



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 10:48 PM BST

PDB ID : 6VYP
Title : Crystal structure of the LSD1/CoREST histone demethylase bound to its nucleosome substrate
Authors : Kim, S.; Zhu, J.; Eek, P.; Yennawar, N.; Song, T.
Deposited on : 2020-02-27
Resolution : 4.99 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

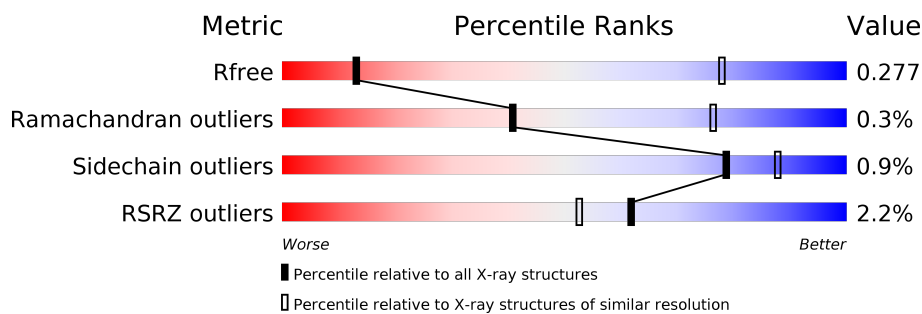
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.99 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.











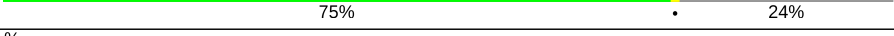
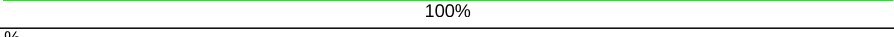
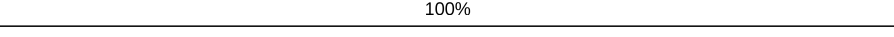
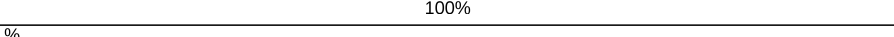
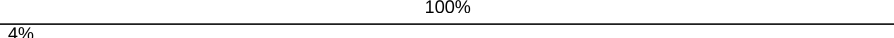
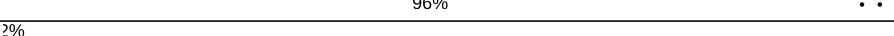
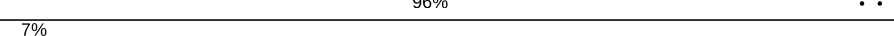
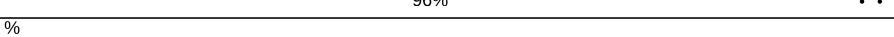
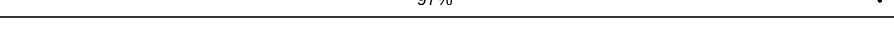
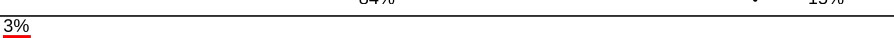
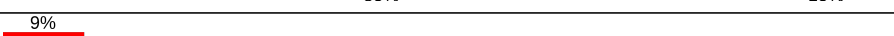
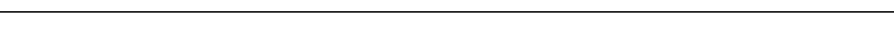

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1140 (6.20-3.80)
Ramachandran outliers	138981	1146 (6.20-3.80)
Sidechain outliers	138945	1122 (6.20-3.80)
RSRZ outliers	127900	1010 (6.22-3.72)

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 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 $\leq 5\%$. 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	135	
1	E	135	
1	a	135	
1	e	135	
2	B	102	
2	F	102	
2	b	102	

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Mol	Chain	Length	Quality of chain
2	f	102	
3	C	129	
3	G	129	
3	c	129	
3	g	129	
4	D	122	
4	H	122	
4	d	122	
4	h	122	
5	I	191	
5	i	191	
6	J	191	
6	j	191	
7	K	684	
7	M	684	
7	k	684	
7	m	684	
8	L	157	
8	N	157	
8	l	157	
8	n	157	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 52996 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 Histone H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	110	Total	C	N	O	S	0	0	0
			893	559	174	156	4			
1	E	110	Total	C	N	O	S	0	0	0
			889	557	174	154	4			
1	a	94	Total	C	N	O	S	0	0	0
			774	489	147	135	3			
1	e	103	Total	C	N	O	S	0	0	0
			836	525	158	149	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	LYS	engineered mutation	UNP A0A310TTQ1
E	4	MET	LYS	engineered mutation	UNP A0A310TTQ1
a	4	MET	LYS	engineered mutation	UNP A0A310TTQ1
e	4	MET	LYS	engineered mutation	UNP A0A310TTQ1

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	81	Total	C	N	O	S	0	0	0
			648	410	126	111	1			
2	F	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			
2	b	80	Total	C	N	O	S	0	0	0
			638	401	125	111	1			
2	f	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			

- Molecule 3 is a protein called Histone H2A type 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	0	0	0
			795	501	155	139			
3	G	105	Total	C	N	O	0	0	0
			809	510	158	141			
3	c	103	Total	C	N	O	0	0	0
			795	501	155	139			
3	g	104	Total	C	N	O	0	0	0
			804	507	157	140			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	99	ARG	GLY	engineered mutation	UNP P06897
C	123	SER	ALA	engineered mutation	UNP P06897
G	99	ARG	GLY	engineered mutation	UNP P06897
G	123	SER	ALA	engineered mutation	UNP P06897
c	99	ARG	GLY	engineered mutation	UNP P06897
c	123	SER	ALA	engineered mutation	UNP P06897
g	99	ARG	GLY	engineered mutation	UNP P06897
g	123	SER	ALA	engineered mutation	UNP P06897

- Molecule 4 is a protein called Histone H2B 1.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	92	Total	C	N	O	S	0	0	0
			719	453	129	135	2			
4	H	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			
4	d	91	Total	C	N	O	S	0	0	0
			708	447	125	134	2			
4	h	93	Total	C	N	O	S	0	0	0
			726	457	130	137	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	29	THR	SER	engineered mutation	UNP P02281
H	29	THR	SER	engineered mutation	UNP P02281
d	29	THR	SER	engineered mutation	UNP P02281
h	29	THR	SER	engineered mutation	UNP P02281

- Molecule 5 is a DNA chain called DNA (191-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	191	Total	C	N	O	P	0	0	0
			3895	1849	710	1145	191			
5	i	191	Total	C	N	O	P	0	0	0
			3895	1849	710	1145	191			

- Molecule 6 is a DNA chain called DNA (191-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	191	Total	C	N	O	P	0	0	0
			3936	1863	735	1147	191			
6	j	191	Total	C	N	O	P	0	0	0
			3936	1863	735	1147	191			

- Molecule 7 is a protein called Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	M	666	Total	C	N	O	S	0	0	0
			5205	3319	902	964	20			
7	m	666	Total	C	N	O	S	0	0	0
			5205	3319	902	964	20			
7	K	666	Total	C	N	O	S	0	0	0
			5205	3319	902	964	20			
7	k	666	Total	C	N	O	S	0	0	0
			5205	3319	902	964	20			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	169	GLY	-	expression tag	UNP O60341
M	170	SER	-	expression tag	UNP O60341
M	608	ALA	ARG	engineered mutation	UNP O60341
M	717	ALA	ASN	engineered mutation	UNP O60341
M	721	ALA	ASP	engineered mutation	UNP O60341
m	169	GLY	-	expression tag	UNP O60341
m	170	SER	-	expression tag	UNP O60341
m	608	ALA	ARG	engineered mutation	UNP O60341
m	717	ALA	ASN	engineered mutation	UNP O60341
m	721	ALA	ASP	engineered mutation	UNP O60341
K	169	GLY	-	expression tag	UNP O60341
K	170	SER	-	expression tag	UNP O60341
K	608	ALA	ARG	engineered mutation	UNP O60341
K	717	ALA	ASN	engineered mutation	UNP O60341
K	721	ALA	ASP	engineered mutation	UNP O60341

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Chain	Residue	Modelled	Actual	Comment	Reference
k	169	GLY	-	expression tag	UNP O60341
k	170	SER	-	expression tag	UNP O60341
k	608	ALA	ARG	engineered mutation	UNP O60341
k	717	ALA	ASN	engineered mutation	UNP O60341
k	721	ALA	ASP	engineered mutation	UNP O60341

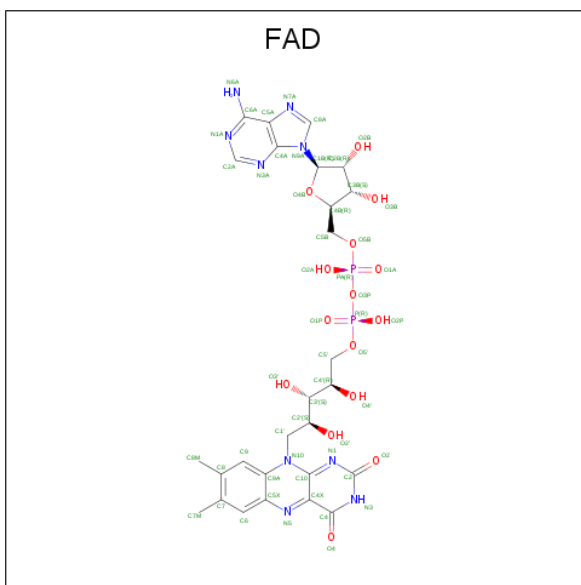
- Molecule 8 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	N	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			
8	n	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			
8	L	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			
8	l	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	284	GLY	-	expression tag	UNP Q9UKL0
N	285	SER	-	expression tag	UNP Q9UKL0
n	284	GLY	-	expression tag	UNP Q9UKL0
n	285	SER	-	expression tag	UNP Q9UKL0
L	284	GLY	-	expression tag	UNP Q9UKL0
L	285	SER	-	expression tag	UNP Q9UKL0
l	284	GLY	-	expression tag	UNP Q9UKL0
l	285	SER	-	expression tag	UNP Q9UKL0

- Molecule 9 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).




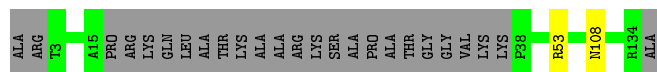
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	M	1	Total 53	C 27	N 9	O 15	P 2	0	0
9	m	1	Total 53	C 27	N 9	O 15	P 2	0	0
9	K	1	Total 53	C 27	N 9	O 15	P 2	0	0
9	k	1	Total 53	C 27	N 9	O 15	P 2	0	0

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.

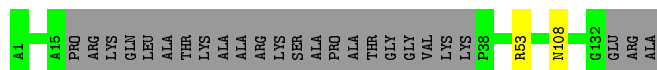
- Molecule 1: Histone H3

Chain A: 



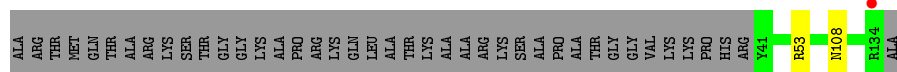
- Molecule 1: Histone H3

Chain E: 



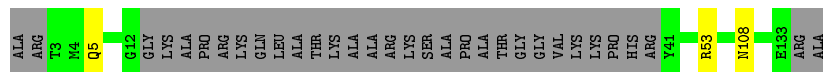
- Molecule 1: Histone H3

Chain a: 




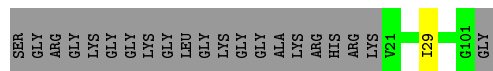
- Molecule 1: Histone H3

Chain e: 



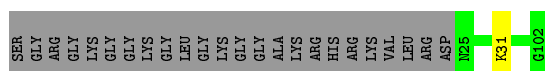
- Molecule 2: Histone H4

Chain B: 

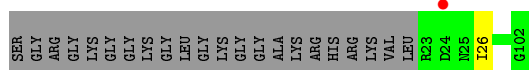
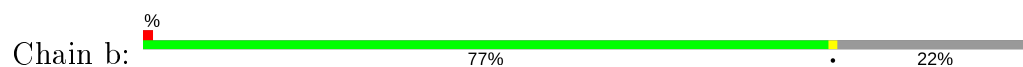


- Molecule 2: Histone H4

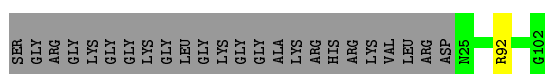
Chain F: 



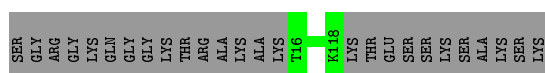
- Molecule 2: Histone H4



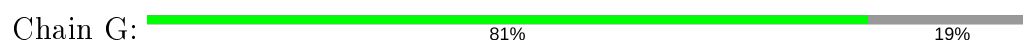
- Molecule 2: Histone H4



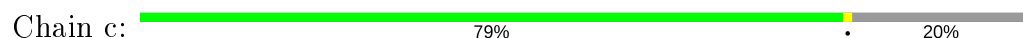
- Molecule 3: Histone H2A type 1



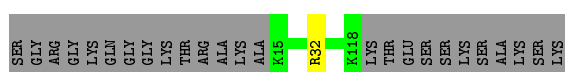
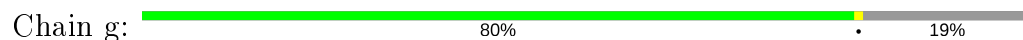
- Molecule 3: Histone H2A type 1



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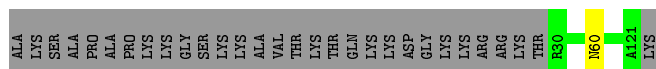


- Molecule 3: Histone H2A type 1



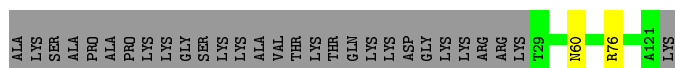
- Molecule 4: Histone H2B 1.1





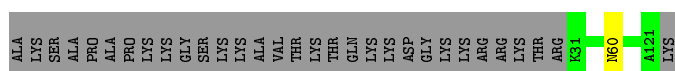
- Molecule 4: Histone H2B 1.1

Chain H: 75% 24%



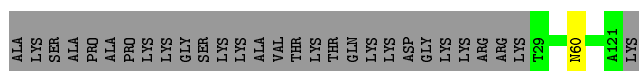
- Molecule 4: Histone H2B 1.1

Chain d: 74% 25%



- Molecule 4: Histone H2B 1.1

Chain h: 75% 24%



- Molecule 5: DNA (191-MER)

Chain I: 100%



- Molecule 5: DNA (191-MER)

Chain i: 100%



- Molecule 6: DNA (191-MER)

Chain J: 100%

There are no outlier residues recorded for this chain.

- Molecule 6: DNA (191-MER)

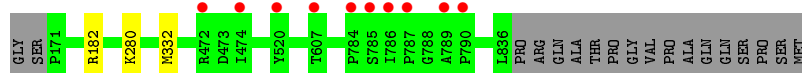
Chain j: 100%



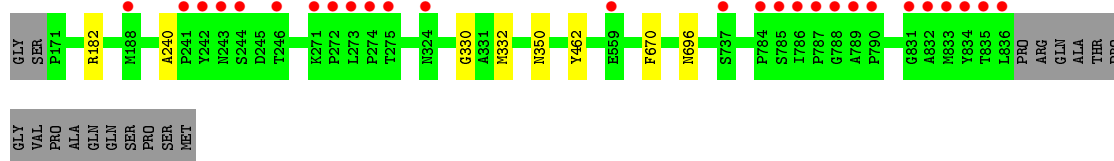
- Molecule 7: Lysine-specific histone demethylase 1A



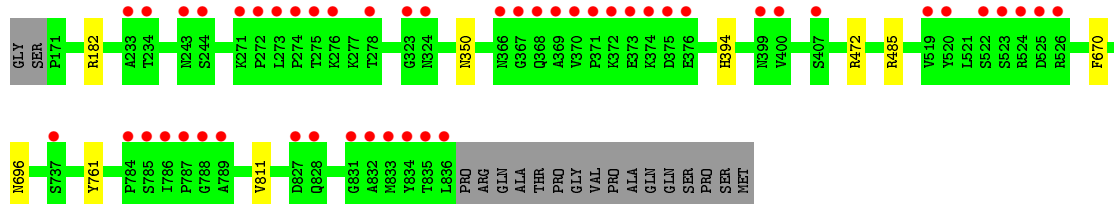
- Molecule 7: Lysine-specific histone demethylase 1A



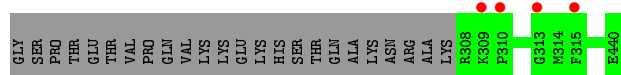
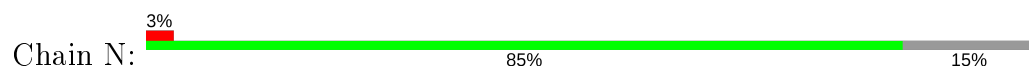
- Molecule 7: Lysine-specific histone demethylase 1A



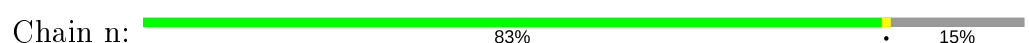
- Molecule 7: Lysine-specific histone demethylase 1A

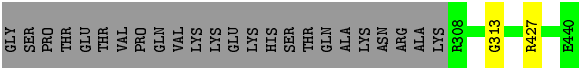


- Molecule 8: REST corepressor 1

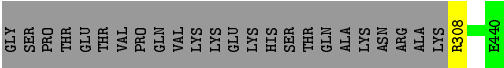
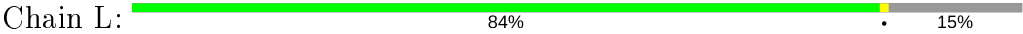


- Molecule 8: REST corepressor 1

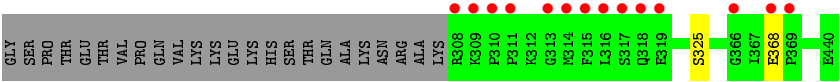
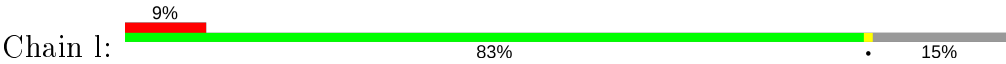




● Molecule 8: REST corepressor 1



● Molecule 8: REST corepressor 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.77Å 335.77Å 174.63Å 90.00° 91.07° 90.00°	Depositor
Resolution (Å)	20.17 – 4.99 20.17 – 4.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.17-4.99) 94.0 (20.17-4.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 4.97Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.229 , 0.277 0.229 , 0.277	Depositor DCC
R_{free} test set	1978 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	309.0	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 334.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.165 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	52996	wwPDB-VP
Average B, all atoms (Å ²)	415.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.23	0/904	0.38	0/1209
1	E	0.24	0/900	0.38	0/1204
1	a	0.23	0/784	0.37	0/1052
1	e	0.23	0/845	0.38	0/1132
2	B	0.23	0/655	0.43	0/878
2	F	0.26	0/626	0.46	0/837
2	b	0.25	0/645	0.41	0/862
2	f	0.23	0/626	0.42	0/837
3	C	0.24	0/805	0.39	0/1088
3	G	0.24	0/819	0.40	0/1106
3	c	0.23	0/805	0.38	0/1088
3	g	0.23	0/814	0.38	0/1099
4	D	0.23	0/730	0.37	0/983
4	H	0.23	0/737	0.38	0/993
4	d	0.23	0/719	0.37	0/969
4	h	0.23	0/737	0.37	0/993
5	I	0.47	0/4365	0.89	0/6729
5	i	0.47	0/4365	0.89	0/6729
6	J	0.47	0/4419	0.88	0/6824
6	j	0.47	0/4419	0.87	0/6824
7	K	0.23	0/5319	0.40	0/7217
7	M	0.24	0/5319	0.40	0/7217
7	k	0.24	0/5319	0.40	0/7217
7	m	0.24	0/5319	0.40	0/7217
8	L	0.23	0/1091	0.36	0/1471
8	N	0.23	0/1091	0.36	0/1471
8	l	0.24	0/1091	0.36	0/1471
8	n	0.23	0/1091	0.36	0/1471
All	All	0.33	0/55359	0.61	0/78188

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 [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	106/135 (78%)	101 (95%)	5 (5%)	0	100	100
1	E	106/135 (78%)	102 (96%)	4 (4%)	0	100	100
1	a	92/135 (68%)	88 (96%)	4 (4%)	0	100	100
1	e	99/135 (73%)	94 (95%)	4 (4%)	1 (1%)	15	54
2	B	79/102 (78%)	74 (94%)	4 (5%)	1 (1%)	12	48
2	F	76/102 (74%)	73 (96%)	2 (3%)	1 (1%)	12	48
2	b	78/102 (76%)	74 (95%)	3 (4%)	1 (1%)	12	48
2	f	76/102 (74%)	74 (97%)	2 (3%)	0	100	100
3	C	101/129 (78%)	97 (96%)	4 (4%)	0	100	100
3	G	103/129 (80%)	99 (96%)	4 (4%)	0	100	100
3	c	101/129 (78%)	97 (96%)	4 (4%)	0	100	100
3	g	102/129 (79%)	97 (95%)	5 (5%)	0	100	100
4	D	90/122 (74%)	86 (96%)	4 (4%)	0	100	100
4	H	91/122 (75%)	87 (96%)	4 (4%)	0	100	100
4	d	89/122 (73%)	85 (96%)	4 (4%)	0	100	100
4	h	91/122 (75%)	87 (96%)	4 (4%)	0	100	100
7	K	664/684 (97%)	633 (95%)	28 (4%)	3 (0%)	29	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	M	664/684 (97%)	626 (94%)	36 (5%)	2 (0%)	41	76
7	k	664/684 (97%)	620 (93%)	41 (6%)	3 (0%)	29	68
7	m	664/684 (97%)	632 (95%)	32 (5%)	0	100	100
8	L	131/157 (83%)	129 (98%)	2 (2%)	0	100	100
8	N	131/157 (83%)	129 (98%)	2 (2%)	0	100	100
8	l	131/157 (83%)	121 (92%)	8 (6%)	2 (2%)	10	46
8	n	131/157 (83%)	122 (93%)	8 (6%)	1 (1%)	19	60
All	All	4660/5316 (88%)	4427 (95%)	218 (5%)	15 (0%)	41	76

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	31	LYS
2	b	26	ILE
1	e	5	GLN
7	M	519	VAL
7	K	240	ALA

5.3.2 Protein sidechains ⓘ

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	94/110 (86%)	92 (98%)	2 (2%)	53	72
1	E	93/110 (84%)	91 (98%)	2 (2%)	52	71
1	a	82/110 (74%)	80 (98%)	2 (2%)	49	69
1	e	89/110 (81%)	87 (98%)	2 (2%)	52	71
2	B	67/78 (86%)	67 (100%)	0	100	100
2	F	63/78 (81%)	63 (100%)	0	100	100
2	b	65/78 (83%)	65 (100%)	0	100	100
2	f	63/78 (81%)	62 (98%)	1 (2%)	62	79
3	C	82/101 (81%)	82 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	83/101 (82%)	83 (100%)	0	100	100
3	c	82/101 (81%)	82 (100%)	0	100	100
3	g	83/101 (82%)	82 (99%)	1 (1%)	71	84
4	D	78/102 (76%)	77 (99%)	1 (1%)	69	82
4	H	79/102 (78%)	77 (98%)	2 (2%)	47	68
4	d	77/102 (76%)	76 (99%)	1 (1%)	69	82
4	h	79/102 (78%)	78 (99%)	1 (1%)	69	82
7	K	563/577 (98%)	558 (99%)	5 (1%)	78	88
7	M	563/577 (98%)	558 (99%)	5 (1%)	78	88
7	k	563/577 (98%)	557 (99%)	6 (1%)	73	85
7	m	563/577 (98%)	560 (100%)	3 (0%)	88	93
8	L	117/138 (85%)	116 (99%)	1 (1%)	78	88
8	N	117/138 (85%)	117 (100%)	0	100	100
8	l	117/138 (85%)	117 (100%)	0	100	100
8	n	117/138 (85%)	116 (99%)	1 (1%)	78	88
All	All	3979/4424 (90%)	3943 (99%)	36 (1%)	78	88

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	M	332	MET
7	m	182	ARG
7	k	670	PHE
7	M	530	ASP
7	m	280	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	27	GLN
3	c	84	GLN
7	K	802	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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
9	FAD	M	900	-	51,58,58	1.22	5 (9%)	60,89,89	2.22	8 (13%)
9	FAD	k	900	-	51,58,58	1.32	7 (13%)	60,89,89	2.25	7 (11%)
9	FAD	m	900	-	51,58,58	1.21	5 (9%)	60,89,89	2.22	8 (13%)
9	FAD	K	900	-	51,58,58	1.23	5 (9%)	60,89,89	2.13	8 (13%)

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
9	FAD	M	900	-	-	15/30/50/50	0/6/6/6
9	FAD	k	900	-	-	18/30/50/50	0/6/6/6
9	FAD	m	900	-	-	15/30/50/50	0/6/6/6
9	FAD	K	900	-	-	13/30/50/50	0/6/6/6

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	M	900	FAD	C4X-C10	5.61	1.44	1.38
9	m	900	FAD	C4X-C10	5.60	1.44	1.38
9	k	900	FAD	C4X-C10	5.57	1.44	1.38
9	K	900	FAD	C4X-C10	5.51	1.44	1.38
9	K	900	FAD	C4-N3	3.68	1.39	1.33

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	m	900	FAD	C4-N3-C2	13.00	126.12	115.14
9	M	900	FAD	C4-N3-C2	12.97	126.09	115.14
9	k	900	FAD	C4-N3-C2	12.92	126.05	115.14
9	K	900	FAD	C4-N3-C2	12.17	125.41	115.14
9	m	900	FAD	C4X-C4-N3	-7.06	113.77	123.43

There are no chirality outliers.

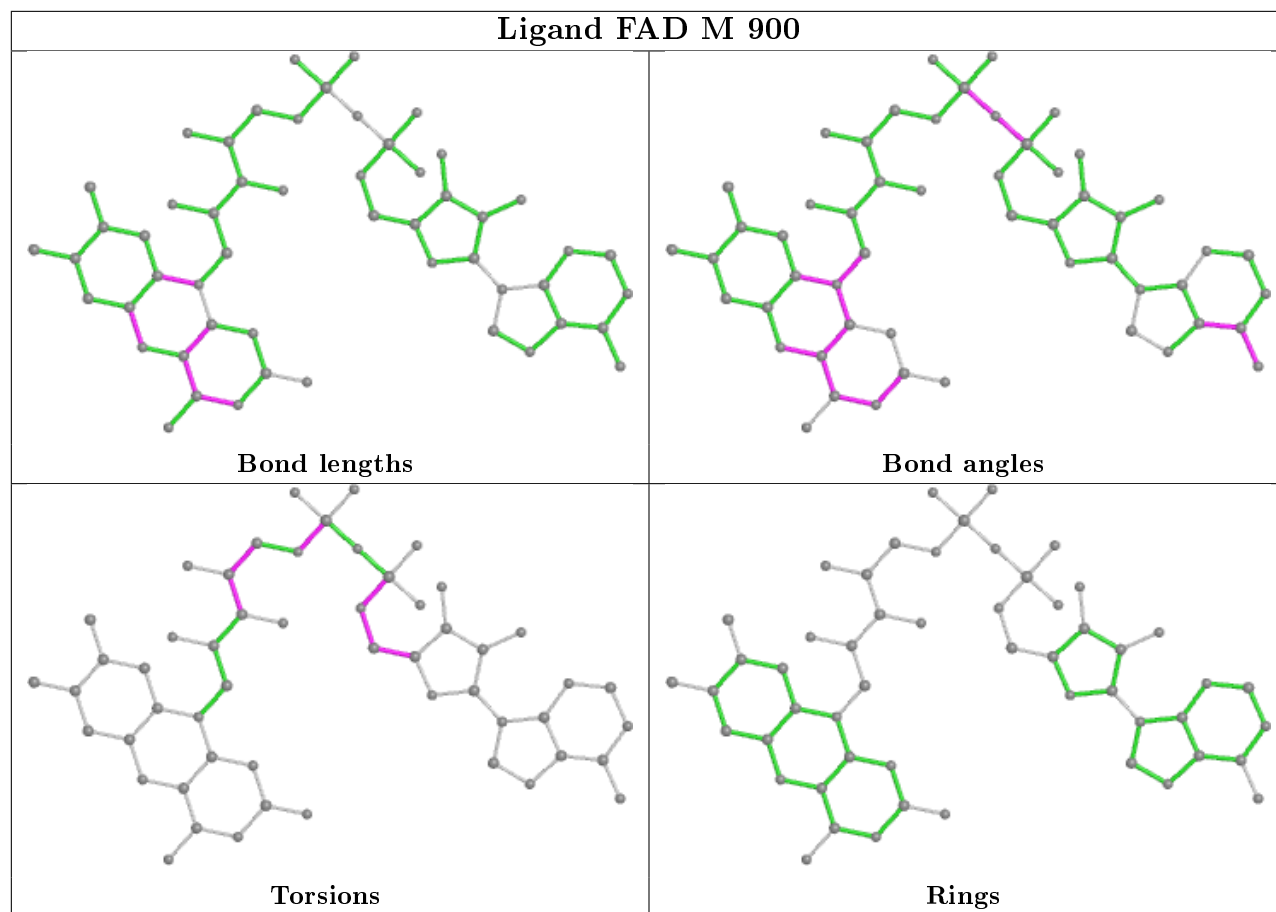
5 of 61 torsion outliers are listed below:

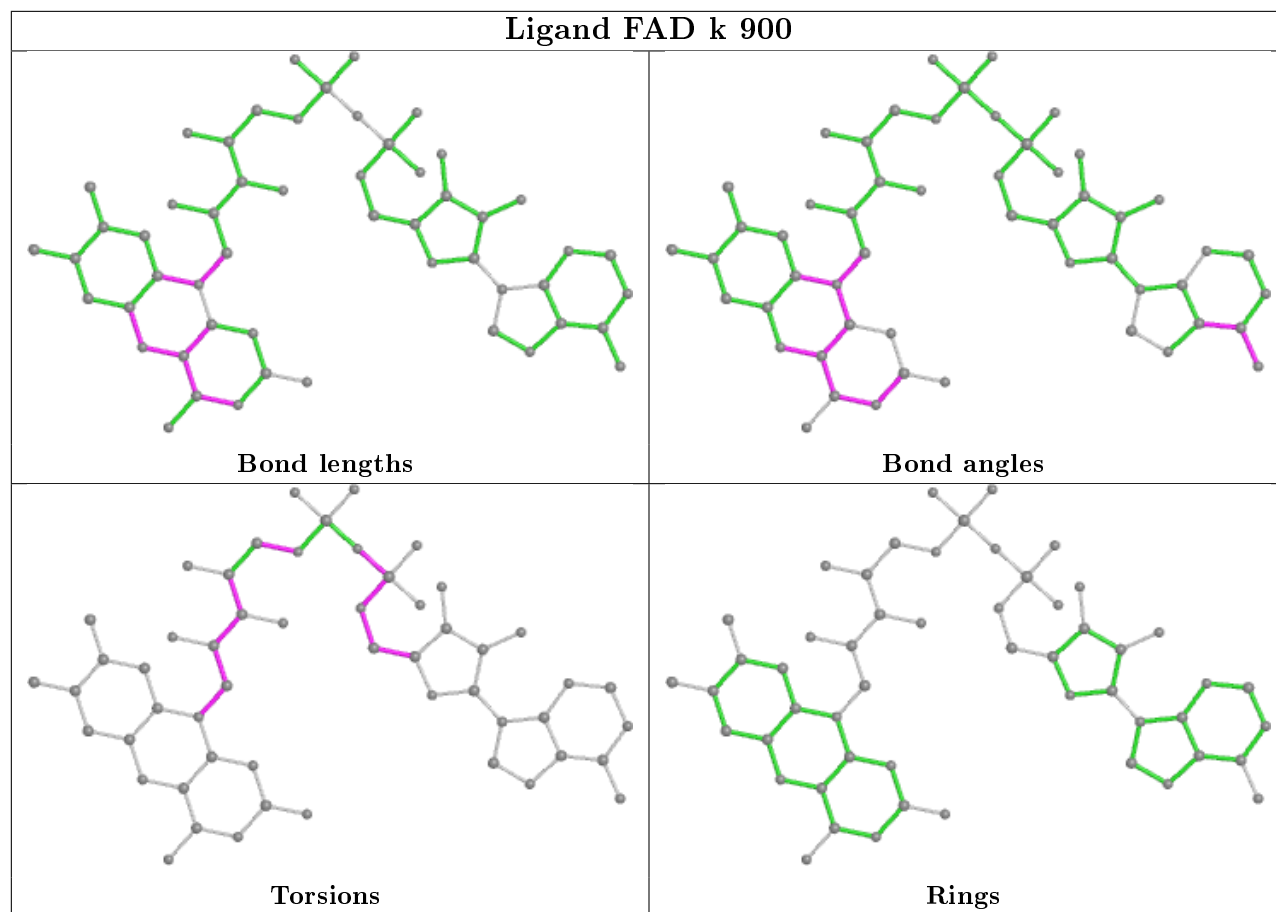
Mol	Chain	Res	Type	Atoms
9	k	900	FAD	C5B-O5B-PA-O2A
9	k	900	FAD	C5B-O5B-PA-O3P
9	k	900	FAD	C2'-C1'-N10-C10
9	k	900	FAD	N10-C1'-C2'-O2'
9	k	900	FAD	N10-C1'-C2'-C3'

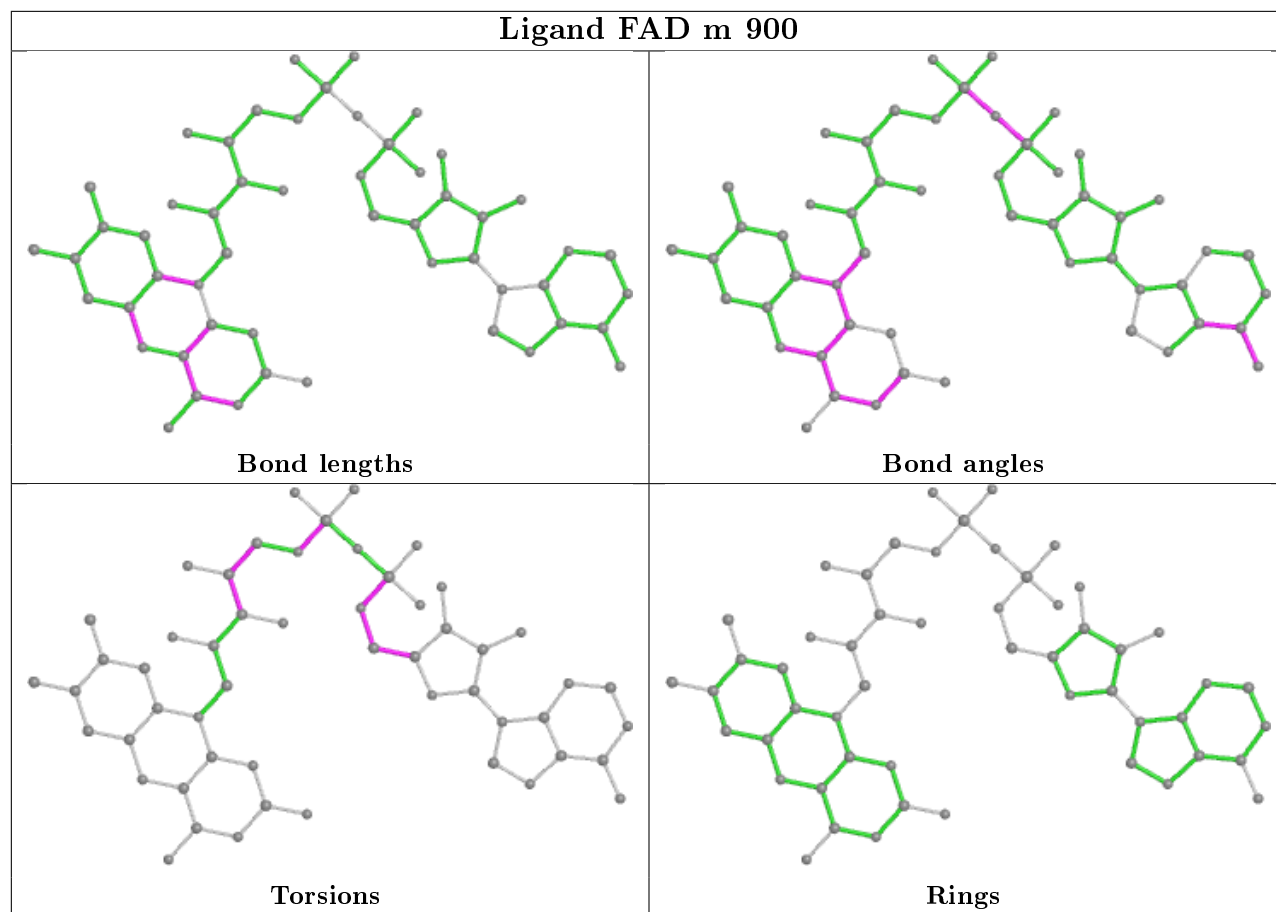
There are no ring outliers.

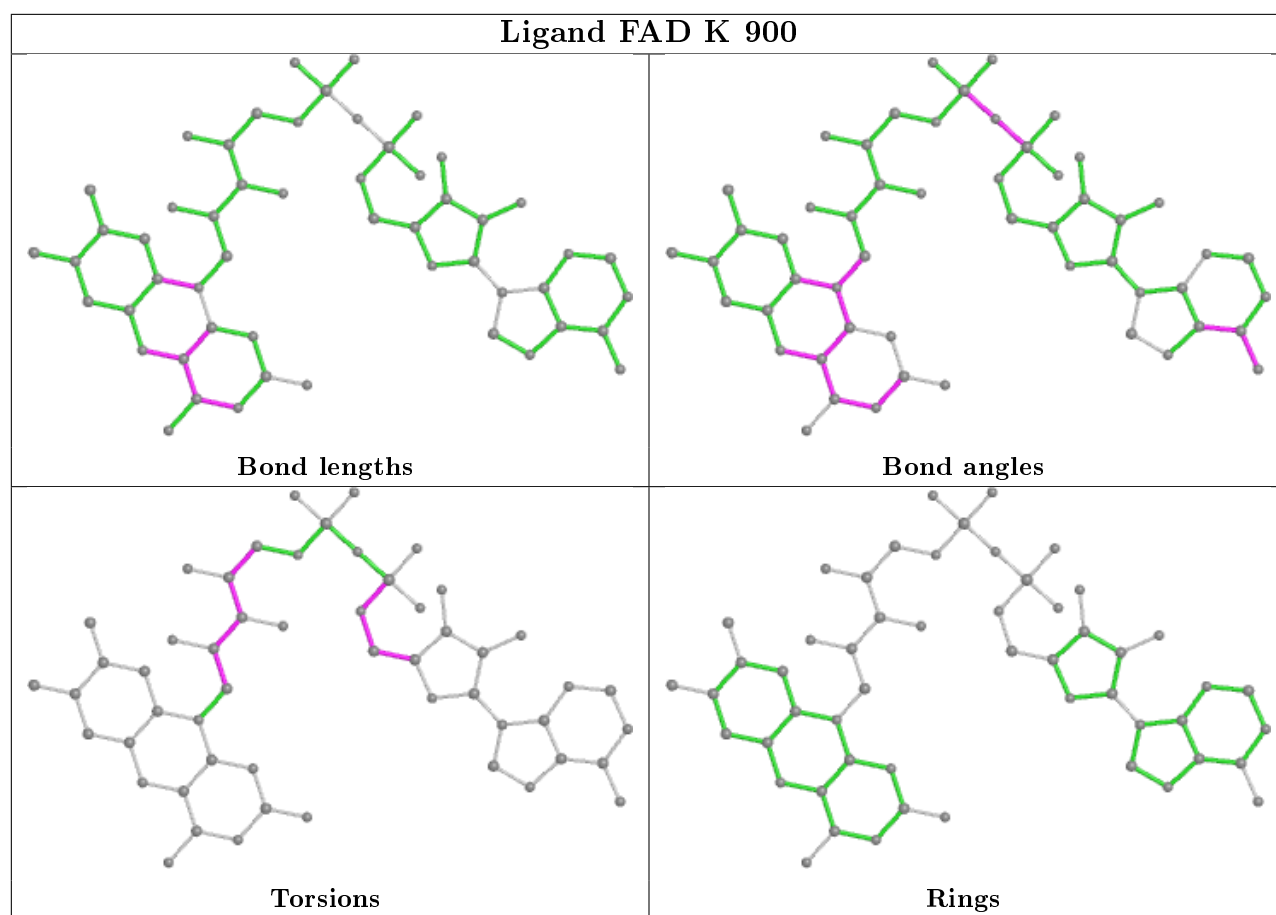
No monomer is involved in short contacts.

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 than 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.









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, 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	110/135 (81%)	-0.40	0 100 100	225, 282, 423, 455	0
1	E	110/135 (81%)	-0.47	0 100 100	262, 317, 371, 412	0
1	a	94/135 (69%)	-0.36	1 (1%) 80 72	243, 299, 353, 407	0
1	e	103/135 (76%)	-0.55	0 100 100	254, 305, 367, 398	0
2	B	81/102 (79%)	-0.38	0 100 100	222, 297, 360, 446	0
2	F	78/102 (76%)	-0.45	0 100 100	265, 319, 367, 377	0
2	b	80/102 (78%)	-0.39	1 (1%) 77 68	231, 289, 322, 369	0
2	f	78/102 (76%)	-0.55	0 100 100	248, 301, 346, 356	0
3	C	103/129 (79%)	-0.39	0 100 100	247, 301, 376, 425	0
3	G	105/129 (81%)	-0.44	0 100 100	234, 302, 348, 393	0
3	c	103/129 (79%)	-0.46	0 100 100	223, 322, 384, 449	0
3	g	104/129 (80%)	-0.46	0 100 100	239, 302, 367, 398	0
4	D	92/122 (75%)	-0.49	0 100 100	249, 303, 358, 394	0
4	H	93/122 (76%)	-0.51	0 100 100	221, 300, 379, 406	0
4	d	91/122 (74%)	-0.44	0 100 100	240, 312, 364, 390	0
4	h	93/122 (76%)	-0.46	0 100 100	220, 301, 366, 396	0
5	I	191/191 (100%)	-0.69	1 (0%) 91 85	316, 421, 650, 720	0
5	i	191/191 (100%)	-0.70	1 (0%) 91 85	321, 434, 669, 808	0
6	J	191/191 (100%)	-0.74	0 100 100	320, 415, 642, 757	0
6	j	191/191 (100%)	-0.69	2 (1%) 82 74	348, 445, 681, 843	0
7	K	666/684 (97%)	-0.33	27 (4%) 37 31	390, 475, 580, 696	0
7	M	666/684 (97%)	-0.48	11 (1%) 70 61	276, 365, 472, 544	0
7	k	666/684 (97%)	-0.07	49 (7%) 14 12	442, 531, 613, 696	0
7	m	666/684 (97%)	-0.53	10 (1%) 73 64	278, 378, 472, 532	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
8	L	133/157 (84%)	-0.49	0 100 100	341, 441, 510, 558	0
8	N	133/157 (84%)	-0.38	4 (3%) 50 40	302, 407, 522, 539	0
8	l	133/157 (84%)	0.10	14 (10%) 6 6	378, 454, 565, 621	0
8	n	133/157 (84%)	-0.48	0 100 100	306, 387, 480, 520	0
All	All	5478/6080 (90%)	-0.42	121 (2%) 62 52	220, 398, 577, 843	0

The worst 5 of 121 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	K	789	ALA	10.5
7	K	785	SER	10.0
7	k	788	GLY	9.9
7	k	789	ALA	9.4
8	l	315	PHE	9.0

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 monosaccharides in this entry.

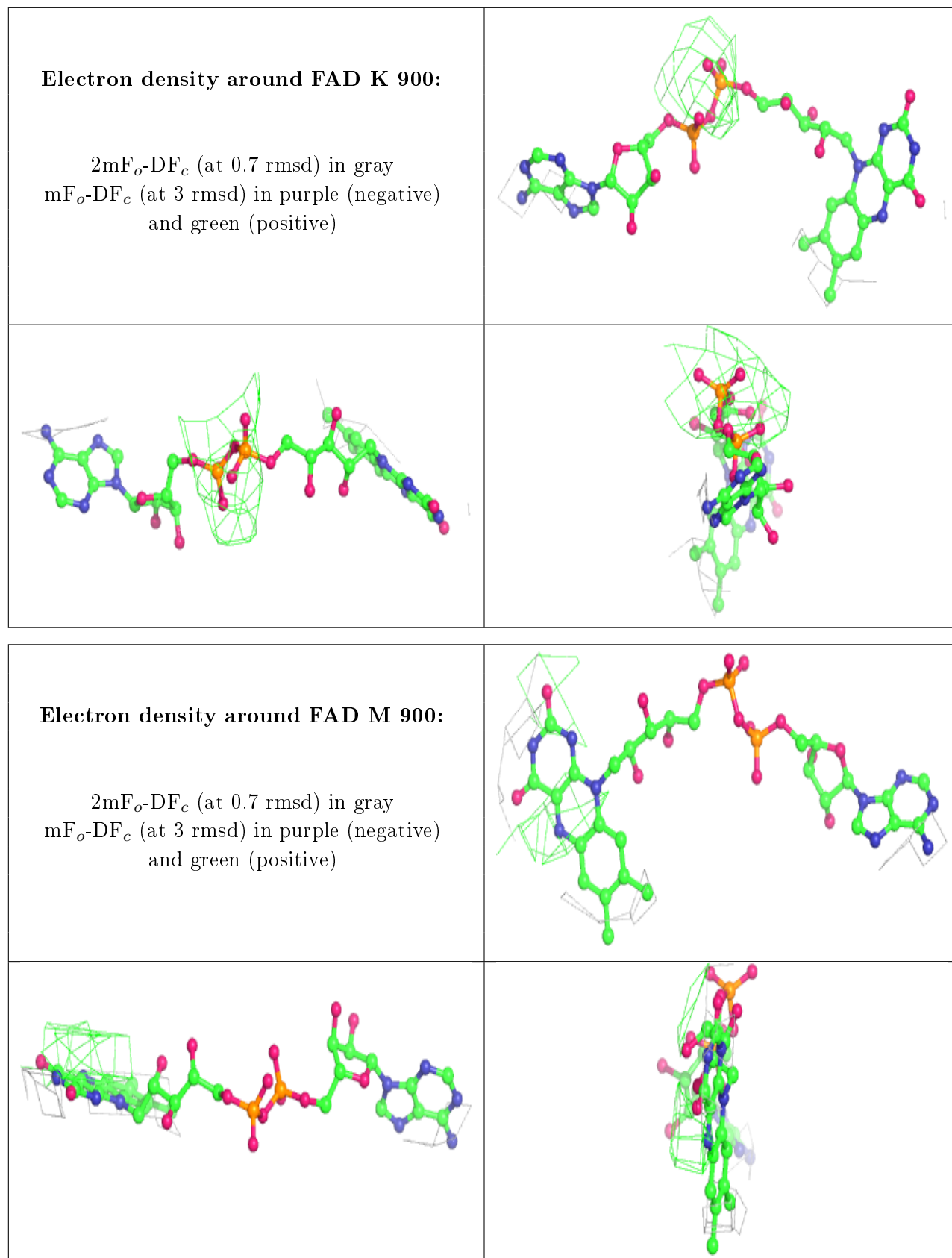
6.4 Ligands [i](#)

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, 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	B-factors(Å ²)	Q<0.9
9	FAD	K	900	53/53	0.84	0.14	460,467,476,477	0
9	FAD	M	900	53/53	0.90	0.18	296,303,312,313	0
9	FAD	k	900	53/53	0.91	0.12	534,540,543,544	0
9	FAD	m	900	53/53	0.93	0.17	326,329,335,336	0

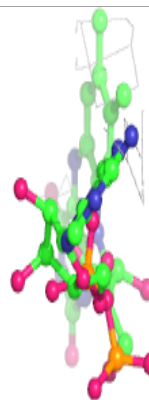
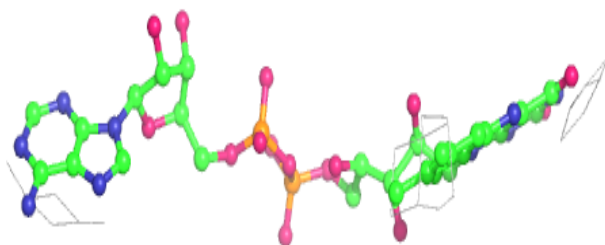
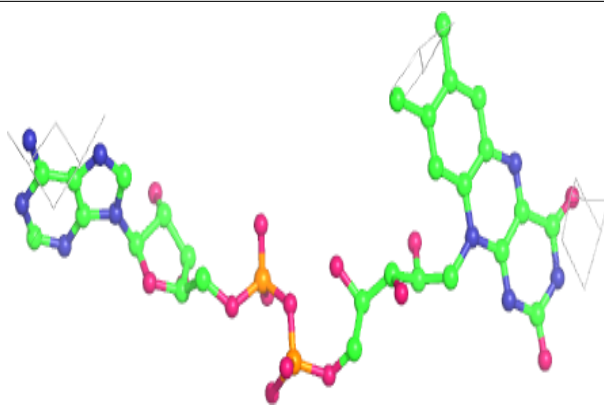
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

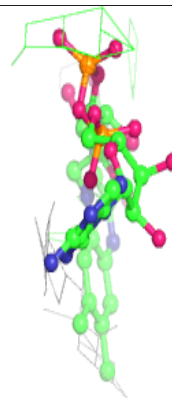
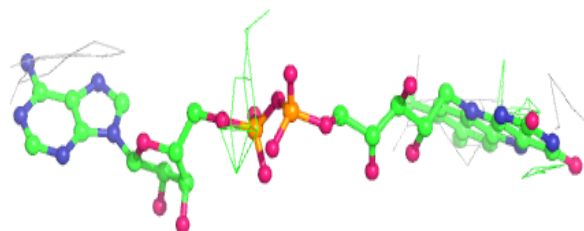
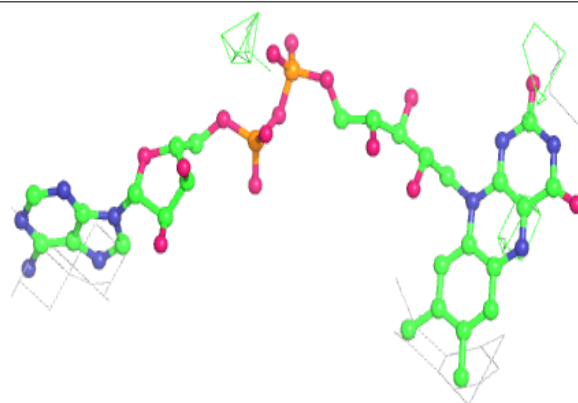


Electron density around FAD k 900:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around FAD m 900:**

$2mF_o - DF_c$ (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.