Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 10:45 AM EDT

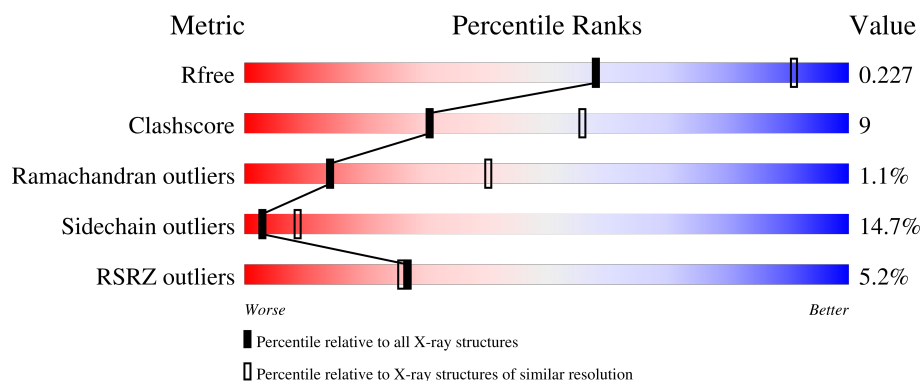|		
PDB ID	:	4GU1
Title	:	Crystal structure of LSD2
Authors	:	Chen, F.; Dong, Z.; Fang, J.; Yang, Y.; Li, Z.; Xu, Y.; Yang, H.; Wang, P.; Fang, R.; Shi, Y.; Xu, Y.
Deposited on	:	2012-08-29
Resolution	:	2.94 Å(reported)

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 2.94 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.227
Clashscore		9
Ramachandran outliers		1.1%
Sidechain outliers		14.7%
RSRZ outliers		5.2%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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	784	4% / 67% / 23% / • / 5%
1	B	784	6% / 65% / 25% / 5% / 5%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 11971 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	746	Total	C	N	O	S	0	0	0
			5915	3775	1013	1086	41			
1	B	746	Total	C	N	O	S	0	0	0
			5915	3775	1013	1086	41			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	PRO	-	expression tag	UNP Q8NB78
A	40	LEU	-	expression tag	UNP Q8NB78
A	41	GLY	-	expression tag	UNP Q8NB78
A	42	SER	-	expression tag	UNP Q8NB78
A	43	GLU	-	expression tag	UNP Q8NB78
A	44	PHE	-	expression tag	UNP Q8NB78
A	45	LYS	-	expression tag	UNP Q8NB78
A	46	GLY	-	expression tag	UNP Q8NB78
A	47	LEU	-	expression tag	UNP Q8NB78
A	48	ARG	-	expression tag	UNP Q8NB78
A	49	ARG	-	expression tag	UNP Q8NB78
A	50	ARG	-	expression tag	UNP Q8NB78
B	39	PRO	-	expression tag	UNP Q8NB78
B	40	LEU	-	expression tag	UNP Q8NB78
B	41	GLY	-	expression tag	UNP Q8NB78
B	42	SER	-	expression tag	UNP Q8NB78
B	43	GLU	-	expression tag	UNP Q8NB78
B	44	PHE	-	expression tag	UNP Q8NB78
B	45	LYS	-	expression tag	UNP Q8NB78
B	46	GLY	-	expression tag	UNP Q8NB78
B	47	LEU	-	expression tag	UNP Q8NB78
B	48	ARG	-	expression tag	UNP Q8NB78
B	49	ARG	-	expression tag	UNP Q8NB78
B	50	ARG	-	expression tag	UNP Q8NB78

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

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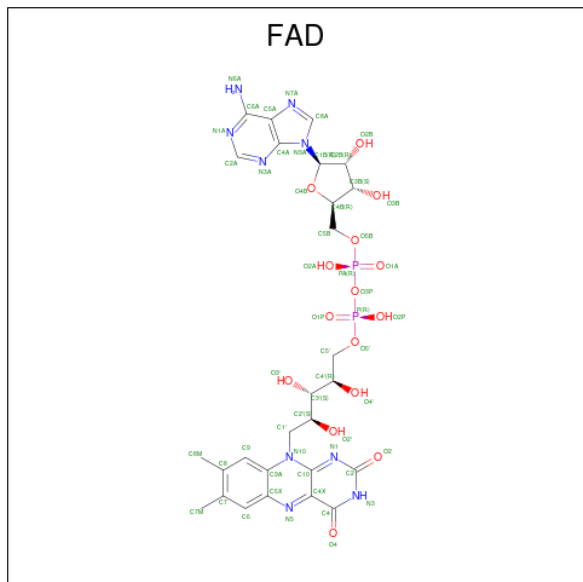
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total 11	O 11	0	0
6	B	12	Total 12	O 12	0	0

3 Residue-property plots ⓘ

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
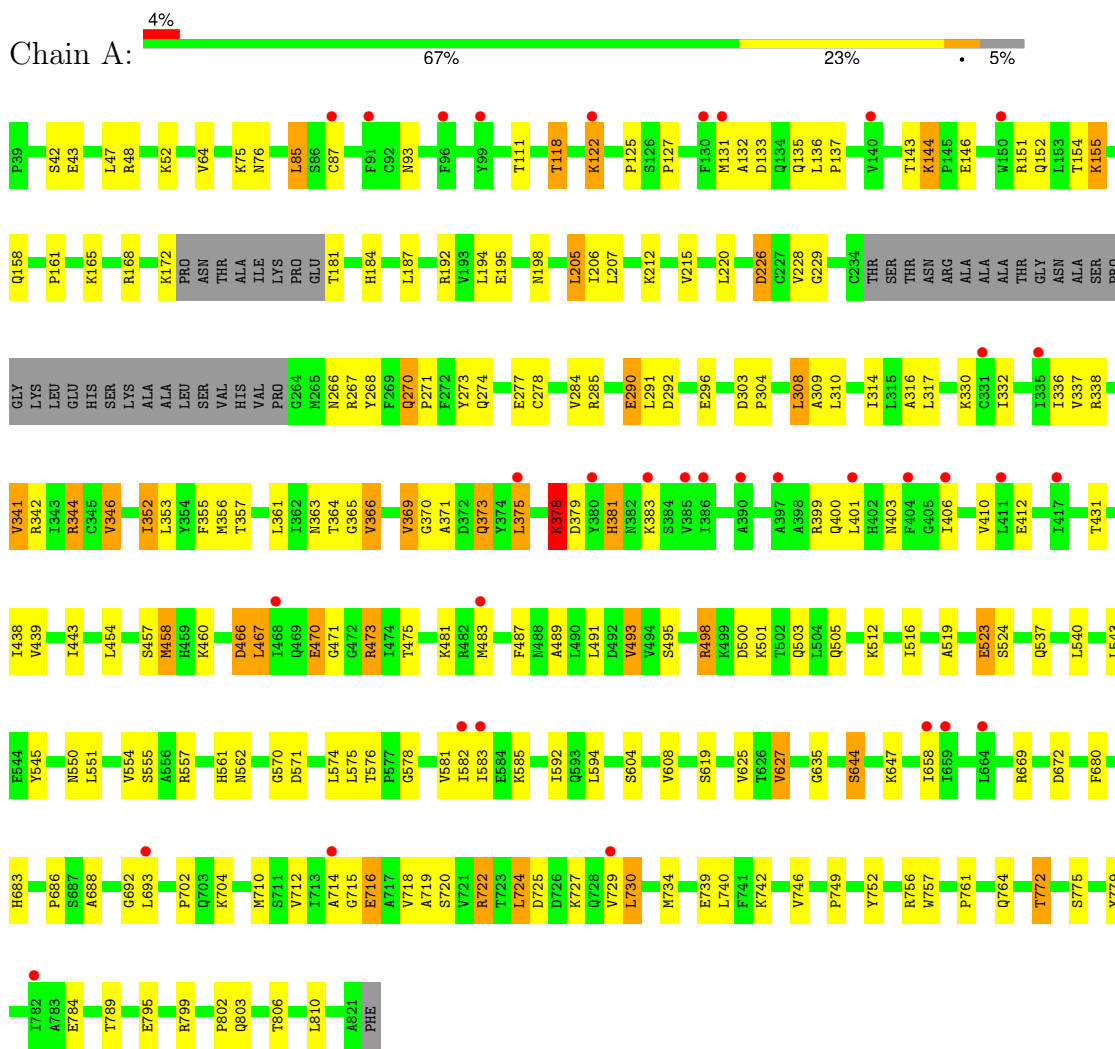
• Molecule 1: Lysine-specific histone demethylase 1B
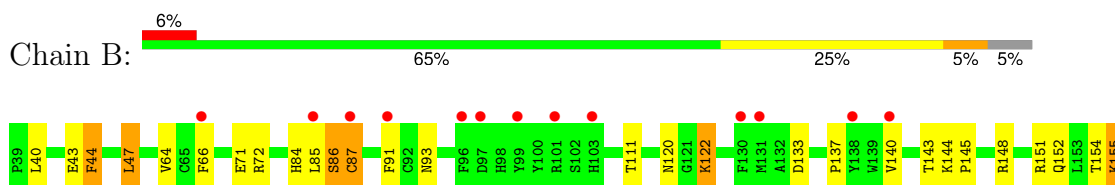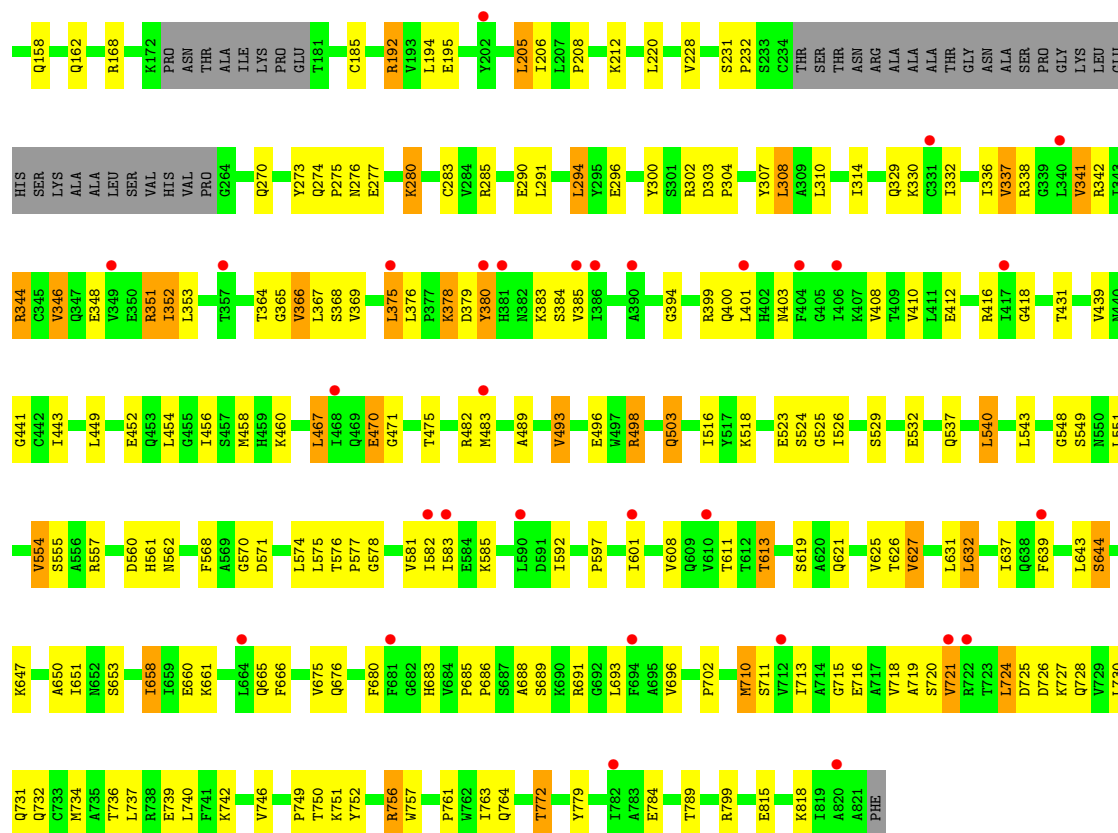
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.16Å 89.22Å 342.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.56 – 2.94 44.61 – 2.94	Depositor EDS
% Data completeness (in resolution range)	97.5 (39.56-2.94) 97.5 (44.61-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.185 , 0.228 0.187 , 0.227	Depositor DCC
R_{free} test set	2926 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	83.1	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.467 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11971	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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: CL, ZN, FAD, NA

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	0.46	0/6060	0.62	0/8203
1	B	0.46	0/6060	0.62	1/8203 (0.0%)
All	All	0.46	0/12120	0.62	1/16406 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	632	LEU	CA-CB-CG	5.22	127.31	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5915	0	5842	106	0
1	B	5915	0	5842	113	0
2	A	53	0	31	4	0
2	B	53	0	31	4	0
3	A	2	0	0	1	0
3	B	2	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	11	0	0	0	0
6	B	12	0	0	0	0
All	All	11971	0	11746	217	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 9.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:ARG:HD3	1:A:557:ARG:HA	1.57	0.87
1:B:192:ARG:HG3	1:B:192:ARG:HH11	1.46	0.80
1:A:458:MET:HE3	1:A:575:LEU:HD13	1.72	0.69
1:A:332:ILE:HG12	1:A:346:VAL:HB	1.75	0.68
1:B:384:SER:HB3	1:B:621:GLN:H	1.60	0.67
1:A:412:GLU:OE2	2:A:901:FAD:O2B	2.10	0.67
1:B:205:LEU:HD21	1:B:341:VAL:HG13	1.76	0.66
1:B:597:PRO:HG2	1:B:613:THR:HB	1.79	0.65
1:A:495:SER:HA	1:A:498:ARG:HG3	1.78	0.64
1:B:378:LYS:H	1:B:378:LYS:HD3	1.67	0.60
1:A:310:LEU:O	1:A:314:ILE:HG13	2.01	0.59
1:B:212:LYS:HB2	1:B:336:ILE:HG22	1.84	0.59
1:B:578:GLY:O	1:B:581:VAL:HG12	2.02	0.59
1:A:132:ALA:HA	1:A:136:LEU:HD12	1.84	0.59
1:A:467:LEU:HD12	1:A:467:LEU:H	1.68	0.58
1:B:454:LEU:HD21	1:B:585:LYS:HG2	1.84	0.58
1:A:205:LEU:HD21	1:A:341:VAL:HG13	1.85	0.58
1:A:550:ASN:HD22	1:A:716:GLU:HG2	1.67	0.58
1:A:724:LEU:H	1:A:724:LEU:HD23	1.68	0.58
1:B:482:ARG:NH1	1:B:532:GLU:OE1	2.37	0.58
1:B:143:THR:HB	1:B:168:ARG:HG3	1.85	0.58
1:A:537:GLN:HG2	1:A:688:ALA:HA	1.86	0.58
1:A:734:MET:HE2	1:A:734:MET:HA	1.85	0.58
1:A:220:LEU:HD13	1:A:228:VAL:HG11	1.86	0.58
1:A:401:LEU:HD22	1:A:406:ILE:HD12	1.86	0.57
1:B:364:THR:HG22	1:B:400:GLN:OE1	2.05	0.57
1:A:226:ASP:OD1	1:A:226:ASP:N	2.32	0.57
1:B:779:TYR:HB2	1:B:799:ARG:HB2	1.86	0.56
1:A:779:TYR:HB2	1:A:799:ARG:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:SER:HB2	1:A:647:LYS:H	1.69	0.56
1:B:412:GLU:OE2	2:B:901:FAD:O2B	2.22	0.56
1:A:454:LEU:HD21	1:A:585:LYS:HG2	1.88	0.56
1:B:220:LEU:HD13	1:B:228:VAL:HG11	1.88	0.56
1:B:730:LEU:HD12	1:B:752:TYR:CZ	2.42	0.55
1:A:330:LYS:NZ	3:A:903:CL:CL	2.77	0.55
1:B:366:VAL:HG21	1:B:585:LYS:HB3	1.89	0.55
1:B:498:ARG:NH2	1:B:560:ASP:OD1	2.40	0.54
1:A:273:TYR:HD2	1:A:277:GLU:HG3	1.72	0.54
1:A:352:ILE:O	1:A:356:MET:HG3	2.08	0.54
1:A:439:VAL:HG21	1:A:458:MET:HE1	1.90	0.54
1:B:348:GLU:OE1	1:B:351:ARG:NH1	2.40	0.54
1:B:337:VAL:HG23	1:B:342:ARG:HG3	1.89	0.54
1:A:460:LYS:HE2	1:A:571:ASP:OD1	2.08	0.54
1:A:122:LYS:NZ	1:B:122:LYS:HG3	2.23	0.53
1:B:412:GLU:OE1	2:B:901:FAD:O3B	2.26	0.53
1:B:467:LEU:H	1:B:467:LEU:HD12	1.73	0.53
1:B:540:LEU:HB3	1:B:691:ARG:HH11	1.72	0.53
1:A:118:THR:HG23	1:A:125:PRO:HG3	1.91	0.53
1:A:493:VAL:HG22	1:A:516:ILE:HD13	1.91	0.52
1:B:724:LEU:HD23	1:B:724:LEU:H	1.74	0.52
1:B:761:PRO:O	1:B:764:GLN:NE2	2.43	0.52
1:A:314:ILE:HD13	1:A:353:LEU:HD12	1.90	0.52
1:B:537:GLN:HG2	1:B:688:ALA:HA	1.90	0.52
1:B:376:LEU:HB3	1:B:380:TYR:HE1	1.75	0.52
1:B:555:SER:HB2	1:B:772:THR:HA	1.90	0.52
1:A:85:LEU:HD23	1:A:136:LEU:HD11	1.92	0.52
1:A:43:GLU:CD	1:A:43:GLU:H	2.13	0.51
1:A:144:LYS:HD3	1:A:168:ARG:HG2	1.92	0.51
1:A:578:GLY:O	1:A:581:VAL:HG12	2.10	0.51
1:B:460:LYS:HE2	1:B:571:ASP:OD1	2.10	0.51
1:A:730:LEU:HD21	1:A:749:PRO:HG2	1.94	0.50
1:B:726:ASP:OD1	1:B:756:ARG:NH1	2.43	0.50
2:B:901:FAD:O5'	2:B:901:FAD:O1A	2.30	0.50
1:A:366:VAL:HG21	1:A:585:LYS:HB3	1.92	0.50
1:B:66:PHE:CE1	1:B:91:PHE:HB3	2.46	0.50
1:A:715:GLY:O	1:A:718:VAL:HG12	2.11	0.50
1:B:661:LYS:HE2	1:B:710:MET:HE1	1.93	0.50
1:A:757:TRP:O	1:A:764:GLN:HA	2.12	0.50
1:B:192:ARG:O	1:B:195:GLU:HB2	2.12	0.50
1:A:761:PRO:O	1:A:764:GLN:NE2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ARG:HG3	1:B:192:ARG:NH1	2.22	0.49
1:B:757:TRP:O	1:B:764:GLN:HA	2.12	0.49
1:A:127:PRO:O	1:A:131:MET:HG2	2.13	0.49
1:B:715:GLY:O	1:B:718:VAL:HG12	2.13	0.49
1:B:493:VAL:HG22	1:B:516:ILE:HD13	1.95	0.49
1:A:304:PRO:HB2	1:A:308:LEU:HD22	1.95	0.48
1:A:719:ALA:O	1:A:722:ARG:HG2	2.14	0.48
1:B:86:SER:OG	1:B:87:CYS:N	2.45	0.48
1:A:344:ARG:HA	1:A:344:ARG:HD3	1.66	0.48
1:A:500:ASP:HB3	1:A:501:LYS:HZ2	1.78	0.48
1:B:576:THR:HG21	1:B:702:PRO:HG2	1.94	0.48
1:B:728:GLN:O	1:B:731:GLN:HG2	2.13	0.48
1:A:471:GLY:HA2	1:A:739:GLU:O	2.14	0.48
1:B:310:LEU:O	1:B:314:ILE:HG13	2.12	0.48
1:A:122:LYS:HZ2	1:B:122:LYS:HG3	1.77	0.48
1:A:730:LEU:HD12	1:A:752:TYR:CZ	2.48	0.48
1:B:467:LEU:HD13	1:B:475:THR:HB	1.96	0.48
1:B:601:ILE:HD12	1:B:637:ILE:HG21	1.95	0.48
1:B:734:MET:HE1	1:B:737:LEU:HD12	1.95	0.48
1:A:369:VAL:HG22	1:A:373:GLN:O	2.14	0.47
1:B:273:TYR:HD2	1:B:277:GLU:HG3	1.79	0.47
1:B:685:PRO:HA	1:B:686:PRO:HD3	1.80	0.47
1:A:576:THR:HG21	1:A:702:PRO:HG2	1.97	0.47
1:B:644:SER:HB2	1:B:647:LYS:H	1.79	0.47
1:B:696:VAL:O	1:B:711:SER:OG	2.24	0.47
1:B:734:MET:CE	1:B:737:LEU:HD12	2.45	0.47
1:B:443:ILE:HG12	1:B:570:GLY:HA3	1.96	0.46
1:B:576:THR:OG1	1:B:577:PRO:HD3	2.15	0.46
1:A:229:GLY:HA3	1:A:309:ALA:HB2	1.97	0.46
1:B:144:LYS:HA	1:B:145:PRO:HD3	1.75	0.46
1:A:555:SER:HB2	1:A:772:THR:HA	1.98	0.46
1:A:523:GLU:OE1	1:A:524:SER:N	2.49	0.46
1:B:364:THR:HB	1:B:365:GLY:H	1.59	0.46
1:A:466:ASP:OD2	1:A:466:ASP:N	2.36	0.46
1:B:489:ALA:O	1:B:493:VAL:HG12	2.16	0.45
1:A:184:HIS:HA	1:A:187:LEU:HD13	1.98	0.45
1:A:342:ARG:O	1:A:346:VAL:HG13	2.16	0.45
1:B:300:TYR:OH	1:B:348:GLU:HG3	2.16	0.45
1:B:310:LEU:HD23	1:B:310:LEU:HA	1.74	0.45
1:A:519:ALA:O	1:A:523:GLU:HB2	2.17	0.45
1:B:439:VAL:HG21	1:B:458:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:PRO:HG3	1:B:152:GLN:NE2	2.31	0.45
1:A:296:GLU:HG3	1:A:355:PHE:CE1	2.52	0.45
1:A:647:LYS:NZ	1:A:784:GLU:O	2.49	0.45
1:A:42:SER:O	1:A:48:ARG:NH1	2.49	0.44
1:A:212:LYS:HB2	1:A:336:ILE:HG22	1.98	0.44
1:A:545:TYR:CD1	1:A:712:VAL:HG11	2.53	0.44
1:A:795:GLU:HB2	2:A:901:FAD:H5'2	2.00	0.44
1:B:133:ASP:O	1:B:338:ARG:HD2	2.17	0.44
1:B:471:GLY:HA2	1:B:739:GLU:O	2.17	0.44
1:B:730:LEU:HD21	1:B:749:PRO:HG2	1.98	0.44
1:A:195:GLU:O	1:A:198:ASN:HB3	2.17	0.44
1:A:692:GLY:HA3	1:A:714:ALA:O	2.17	0.44
1:A:366:VAL:HG11	1:A:454:LEU:HG	1.99	0.44
1:B:155:LYS:O	1:B:155:LYS:HD3	2.18	0.44
1:A:467:LEU:HD13	1:A:475:THR:HB	1.99	0.44
1:A:161:PRO:O	1:A:165:LYS:HB2	2.17	0.44
1:B:375:LEU:HD22	1:B:403:ASN:HB3	2.00	0.44
1:B:561:HIS:CG	1:B:562:ASN:N	2.85	0.44
1:A:378:LYS:HA	1:A:381:HIS:CE1	2.52	0.44
1:B:493:VAL:HG11	1:B:516:ILE:HG21	2.00	0.44
1:A:220:LEU:HD13	1:A:228:VAL:CG1	2.47	0.44
1:A:270:GLN:HA	1:A:271:PRO:HD3	1.84	0.44
1:A:443:ILE:HG12	1:A:570:GLY:HA3	1.99	0.44
1:B:470:GLU:HA	1:B:471:GLY:HA2	1.70	0.44
1:B:548:GLY:O	1:B:658:ILE:N	2.46	0.43
1:A:303:ASP:HA	1:A:304:PRO:HD3	1.81	0.43
1:A:803:GLN:O	2:A:901:FAD:O3'	2.36	0.43
1:B:666:PHE:HZ	1:B:734:MET:HE3	1.83	0.43
1:B:376:LEU:HB3	1:B:380:TYR:CE1	2.52	0.43
1:A:266:ASN:OD1	1:A:268:TYR:N	2.36	0.43
1:A:270:GLN:HG2	1:A:443:ILE:HG23	2.00	0.43
1:A:500:ASP:HB3	1:A:501:LYS:NZ	2.33	0.43
1:B:660:GLU:HB3	1:B:713:ILE:HG12	1.99	0.43
1:B:523:GLU:OE1	1:B:524:SER:N	2.51	0.43
1:A:493:VAL:HG11	1:A:516:ILE:HG21	2.00	0.43
1:B:551:LEU:HA	1:B:554:VAL:HG13	2.00	0.43
1:B:639:PHE:CE1	1:B:643:LEU:HD11	2.53	0.43
1:A:133:ASP:O	1:A:338:ARG:HD2	2.19	0.43
1:B:721:VAL:HA	1:B:724:LEU:HD21	2.00	0.43
1:B:383:LYS:HA	1:B:621:GLN:OE1	2.19	0.43
1:A:137:PRO:HG3	1:A:152:GLN:NE2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:HG12	1:A:316:ALA:HB1	2.00	0.43
1:B:220:LEU:HD13	1:B:228:VAL:CG1	2.48	0.43
1:B:524:SER:OG	1:B:526:ILE:HG22	2.19	0.43
1:A:470:GLU:HA	1:A:471:GLY:HA2	1.69	0.42
1:A:720:SER:O	1:A:724:LEU:HD21	2.18	0.42
1:B:342:ARG:O	1:B:346:VAL:HG13	2.19	0.42
1:A:364:THR:HG22	1:A:400:GLN:OE1	2.17	0.42
1:B:332:ILE:HG12	1:B:346:VAL:HB	2.00	0.42
1:B:650:ALA:O	1:B:653:SER:HB3	2.19	0.42
1:A:561:HIS:CG	1:A:562:ASN:N	2.87	0.42
1:B:307:TYR:CE1	1:B:352:ILE:HD12	2.54	0.42
1:A:42:SER:N	1:A:43:GLU:OE1	2.53	0.42
1:A:192:ARG:O	1:A:195:GLU:HB2	2.19	0.42
1:B:503:GLN:HG3	1:B:557:ARG:NH1	2.34	0.42
1:B:815:GLU:OE2	1:B:818:LYS:HE3	2.19	0.42
1:A:551:LEU:HA	1:A:554:VAL:HG13	2.02	0.42
1:B:275:PRO:O	1:B:276:ASN:HB2	2.19	0.42
1:B:575:LEU:HD12	1:B:577:PRO:HD2	2.01	0.42
1:A:375:LEU:HD22	1:A:403:ASN:HB3	2.02	0.42
1:A:627:VAL:HG22	2:A:901:FAD:C8A	2.50	0.42
1:B:294:LEU:HD12	1:B:294:LEU:HA	1.84	0.42
1:A:207:LEU:HD23	1:A:207:LEU:HA	1.85	0.42
1:A:215:VAL:HG21	1:A:317:LEU:HD21	2.02	0.42
1:B:344:ARG:HD3	1:B:344:ARG:HA	1.84	0.42
1:A:364:THR:HB	1:A:365:GLY:H	1.61	0.42
1:A:810:LEU:HD23	1:A:810:LEU:HA	1.83	0.42
1:B:441:GLY:HA3	1:B:568:PHE:O	2.20	0.42
1:B:661:LYS:HG2	1:B:710:MET:HE3	2.02	0.41
1:B:231:SER:HA	1:B:232:PRO:HD3	1.90	0.41
1:B:280:LYS:HD2	1:B:283:CYS:SG	2.59	0.41
1:B:416:ARG:NH1	1:B:418:GLY:O	2.53	0.41
1:A:308:LEU:HD12	1:A:308:LEU:HA	1.77	0.41
1:A:489:ALA:O	1:A:493:VAL:HG12	2.20	0.41
1:B:208:PRO:HB3	1:B:303:ASP:OD2	2.20	0.41
1:B:314:ILE:HD13	1:B:353:LEU:HD12	2.02	0.41
1:B:632:LEU:HD13	1:B:651:ILE:HD13	2.02	0.41
1:B:627:VAL:HG22	2:B:901:FAD:C8A	2.50	0.41
1:A:143:THR:HB	1:A:168:ARG:HG3	2.00	0.41
1:A:491:LEU:HD23	1:A:491:LEU:HA	1.92	0.41
1:A:290:GLU:HB3	1:A:292:ASP:OD2	2.20	0.41
1:B:385:VAL:HG21	1:B:401:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:ARG:HH11	1:A:473:ARG:HB3	1.85	0.41
1:B:330:LYS:NZ	3:B:903:CL:CL	2.82	0.41
1:B:366:VAL:HG11	1:B:454:LEU:HG	2.01	0.41
1:B:631:LEU:HD13	1:B:631:LEU:HA	1.79	0.41
1:A:85:LEU:HD12	1:A:85:LEU:HA	1.87	0.41
1:A:512:LYS:HA	1:A:512:LYS:HD2	1.82	0.41
1:A:669:ARG:HD3	1:A:672:ASP:OD2	2.21	0.41
1:B:666:PHE:CZ	1:B:734:MET:HE3	2.56	0.41
1:B:44:PHE:HB2	1:B:47:LEU:CD1	2.51	0.40
1:B:543:LEU:HD12	1:B:543:LEU:HA	1.89	0.40
1:B:719:ALA:C	1:B:721:VAL:H	2.24	0.40
1:A:357:THR:HG23	1:A:363:ASN:HB2	2.01	0.40
1:A:438:ILE:HD13	1:B:43:GLU:HG2	2.04	0.40
1:A:802:PRO:HB2	1:A:803:GLN:HG3	2.03	0.40
1:B:524:SER:O	1:B:526:ILE:N	2.54	0.40
1:B:665:GLN:HE21	1:B:750:THR:HB	1.85	0.40
1:A:135:GLN:NE2	1:A:155:LYS:NZ	2.70	0.40
1:A:370:GLY:HA2	1:A:371:ALA:HA	1.90	0.40
1:B:43:GLU:CD	1:B:43:GLU:H	2.25	0.40
1:B:84:HIS:CE1	1:B:86:SER:O	2.75	0.40
1:A:487:PHE:CE1	1:A:540:LEU:HD12	2.56	0.40
1:B:304:PRO:HB2	1:B:308:LEU:HD22	2.03	0.40
1:B:394:GLY:HA2	1:B:626:THR:HG21	2.03	0.40
1:B:730:LEU:HD12	1:B:752:TYR:CE1	2.56	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	740/784 (94%)	681 (92%)	52 (7%)	7 (1%)	17	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	740/784 (94%)	674 (91%)	57 (8%)	9 (1%)	13	38
All	All	1480/1568 (94%)	1355 (92%)	109 (7%)	16 (1%)	14	40

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	ASN
1	A	369	VAL
1	A	635	GLY
1	B	155	LYS
1	B	525	GLY
1	B	721	VAL
1	A	75	LYS
1	A	155	LYS
1	A	523	GLU
1	B	369	VAL
1	B	676	GLN
1	A	378	LYS
1	B	720	SER
1	B	270	GLN
1	A	686	PRO
1	B	763	ILE

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	640/669 (96%)	549 (86%)	91 (14%)	3	9
1	B	640/669 (96%)	543 (85%)	97 (15%)	3	8
All	All	1280/1338 (96%)	1092 (85%)	188 (15%)	3	9

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	52	LYS
1	A	64	VAL
1	A	76	ASN
1	A	85	LEU
1	A	87	CYS
1	A	93	ASN
1	A	111	THR
1	A	118	THR
1	A	122	LYS
1	A	144	LYS
1	A	146	GLU
1	A	151	ARG
1	A	154	THR
1	A	158	GLN
1	A	172	LYS
1	A	181	THR
1	A	194	LEU
1	A	205	LEU
1	A	206	ILE
1	A	226	ASP
1	A	267	ARG
1	A	270	GLN
1	A	274	GLN
1	A	278	CYS
1	A	284	VAL
1	A	285	ARG
1	A	290	GLU
1	A	291	LEU
1	A	308	LEU
1	A	337	VAL
1	A	341	VAL
1	A	344	ARG
1	A	346	VAL
1	A	352	ILE
1	A	361	LEU
1	A	366	VAL
1	A	373	GLN
1	A	375	LEU
1	A	378	LYS
1	A	379	ASP
1	A	381	HIS
1	A	383	LYS

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Mol	Chain	Res	Type
1	A	399	ARG
1	A	410	VAL
1	A	431	THR
1	A	457	SER
1	A	458	MET
1	A	466	ASP
1	A	467	LEU
1	A	470	GLU
1	A	473	ARG
1	A	481	LYS
1	A	483	MET
1	A	493	VAL
1	A	498	ARG
1	A	503	GLN
1	A	505	GLN
1	A	543	LEU
1	A	574	LEU
1	A	582	ILE
1	A	583	ILE
1	A	592	ILE
1	A	594	LEU
1	A	604	SER
1	A	608	VAL
1	A	619	SER
1	A	625	VAL
1	A	627	VAL
1	A	644	SER
1	A	658	ILE
1	A	680	PHE
1	A	683	HIS
1	A	693	LEU
1	A	704	LYS
1	A	710	MET
1	A	716	GLU
1	A	722	ARG
1	A	724	LEU
1	A	725	ASP
1	A	727	LYS
1	A	729	VAL
1	A	730	LEU
1	A	740	LEU
1	A	742	LYS

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Mol	Chain	Res	Type
1	A	746	VAL
1	A	756	ARG
1	A	772	THR
1	A	775	SER
1	A	789	THR
1	A	806	THR
1	B	40	LEU
1	B	44	PHE
1	B	47	LEU
1	B	64	VAL
1	B	71	GLU
1	B	72	ARG
1	B	85	LEU
1	B	86	SER
1	B	87	CYS
1	B	93	ASN
1	B	111	THR
1	B	122	LYS
1	B	140	VAL
1	B	148	ARG
1	B	151	ARG
1	B	154	THR
1	B	158	GLN
1	B	162	GLN
1	B	185	CYS
1	B	192	ARG
1	B	194	LEU
1	B	205	LEU
1	B	206	ILE
1	B	274	GLN
1	B	280	LYS
1	B	285	ARG
1	B	290	GLU
1	B	291	LEU
1	B	294	LEU
1	B	296	GLU
1	B	302	ARG
1	B	308	LEU
1	B	329	GLN
1	B	337	VAL
1	B	341	VAL
1	B	344	ARG

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Mol	Chain	Res	Type
1	B	346	VAL
1	B	351	ARG
1	B	352	ILE
1	B	366	VAL
1	B	367	LEU
1	B	368	SER
1	B	375	LEU
1	B	378	LYS
1	B	379	ASP
1	B	380	TYR
1	B	399	ARG
1	B	408	VAL
1	B	410	VAL
1	B	431	THR
1	B	449	LEU
1	B	452	GLU
1	B	456	ILE
1	B	467	LEU
1	B	470	GLU
1	B	483	MET
1	B	493	VAL
1	B	496	GLU
1	B	498	ARG
1	B	503	GLN
1	B	518	LYS
1	B	529	SER
1	B	540	LEU
1	B	549	SER
1	B	554	VAL
1	B	574	LEU
1	B	582	ILE
1	B	583	ILE
1	B	592	ILE
1	B	608	VAL
1	B	611	THR
1	B	613	THR
1	B	619	SER
1	B	625	VAL
1	B	627	VAL
1	B	644	SER
1	B	658	ILE
1	B	675	VAL

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Mol	Chain	Res	Type
1	B	680	PHE
1	B	683	HIS
1	B	689	SER
1	B	693	LEU
1	B	710	MET
1	B	716	GLU
1	B	724	LEU
1	B	725	ASP
1	B	727	LYS
1	B	732	GLN
1	B	736	THR
1	B	740	LEU
1	B	742	LYS
1	B	746	VAL
1	B	751	LYS
1	B	756	ARG
1	B	772	THR
1	B	784	GLU
1	B	789	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	347	GLN

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 ⓘ

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	#$|Z| > 2$
2	FAD	A	901	-	54,58,58	1.23	4 (7%)	71,89,89	1.51	11 (15%)
2	FAD	B	901	-	54,58,58	2.11	19 (35%)	71,89,89	1.74	17 (23%)

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
2	FAD	A	901	-	-	3/30/50/50	0/6/6/6
2	FAD	B	901	-	-	9/30/50/50	0/6/6/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	FAD	PA-O3P	-8.07	1.50	1.59
2	B	901	FAD	P-O3P	-4.52	1.54	1.59
2	A	901	FAD	C4X-N5	4.47	1.40	1.30
2	B	901	FAD	PA-O5B	-3.50	1.45	1.59
2	A	901	FAD	C10-N1	3.22	1.39	1.33
2	B	901	FAD	C4A-N3A	-2.87	1.31	1.35
2	A	901	FAD	P-O2P	2.80	1.68	1.55
2	B	901	FAD	O4B-C4B	-2.71	1.39	1.45
2	B	901	FAD	C9A-C5X	-2.68	1.37	1.41
2	B	901	FAD	C5A-N7A	-2.54	1.30	1.39
2	B	901	FAD	C4X-C10	-2.46	1.36	1.44
2	B	901	FAD	O4'-C4'	-2.39	1.38	1.43
2	B	901	FAD	C4'-C3'	-2.38	1.49	1.53
2	B	901	FAD	C4X-N5	2.26	1.35	1.30
2	B	901	FAD	C5X-N5	-2.23	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	FAD	C4X-C4	-2.22	1.36	1.44
2	A	901	FAD	O4B-C1B	2.21	1.43	1.40
2	B	901	FAD	PA-O1A	-2.18	1.43	1.50
2	B	901	FAD	C9A-N10	-2.16	1.37	1.41
2	B	901	FAD	C6-C7	-2.12	1.36	1.39
2	B	901	FAD	P-O1P	-2.12	1.43	1.50
2	B	901	FAD	O5B-C5B	-2.12	1.36	1.44
2	B	901	FAD	C1B-N9A	-2.07	1.44	1.49

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	FAD	C4B-O4B-C1B	-6.86	103.65	109.92
2	A	901	FAD	N3A-C2A-N1A	-5.10	121.75	128.67
2	A	901	FAD	C4B-O4B-C1B	-5.07	105.28	109.92
2	B	901	FAD	N3A-C2A-N1A	-4.93	121.98	128.67
2	B	901	FAD	C4-N3-C2	-4.28	118.03	125.64
2	A	901	FAD	O2A-PA-O3P	-4.04	96.36	107.27
2	A	901	FAD	C10-C4X-N5	-3.08	118.51	124.81
2	B	901	FAD	C5X-C9A-N10	3.08	120.75	117.97
2	A	901	FAD	C4-N3-C2	-2.99	120.33	125.64
2	B	901	FAD	C4X-C10-N10	2.96	120.71	116.48
2	B	901	FAD	O3B-C3B-C2B	-2.80	102.84	111.82
2	B	901	FAD	C4X-C4-N3	2.74	120.23	113.25
2	B	901	FAD	O2A-PA-O3P	-2.74	99.88	107.27
2	B	901	FAD	C4-C4X-C10	2.73	121.61	116.93
2	B	901	FAD	O4-C4-C4X	-2.73	119.33	126.53
2	B	901	FAD	C4X-C10-N1	-2.60	118.22	124.59
2	A	901	FAD	C4X-C4-N3	2.49	119.60	113.25
2	A	901	FAD	C4X-C10-N10	2.42	119.94	116.48
2	A	901	FAD	C4A-C5A-N7A	-2.30	106.91	109.34
2	A	901	FAD	C4-C4X-N5	2.26	121.33	118.21
2	A	901	FAD	C9A-C5X-N5	-2.24	120.08	122.45
2	B	901	FAD	C4'-C3'-C2'	-2.15	109.99	113.57
2	B	901	FAD	C9A-N10-C10	-2.11	117.54	120.75
2	B	901	FAD	C10-C4X-N5	-2.07	120.58	124.81
2	B	901	FAD	C4A-C5A-N7A	-2.07	107.15	109.34
2	A	901	FAD	O3P-PA-O1A	2.04	116.84	110.70
2	B	901	FAD	C6-C5X-C9A	2.03	121.83	119.05
2	B	901	FAD	O4B-C4B-C5B	-2.00	102.93	109.33

There are no chirality outliers.

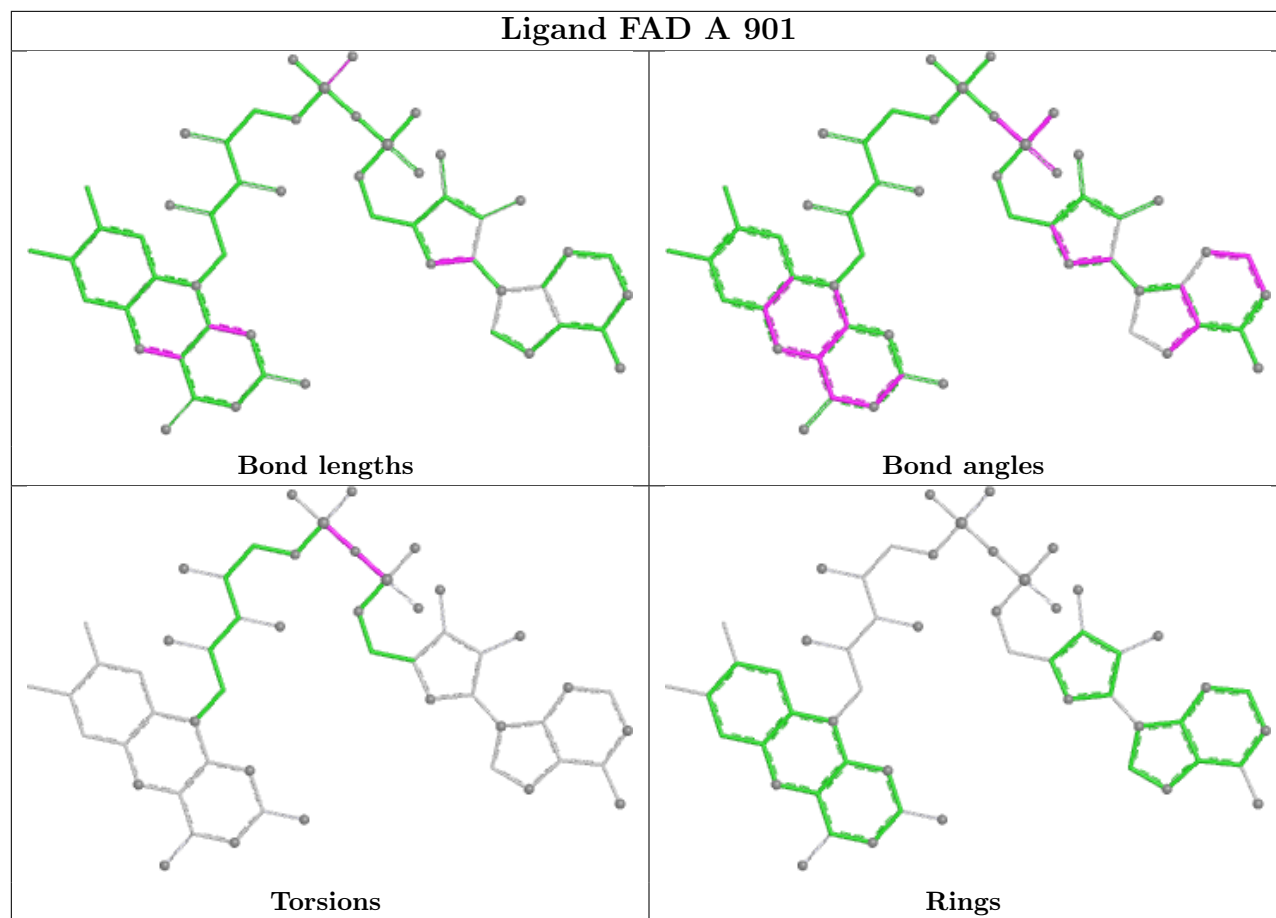All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	FAD	C5B-O5B-PA-O3P
2	B	901	FAD	C3'-C4'-C5'-O5'
2	B	901	FAD	O4'-C4'-C5'-O5'
2	B	901	FAD	C5'-O5'-P-O1P
2	B	901	FAD	C5'-O5'-P-O2P
2	B	901	FAD	C5'-O5'-P-O3P
2	A	901	FAD	PA-O3P-P-O5'
2	B	901	FAD	PA-O3P-P-O5'
2	A	901	FAD	P-O3P-PA-O1A
2	B	901	FAD	O4B-C4B-C5B-O5B
2	B	901	FAD	PA-O3P-P-O2P
2	A	901	FAD	P-O3P-PA-O2A

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	FAD	4	0
2	B	901	FAD	4	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 901

Bond lengths

Bond angles

Torsions

Rings

Ligand FAD B 901

Bond lengths

Bond angles

Torsions

Rings
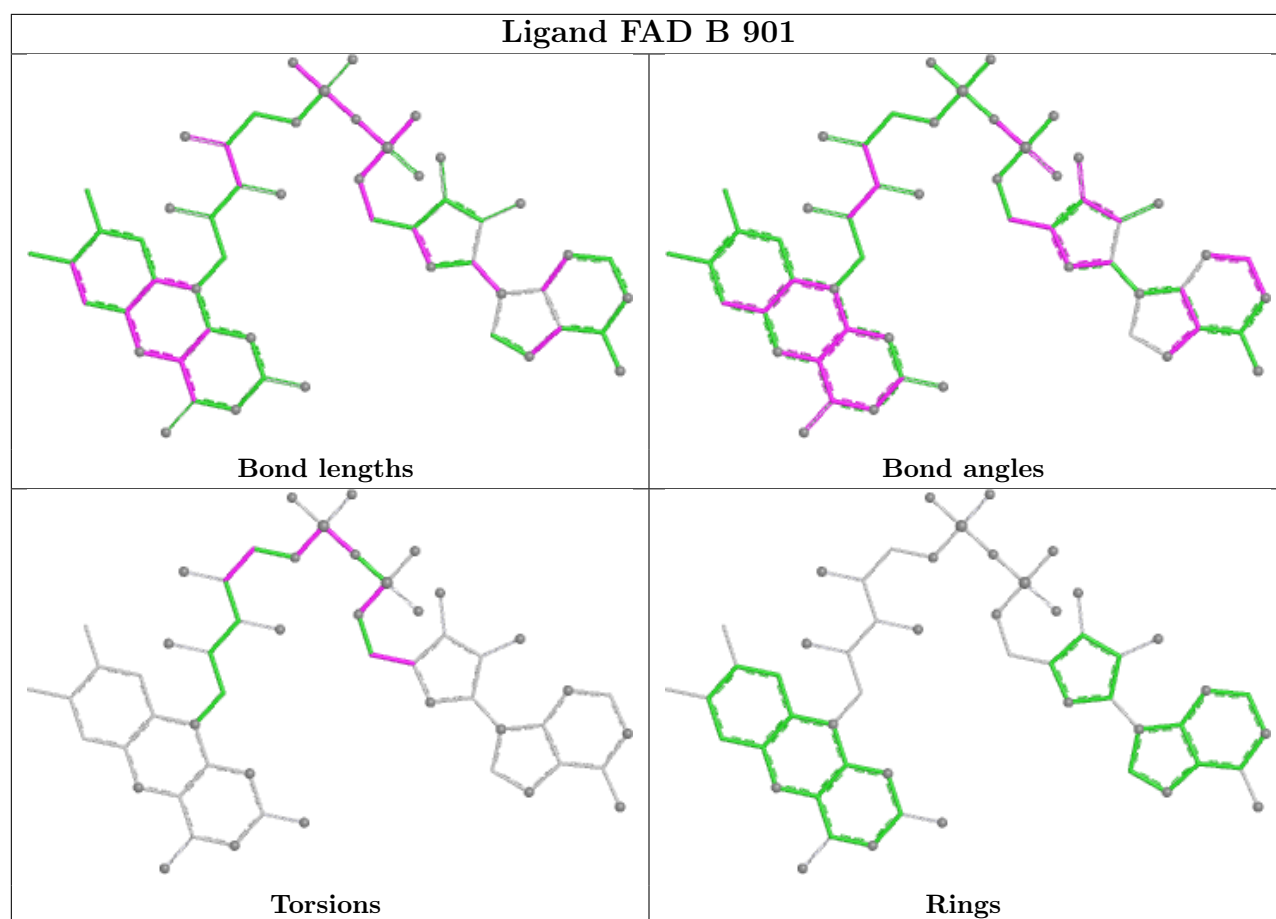
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	746/784 (95%)	0.70	34 (4%)	32	32	54, 79, 116, 161	0
1	B	746/784 (95%)	0.72	44 (5%)	22	20	56, 80, 117, 153	0
All	All	1492/1568 (95%)	0.71	78 (5%)	27	26	54, 80, 117, 161	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380	TYR	6.9
1	A	380	TYR	4.2
1	B	375	LEU	3.8
1	A	87	CYS	3.8
1	A	122	LYS	3.4
1	B	131	MET	3.3
1	A	96	PHE	3.2
1	A	406	ILE	3.2
1	A	375	LEU	3.1
1	A	401	LEU	3.0
1	B	130	PHE	3.0
1	B	381	HIS	3.0
1	A	386	ILE	2.9
1	B	103	HIS	2.9
1	A	729	VAL	2.8
1	B	782	ILE	2.7
1	A	483	MET	2.7
1	A	91	PHE	2.7
1	B	722	ARG	2.7
1	A	664	LEU	2.6
1	A	140	VAL	2.6
1	B	385	VAL	2.6
1	B	87	CYS	2.6
1	B	582	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	385	VAL	2.5
1	B	97	ASP	2.5
1	B	610	VAL	2.5
1	B	101	ARG	2.5
1	B	664	LEU	2.5
1	B	357	THR	2.4
1	B	404	PHE	2.4
1	A	658	ILE	2.4
1	B	468	ILE	2.4
1	A	404	PHE	2.4
1	B	417	ILE	2.4
1	B	99	TYR	2.4
1	A	130	PHE	2.4
1	B	96	PHE	2.4
1	A	583	ILE	2.4
1	A	390	ALA	2.3
1	A	411	LEU	2.3
1	B	681	PHE	2.3
1	B	349	VAL	2.3
1	B	91	PHE	2.3
1	A	383	LYS	2.3
1	B	386	ILE	2.2
1	B	406	ILE	2.2
1	B	694	PHE	2.2
1	A	335	ILE	2.2
1	B	601	ILE	2.2
1	B	483	MET	2.2
1	B	583	ILE	2.2
1	A	468	ILE	2.2
1	A	582	ILE	2.2
1	A	150	TRP	2.2
1	A	131	MET	2.2
1	A	99	TYR	2.2
1	B	140	VAL	2.2
1	A	693	LEU	2.1
1	B	721	VAL	2.1
1	B	639	PHE	2.1
1	A	782	ILE	2.1
1	B	331	CYS	2.1
1	B	401	LEU	2.1
1	B	820	ALA	2.1
1	A	331	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	397	ALA	2.1
1	A	714	ALA	2.1
1	B	138	TYR	2.1
1	B	712	VAL	2.1
1	B	590	LEU	2.1
1	B	85	LEU	2.1
1	A	659	ILE	2.0
1	B	390	ALA	2.0
1	B	340	LEU	2.0
1	B	66	PHE	2.0
1	A	417	ILE	2.0
1	B	202	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	NA	A	904	1/1	0.85	0.19	88,88,88,88	0
3	CL	B	903	1/1	0.86	0.20	98,98,98,98	0
4	NA	B	904	1/1	0.86	0.20	86,86,86,86	0
3	CL	A	903	1/1	0.88	0.19	102,102,102,102	0
3	CL	A	902	1/1	0.90	0.38	104,104,104,104	0
3	CL	B	902	1/1	0.93	0.18	102,102,102,102	0
5	ZN	A	907	1/1	0.94	0.17	106,106,106,106	0
2	FAD	B	901	53/53	0.98	0.25	54,71,79,80	0
2	FAD	A	901	53/53	0.98	0.26	51,68,77,80	0
5	ZN	B	907	1/1	0.98	0.18	101,101,101,101	0
5	ZN	A	905	1/1	0.99	0.26	72,72,72,72	0

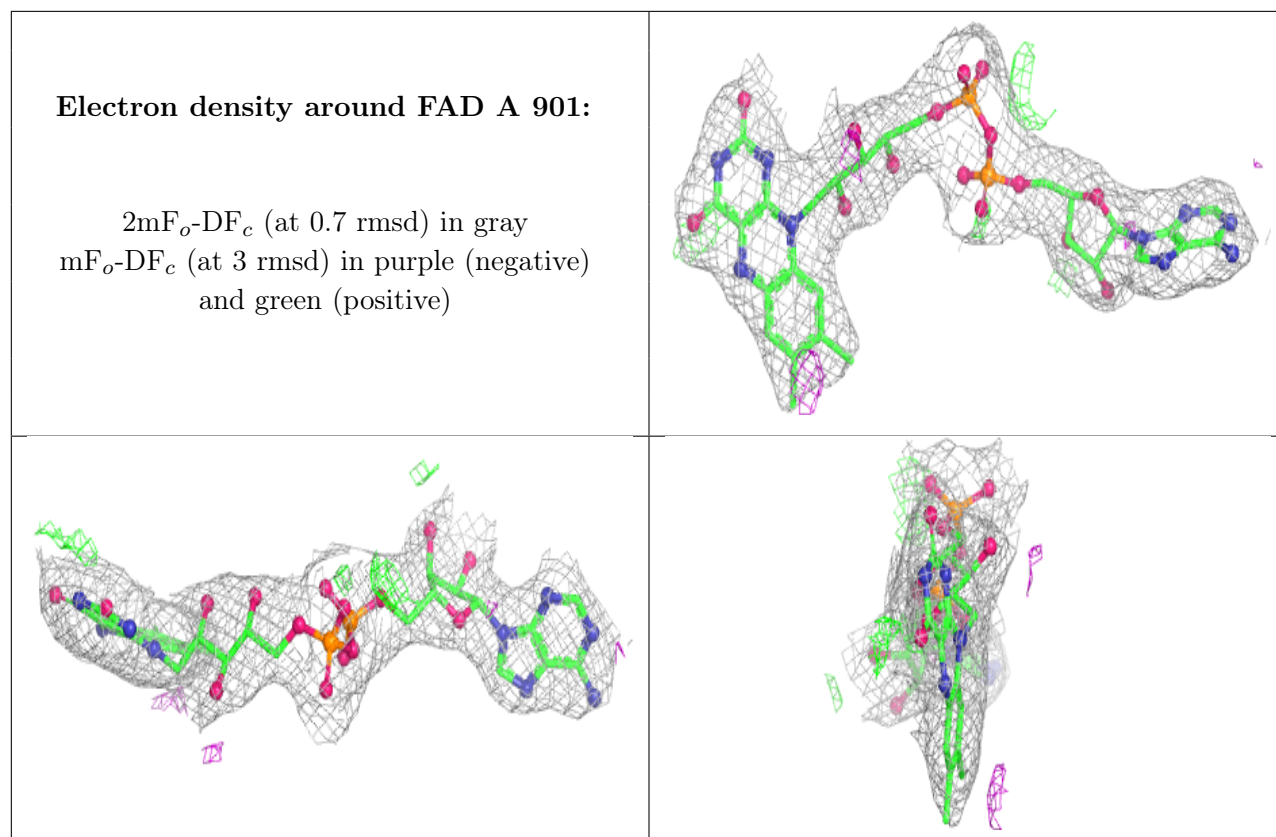*Continued on next page...*

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	B	905	1/1	0.99	0.25	73,73,73,73	0
5	ZN	A	906	1/1	0.99	0.23	96,96,96,96	0
5	ZN	B	906	1/1	1.00	0.20	98,98,98,98	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 901:

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

Electron density around FAD A 901:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.