Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:32 AM EDT

PDB ID	:	4FWJ
Title	:	Native structure of LSD2/AOF1/KDM1b in spacegroup of I222 at 2.9A
Authors	:	Zhang, Q.; Chen, Z.
Deposited on	:	2012-07-01
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

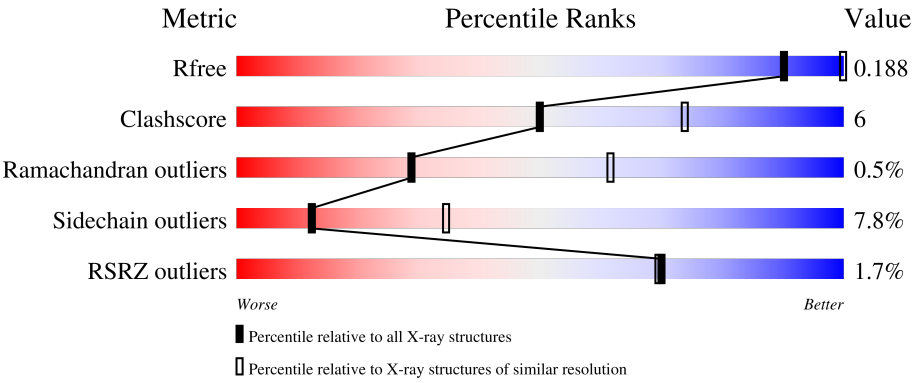
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

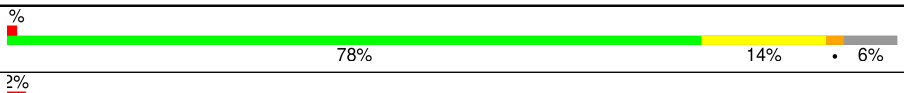
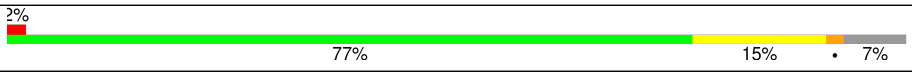
The reported resolution of this entry is 2.90 Å.

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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	796	
1	B	796	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12080 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	750	Total	C	N	O	S	0	1	0
			5800	3712	992	1054	42			
1	B	742	Total	C	N	O	S	0	2	0
			5698	3641	962	1053	42			

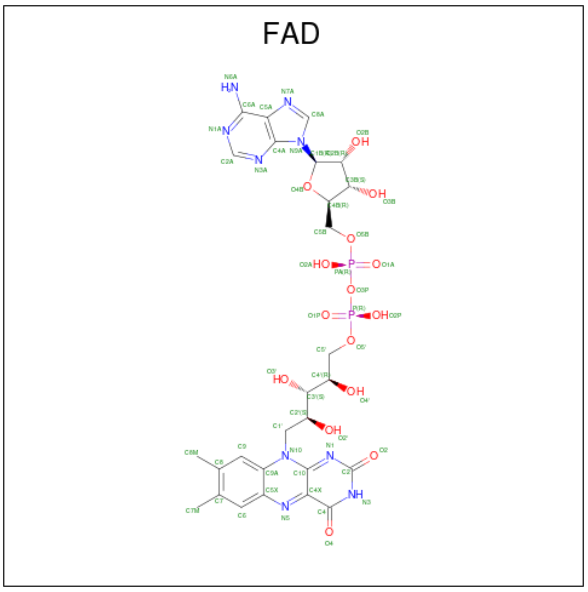
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLY	-	expression tag	UNP Q8NB78
A	28	HIS	-	expression tag	UNP Q8NB78
A	29	MET	-	expression tag	UNP Q8NB78
B	27	GLY	-	expression tag	UNP Q8NB78
B	28	HIS	-	expression tag	UNP Q8NB78
B	29	MET	-	expression tag	UNP Q8NB78

- Molecule 2 is ZINC ION (three-letter code: 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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

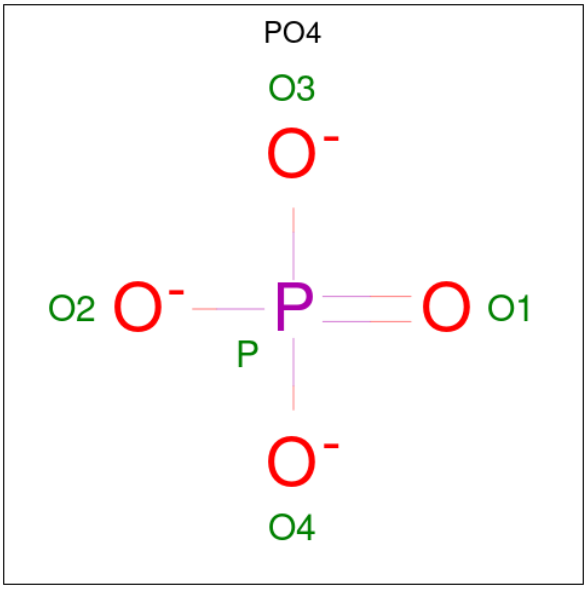


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 5 4 1	0	0

- Molecule 6 is water.

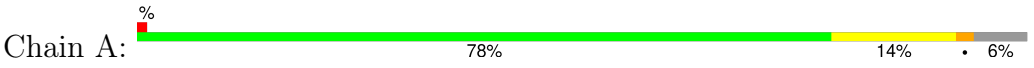
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	284	Total O 284 284	0	0
6	B	180	Total O 180 180	0	0

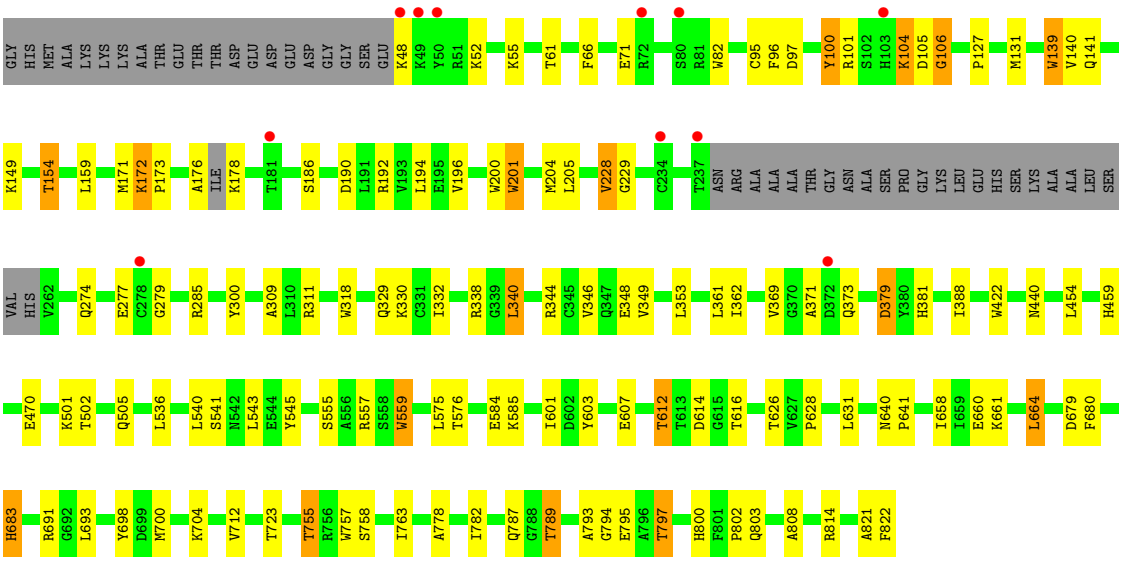
3 Residue-property plots (i)

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: Lysine-specific histone demethylase 1B

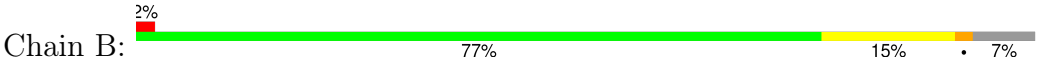
Chain A:

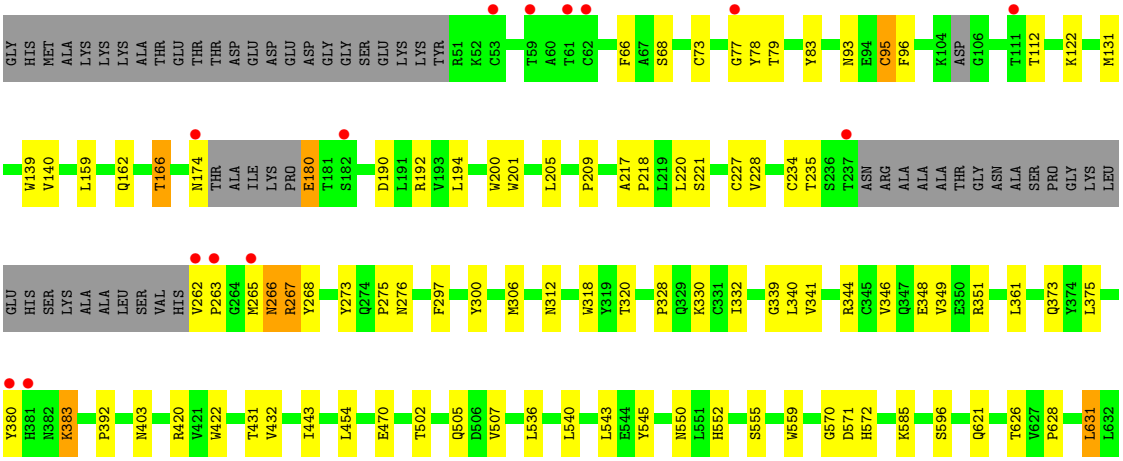


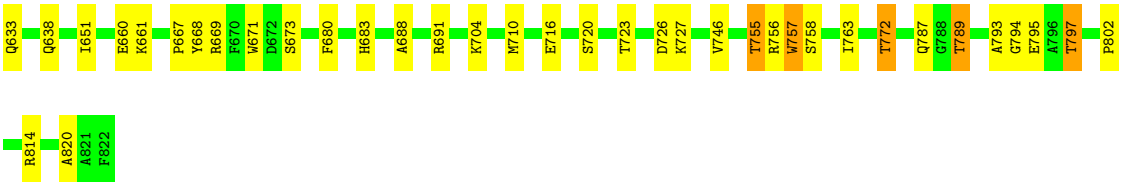


• Molecule 1: Lysine-specific histone demethylase 1B

Chain B:






Q633
Q638
I651
E660
K661
P667
Y668
R669
F670
W671
D672
S673
F680
H683
A688
R691
K704
M710
E716
S720
T723
D726
K727
V746
T755
R756
W757
S758
I763
T772
Q787
G788
T789
A793
G794
E795
A796
T797
P802
R814
A820
A821
F822

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	144.32Å 170.93Å 202.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 49.74 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.90) 99.6 (49.74-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.186 , 0.222 0.189 , 0.188	Depositor DCC
R_{free} test set	2818 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12080	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 2.87% 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: PO4, K, ZN, 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	0.54	7/5947 (0.1%)	0.62	1/8067 (0.0%)
1	B	0.54	8/5846 (0.1%)	0.61	2/7941 (0.0%)
All	All	0.54	15/11793 (0.1%)	0.61	3/16008 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	422	TRP	CD2-CE2	6.24	1.48	1.41
1	A	559	TRP	CD2-CE2	5.92	1.48	1.41
1	A	757	TRP	CD2-CE2	5.46	1.48	1.41
1	A	139	TRP	CD2-CE2	5.29	1.47	1.41
1	B	318	TRP	CD2-CE2	5.29	1.47	1.41
1	B	671	TRP	CD2-CE2	5.25	1.47	1.41
1	A	82	TRP	CD2-CE2	5.22	1.47	1.41
1	A	201	TRP	CD2-CE2	5.22	1.47	1.41
1	A	318	TRP	CD2-CE2	5.22	1.47	1.41
1	B	200	TRP	CD2-CE2	5.15	1.47	1.41
1	B	201	TRP	CD2-CE2	5.13	1.47	1.41
1	B	757	TRP	CD2-CE2	5.11	1.47	1.41
1	B	559	TRP	CD2-CE2	5.07	1.47	1.41
1	A	422	TRP	CD2-CE2	5.05	1.47	1.41
1	B	139	TRP	CD2-CE2	5.02	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	340	LEU	CA-CB-CG	6.75	130.83	115.30
1	B	631	LEU	CA-CB-CG	-5.64	102.32	115.30
1	A	664	LEU	CA-CB-CG	5.52	128.00	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	95	CYS	Peptide

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	5800	0	5607	61	0
1	B	5698	0	5408	70	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	53	0	31	2	0
3	B	53	0	31	3	0
4	A	1	0	0	0	0
5	B	5	0	0	0	0
6	A	284	0	0	4	0
6	B	180	0	0	0	0
All	All	12080	0	11077	131	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 6.

All (131) 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:B:95:CYS:O	1:B:96[B]:PHE:HD1	1.26	1.19
1:B:332:ILE:HD12	1:B:346:VAL:HG13	1.30	1.12
1:B:95:CYS:O	1:B:96[B]:PHE:CD1	2.15	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:THR:CG2	1:A:814:ARG:HH22	1.80	0.95
1:B:797:THR:CG2	1:B:814:ARG:HH22	1.83	0.91
1:B:660:GLU:OE1	1:B:755:THR:HG22	1.72	0.89
1:B:266:ASN:HD22	1:B:268:TYR:H	1.19	0.86
1:A:502:THR:H	1:A:505:GLN:HE21	1.27	0.82
1:B:332:ILE:CD1	1:B:346:VAL:HG13	2.09	0.81
1:B:266:ASN:ND2	1:B:268:TYR:H	1.80	0.80
1:B:550:ASN:HD22	1:B:552:HIS:H	1.33	0.76
1:A:104:LYS:O	1:A:106:GLY:N	2.19	0.74
1:A:797:THR:HG23	1:A:814:ARG:HH22	1.53	0.74
1:B:220:LEU:HD13	1:B:228:VAL:HG11	1.72	0.72
1:B:795:GLU:HG2	1:B:802:PRO:O	1.90	0.70
1:B:797:THR:HG23	1:B:814:ARG:HH22	1.56	0.69
1:A:793:ALA:HA	1:A:797:THR:HG21	1.74	0.69
1:B:502:THR:H	1:B:505:GLN:HE21	1.39	0.69
1:B:190:ASP:OD1	1:B:192:ARG:HD3	1.92	0.68
1:B:755:THR:HG23	1:B:757:TRP:CD1	2.28	0.68
1:B:755:THR:CG2	1:B:757:TRP:CD1	2.78	0.67
1:A:808:ALA:HB2	3:A:904:FAD:H5'2	1.78	0.66
1:A:698:TYR:HB3	1:A:700:MET:CE	2.26	0.66
1:A:172:LYS:CB	1:A:173:PRO:CD	2.73	0.66
1:B:266:ASN:HD22	1:B:266:ASN:C	2.00	0.65
1:B:550:ASN:ND2	1:B:552:HIS:H	1.94	0.64
1:A:274:GLN:O	1:A:277:GLU:HB2	1.99	0.62
1:A:440:ASN:CB	6:A:1263:HOH:O	2.48	0.61
1:B:332:ILE:HD12	1:B:346:VAL:CG1	2.20	0.61
1:B:228:VAL:CG1	1:B:228:VAL:O	2.49	0.60
1:A:794:GLY:O	1:A:797:THR:HB	2.02	0.60
1:A:229:GLY:HA3	1:A:309:ALA:HB2	1.84	0.59
1:B:228:VAL:O	1:B:228:VAL:HG12	2.01	0.59
1:B:794:GLY:O	1:B:797:THR:HB	2.02	0.59
1:A:612:THR:HG22	1:A:616:THR:H	1.67	0.59
1:B:787:GLN:O	1:B:789:THR:HG22	2.02	0.59
1:B:162:GLN:O	1:B:166:THR:HB	2.02	0.58
1:A:603:TYR:CZ	1:A:641:PRO:HD2	2.39	0.58
1:A:541:SER:HB3	1:A:691:ARG:HG2	1.85	0.57
1:B:380:TYR:HD1	1:B:820:ALA:O	1.87	0.57
1:B:383:LYS:HA	1:B:621:GLN:NE2	2.20	0.57
1:A:388:ILE:CD1	1:A:601:ILE:HD11	2.34	0.56
1:A:584:GLU:HG2	6:A:1196:HOH:O	2.05	0.56
1:A:795:GLU:HG2	1:A:802:PRO:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:PRO:O	1:B:332:ILE:HG12	2.06	0.56
1:B:669:ARG:NH2	1:B:704:LYS:HG3	2.21	0.56
1:A:454:LEU:HD21	1:A:585:LYS:HG2	1.88	0.55
1:A:139:TRP:CE2	1:A:340:LEU:HD13	2.42	0.55
1:B:383:LYS:HA	1:B:621:GLN:HE22	1.71	0.55
1:B:420:ARG:HB2	3:B:904:FAD:H4'	1.89	0.54
1:B:793:ALA:HA	1:B:797:THR:HG21	1.88	0.54
1:B:660:GLU:OE1	1:B:755:THR:CG2	2.50	0.54
1:A:459:HIS:HE1	1:A:679:ASP:OD1	1.91	0.53
3:B:904:FAD:O1A	3:B:904:FAD:H5'2	2.08	0.53
1:B:688:ALA:O	1:B:691:ARG:HB2	2.08	0.53
1:B:375:LEU:HD12	1:B:403:ASN:HB3	1.90	0.53
1:B:755:THR:CG2	1:B:757:TRP:HD1	2.20	0.53
1:A:661:LYS:H	1:A:755:THR:CG2	2.21	0.53
1:B:667:PRO:HB2	1:B:668:TYR:CD2	2.44	0.53
1:B:755:THR:HG21	1:B:757:TRP:HD1	1.74	0.52
1:A:658:ILE:HG12	1:A:758:SER:HB3	1.90	0.52
1:B:217:ALA:HB3	1:B:218:PRO:HD3	1.92	0.52
1:A:501:LYS:O	1:A:557:ARG:NH1	2.43	0.52
1:A:300:TYR:OH	1:A:348:GLU:HG3	2.09	0.51
1:B:661:LYS:H	1:B:755:THR:HB	1.75	0.51
1:A:332:ILE:HG12	1:A:346:VAL:HG13	1.93	0.51
1:B:392:PRO:HG2	3:B:904:FAD:H5'1	1.92	0.51
1:B:755:THR:HG21	1:B:757:TRP:CD1	2.43	0.51
1:B:626:THR:HG22	1:B:793:ALA:HB3	1.92	0.51
1:A:626:THR:HG22	1:A:793:ALA:HB3	1.93	0.51
1:A:808:ALA:CB	3:A:904:FAD:H5'2	2.41	0.51
1:A:698:TYR:HB3	1:A:700:MET:HE2	1.93	0.50
1:A:628:PRO:HG2	1:A:763:ILE:HA	1.93	0.50
1:B:470:GLU:OE1	1:B:683:HIS:HE1	1.95	0.50
1:A:190:ASP:OD1	1:A:192:ARG:HD3	2.11	0.50
1:A:285:ARG:O	1:A:311:ARG:NH2	2.43	0.49
1:A:603:TYR:CE1	1:A:641:PRO:HD2	2.47	0.49
1:B:83:TYR:HE2	1:B:93:ASN:HD22	1.61	0.49
1:A:821:ALA:O	1:A:822:PHE:CB	2.61	0.49
1:B:77:GLY:O	1:B:79:THR:N	2.46	0.49
1:A:797:THR:HG21	1:A:814:ARG:HH22	1.74	0.49
1:A:176:ALA:HB2	1:A:178:LYS:N	2.27	0.49
1:A:545:TYR:CD1	1:A:712:VAL:HG11	2.48	0.49
1:B:339:GLY:HA3	1:B:341:VAL:HG12	1.94	0.49
1:B:454:LEU:HD21	1:B:585:LYS:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:VAL:HG13	1:A:228:VAL:O	2.13	0.48
1:B:797:THR:CG2	1:B:797:THR:O	2.63	0.47
1:A:66:PHE:HZ	1:A:131:MET:HB3	1.80	0.47
1:B:443:ILE:HG13	1:B:570:GLY:HA3	1.96	0.46
1:B:797:THR:HG21	1:B:814:ARG:HH22	1.76	0.46
1:B:661:LYS:HE2	1:B:710[A]:MET:SD	2.56	0.46
1:A:228:VAL:O	1:A:228:VAL:CG1	2.64	0.46
1:B:667:PRO:HB2	1:B:668:TYR:HD2	1.79	0.46
1:A:787:GLN:O	1:A:789:THR:HG23	2.16	0.45
1:B:209:PRO:CG	1:B:306:MET:HG3	2.46	0.45
1:A:349:VAL:O	1:A:353:LEU:HB2	2.15	0.45
1:A:555:SER:O	1:A:559:TRP:HB3	2.15	0.45
1:B:555:SER:HB2	1:B:772:THR:HA	1.98	0.45
1:A:388:ILE:HD13	1:A:601:ILE:HD11	1.97	0.45
1:B:267:ARG:NH2	1:B:571:ASP:OD2	2.50	0.45
1:A:501:LYS:HA	1:A:505:GLN:NE2	2.32	0.45
1:B:628:PRO:HG2	1:B:763:ILE:HA	1.99	0.45
1:A:154:THR:HB	6:A:1029:HOH:O	2.18	0.44
1:A:640:ASN:HD22	1:A:641:PRO:HA	1.83	0.44
1:B:266:ASN:ND2	1:B:266:ASN:C	2.68	0.44
1:A:96:PHE:HB3	1:A:100:TYR:CE1	2.51	0.44
1:A:470:GLU:OE1	1:A:683:HIS:HE1	2.01	0.44
1:B:297:PHE:HB3	1:B:300:TYR:HD2	1.83	0.43
1:A:285:ARG:HD3	6:A:1061:HOH:O	2.18	0.43
1:A:200:TRP:HD1	1:B:273:TYR:OH	2.02	0.43
1:B:122:LYS:HD2	1:B:227:CYS:SG	2.59	0.43
1:B:380:TYR:CD1	1:B:820:ALA:O	2.70	0.42
1:A:196:VAL:HG22	1:A:201:TRP:CE2	2.54	0.42
1:B:66:PHE:HZ	1:B:131:MET:HB3	1.83	0.42
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.92	0.42
1:A:379:ASP:OD1	1:A:381:HIS:HD2	2.01	0.42
1:B:262:VAL:HB	1:B:263:PRO:HD3	2.02	0.42
1:B:348:GLU:OE1	1:B:351:ARG:HD3	2.20	0.42
1:A:660:GLU:HB3	1:A:755:THR:HG22	2.01	0.42
1:A:661:LYS:H	1:A:755:THR:HG22	1.84	0.42
1:B:180:GLU:O	1:B:180:GLU:HG2	2.20	0.41
1:B:275:PRO:O	1:B:276:ASN:CB	2.68	0.41
1:A:127:PRO:O	1:A:131:MET:HG2	2.20	0.41
1:A:778:ALA:O	1:A:782:ILE:HG13	2.20	0.41
1:B:633:GLN:HG3	1:B:651:ILE:HG22	2.03	0.41
1:A:802:PRO:HB2	1:A:803:GLN:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLN:HE22	1:A:332:ILE:HG21	1.86	0.41
1:A:172:LYS:CB	1:A:173:PRO:HD3	2.51	0.41
1:B:68:SER:HA	1:B:73:CYS:SG	2.62	0.40
1:B:228:VAL:HG13	1:B:312:ASN:HD22	1.86	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	745/796 (94%)	699 (94%)	40 (5%)	6 (1%)	19 51
1	B	736/796 (92%)	699 (95%)	35 (5%)	2 (0%)	41 71
All	All	1481/1592 (93%)	1398 (94%)	75 (5%)	8 (0%)	29 61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	105	ASP
1	A	172	LYS
1	A	371	ALA
1	B	78	TYR
1	B	95	CYS
1	A	279	GLY
1	A	106	GLY

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	602/678 (89%)	555 (92%)	47 (8%)	12	34
1	B	589/678 (87%)	543 (92%)	46 (8%)	12	34
All	All	1191/1356 (88%)	1098 (92%)	93 (8%)	12	34

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	52	LYS
1	A	55	LYS
1	A	61	THR
1	A	71	GLU
1	A	97	ASP
1	A	100	TYR
1	A	101	ARG
1	A	140	VAL
1	A	149	LYS
1	A	154	THR
1	A	159	LEU
1	A	171	MET
1	A	186	SER
1	A	194	LEU
1	A	204	MET
1	A	205	LEU
1	A	228	VAL
1	A	329	GLN
1	A	330	LYS
1	A	338	ARG
1	A	340	LEU
1	A	344	ARG
1	A	361	LEU
1	A	362	ILE
1	A	369	VAL
1	A	373	GLN
1	A	379	ASP
1	A	536	LEU
1	A	540	LEU
1	A	543	LEU
1	A	575	LEU
1	A	576	THR

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Mol	Chain	Res	Type
1	A	607	GLU
1	A	612	THR
1	A	614	ASP
1	A	631	LEU
1	A	664	LEU
1	A	680	PHE
1	A	683	HIS
1	A	693	LEU
1	A	704	LYS
1	A	723	THR
1	A	755	THR
1	A	789	THR
1	A	797	THR
1	A	800	HIS
1	B	112	THR
1	B	140	VAL
1	B	159	LEU
1	B	166	THR
1	B	174	ASN
1	B	180	GLU
1	B	194	LEU
1	B	205	LEU
1	B	221	SER
1	B	234	CYS
1	B	235	THR
1	B	265	MET
1	B	266	ASN
1	B	267	ARG
1	B	320	THR
1	B	330	LYS
1	B	344	ARG
1	B	349	VAL
1	B	361	LEU
1	B	373	GLN
1	B	383	LYS
1	B	431	THR
1	B	432	VAL
1	B	507	VAL
1	B	536	LEU
1	B	540	LEU
1	B	543	LEU
1	B	545	TYR

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Mol	Chain	Res	Type
1	B	572	HIS
1	B	596	SER
1	B	631	LEU
1	B	638	GLN
1	B	673	SER
1	B	680	PHE
1	B	716	GLU
1	B	720	SER
1	B	723	THR
1	B	726	ASP
1	B	727	LYS
1	B	746	VAL
1	B	755	THR
1	B	756	ARG
1	B	758	SER
1	B	772	THR
1	B	789	THR
1	B	797	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	141	GLN
1	A	381	HIS
1	A	459	HIS
1	A	488	ASN
1	A	503	GLN
1	A	505	GLN
1	A	640	ASN
1	A	683	HIS
1	A	800	HIS
1	B	93	ASN
1	B	158	GLN
1	B	174	ASN
1	B	184	HIS
1	B	266	ASN
1	B	486	HIS
1	B	505	GLN
1	B	550	ASN
1	B	561	HIS
1	B	621	GLN

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Mol	Chain	Res	Type
1	B	640	ASN
1	B	683	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	FAD	A	904	-	54,58,58	1.24	3 (5%)	71,89,89	1.61	9 (12%)
5	PO4	B	905	-	4,4,4	0.91	0	6,6,6	0.48	0
3	FAD	B	904	-	54,58,58	1.21	4 (7%)	71,89,89	1.88	15 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	A	904	-	-	9/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FAD	B	904	-	-	15/30/50/50	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	904	FAD	C4X-N5	4.12	1.39	1.30
3	A	904	FAD	C4X-N5	4.07	1.39	1.30
3	A	904	FAD	C10-N1	3.68	1.40	1.33
3	A	904	FAD	P-O3P	3.47	1.63	1.59
3	B	904	FAD	C1'-C2'	3.22	1.57	1.52
3	B	904	FAD	C10-N1	2.97	1.39	1.33
3	B	904	FAD	O4B-C1B	2.34	1.44	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	904	FAD	C4B-O4B-C1B	-7.19	103.34	109.92
3	B	904	FAD	C4'-C3'-C2'	-6.57	102.64	113.57
3	B	904	FAD	C1'-C2'-C3'	5.43	124.39	109.66
3	B	904	FAD	N3A-C2A-N1A	-5.31	121.46	128.67
3	A	904	FAD	N3A-C2A-N1A	-5.03	121.84	128.67
3	B	904	FAD	C4B-O4B-C1B	-4.71	105.61	109.92
3	B	904	FAD	C5'-C4'-C3'	3.76	119.32	112.22
3	A	904	FAD	C4-N3-C2	-3.26	119.86	125.64
3	A	904	FAD	C10-C4X-N5	-3.21	118.26	124.81
3	B	904	FAD	C2'-C1'-N10	3.20	125.33	110.20
3	B	904	FAD	C4-N3-C2	-3.12	120.10	125.64
3	A	904	FAD	C4X-C10-N10	2.88	120.61	116.48
3	A	904	FAD	C9A-C5X-N5	-2.82	119.46	122.45
3	A	904	FAD	C4-C4X-N5	2.81	122.09	118.21
3	A	904	FAD	O5B-PA-O1A	2.75	119.84	108.94
3	B	904	FAD	C9A-C5X-N5	-2.72	119.57	122.45
3	A	904	FAD	C4X-C4-N3	2.64	119.97	113.25
3	B	904	FAD	O2P-P-O3P	-2.57	100.33	107.27
3	B	904	FAD	C4X-C4-N3	2.32	119.15	113.25
3	B	904	FAD	C5X-C9A-N10	2.25	120.00	117.97
3	B	904	FAD	C4X-C10-N10	2.16	119.58	116.48
3	B	904	FAD	C4-C4X-C10	2.16	120.63	116.93
3	B	904	FAD	O2A-PA-O3P	-2.11	101.57	107.27
3	B	904	FAD	C10-C4X-N5	-2.02	120.69	124.81

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	904	FAD	C5B-O5B-PA-O1A
3	A	904	FAD	C5B-O5B-PA-O2A
3	A	904	FAD	C5B-O5B-PA-O3P
3	A	904	FAD	C3'-C4'-C5'-O5'
3	A	904	FAD	O4'-C4'-C5'-O5'
3	B	904	FAD	N10-C1'-C2'-O2'
3	B	904	FAD	N10-C1'-C2'-C3'
3	B	904	FAD	C1'-C2'-C3'-O3'
3	B	904	FAD	C1'-C2'-C3'-C4'
3	B	904	FAD	O3'-C3'-C4'-O4'
3	B	904	FAD	O3'-C3'-C4'-C5'
3	B	904	FAD	C3'-C4'-C5'-O5'
3	B	904	FAD	O4'-C4'-C5'-O5'
3	B	904	FAD	C2'-C3'-C4'-O4'
3	B	904	FAD	O2'-C2'-C3'-C4'
3	A	904	FAD	O4B-C4B-C5B-O5B
3	A	904	FAD	C3B-C4B-C5B-O5B
3	B	904	FAD	C2'-C3'-C4'-C5'
3	B	904	FAD	O2'-C2'-C3'-O3'
3	B	904	FAD	C3B-C4B-C5B-O5B
3	B	904	FAD	O4B-C4B-C5B-O5B
3	B	904	FAD	C5'-O5'-P-O1P
3	A	904	FAD	PA-O3P-P-O1P
3	A	904	FAD	PA-O3P-P-O5'

There are no ring outliers.

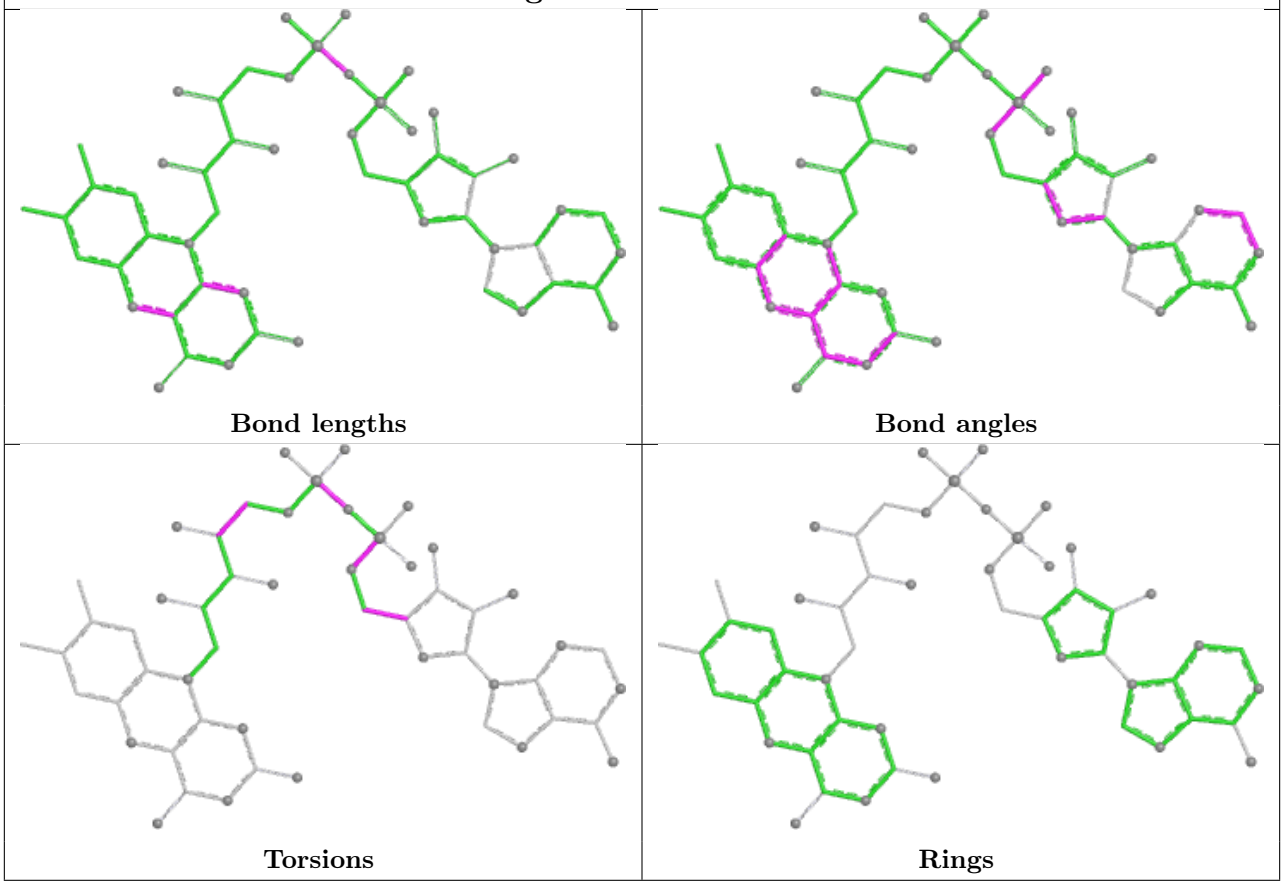
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	904	FAD	2	0
3	B	904	FAD	3	0

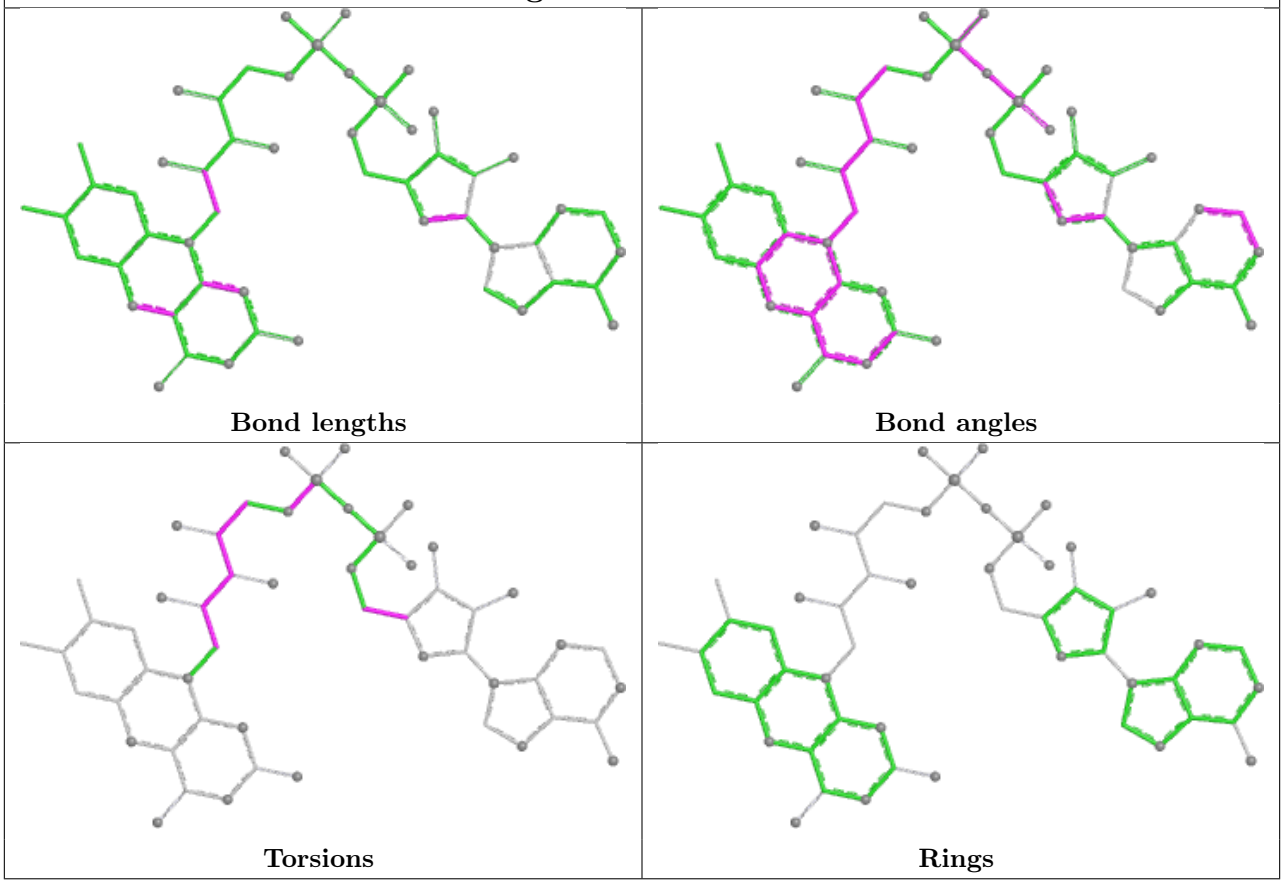
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 904



Ligand FAD B 904



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, 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	750/796 (94%)	-0.39	11 (1%)	73	73	21, 36, 77, 179	1 (0%)
1	B	742/796 (93%)	-0.26	14 (1%)	66	65	26, 46, 106, 269	1 (0%)
All	All	1492/1592 (93%)	-0.33	25 (1%)	70	69	21, 41, 99, 269	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	VAL	6.5
1	B	237	THR	6.1
1	A	50	TYR	4.6
1	A	237	THR	3.7
1	A	48	LYS	3.5
1	B	174	ASN	2.9
1	A	49	LYS	2.9
1	B	265	MET	2.9
1	B	61	THR	2.9
1	B	380	TYR	2.9
1	A	278	CYS	2.8
1	B	263	PRO	2.8
1	B	77	GLY	2.7
1	B	182	SER	2.6
1	A	80	SER	2.6
1	B	53	CYS	2.6
1	B	111	THR	2.5
1	B	381	HIS	2.5
1	A	234	CYS	2.4
1	A	72	ARG	2.2
1	A	372	ASP	2.2
1	A	181	THR	2.1
1	B	59	THR	2.1
1	B	62	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	103	HIS	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 monosaccharides in this entry.

6.4 Ligands (i)

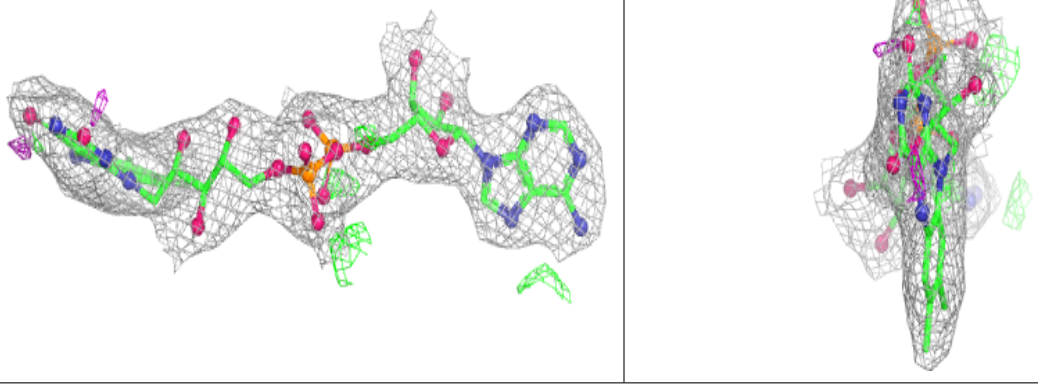
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

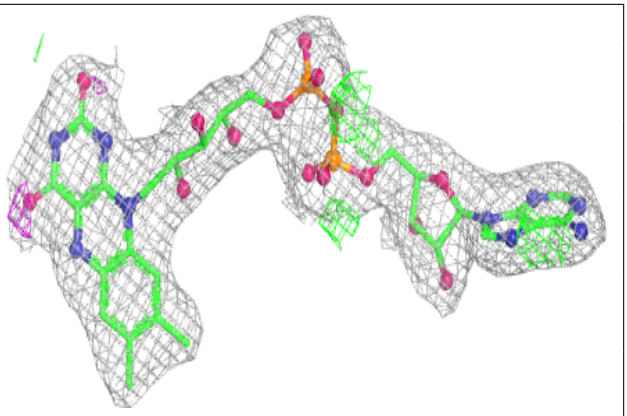
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	903	1/1	0.92	0.05	102,102,102,102	0
4	K	A	905	1/1	0.95	0.04	57,57,57,57	0
2	ZN	A	902	1/1	0.98	0.06	52,52,52,52	0
3	FAD	A	904	53/53	0.98	0.15	20,22,25,26	0
3	FAD	B	904	53/53	0.98	0.14	27,31,34,36	0
2	ZN	B	902	1/1	0.98	0.03	88,88,88,88	0
5	PO4	B	905	5/5	0.98	0.12	42,45,48,48	0
2	ZN	A	901	1/1	0.99	0.05	59,59,59,59	0
2	ZN	A	903	1/1	0.99	0.03	62,62,62,62	0
2	ZN	B	901	1/1	0.99	0.06	51,51,51,51	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 A 904:

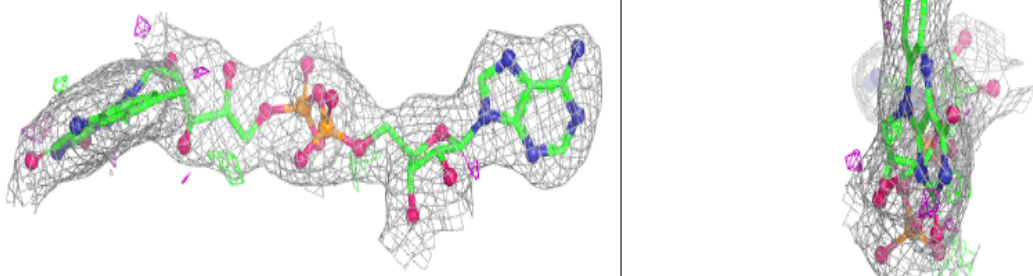
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

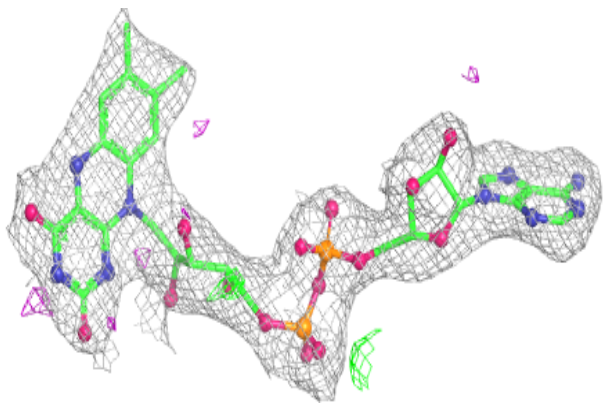




Electron density around FAD B 904:

$2mF_o$-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.