:FAD:HM83	2.26	0.65
1:A:562:GLY:O	4:A:904:E11:HAU	1.99	0.62
1:A:661:LYS:HB3	1:A:704:LEU:HD21	1.83	0.61
1:A:666:PHE:O	1:A:701:PRO:HG2	2.02	0.59
1:A:331:ALA:HA	3:A:901:FAD:N5	2.19	0.56
1:A:564:HIS:C	1:A:565:LEU:HD12	2.28	0.54
1:A:391:TYR:CD1	1:A:395:GLN:HG3	2.45	0.52
1:A:421:LYS:NZ	2:B:320:ASP:OD1	2.45	0.50
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.93	0.49
1:A:385:LEU:HD23	1:A:415:VAL:HG12	1.94	0.49
1:A:563:SER:HA	4:A:904:E11:HAS	1.94	0.49
1:A:485:ARG:HG3	1:A:486:ASP:N	2.27	0.48
1:A:325:TYR:CE2	1:A:665:CYS:HB3	2.49	0.48
1:A:385:LEU:O	1:A:388:ALA:HB3	2.13	0.48
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.48	0.47
1:A:384:ARG:NH2	2:B:312:LYS:O	2.48	0.47
1:A:439:GLU:HG3	2:B:352:ILE:HD13	1.96	0.46
1:A:331:ALA:HA	3:A:901:FAD:C4X	2.45	0.46
2:B:423:ASN:O	2:B:426:ARG:NH1	2.49	0.45
1:A:373:GLU:O	1:A:377:MET:HG2	2.17	0.45
1:A:662:VAL:HG13	1:A:748:VAL:HG22	1.97	0.45
1:A:209:VAL:HG13	1:A:242:TYR:HD1	1.82	0.44
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.47	0.44
1:A:360:CYS:SG	1:A:677:LEU:CD1	3.05	0.44
1:A:548:SER:O	1:A:552:TRP:HB3	2.17	0.44
1:A:205:GLN:O	1:A:209:VAL:HG23	2.18	0.44
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:ILE:HG22	2:B:376:ILE:O	2.18	0.43
1:A:197:PRO:HA	1:A:200:ILE:HG22	2.01	0.43
2:B:417:VAL:O	2:B:420:PHE:HB3	2.20	0.42
1:A:401:LEU:O	1:A:402:ASN:HB2	2.20	0.41
1:A:448:MET:HE3	1:A:498:ALA:HB2	2.01	0.41
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.20	0.41
1:A:563:SER:O	1:A:565:LEU:CD1	2.69	0.41
1:A:308:GLU:OE1	3:A:901:FAD:O3B	2.37	0.41
1:A:196:PHE:N	1:A:197:PRO:HD3	2.36	0.41
1:A:296:GLN:O	1:A:299:SER:HB3	2.20	0.41
2:B:330:ALA:HA	2:B:333:THR:HB	2.03	0.41
1:A:366:ASN:OD1	1:A:367:GLY:N	2.54	0.41
1:A:627:LEU:O	1:A:631:LYS:HG3	2.20	0.41
1:A:360:CYS:SG	1:A:677:LEU:HD12	2.62	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%)	636 (96%)	28 (4%)	0	100	100
2	B	131/178 (74%)	124 (95%)	7 (5%)	0	100	100
All	All	795/908 (88%)	760 (96%)	35 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	562 (99%)	4 (1%)	88 97
2	B	117/156 (75%)	117 (100%)	0	100 100
All	All	683/779 (88%)	679 (99%)	4 (1%)	90 98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	485	ARG
1	A	538	PHE
1	A	571	TYR
1	A	668	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	5	52,58,58	1.30	8 (15%)	52,89,89	2.72	15 (28%)
4	E11	A	902	-	37,38,38	1.26	3 (8%)	49,51,51	2.49	17 (34%)
4	E11	A	903	-	37,38,38	1.18	3 (8%)	49,51,51	2.37	14 (28%)
4	E11	A	904	-	37,38,38	1.34	5 (13%)	49,51,51	2.36	16 (32%)
4	E11	A	905	-	37,38,38	1.51	7 (18%)	49,51,51	2.60	15 (30%)
4	E11	A	906	-	37,38,38	1.31	4 (10%)	49,51,51	2.85	21 (42%)

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	5	-	0/30/50/50	0/6/6/6
4	E11	A	902	-	-	0/19/29/29	0/4/4/4
4	E11	A	903	-	-	0/19/29/29	0/4/4/4
4	E11	A	904	-	-	0/19/29/29	0/4/4/4
4	E11	A	905	-	-	0/19/29/29	0/4/4/4
4	E11	A	906	-	-	0/19/29/29	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	E11	C6-C5	-4.57	1.39	1.44
3	A	901	FAD	C2B-C1B	-2.88	1.49	1.53
3	A	901	FAD	C6-C5X	-2.60	1.37	1.41
4	A	903	E11	C6-C5	-2.51	1.41	1.44
4	A	906	E11	C6-C5	-2.32	1.42	1.44
4	A	905	E11	OAL-CAD	2.13	1.40	1.37
4	A	904	E11	CBB-CBC	2.14	1.55	1.51
4	A	904	E11	OAK-CAE	2.18	1.40	1.37
3	A	901	FAD	C8-C7	2.34	1.47	1.41
4	A	903	E11	CAC-CAD	2.35	1.40	1.36
3	A	901	FAD	C5A-C4A	2.42	1.46	1.40
4	A	906	E11	CBB-NAY	2.43	1.52	1.47
3	A	901	FAD	C9A-C5X	2.44	1.47	1.42
4	A	902	E11	CAC-CAD	2.44	1.40	1.36
4	A	904	E11	C6-N1	2.49	1.36	1.33
4	A	902	E11	CAF-CAE	2.50	1.41	1.36
4	A	905	E11	C2-NAN	2.52	1.38	1.34
4	A	904	E11	CAC-CAD	2.55	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	906	E11	CAF-CAE	2.68	1.41	1.36
4	A	905	E11	CBB-CBC	2.73	1.56	1.51
3	A	901	FAD	C9A-N10	2.74	1.42	1.38
4	A	903	E11	C6-N1	2.78	1.36	1.33
4	A	905	E11	CBB-NAY	2.82	1.52	1.47
4	A	905	E11	CAF-CAE	2.90	1.41	1.36
3	A	901	FAD	C4X-C10	3.00	1.46	1.40
4	A	905	E11	CAC-CAD	3.00	1.41	1.36
4	A	904	E11	CAF-CAE	3.15	1.42	1.36
4	A	905	E11	C6-N1	3.22	1.37	1.33
4	A	906	E11	C6-N1	3.23	1.37	1.33
3	A	901	FAD	C10-N10	3.28	1.43	1.39

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	FAD	N3A-C2A-N1A	-9.77	121.20	128.87
4	A	902	E11	CAF-C5-C6	-7.78	120.47	124.87
4	A	906	E11	OAL-CAD-CAC	-6.93	116.43	125.26
3	A	901	FAD	C1B-N9A-C4A	-6.92	119.08	126.81
3	A	901	FAD	C4X-C10-N10	-6.28	115.96	120.52
4	A	903	E11	N3-C2-N1	-5.39	118.12	126.18
4	A	906	E11	OAK-CAE-CAF	-5.32	118.48	125.26
4	A	905	E11	N3-C2-N1	-5.20	118.40	126.18
4	A	903	E11	CAW-CAV-NAM	-5.15	102.22	110.53
4	A	904	E11	N3-C2-N1	-4.96	118.76	126.18
4	A	906	E11	N3-C2-N1	-4.64	119.24	126.18
4	A	903	E11	CAF-C5-C6	-4.62	122.26	124.87
4	A	904	E11	C5-C6-N1	-4.59	116.27	122.42
4	A	906	E11	CBA-CAV-NAM	-4.58	103.14	110.53
4	A	905	E11	CAF-C5-C6	-4.57	122.28	124.87
4	A	902	E11	C5-C6-N1	-4.43	116.48	122.42
4	A	902	E11	OAK-CAE-CAF	-3.84	120.37	125.26
4	A	905	E11	C5-C4-N3	-3.82	119.38	122.89
3	A	901	FAD	C4-C4X-C10	-3.78	117.52	119.94
4	A	905	E11	C5-C6-N1	-3.78	117.35	122.42
3	A	901	FAD	N3-C2-N1	-3.70	121.46	127.69
4	A	904	E11	OAK-CAE-CAF	-3.44	120.87	125.26
4	A	904	E11	C5-C4-N3	-3.42	119.75	122.89
4	A	903	E11	C5-C6-N1	-3.25	118.07	122.42
3	A	901	FAD	C4B-O4B-C1B	-3.23	106.22	109.64
4	A	902	E11	N3-C2-N1	-3.18	121.43	126.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	904	E11	CAF-C5-C6	-3.12	123.11	124.87
4	A	905	E11	CBA-CAV-CAW	-3.01	105.86	110.87
4	A	906	E11	CAP-CAO-NAN	-2.95	103.41	111.36
4	A	902	E11	OAL-CAD-CAC	-2.95	121.50	125.26
3	A	901	FAD	C4X-C4-N3	-2.91	119.72	123.52
4	A	902	E11	CAO-NAN-C2	-2.89	118.69	123.62
4	A	903	E11	C5-C4-N3	-2.88	120.25	122.89
4	A	906	E11	C5-C6-N1	-2.84	118.61	122.42
4	A	902	E11	C5-C4-N3	-2.58	120.53	122.89
4	A	904	E11	CAP-CAO-NAN	-2.49	104.65	111.36
3	A	901	FAD	O5'-P-O1P	-2.34	99.65	109.21
4	A	903	E11	C6-NAM-CAV	-2.24	120.55	124.34
4	A	902	E11	CAP-CAO-NAN	-2.17	105.51	111.36
4	A	906	E11	CAF-C5-C6	-2.17	123.64	124.87
4	A	906	E11	CBA-CAV-CAW	2.03	114.25	110.87
4	A	903	E11	C2-N3-C4	2.03	121.41	115.97
3	A	901	FAD	O2A-PA-O3P	2.03	113.98	105.27
4	A	905	E11	C2-N3-C4	2.05	121.45	115.97
4	A	904	E11	CAU-NAR-CAS	2.09	115.22	109.71
4	A	903	E11	CBD-CBC-CBH	2.10	121.62	118.15
4	A	904	E11	CAO-NAN-C2	2.14	127.27	123.62
4	A	902	E11	NAN-C2-N3	2.15	121.37	117.24
3	A	901	FAD	O2P-P-O1P	2.19	123.95	112.56
4	A	903	E11	CBA-CAV-NAM	2.23	114.14	110.53
4	A	906	E11	CBB-NAY-CAX	2.32	116.41	111.09
4	A	903	E11	CAZ-NAY-CAX	2.32	114.08	108.87
4	A	904	E11	CAW-CAV-NAM	2.35	114.33	110.53
4	A	906	E11	CBB-CBC-CBH	2.35	125.19	120.78
4	A	905	E11	NAN-C2-N3	2.39	121.83	117.24
4	A	905	E11	CAZ-CBA-CAV	2.43	114.03	110.29
4	A	904	E11	CAZ-CBA-CAV	2.43	114.04	110.29
4	A	902	E11	CAZ-CBA-CAV	2.48	114.11	110.29
3	A	901	FAD	C2A-N1A-C6A	2.49	123.22	118.77
3	A	901	FAD	C1'-N10-C9A	2.67	121.92	118.83
4	A	906	E11	C6-C5-C4	2.70	117.38	115.83
4	A	904	E11	NAN-C2-N3	2.72	122.45	117.24
3	A	901	FAD	N6A-C6A-N1A	2.81	123.22	118.52
4	A	904	E11	OAK-CAE-CAD	2.82	119.21	115.41
4	A	902	E11	CAU-NAR-CAS	2.82	117.13	109.71
4	A	902	E11	OAK-CAE-CAD	2.82	119.21	115.41
4	A	904	E11	CBC-CBB-NAY	2.95	118.84	113.17
4	A	906	E11	NAN-C2-N3	3.07	123.12	117.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	905	E11	CAW-CAX-NAY	3.21	116.35	110.97
4	A	902	E11	OAL-CAD-CAE	3.23	119.76	115.41
4	A	906	E11	CBI-OAL-CAD	3.27	122.30	117.53
4	A	903	E11	NAN-C2-N3	3.33	123.64	117.24
4	A	906	E11	CAO-NAN-C2	3.42	129.46	123.62
4	A	905	E11	CAZ-NAY-CAX	3.45	116.59	108.87
4	A	902	E11	CAW-CAX-NAY	3.54	116.90	110.97
4	A	906	E11	CAZ-NAY-CAX	3.68	117.11	108.87
4	A	903	E11	C6-C5-C4	3.71	117.96	115.83
3	A	901	FAD	C4X-N5-C5X	3.81	121.21	116.72
4	A	902	E11	CBI-OAL-CAD	4.07	123.47	117.53
4	A	906	E11	CAX-CAW-CAV	4.44	117.12	110.29
4	A	906	E11	CBJ-OAK-CAE	4.56	124.18	117.53
4	A	905	E11	CBA-CAZ-NAY	4.61	118.69	110.97
4	A	906	E11	CAW-CAX-NAY	4.64	118.74	110.97
4	A	906	E11	OAK-CAE-CAD	5.05	122.22	115.41
4	A	902	E11	CBJ-OAK-CAE	5.19	125.10	117.53
4	A	904	E11	C6-C5-C4	5.34	118.89	115.83
4	A	904	E11	CBJ-OAK-CAE	5.37	125.36	117.53
4	A	905	E11	CBJ-OAK-CAE	5.42	125.44	117.53
4	A	905	E11	CBC-CBB-NAY	5.52	123.78	113.17
4	A	906	E11	CBC-CBB-NAY	5.77	124.28	113.17
4	A	905	E11	C6-C5-C4	5.99	119.27	115.83
4	A	906	E11	OAL-CAD-CAE	6.28	123.87	115.41
4	A	903	E11	CBI-OAL-CAD	6.81	127.46	117.53
4	A	903	E11	CBJ-OAK-CAE	7.17	127.99	117.53
4	A	902	E11	C6-C5-C4	7.46	120.11	115.83
4	A	904	E11	CBI-OAL-CAD	7.51	128.49	117.53
4	A	905	E11	CBI-OAL-CAD	7.98	129.17	117.53
3	A	901	FAD	C4-N3-C2	8.48	122.23	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	FAD	5	0
4	A	904	E11	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	666/730 (91%)	0.23	5 (0%) 87 81	34, 64, 102, 130	0
2	B	133/178 (74%)	0.48	6 (4%) 37 26	58, 93, 127, 140	0
All	All	799/908 (87%)	0.27	11 (1%) 78 69	34, 69, 108, 140	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	376	ILE	4.3
1	A	403	ASN	3.1
2	B	378	LYS	2.8
2	B	374	GLU	2.3
1	A	373	GLU	2.2
1	A	273	LEU	2.2
1	A	350	ASN	2.2
1	A	401	LEU	2.1
2	B	415	VAL	2.1
2	B	308	ARG	2.1
2	B	383	TRP	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	E11	A	904	35/35	0.92	0.35	8.22	74,103,154,164	0
5	NA	A	907	1/1	0.85	0.42	6.90	55,55,55,55	0
4	E11	A	903	35/35	0.94	0.30	2.22	65,94,121,124	0
4	E11	A	902	35/35	0.96	0.23	0.11	57,76,96,98	0
3	FAD	A	901	53/53	0.98	0.21	-0.63	33,43,54,65	0
4	E11	A	905	35/35	0.89	0.45	-	95,122,140,145	0
4	E11	A	906	35/35	0.73	0.57	-	125,153,172,177	0

6.5 Other polymers

There are no such residues in this entry.