



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:39 PM UTC

PDB ID : 7XE2 / pdb_00007xe2
Title : Crystal structure of LSD2 in complex with trans-4-Br-PCPA
Authors : Niwa, H.; Sato, S.; Umehara, T.
Deposited on : 2022-03-29
Resolution : 2.05 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

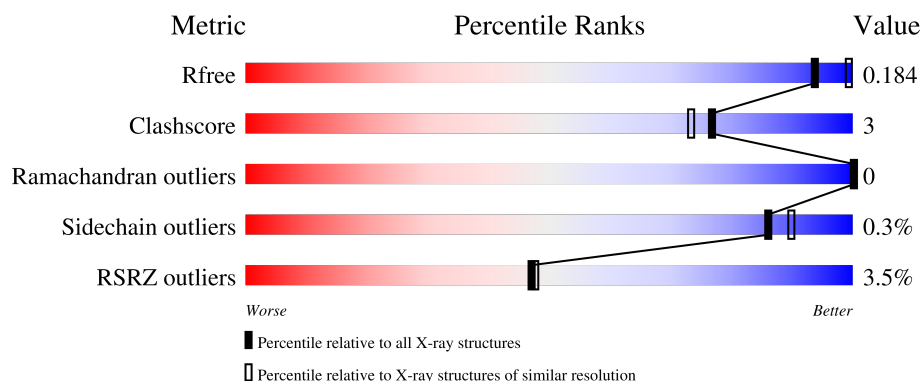
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

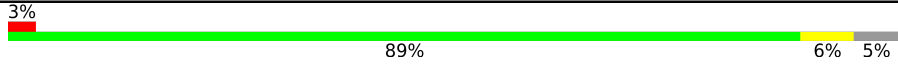
The reported resolution of this entry is 2.05 Å.

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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 of 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	793	
1	B	793	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13126 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.

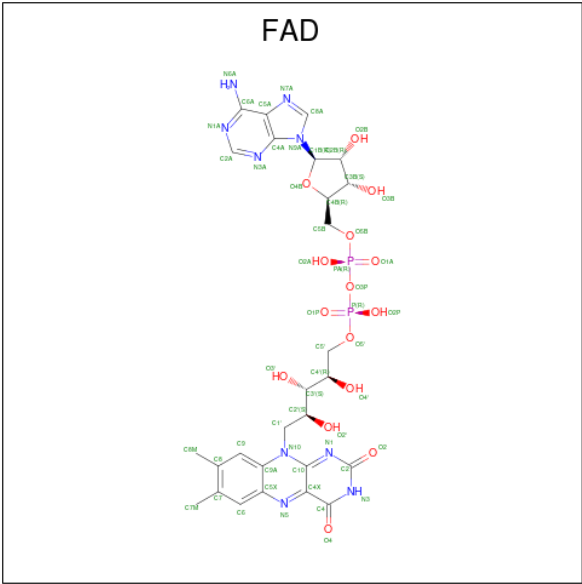
- Molecule 1 is a protein called Lysine-specific histone demethylase 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	751	Total	C	N	O	S	0	5	0
			5970	3813	1017	1098	42			
1	B	741	Total	C	N	O	S	0	2	0
			5872	3748	1001	1082	41			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

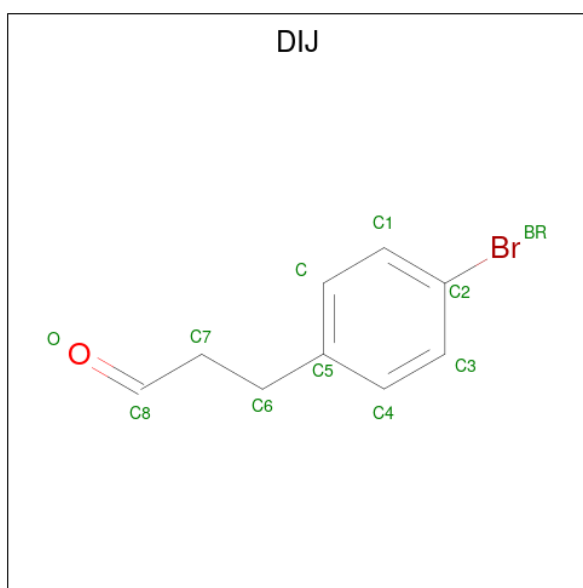
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is 3-(4-bromophenyl)propanal (CCD ID: DIJ) (formula: C₉H₉BrO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Br	C	O	0	1
			11	1	9	1		
4	A	1	Total	Br	C	O	0	1
			11	1	9	1		
4	B	1	Total	Br	C	O	0	1
			11	1	9	1		
4	B	1	Total	Br	C	O	0	1
			11	1	9	1		

- Molecule 5 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	587	Total	O	0	0
			587	587		
8	B	382	Total	O	0	0
			382	382		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	143.58Å 170.08Å 201.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.56 – 2.05 46.56 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.56-2.05) 99.7 (46.56-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158+SVN	Depositor
R, R_{free}	0.167 , 0.194 (Not available) , 0.184	Depositor DCC
R_{free} test set	7597 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.8	Xtriage
Anisotropy	0.623	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13126	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, FAD, GOL, DIJ, PGE, ZN

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	0.36	0/6133	0.51	0/8310
1	B	0.30	0/6022	0.47	0/8158
All	All	0.33	0/12155	0.49	0/16468

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	5970	0	5887	32	0
1	B	5872	0	5772	37	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	106	0	62	1	0
3	B	106	0	62	1	0
4	A	22	0	0	3	0
4	B	22	0	0	4	0
5	A	13	0	5	0	0
6	A	10	0	14	2	0
7	A	24	0	32	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	6	0	8	2	0
8	A	587	0	0	6	0
8	B	382	0	0	6	0
All	All	13126	0	11842	70	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 (70) 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)
4:B:907[B]:DIJ:O	8:B:1001:HOH:O	1.95	0.84
1:B:306:MET:HE1	1:B:344:ARG:HG3	1.62	0.81
1:B:306:MET:HE3	1:B:345:CYS:HA	1.71	0.73
4:B:907[B]:DIJ:O	8:B:1002:HOH:O	2.08	0.71
4:A:907[B]:DIJ:O	8:A:1002:HOH:O	2.07	0.70
1:A:719:ALA:O	1:A:722[B]:ARG:HG2	1.94	0.68
1:B:550:ASN:HD22	1:B:716:GLU:HG3	1.58	0.68
1:A:638[B]:GLN:NE2	8:A:1009:HOH:O	2.30	0.65
1:A:234[A]:CYS:HB3	1:A:237:THR:HB	1.84	0.60
1:A:200:TRP:CD1	1:B:273:TYR:HH	2.21	0.59
1:B:234:CYS:HB2	1:B:237:THR:HB	1.84	0.58
1:B:541:SER:HB3	1:B:691:ARG:HG2	1.85	0.57
1:B:303:ASP:OD1	8:B:1003:HOH:O	2.18	0.57
1:B:514:GLU:HG2	7:B:908:GOL:H31	1.86	0.56
1:A:156:GLU:OE1	1:A:156:GLU:N	2.36	0.56
1:B:122:LYS:HD2	1:B:227:CYS:SG	2.45	0.55
1:A:200:TRP:HD1	1:B:273:TYR:HH	1.56	0.52
1:A:55:LYS:HD3	1:B:224:TYR:CZ	2.44	0.52
1:A:722[B]:ARG:HD2	8:A:1500:HOH:O	2.08	0.52
1:B:715:GLY:HA3	8:B:1010:HOH:O	2.10	0.51
1:B:101:ARG:HB3	1:B:103:HIS:CE1	2.46	0.51
1:B:64:VAL:HG23	1:B:76:ASN:HB3	1.93	0.50
1:A:293:GLU:OE2	1:A:311:ARG:HD3	2.13	0.49
7:A:912:GOL:O2	1:B:122:LYS:HD3	2.12	0.49
1:A:48:LYS:HE3	1:A:50:TYR:CE1	2.48	0.49
4:A:907[B]:DIJ:O	8:A:1004:HOH:O	2.20	0.48
1:B:688:ALA:O	1:B:691:ARG:HB2	2.13	0.47
1:A:512:LYS:NZ	8:A:1018:HOH:O	2.44	0.47
1:B:280:LYS:NZ	1:B:283:CYS:SG	2.80	0.47
1:B:334:HIS:HD2	8:B:1338:HOH:O	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:HIS:CD2	1:B:740:LEU:HD21	2.49	0.47
1:A:224:TYR:CE2	6:A:909:PGE:H3	2.49	0.47
1:B:234:CYS:CB	1:B:237:THR:HB	2.45	0.47
1:A:229:GLY:HA2	1:A:305:THR:HG23	1.96	0.46
1:A:280:LYS:HE3	1:A:283:CYS:SG	2.55	0.46
1:B:226:ASP:OD1	1:B:226:ASP:N	2.47	0.46
1:A:224:TYR:HD2	6:A:909:PGE:H62	1.79	0.46
1:A:609:GLN:OE1	8:A:1005:HOH:O	2.21	0.46
1:A:212:LYS:HA	1:A:234[B]:CYS:SG	2.55	0.45
1:A:628:PRO:HG2	1:A:763:ILE:HA	1.98	0.45
1:B:628:PRO:HG2	1:B:763:ILE:HA	1.99	0.45
1:B:315:LEU:HG	1:B:356:MET:HE1	1.98	0.45
1:A:146:GLU:OE1	1:A:146:GLU:N	2.43	0.45
1:B:440:ASN:HD21	4:B:905[A]:DIJ:C3	2.30	0.45
1:B:513:ILE:HG22	7:B:908:GOL:H12	1.99	0.45
1:B:436:ALA:HA	3:B:904[A]:FAD:N5	2.32	0.44
1:B:504:LEU:H	1:B:504:LEU:HD12	1.82	0.44
1:B:800:HIS:HD2	8:B:1187:HOH:O	2.00	0.44
1:A:53:CYS:SG	1:A:84:HIS:HB2	2.57	0.44
1:B:512:LYS:HA	1:B:512:LYS:HD2	1.74	0.44
1:A:575:LEU:HD12	1:A:577:PRO:HD2	2.00	0.43
1:A:202:TYR:CE1	7:A:912:GOL:H32	2.54	0.43
1:B:54:GLU:OE1	1:B:81:ARG:NH1	2.51	0.43
1:A:348:GLU:OE1	1:A:351:ARG:HD3	2.19	0.43
1:B:730:LEU:HD22	1:B:752:TYR:CE1	2.53	0.42
1:B:713:ILE:HD13	1:B:721:VAL:HG11	2.00	0.42
1:A:440:ASN:ND2	4:A:907[B]:DIJ:C1	2.82	0.42
1:A:514:GLU:HG2	1:A:518:LYS:HE2	2.01	0.42
1:A:803:GLN:O	3:A:906[B]:FAD:H1'2	2.20	0.42
1:B:378:LYS:HD2	1:B:381:HIS:ND1	2.34	0.42
1:B:229:GLY:HA3	1:B:309:ALA:HB2	2.01	0.41
1:A:383:LYS:HA	1:A:621:GLN:OE1	2.19	0.41
1:B:454:LEU:HD13	1:B:581:VAL:HG12	2.02	0.41
1:A:388:ILE:HD13	1:A:601:ILE:HD11	2.03	0.41
1:B:440:ASN:ND2	4:B:907[B]:DIJ:C1	2.83	0.41
1:A:512:LYS:HA	1:A:512:LYS:HD2	1.92	0.41
1:A:234[B]:CYS:HB2	1:A:237:THR:HB	2.02	0.41
1:A:172:LYS:O	1:A:175:THR:HB	2.21	0.40
1:A:102:SER:HA	1:A:107:TYR:CD1	2.56	0.40
1:B:479:ILE:HG12	1:B:482:ARG:HH12	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	750/793 (95%)	732 (98%)	18 (2%)	0	100	100
1	B	737/793 (93%)	717 (97%)	20 (3%)	0	100	100
All	All	1487/1586 (94%)	1449 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	648/676 (96%)	646 (100%)	2 (0%)	86	90
1	B	634/676 (94%)	632 (100%)	2 (0%)	86	90
All	All	1282/1352 (95%)	1278 (100%)	4 (0%)	86	90

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

Mol	Chain	Res	Type
1	A	680	PHE
1	A	707	SER
1	B	283	CYS
1	B	680	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	GLN
1	A	199	HIS
1	A	334	HIS
1	A	400	GLN
1	A	440	ASN
1	A	609	GLN
1	B	93	ASN
1	B	440	ASN
1	B	503	GLN
1	B	552	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 6 are monoatomic - leaving 15 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	$\# Z > 2$
4	DIJ	B	905[A]	3	10,11,11	0.16	0	13,13,13	0.26	0
4	DIJ	B	907[B]	3	10,11,11	0.22	0	13,13,13	0.24	0
3	FAD	A	906[B]	4	58,58,58	0.79	3 (5%)	85,89,89	1.11	7 (8%)
3	FAD	B	904[A]	4	58,58,58	1.14	3 (5%)	85,89,89	1.57	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PGE	A	909	-	9,9,9	0.58	0	8,8,8	0.75	0
3	FAD	A	904[A]	4	58,58,58	1.14	3 (5%)	85,89,89	1.50	6 (7%)
7	GOL	A	911	-	5,5,5	1.16	0	5,5,5	1.04	0
7	GOL	A	912	-	5,5,5	0.76	0	5,5,5	0.96	0
3	FAD	B	906[B]	4	58,58,58	0.77	3 (5%)	85,89,89	1.16	7 (8%)
4	DIJ	A	907[B]	3	10,11,11	0.24	0	13,13,13	0.26	0
7	GOL	A	910	-	5,5,5	0.59	0	5,5,5	1.27	1 (20%)
7	GOL	A	913	-	5,5,5	1.13	1 (20%)	5,5,5	1.15	0
5	FLC	A	908	-	12,12,12	1.20	1 (8%)	17,17,17	1.11	1 (5%)
4	DIJ	A	905[A]	3	10,11,11	0.17	0	13,13,13	0.26	0
7	GOL	B	908	-	5,5,5	0.97	0	5,5,5	1.15	0

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	DIJ	B	905[A]	3	-	0/4/4/4	0/1/1/1
4	DIJ	B	907[B]	3	-	2/4/4/4	0/1/1/1
3	FAD	A	906[B]	4	-	5/34/50/50	0/6/6/6
3	FAD	B	904[A]	4	-	1/34/50/50	0/6/6/6
6	PGE	A	909	-	-	6/7/7/7	-
3	FAD	A	904[A]	4	-	1/34/50/50	0/6/6/6
7	GOL	A	911	-	-	2/4/4/4	-
7	GOL	A	912	-	-	1/4/4/4	-
3	FAD	B	906[B]	4	-	3/34/50/50	0/6/6/6
4	DIJ	A	907[B]	3	-	2/4/4/4	0/1/1/1
7	GOL	A	910	-	-	1/4/4/4	-
7	GOL	A	913	-	-	1/4/4/4	-
5	FLC	A	908	-	-	2/16/16/16	-
4	DIJ	A	905[A]	3	-	0/4/4/4	0/1/1/1
7	GOL	B	908	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	904[A]	FAD	C4X-N5	7.44	1.46	1.30
3	A	904[A]	FAD	C4X-N5	7.43	1.46	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	906[B]	FAD	C4X-N5	4.38	1.40	1.30
3	B	906[B]	FAD	C4X-N5	4.08	1.39	1.30
3	B	904[A]	FAD	C4X-C4	2.83	1.55	1.44
3	A	904[A]	FAD	C4X-C4	2.77	1.54	1.44
5	A	908	FLC	CB-CBC	2.62	1.56	1.53
3	B	904[A]	FAD	C4X-C10	2.53	1.51	1.44
3	B	906[B]	FAD	C4X-C10	-2.52	1.36	1.44
3	A	906[B]	FAD	C4X-C10	-2.51	1.36	1.44
3	A	904[A]	FAD	C4X-C10	2.49	1.51	1.44
3	A	906[B]	FAD	C10-N1	2.17	1.37	1.33
3	B	906[B]	FAD	C10-N1	2.08	1.37	1.33
7	A	913	GOL	C1-C2	2.08	1.59	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	904[A]	FAD	C4-C4X-N5	-9.19	105.50	118.21
3	A	904[A]	FAD	C4-C4X-N5	-8.78	106.08	118.21
3	B	904[A]	FAD	C10-C4X-N5	-7.92	108.64	124.81
3	A	904[A]	FAD	C10-C4X-N5	-6.55	111.43	124.81
3	A	904[A]	FAD	C4-C4X-C10	-4.60	109.04	116.93
3	B	906[B]	FAD	C9A-C5X-N5	-4.45	117.73	122.45
3	A	906[B]	FAD	C9A-C5X-N5	-4.41	117.77	122.45
3	B	906[B]	FAD	C4X-C10-N10	4.35	122.70	116.48
3	B	906[B]	FAD	C10-C4X-N5	-4.18	116.28	124.81
3	B	904[A]	FAD	C4-C4X-C10	-3.94	110.17	116.93
3	A	906[B]	FAD	C4X-C10-N10	3.83	121.96	116.48
3	A	906[B]	FAD	C10-C4X-N5	-3.82	117.02	124.81
3	B	906[B]	FAD	C4-C4X-C10	3.34	122.67	116.93
3	A	906[B]	FAD	C4-C4X-C10	3.19	122.40	116.93
3	B	904[A]	FAD	C10-N1-C2	2.81	122.94	116.85
3	B	906[B]	FAD	C10-N1-C2	2.62	122.52	116.85
3	B	906[B]	FAD	C6-C5X-N5	2.58	122.73	118.44
3	A	906[B]	FAD	C6-C5X-N5	2.57	122.70	118.44
3	B	904[A]	FAD	C9A-C5X-N5	-2.49	119.81	122.45
3	B	906[B]	FAD	C4X-C10-N1	-2.42	118.64	124.59
3	A	904[A]	FAD	C9A-C5X-N5	-2.30	120.01	122.45
3	A	904[A]	FAD	C10-N1-C2	2.28	121.77	116.85
3	A	906[B]	FAD	C10-N1-C2	2.27	121.76	116.85
7	A	910	GOL	C3-C2-C1	-2.20	103.73	111.80
3	A	906[B]	FAD	C4X-C10-N1	-2.11	119.42	124.59
5	A	908	FLC	OB1-CBC-CB	-2.08	118.06	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	904[A]	FAD	C5X-N5-C4X	2.05	121.41	118.09
3	A	904[A]	FAD	O2P-P-O1P	2.04	121.95	112.44

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	906[B]	FAD	PA-O3P-P-O5'
3	B	904[A]	FAD	PA-O3P-P-O5'
3	B	906[B]	FAD	PA-O3P-P-O5'
7	A	911	GOL	C1-C2-C3-O3
7	A	911	GOL	O2-C2-C3-O3
6	A	909	PGE	O2-C3-C4-O3
6	A	909	PGE	C1-C2-O2-C3
7	A	913	GOL	O1-C1-C2-C3
7	B	908	GOL	O1-C1-C2-C3
6	A	909	PGE	O1-C1-C2-O2
7	B	908	GOL	O1-C1-C2-O2
6	A	909	PGE	C3-C4-O3-C5
6	A	909	PGE	C6-C5-O3-C4
3	B	906[B]	FAD	P-O3P-PA-O1A
6	A	909	PGE	O3-C5-C6-O4
3	A	906[B]	FAD	P-O3P-PA-O1A
4	A	907[B]	DIJ	C-C5-C6-C7
4	B	907[B]	DIJ	C4-C5-C6-C7
4	B	907[B]	DIJ	C-C5-C6-C7
4	A	907[B]	DIJ	C4-C5-C6-C7
7	A	910	GOL	O1-C1-C2-O2
3	A	906[B]	FAD	O4'-C4'-C5'-O5'
7	A	912	GOL	C1-C2-C3-O3
3	A	906[B]	FAD	O4B-C4B-C5B-O5B
3	A	906[B]	FAD	P-O3P-PA-O2A
5	A	908	FLC	CB-CG-CGC-OG1
5	A	908	FLC	CB-CG-CGC-OG2
3	B	906[B]	FAD	P-O3P-PA-O2A
3	A	904[A]	FAD	O4B-C4B-C5B-O5B

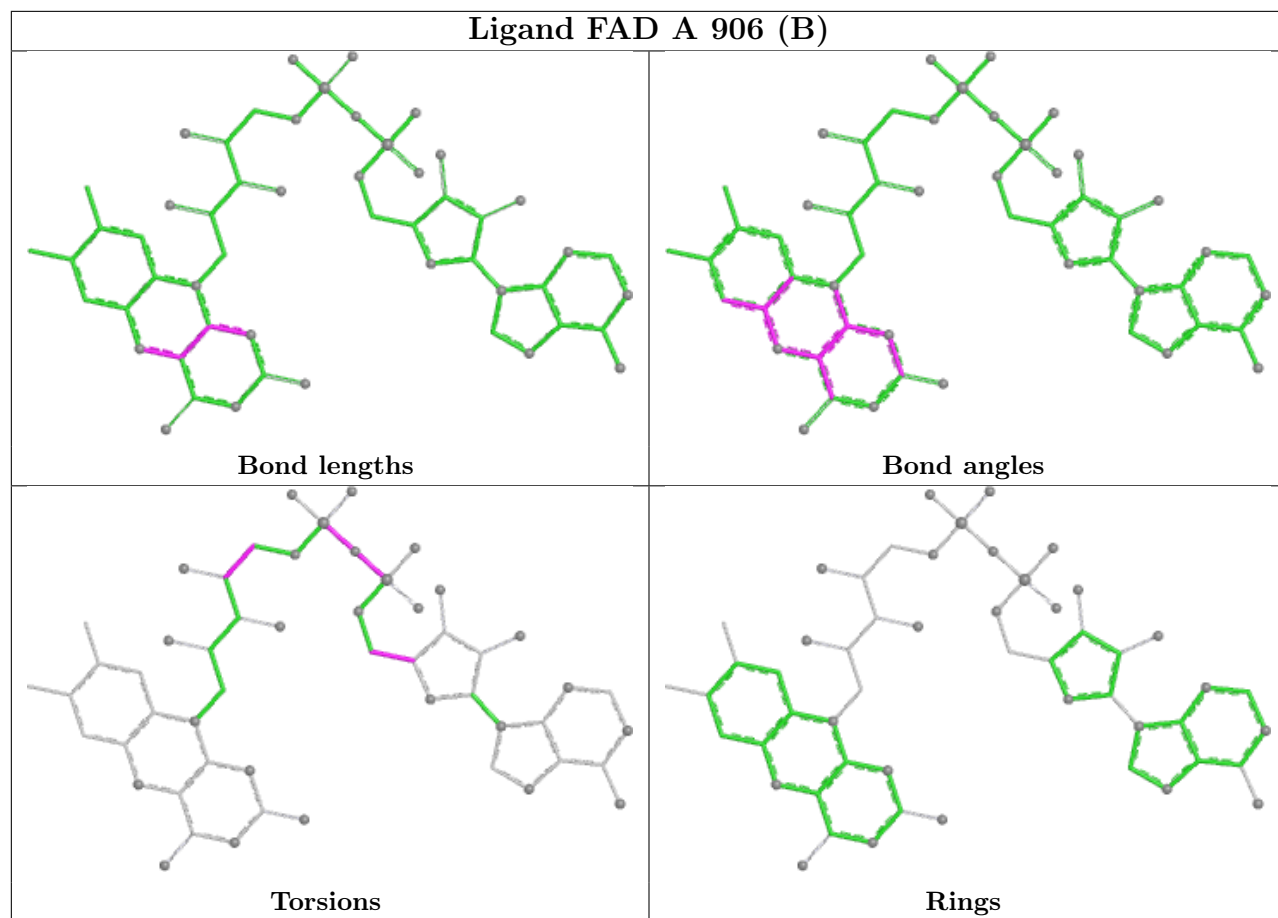
There are no ring outliers.

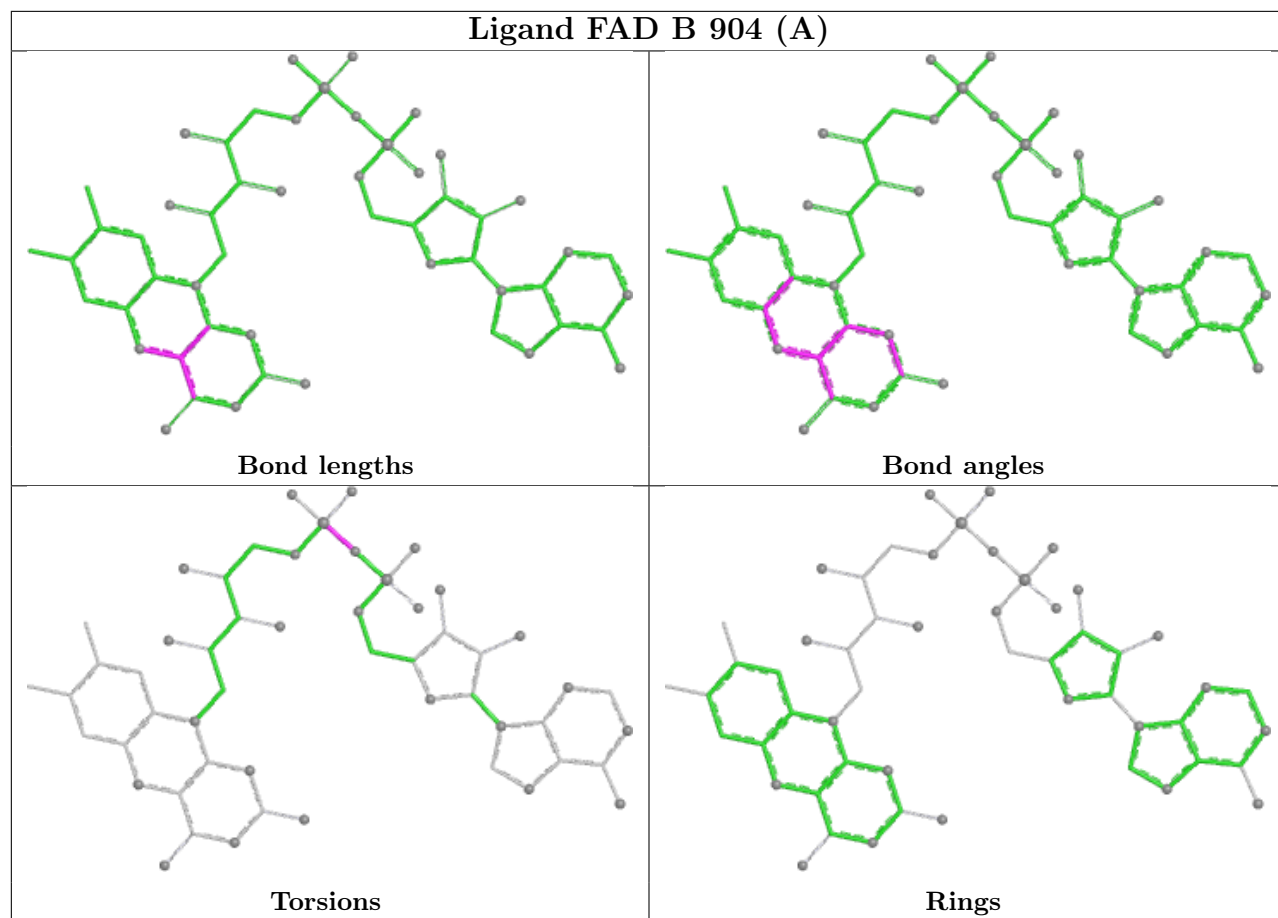
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	905[A]	DIJ	1	0
4	B	907[B]	DIJ	3	0
3	A	906[B]	FAD	1	0
3	B	904[A]	FAD	1	0
6	A	909	PGE	2	0
7	A	912	GOL	2	0
4	A	907[B]	DIJ	3	0
7	B	908	GOL	2	0

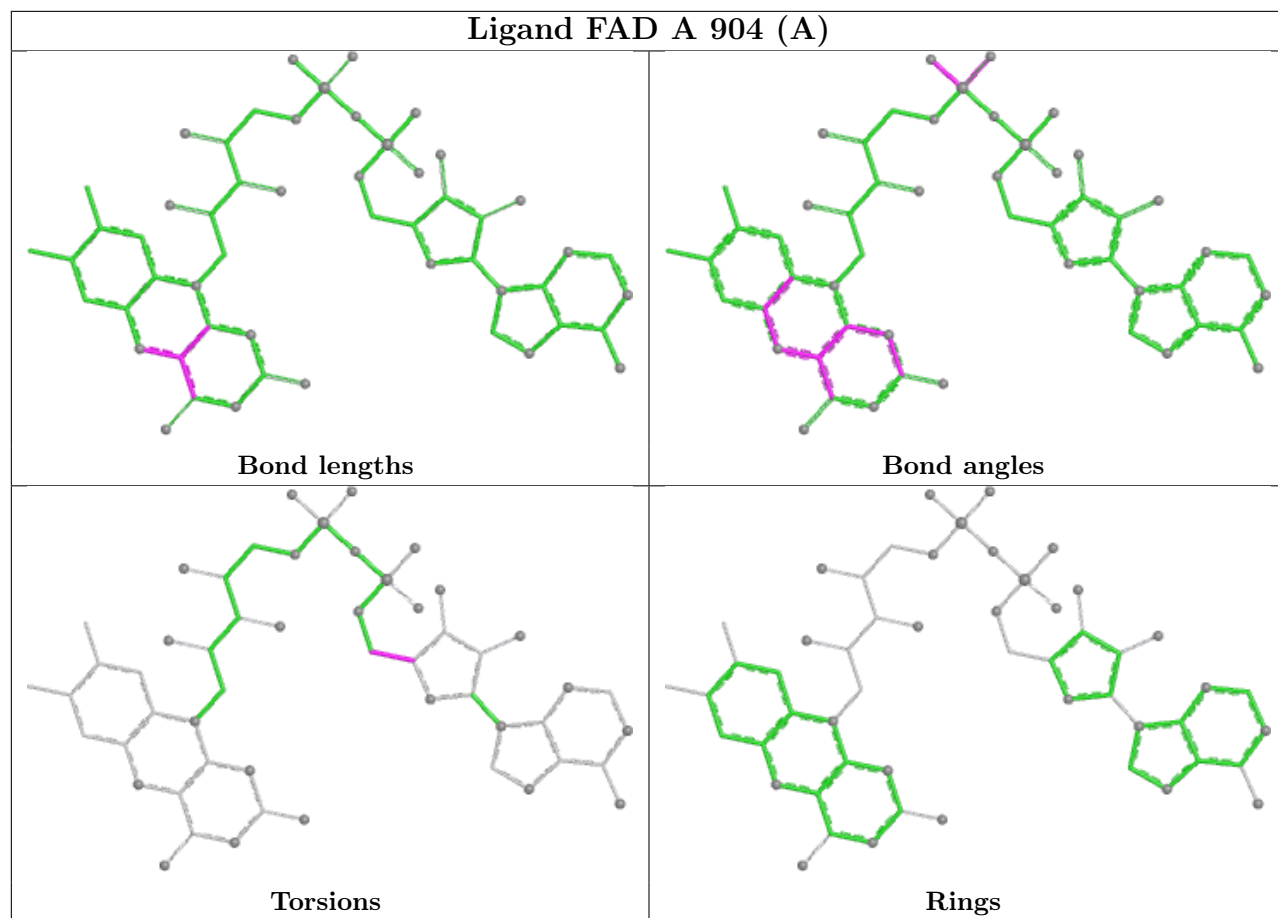
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

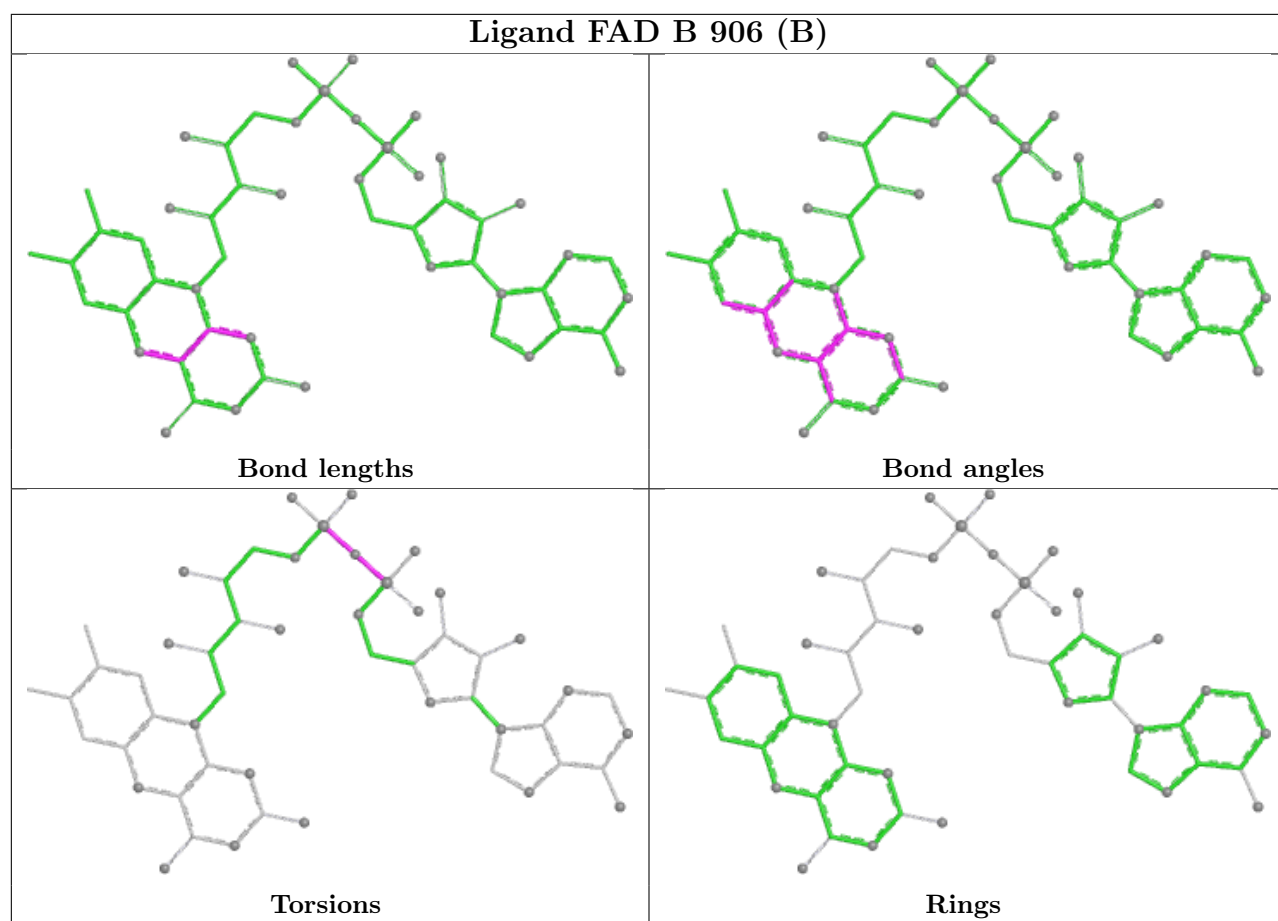
Ligand FAD A 906 (B)





Ligand FAD A 904 (A)





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	751/793 (94%)	-0.26	27 (3%) 46 46	20, 37, 72, 114	5 (0%)
1	B	741/793 (93%)	0.21	25 (3%) 48 48	24, 48, 91, 126	2 (0%)
All	All	1492/1586 (94%)	-0.03	52 (3%) 47 48	20, 43, 83, 126	7 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	TYR	5.9
1	A	173	PRO	5.0
1	A	237	THR	4.9
1	A	174	ASN	4.5
1	A	175	THR	4.1
1	A	381	HIS	4.1
1	B	822	PHE	3.6
1	B	237	THR	3.5
1	A	262	VAL	3.5
1	B	239	ARG	3.5
1	A	380	TYR	3.5
1	A	170	GLY	3.4
1	A	263	PRO	3.3
1	B	236	SER	3.2
1	A	181	THR	3.2
1	A	182	SER	3.1
1	B	103	HIS	3.1
1	B	380	TYR	3.1
1	A	47	GLU	3.0
1	B	279	GLY	3.0
1	A	171	MET	3.0
1	A	382	ASN	2.9
1	A	238	ASN	2.9
1	A	50	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	183	ASP	2.8
1	A	239	ARG	2.8
1	A	236	SER	2.8
1	A	180	GLU	2.8
1	A	264	GLY	2.8
1	A	688	ALA	2.6
1	B	564	PHE	2.6
1	A	370	GLY	2.6
1	B	479	ILE	2.6
1	B	78	TYR	2.5
1	B	100	TYR	2.5
1	B	278	CYS	2.4
1	B	56	ALA	2.4
1	A	564	PHE	2.4
1	B	238	ASN	2.4
1	B	521	ILE	2.4
1	A	49	LYS	2.4
1	B	49	LYS	2.4
1	B	520	PHE	2.3
1	B	172	LYS	2.3
1	B	523	GLU	2.2
1	A	172	LYS	2.2
1	B	200	TRP	2.2
1	B	370	GLY	2.2
1	A	295	TYR	2.1
1	B	716	GLU	2.0
1	B	369	VAL	2.0
1	B	69	ALA	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 oligosaccharides 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,

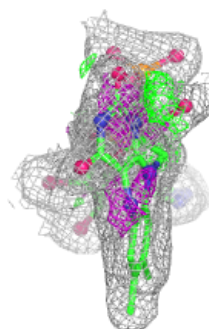
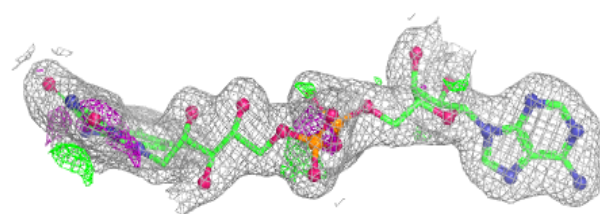
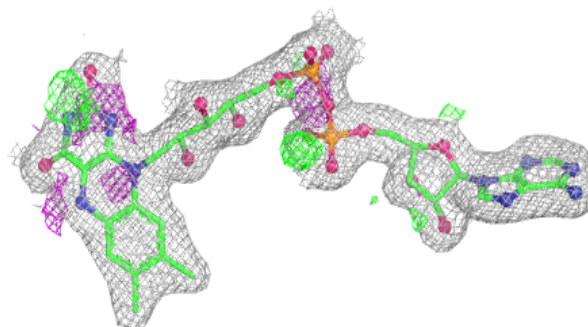
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DIJ	B	907[B]	11/11	0.69	0.24	39,43,47,73	11
7	GOL	A	911	6/6	0.80	0.21	58,65,72,74	0
6	PGE	A	909	10/10	0.82	0.16	44,62,67,77	0
4	DIJ	A	907[B]	11/11	0.84	0.19	30,31,39,66	11
7	GOL	A	913	6/6	0.87	0.18	43,45,48,48	6
7	GOL	A	910	6/6	0.89	0.14	53,59,63,69	0
7	GOL	B	908	6/6	0.89	0.15	43,66,68,75	0
4	DIJ	B	905[A]	11/11	0.90	0.14	38,43,52,68	11
5	FLC	A	908	13/13	0.91	0.09	44,56,61,65	0
4	DIJ	A	905[A]	11/11	0.94	0.11	26,32,38,62	11
7	GOL	A	912	6/6	0.95	0.17	40,43,46,56	0
3	FAD	B	906[B]	53/53	0.96	0.07	28,34,37,38	53
2	ZN	B	903	1/1	0.96	0.06	78,78,78,78	0
3	FAD	B	904[A]	53/53	0.97	0.07	28,34,38,38	53
3	FAD	A	906[B]	53/53	0.98	0.04	21,25,27,29	53
2	ZN	A	903	1/1	0.98	0.04	48,48,48,48	0
2	ZN	A	901	1/1	0.99	0.03	35,35,35,35	0
3	FAD	A	904[A]	53/53	0.99	0.04	21,25,28,29	53
2	ZN	B	901	1/1	0.99	0.04	43,43,43,43	0
2	ZN	B	902	1/1	0.99	0.03	66,66,66,66	0
2	ZN	A	902	1/1	1.00	0.01	36,36,36,36	0

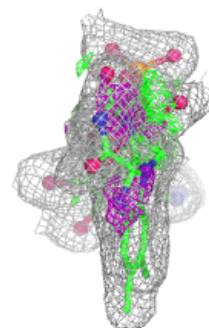
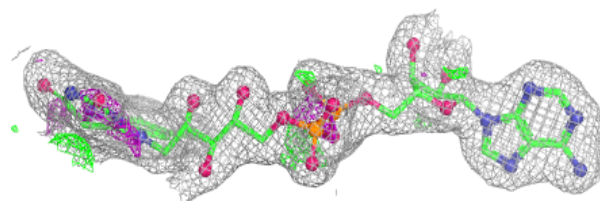
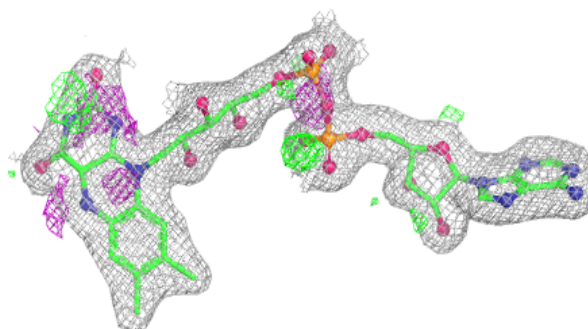
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 906 (B):

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

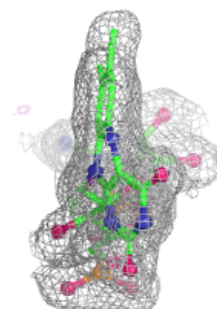
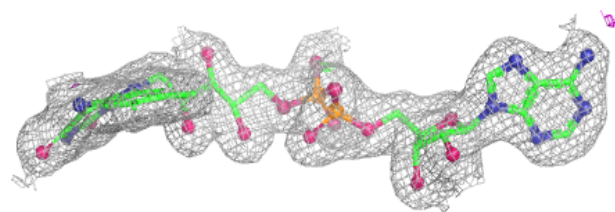
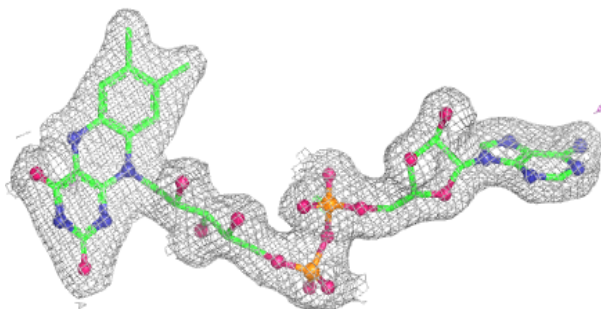
**Electron density around FAD B 904 (A):**

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

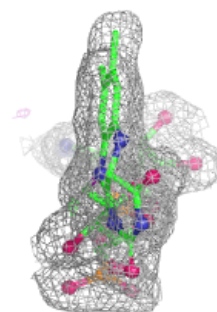
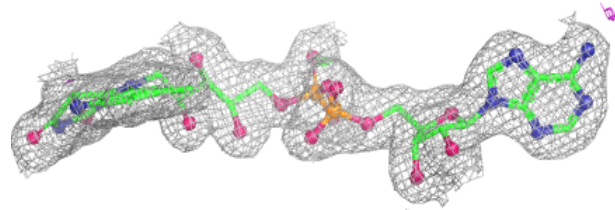
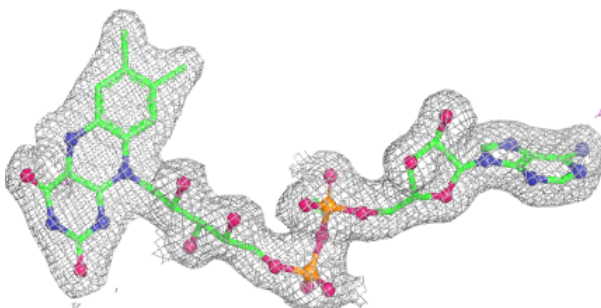


Electron density around FAD A 906 (B):

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

**Electron density around FAD A 904 (A):**

$2mF_o-DF_c$ (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.