



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:47 PM UTC

PDB ID : 1DDG / pdb_00001ddg
Title : CRYSTAL STRUCTURE OF SIR-FP60
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Deposited on : 1999-11-10
Resolution : 2.01 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

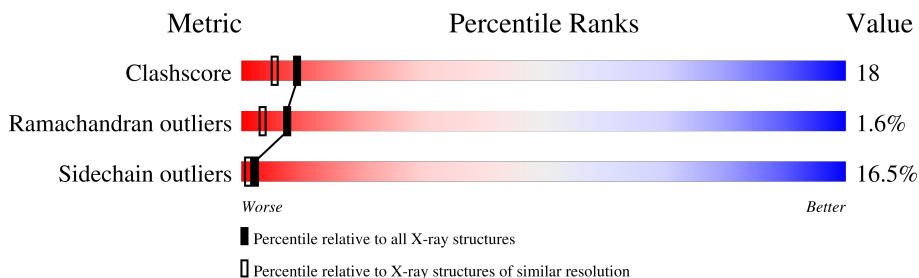
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.01 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	374	
1	B	374	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	600	X	-	-	-
2	FAD	B	601	X	-	-	-

2 Entry composition [i](#)

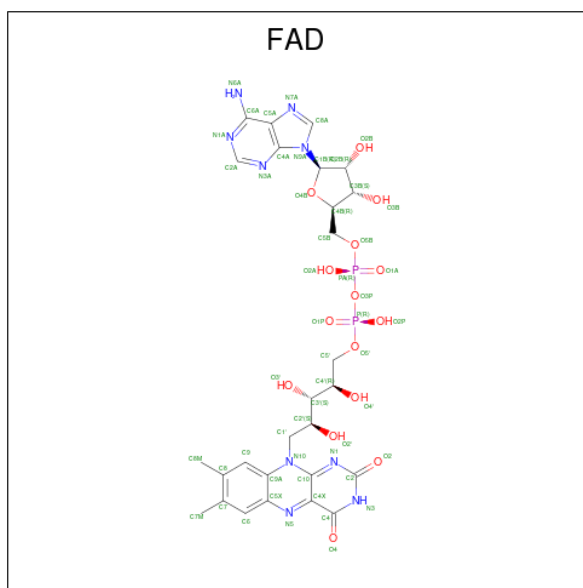
There are 4 unique types of molecules in this entry. The entry contains 6697 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SULFITE REDUCTASE (NADPH) FLAVOPROTEIN ALPHA-COMPONENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	374	Total	C	N	O	S	0	4	0
			3028	1915	532	575	6			
1	B	374	Total	C	N	O	S	0	3	0
			3010	1906	523	575	6			

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



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 SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

- Molecule 4 is water.

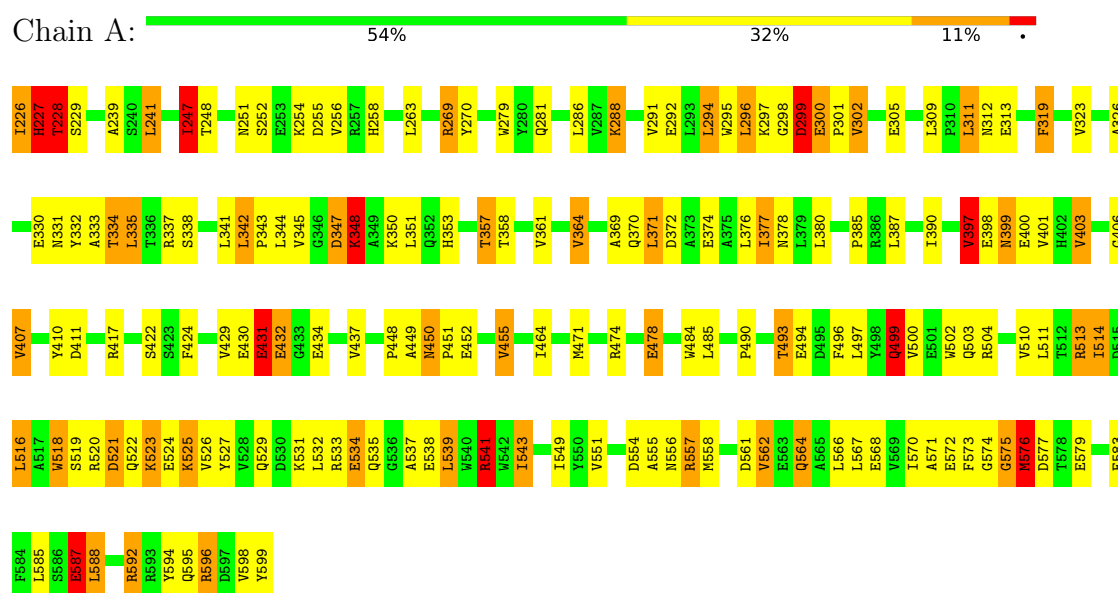
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	271	Total	O	0	0
			271	271		
4	B	277	Total	O	0	0
			277	277		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: SULFITE REDUCTASE (NADPH) FLAVOPROTEIN ALPHA-COMPONENT



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	34.84Å 82.54Å 105.36Å 79.71° 83.05° 89.90°	Depositor
Resolution (Å)	10.00 – 2.01	Depositor
% Data completeness (in resolution range)	91.0 (10.00-2.01)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97, REFMAC	Depositor
R, R_{free}	0.206 , 0.289	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6697	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, SO4

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	0.48	2/3095 (0.1%)	1.57	48/4206 (1.1%)
1	B	0.57	1/3077 (0.0%)	1.47	28/4185 (0.7%)
All	All	0.53	3/6172 (0.0%)	1.52	76/8391 (0.9%)

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
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	599	TYR	C-OXT	19.23	1.62	1.23
1	A	599	TYR	C-OXT	5.93	1.35	1.23
1	A	398	GLU	N-CA	5.17	1.52	1.46

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	397	VAL	CA-C-N	-17.09	101.14	121.64
1	B	397	VAL	C-N-CA	-17.09	101.14	121.64
1	A	398	GLU	CA-C-N	13.78	147.85	121.54
1	A	398	GLU	C-N-CA	13.78	147.85	121.54
1	B	431	GLU	CA-C-N	-12.34	104.78	123.17
1	B	431	GLU	C-N-CA	-12.34	104.78	123.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	VAL	O-C-N	-12.02	106.72	122.47
1	A	372	ASP	CA-CB-CG	11.86	124.46	112.60
1	A	397	VAL	CA-C-N	-11.10	100.33	121.54
1	A	397	VAL	C-N-CA	-11.10	100.33	121.54
1	B	397	VAL	O-C-N	-10.81	108.31	122.47
1	A	399	ASN	CA-CB-CG	-9.77	102.83	112.60
1	A	541	ARG	CD-NE-CZ	9.50	137.70	124.40
1	A	269	ARG	CD-NE-CZ	9.29	137.41	124.40
1	B	401	VAL	CB-CA-C	-8.21	98.34	110.33
1	A	406	GLY	CA-C-N	-7.87	113.01	122.93
1	A	406	GLY	C-N-CA	-7.87	113.01	122.93
1	B	249	GLY	CA-C-N	7.87	136.58	121.54
1	B	249	GLY	C-N-CA	7.87	136.58	121.54
1	B	401	VAL	N-CA-CB	7.60	122.61	111.52
1	A	347	ASP	CA-C-N	7.41	135.69	121.54
1	A	347	ASP	C-N-CA	7.41	135.69	121.54
1	A	432	GLU	O-C-N	7.15	129.53	121.88
1	A	247	ILE	CB-CA-C	7.01	118.64	110.93
1	A	432	GLU	CA-C-N	6.98	128.05	120.44
1	A	432	GLU	C-N-CA	6.98	128.05	120.44
1	A	543	ILE	CB-CA-C	-6.96	102.97	111.88
1	B	589	ARG	CD-NE-CZ	6.93	134.10	124.40
1	A	575	GLY	CA-C-N	6.89	134.71	121.54
1	A	575	GLY	C-N-CA	6.89	134.71	121.54
1	A	255	ASP	CA-CB-CG	6.86	119.46	112.60
1	A	403	VAL	CB-CA-C	6.63	121.50	110.30
1	B	383	LEU	CA-CB-CG	6.38	138.64	116.30
1	A	410	TYR	CA-C-N	-6.36	112.13	122.81
1	A	410	TYR	C-N-CA	-6.36	112.13	122.81
1	A	403	VAL	N-CA-CB	-6.05	101.16	112.36
1	B	299	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	301	PRO	CA-C-O	6.00	128.51	121.31
1	B	555	ALA	CA-C-N	5.99	129.12	120.79
1	B	555	ALA	C-N-CA	5.99	129.12	120.79
1	A	410	TYR	O-C-N	-5.87	117.10	123.26
1	A	449	ALA	N-CA-C	-5.77	102.87	110.43
1	B	496	PHE	CA-CB-CG	5.77	119.57	113.80
1	A	241	LEU	O-C-N	-5.74	114.88	122.57
1	A	499	GLN	CA-CB-CG	5.72	125.54	114.10
1	B	431	GLU	CA-CB-CG	-5.67	102.76	114.10
1	A	319	PHE	CA-CB-CG	-5.63	108.17	113.80
1	B	432	GLU	CA-C-N	5.62	128.37	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	432	GLU	C-N-CA	5.62	128.37	121.06
1	B	384	THR	CB-CA-C	5.58	117.57	109.20
1	A	497	LEU	CA-C-N	5.56	130.46	122.40
1	A	497	LEU	C-N-CA	5.56	130.46	122.40
1	A	227	HIS	CA-C-N	5.47	131.99	121.54
1	A	227	HIS	C-N-CA	5.47	131.99	121.54
1	B	437	VAL	N-CA-CB	-5.46	101.70	111.92
1	A	247	ILE	N-CA-CB	-5.44	105.29	112.36
1	A	247	ILE	CA-C-O	5.41	124.08	119.38
1	A	431	GLU	CA-C-O	5.37	127.46	120.11
1	A	449	ALA	CA-C-O	-5.33	116.01	121.87
1	B	467	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	296	LEU	CA-C-O	-5.32	115.13	121.56
1	B	518	TRP	CA-C-N	5.31	127.71	120.54
1	B	518	TRP	C-N-CA	5.31	127.71	120.54
1	A	587	GLU	CA-C-N	5.30	127.38	120.28
1	A	587	GLU	C-N-CA	5.30	127.38	120.28
1	A	499	GLN	CA-C-O	-5.18	115.06	120.55
1	A	417	ARG	CD-NE-CZ	5.15	131.61	124.40
1	B	441	HIS	CA-C-N	-5.12	115.35	123.23
1	B	441	HIS	C-N-CA	-5.12	115.35	123.23
1	B	388	TYR	CA-CB-CG	-5.11	104.70	113.90
1	A	525	LYS	CA-C-N	-5.11	116.51	123.10
1	A	525	LYS	C-N-CA	-5.11	116.51	123.10
1	A	518	TRP	CA-C-N	5.05	131.19	121.54
1	A	518	TRP	C-N-CA	5.05	131.19	121.54
1	B	252	SER	CA-C-N	-5.05	113.25	122.38
1	B	252	SER	C-N-CA	-5.05	113.25	122.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	448	PRO	Peptide
1	B	430	GLU	Peptide

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	3028	0	2958	128	0
1	B	3010	0	2935	92	0
2	A	53	0	31	1	0
2	B	53	0	30	0	0
3	B	5	0	0	0	0
4	A	271	0	0	21	0
4	B	277	0	0	17	0
All	All	6697	0	5954	220	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 18.

All (220) 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:571:ALA:HB1	1:A:576:MET:HG2	1.55	0.87
1:A:302:VAL:HG11	1:A:377:ILE:HD13	1.62	0.81
1:A:347:ASP:HB3	1:A:350:LYS:HD3	1.63	0.79
1:A:361:VAL:HB	4:A:764:HOH:O	1.83	0.78
1:A:344:LEU:HD22	1:A:350:LYS:HB3	1.66	0.77
1:A:490:PRO:HA	1:A:519:SER:HB3	1.67	0.77
1:B:453:THR:HG21	4:B:649:HOH:O	1.84	0.77
1:B:357:THR:HG21	4:B:821:HOH:O	1.84	0.77
1:A:592:ARG:HH11	1:A:592:ARG:HB2	1.49	0.75
1:A:471:MET:HE2	1:A:511:LEU:HD13	1.66	0.75
1:B:520:ARG:HE	1:B:523:LYS:NZ	1.86	0.74
1:A:566:LEU:O	1:A:570:ILE:HD12	1.87	0.74
1:B:308:THR:HB	4:B:800:HOH:O	1.86	0.74
1:A:344:LEU:O	1:A:347:ASP:HB2	1.89	0.72
1:A:338:SER:OG	1:A:341:LEU:HB2	1.89	0.72
1:B:374:GLU:OE2	4:B:706:HOH:O	2.08	0.72
1:A:558:MET:HE2	1:A:562:VAL:HG21	1.71	0.71
1:A:299:ASP:O	1:A:311:LEU:HB2	1.90	0.71
1:B:227:HIS:O	1:B:228:THR:O	2.09	0.71
1:B:357:THR:HG22	1:B:358:THR:OG1	1.90	0.70
1:A:226:ILE:O	1:A:227:HIS:HB2	1.90	0.70
1:A:543:ILE:HD12	1:A:549:ILE:HD11	1.74	0.70
1:A:500:VAL:O	1:A:504:ARG:HG3	1.92	0.69
1:A:500:VAL:HG23	4:A:703:HOH:O	1.92	0.69
1:B:589:ARG:HD2	4:B:864:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LEU:HB3	1:A:514:ILE:HG23	1.76	0.68
1:A:592:ARG:HB2	1:A:592:ARG:NH1	2.09	0.67
1:A:551:VAL:HB	1:A:596:ARG:HG2	1.75	0.67
1:A:263:LEU:HD11	1:A:401[B]:VAL:HG22	1.76	0.67
1:B:404:THR:HA	4:B:866:HOH:O	1.94	0.66
1:B:504:ARG:HA	1:B:507:LYS:HE2	1.77	0.66
1:A:514:ILE:HG21	4:A:865:HOH:O	1.96	0.66
1:B:290:LEU:HD22	1:B:294:LEU:HD22	1.76	0.66
1:A:227:HIS:O	1:A:228:THR:HB	1.96	0.66
1:B:226:ILE:HG23	1:B:227:HIS:N	2.11	0.66
1:B:520:ARG:HE	1:B:523:LYS:HZ1	1.43	0.66
1:A:331:ASN:O	1:A:335:LEU:HB2	1.96	0.66
1:B:286:LEU:HD22	1:B:361[A]:VAL:HG21	1.78	0.65
1:A:490:PRO:HB3	1:A:520:ARG:HD2	1.77	0.65
1:A:286:LEU:HD11	1:A:361:VAL:HG21	1.78	0.64
1:A:312:ASN:HB3	4:A:642:HOH:O	1.98	0.63
1:B:404:THR:HG23	4:B:866:HOH:O	1.99	0.63
1:A:270:TYR:CE2	1:A:401[B]:VAL:HG13	2.34	0.62
1:A:353:HIS:O	1:A:357:THR:HB	1.99	0.62
1:A:228:THR:HA	4:A:786:HOH:O	2.00	0.62
1:A:357:THR:HG22	1:A:358:THR:OG1	1.99	0.61
1:B:551:VAL:HB	1:B:596:ARG:HG2	1.83	0.61
1:A:281:GLN:HG2	1:A:424:PHE:CE1	2.36	0.61
1:B:523:LYS:HA	4:B:852:HOH:O	2.01	0.61
1:B:297:LYS:HG3	1:B:299:ASP:OD1	2.02	0.60
1:B:411:ASP:HB2	4:B:868:HOH:O	2.01	0.60
1:A:397:VAL:HG13	1:A:400:GLU:HB2	1.84	0.60
1:A:543:ILE:CD1	1:A:549:ILE:HD11	2.32	0.59
1:B:531:LYS:HA	1:B:531:LYS:HZ2	1.67	0.58
1:B:254:LYS:NZ	1:B:489:ASN:HD21	2.02	0.57
1:A:557[A]:ARG:HG3	1:A:558:MET:N	2.20	0.57
1:B:268:LEU:HD21	1:B:439:ILE:HD11	1.87	0.57
1:A:576:MET:O	1:A:577:ASP:HB3	2.06	0.56
1:A:571:ALA:HA	1:A:576:MET:HA	1.87	0.56
1:B:258:HIS:HA	4:B:866:HOH:O	2.06	0.55
1:B:450:ASN:O	1:B:453:THR:HG23	2.06	0.55
1:A:523:LYS:HD2	1:A:523:LYS:H	1.71	0.55
1:A:573:PHE:HB3	4:A:826:HOH:O	2.07	0.55
1:B:353:HIS:O	1:B:357:THR:HB	2.06	0.54
1:B:296:LEU:HD13	1:B:311:LEU:HD11	1.89	0.54
1:B:524:GLU:O	1:B:524:GLU:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LYS:HD2	4:A:802:HOH:O	2.08	0.54
1:B:522:GLN:O	1:B:523:LYS:HB2	2.06	0.54
1:A:568:GLU:O	1:A:572:GLU:HB2	2.08	0.53
1:B:482:LYS:H	1:B:482:LYS:CE	2.20	0.53
1:B:227:HIS:CE1	1:B:228:THR:HG22	2.43	0.53
1:A:485:LEU:O	1:A:514:ILE:HA	2.08	0.53
1:A:513:ARG:CZ	1:A:538:GLU:HG2	2.39	0.53
1:B:306:GLY:HA2	4:B:763:HOH:O	2.09	0.53
1:A:537:ALA:HB2	1:A:573:PHE:CE2	2.42	0.53
1:A:516:LEU:HG	1:A:518:TRP:CZ2	2.44	0.52
1:A:490:PRO:HA	1:A:519:SER:CB	2.39	0.52
1:A:522:GLN:NE2	1:A:526:VAL:HG23	2.24	0.52
1:A:558:MET:HE2	1:A:562:VAL:CG2	2.38	0.52
1:B:227:HIS:HE1	4:B:745:HOH:O	1.92	0.52
1:B:531:LYS:HZ2	1:B:531:LYS:CA	2.23	0.52
1:B:532:LEU:HD22	1:B:539:LEU:HD21	1.92	0.51
1:A:374:GLU:HG2	4:A:704:HOH:O	2.11	0.51
1:B:525:LYS:HB2	1:B:527:TYR:CE2	2.45	0.51
1:A:351:LEU:HG	4:A:664:HOH:O	2.10	0.51
1:A:534:GLU:OE1	1:A:535:GLN:HG2	2.11	0.51
1:A:493:THR:HB	4:A:753:HOH:O	2.10	0.51
1:A:555:ALA:HB2	1:A:598:VAL:HB	1.94	0.50
1:B:460:PRO:HG2	1:B:558:MET:HG3	1.92	0.50
1:A:298:GLY:O	1:A:312:ASN:OD1	2.30	0.50
1:A:343:PRO:O	1:A:347:ASP:OD2	2.29	0.50
1:A:294:LEU:O	1:A:295:TRP:HB2	2.10	0.49
1:A:575:GLY:O	1:A:576:MET:O	2.29	0.49
1:B:374:GLU:OE1	1:B:374:GLU:CA	2.60	0.49
1:A:286:LEU:CD1	1:A:361:VAL:HG21	2.43	0.49
1:B:540:TRP:CE2	1:B:574:GLY:HA2	2.47	0.49
1:A:279:TRP:CH2	1:A:385:PRO:HD3	2.47	0.49
1:A:514:ILE:HG12	4:A:865:HOH:O	2.12	0.49
1:A:592:ARG:HD2	4:A:628:HOH:O	2.12	0.49
1:A:288:LYS:NZ	1:A:292:GLU:OE1	2.46	0.49
1:A:333:ALA:HA	1:A:338:SER:OG	2.12	0.49
1:B:374:GLU:OE1	1:B:374:GLU:HA	2.12	0.48
1:B:370:GLN:H	1:B:370:GLN:CD	2.21	0.48
1:A:587:GLU:HG3	1:A:588:LEU:N	2.27	0.48
1:B:268:LEU:HD21	1:B:439:ILE:CG1	2.44	0.48
1:B:359:PRO:HG3	1:B:410:TYR:OH	2.14	0.48
1:A:431:GLU:HA	1:A:431:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLU:N	4:A:784:HOH:O	2.47	0.47
1:B:338:SER:OG	1:B:341:LEU:HB2	2.14	0.47
1:B:493:THR:HG23	1:B:494:GLU:OE2	2.15	0.47
1:A:309:LEU:HD13	1:A:313:GLU:HG2	1.96	0.47
1:B:250:ARG:HG2	4:B:861:HOH:O	2.14	0.47
1:A:296:LEU:HD13	1:A:311:LEU:HD11	1.95	0.47
1:B:227:HIS:ND1	1:B:228:THR:HG22	2.29	0.47
1:A:241:LEU:HD23	1:A:429:VAL:HB	1.96	0.47
1:A:302:VAL:CG1	1:A:377:ILE:HD13	2.41	0.47
1:A:335:LEU:HD23	1:A:371:LEU:HD11	1.97	0.47
1:A:371:LEU:HD12	1:A:371:LEU:HA	1.75	0.47
1:A:485:LEU:O	1:A:514:ILE:HG22	2.15	0.47
1:B:384:THR:HG22	1:B:386:ARG:NH1	2.30	0.46
1:A:397:VAL:CG1	1:A:400:GLU:HB2	2.45	0.46
1:A:574:GLY:N	4:A:826:HOH:O	2.48	0.46
1:A:247:ILE:HD13	1:A:258:HIS:HB3	1.98	0.46
1:B:286:LEU:CD2	1:B:361[A]:VAL:HG21	2.45	0.46
1:A:347:ASP:HB3	1:A:350:LYS:CD	2.40	0.46
1:B:252:SER:HB2	1:B:494:GLU:HB3	1.98	0.46
1:B:290:LEU:HG	1:B:361[A]:VAL:HG22	1.98	0.46
1:A:338:SER:O	1:A:342:LEU:HD22	2.15	0.46
1:A:228:THR:HG22	4:A:829:HOH:O	2.16	0.46
1:A:270:TYR:CE1	1:A:390:ILE:HG21	2.51	0.46
1:A:450:ASN:HA	1:A:451:PRO:HD2	1.65	0.46
1:A:579:GLU:O	1:A:583:GLU:HG3	2.14	0.46
1:A:592:ARG:HG3	1:A:595:GLN:NE2	2.30	0.46
1:B:591:GLU:O	1:B:592:ARG:HB2	2.16	0.46
1:B:471:MET:HE3	1:B:510:VAL:HG22	1.98	0.46
1:A:533:ARG:NH2	4:A:788:HOH:O	2.50	0.45
1:B:507:LYS:HE2	1:B:507:LYS:HB3	1.60	0.45
1:A:564:GLN:NE2	1:A:568:GLU:OE2	2.50	0.45
1:B:450:ASN:HB3	1:B:453:THR:CG2	2.47	0.45
1:A:319:PHE:CE2	1:A:377:ILE:HG12	2.51	0.45
1:A:407:VAL:HA	1:A:422:SER:HB2	1.99	0.45
1:B:290:LEU:HD22	1:B:294:LEU:CD2	2.46	0.45
1:A:471:MET:HG3	1:A:502:TRP:HZ3	1.81	0.45
1:A:592:ARG:NH1	4:A:619:HOH:O	2.50	0.45
1:A:342:LEU:HD12	1:A:345:VAL:HG21	1.98	0.45
1:B:538:GLU:OE2	1:B:541:ARG:NH1	2.50	0.45
1:A:269:ARG:NH1	4:A:794:HOH:O	2.49	0.44
1:A:348:LYS:N	4:A:664:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ALA:O	1:A:541:ARG:NH1	2.50	0.44
1:A:525:LYS:HB3	1:A:527:TYR:CE2	2.52	0.44
1:A:455:VAL:HG13	1:A:474:ARG:NH1	2.32	0.44
1:B:228:THR:HG23	1:B:230:PRO:HD3	1.99	0.44
1:B:482:LYS:HE2	1:B:482:LYS:HB2	1.65	0.44
1:B:523:LYS:HA	1:B:523:LYS:HD2	1.57	0.44
1:A:288:LYS:HE3	4:A:685:HOH:O	2.18	0.44
1:B:450:ASN:HB3	1:B:453:THR:HG22	2.00	0.44
1:A:478:GLU:OE1	1:A:478:GLU:HA	2.10	0.44
1:B:270:TYR:CE2	1:B:390:ILE:HG21	2.52	0.44
1:B:297:LYS:HE3	1:B:299:ASP:OD1	2.18	0.44
1:A:323:VAL:HG22	2:A:600:FAD:H51A	2.00	0.44
1:B:407[B]:VAL:HA	1:B:422:SER:HB2	1.99	0.44
1:B:595:GLN:NE2	4:B:676:HOH:O	2.50	0.44
1:A:263:LEU:HD21	1:A:401[B]:VAL:CG2	2.48	0.43
1:B:579:GLU:O	1:B:582:ASP:HB2	2.18	0.43
1:A:228:THR:HG23	1:A:229:SER:N	2.33	0.43
1:A:302:VAL:HG11	1:A:377:ILE:CD1	2.42	0.43
1:A:554:ASP:O	1:A:558:MET:HB3	2.19	0.43
1:B:543:ILE:CD1	1:B:549:ILE:HD11	2.48	0.43
1:A:572:GLU:HB3	1:A:573:PHE:CD1	2.53	0.43
1:B:255:ASP:HB3	1:B:407[B]:VAL:HG12	2.00	0.43
1:B:376:LEU:O	1:B:379:LEU:HB3	2.18	0.43
1:A:239:ALA:O	1:A:434:GLU:HA	2.19	0.43
1:A:252:SER:HB2	1:A:494:GLU:HB3	2.00	0.43
1:B:490:PRO:HA	1:B:519:SER:HB2	1.99	0.43
1:B:531:LYS:HE3	4:B:878:HOH:O	2.18	0.43
1:A:496:PHE:CG	1:A:499:GLN:HB3	2.54	0.43
1:A:499:GLN:O	1:A:503:GLN:HG3	2.19	0.43
1:B:407[B]:VAL:O	1:B:407[B]:VAL:HG13	2.19	0.43
1:A:484:TRP:CD1	1:A:513:ARG:HB2	2.54	0.43
1:A:288:LYS:NZ	4:A:841:HOH:O	2.52	0.42
1:B:279:TRP:CH2	1:B:385:PRO:HD3	2.54	0.42
1:A:523:LYS:H	1:A:523:LYS:CD	2.31	0.42
1:A:532:LEU:HD23	1:A:539:LEU:HD21	2.00	0.42
1:A:541:ARG:HH11	1:A:541:ARG:HB2	1.84	0.42
1:A:241:LEU:O	1:A:432:GLU:N	2.48	0.42
1:A:585:LEU:HD11	1:A:594:TYR:CD2	2.55	0.42
1:B:431:GLU:HA	4:B:623:HOH:O	2.18	0.42
1:B:440:GLU:HG2	4:B:847:HOH:O	2.18	0.42
1:B:479:ALA:HA	1:B:480:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LYS:HZ3	1:A:348:LYS:HG3	1.64	0.42
1:B:397:VAL:HG11	1:B:402:HIS:CE1	2.54	0.42
1:B:555:ALA:O	1:B:559:ALA:HB3	2.19	0.42
1:B:520:ARG:HE	1:B:523:LYS:HZ3	1.64	0.42
1:B:564:GLN:O	1:B:568:GLU:HG3	2.20	0.42
1:B:319:PHE:CE2	1:B:377:ILE:HG13	2.55	0.42
1:A:464:ILE:HD11	1:A:502:TRP:CZ2	2.54	0.41
1:B:250:ARG:H	1:B:250:ARG:HG3	1.53	0.41
1:B:270:TYR:CE1	1:B:401:VAL:HG13	2.55	0.41
1:A:299:ASP:O	1:A:300:GLU:HB2	2.20	0.41
1:B:268:LEU:HD21	1:B:439:ILE:CD1	2.49	0.41
1:A:326:ALA:HB1	1:A:351:LEU:HB3	2.01	0.41
1:A:332:TYR:OH	1:A:364:VAL:HB	2.20	0.41
1:B:228:THR:HG23	1:B:229:SER:N	2.35	0.41
1:B:357:THR:HG22	1:B:358:THR:HG1	1.83	0.41
1:B:556:ASN:ND2	1:B:556:ASN:H	2.18	0.41
1:A:518:TRP:HB2	1:A:521:ASP:HB2	2.03	0.41
1:A:248:THR:HG23	1:A:256:VAL:HB	2.02	0.41
1:A:294:LEU:HD12	1:A:369:ALA:O	2.21	0.41
1:A:431:GLU:O	1:A:432:GLU:HB2	2.21	0.41
1:B:246:LYS:HA	1:B:257:ARG:HD3	2.02	0.41
1:B:311:LEU:HD22	1:B:315:LEU:HD22	2.02	0.41
1:B:471:MET:CE	1:B:510:VAL:HG22	2.51	0.41
1:A:374:GLU:O	1:A:378:ASN:HB2	2.21	0.41
1:B:485:LEU:O	1:B:514:ILE:HA	2.20	0.41
1:A:534:GLU:O	1:A:534:GLU:HG2	2.21	0.40
1:A:279:TRP:CZ3	1:A:385:PRO:HD3	2.56	0.40
1:A:529:GLN:HA	1:A:532:LEU:HD12	2.03	0.40
1:B:482:LYS:H	1:B:482:LYS:HE2	1.86	0.40
1:B:504:ARG:HG2	1:B:507:LYS:HE3	2.04	0.40
1:A:330:GLU:O	1:A:334:THR:HB	2.22	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	376/374 (100%)	353 (94%)	14 (4%)	9 (2%)	4	2
1	B	375/374 (100%)	358 (96%)	14 (4%)	3 (1%)	16	11
All	All	751/748 (100%)	711 (95%)	28 (4%)	12 (2%)	7	3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	HIS
1	A	228	THR
1	A	299	ASP
1	A	399	ASN
1	A	430	GLU
1	A	576	MET
1	B	228	THR
1	B	250	ARG
1	A	300	GLU
1	A	348	LYS
1	B	522	GLN
1	A	450	ASN

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	320/316 (101%)	261 (82%)	59 (18%)	1	1
1	B	319/316 (101%)	272 (85%)	47 (15%)	3	2
All	All	639/632 (101%)	533 (83%)	106 (17%)	2	1

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226	ILE

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Mol	Chain	Res	Type
1	A	228	THR
1	A	247	ILE
1	A	251	ASN
1	A	288	LYS
1	A	291	VAL
1	A	294	LEU
1	A	297	LYS
1	A	299	ASP
1	A	302	VAL
1	A	305	GLU
1	A	311	LEU
1	A	334	THR
1	A	335	LEU
1	A	337	ARG
1	A	342	LEU
1	A	348	LYS
1	A	357	THR
1	A	364	VAL
1	A	370	GLN
1	A	371	LEU
1	A	376	LEU
1	A	377	ILE
1	A	380	LEU
1	A	387	LEU
1	A	397	VAL
1	A	403	VAL
1	A	407	VAL
1	A	411	ASP
1	A	431	GLU
1	A	437	VAL
1	A	452	GLU
1	A	455	VAL
1	A	478	GLU
1	A	493	THR
1	A	499	GLN
1	A	510	VAL
1	A	513	ARG
1	A	514	ILE
1	A	516	LEU
1	A	521	ASP
1	A	523	LYS
1	A	524	GLU

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Mol	Chain	Res	Type
1	A	531	LYS
1	A	534	GLU
1	A	539	LEU
1	A	541	ARG
1	A	556	ASN
1	A	557[A]	ARG
1	A	557[B]	ARG
1	A	561	ASP
1	A	562	VAL
1	A	564	GLN
1	A	567	LEU
1	A	576	MET
1	A	587	GLU
1	A	588	LEU
1	A	592	ARG
1	A	596	ARG
1	B	226	ILE
1	B	227	HIS
1	B	248	THR
1	B	250	ARG
1	B	253	GLU
1	B	286	LEU
1	B	290	LEU
1	B	292	GLU
1	B	294	LEU
1	B	311	LEU
1	B	315	LEU
1	B	320	GLU
1	B	327[A]	ASN
1	B	327[B]	ASN
1	B	341	LEU
1	B	342	LEU
1	B	348	LYS
1	B	357	THR
1	B	364	VAL
1	B	372	ASP
1	B	374	GLU
1	B	376	LEU
1	B	377	ILE
1	B	380	LEU
1	B	383	LEU
1	B	384	THR

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Mol	Chain	Res	Type
1	B	398	GLU
1	B	401	VAL
1	B	437	VAL
1	B	452	GLU
1	B	453	THR
1	B	482	LYS
1	B	493	THR
1	B	507	LYS
1	B	510	VAL
1	B	519	SER
1	B	523	LYS
1	B	524	GLU
1	B	525	LYS
1	B	531	LYS
1	B	539	LEU
1	B	545	ASP
1	B	557	ARG
1	B	560	LYS
1	B	564	GLN
1	B	583	GLU
1	B	588	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	316	GLN
1	A	441	HIS
1	A	499	GLN
1	A	503	GLN
1	A	556	ASN
1	A	564	GLN
1	B	227	HIS
1	B	489	ASN
1	B	499	GLN
1	B	503	GLN
1	B	556	ASN

5.3.3 RNA ⓘ

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](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FAD	B	601	-	58,58,58	2.74	18 (31%)	85,89,89	2.54	29 (34%)
3	SO4	B	602	-	4,4,4	0.71	0	6,6,6	0.18	0
2	FAD	A	600	-	58,58,58	2.87	19 (32%)	85,89,89	2.68	27 (31%)

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	B	601	-	3/3/9/9	5/34/50/50	0/6/6/6
2	FAD	A	600	-	2/2/9/9	2/34/50/50	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	P-O3P	-15.40	1.42	1.59
2	B	601	FAD	P-O3P	-15.06	1.43	1.59
2	A	600	FAD	C1'-C2'	4.77	1.59	1.52
2	B	601	FAD	C1'-C2'	4.52	1.58	1.52
2	B	601	FAD	PA-O2A	-4.31	1.35	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	PA-O2A	-4.15	1.36	1.55
2	A	600	FAD	O4'-C4'	4.05	1.51	1.43
2	A	600	FAD	C5'-C4'	4.00	1.57	1.51
2	A	600	FAD	C4A-N9A	3.71	1.45	1.37
2	B	601	FAD	O4'-C4'	3.56	1.50	1.43
2	B	601	FAD	C4A-N9A	3.51	1.45	1.37
2	A	600	FAD	P-O1P	-3.50	1.38	1.50
2	A	600	FAD	O4B-C1B	3.47	1.50	1.42
2	B	601	FAD	C5'-C4'	3.41	1.56	1.51
2	A	600	FAD	C5A-N7A	-3.38	1.32	1.39
2	B	601	FAD	C5A-N7A	-3.38	1.32	1.39
2	B	601	FAD	P-O1P	-3.24	1.39	1.50
2	A	600	FAD	O2-C2	-3.10	1.18	1.24
2	A	600	FAD	P-O5'	-2.97	1.47	1.59
2	B	601	FAD	C1'-N10	-2.93	1.40	1.47
2	A	600	FAD	C5X-N5	-2.93	1.34	1.39
2	B	601	FAD	P-O5'	-2.90	1.48	1.59
2	A	600	FAD	C1'-N10	-2.83	1.41	1.47
2	A	600	FAD	C2B-C3B	2.77	1.60	1.53
2	B	601	FAD	O2-C2	-2.55	1.19	1.24
2	B	601	FAD	PA-O5B	-2.53	1.49	1.59
2	B	601	FAD	C5X-N5	-2.47	1.34	1.39
2	A	600	FAD	C5A-C6A	2.40	1.47	1.41
2	B	601	FAD	O4B-C1B	2.37	1.47	1.42
2	B	601	FAD	C5A-C6A	2.35	1.47	1.41
2	A	600	FAD	C2'-C3'	-2.34	1.49	1.53
2	A	600	FAD	PA-O5B	-2.29	1.50	1.59
2	A	600	FAD	O3B-C3B	-2.29	1.37	1.43
2	B	601	FAD	C2'-C3'	-2.21	1.49	1.53
2	A	600	FAD	O5'-C5'	2.09	1.52	1.44
2	B	601	FAD	C8-C7	2.04	1.45	1.40
2	B	601	FAD	C5A-C4A	2.02	1.42	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	O4B-C1B-N9A	12.28	131.67	108.09
2	A	600	FAD	O4B-C1B-N9A	9.31	125.96	108.09
2	A	600	FAD	O4B-C1B-C2B	-8.10	89.28	106.62
2	A	600	FAD	C4A-N9A-C8A	-7.95	97.40	105.74
2	A	600	FAD	O2B-C2B-C3B	-7.55	87.62	111.82
2	A	600	FAD	C3B-C2B-C1B	-7.23	87.80	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4A-N9A-C8A	-6.92	98.47	105.74
2	B	601	FAD	O2B-C2B-C3B	-6.86	89.81	111.82
2	A	600	FAD	C2B-C3B-C4B	-6.81	89.44	102.61
2	B	601	FAD	C4B-O4B-C1B	-4.82	98.81	109.47
2	B	601	FAD	C2A-N1A-C6A	4.37	125.91	118.73
2	A	600	FAD	O4'-C4'-C5'	-4.14	100.86	109.99
2	A	600	FAD	O3'-C3'-C4'	4.07	118.18	108.93
2	B	601	FAD	O4B-C4B-C3B	-3.84	97.54	105.15
2	A	600	FAD	N3A-C2A-N1A	-3.83	122.78	128.58
2	B	601	FAD	O3'-C3'-C4'	3.70	117.34	108.93
2	B	601	FAD	C8M-C8-C9	3.69	126.08	119.57
2	B	601	FAD	N3A-C2A-N1A	-3.45	123.36	128.58
2	B	601	FAD	O4B-C1B-C2B	-3.43	99.29	106.62
2	B	601	FAD	C10-N1-C2	3.38	124.17	116.85
2	B	601	FAD	C4X-C10-N1	-3.29	116.52	124.59
2	A	600	FAD	C5A-C4A-N9A	3.17	109.26	105.81
2	A	600	FAD	C5A-C4A-N3A	-3.09	122.46	126.72
2	A	600	FAD	C4B-O4B-C1B	-3.07	102.68	109.47
2	A	600	FAD	C4X-C10-N1	-3.01	117.20	124.59
2	B	601	FAD	O4'-C4'-C5'	-3.01	103.35	109.99
2	B	601	FAD	C3B-C2B-C1B	2.99	107.13	101.46
2	A	600	FAD	C5'-C4'-C3'	-2.99	106.57	112.22
2	B	601	FAD	C7M-C7-C6	2.98	124.83	119.57
2	B	601	FAD	C5'-C4'-C3'	-2.97	106.61	112.22
2	B	601	FAD	C4-N3-C2	-2.88	120.53	125.64
2	A	600	FAD	N9A-C8A-N7A	2.83	117.95	113.94
2	A	600	FAD	O2A-PA-O1A	2.83	125.60	112.44
2	A	600	FAD	O2B-C2B-C1B	2.76	119.62	110.10
2	B	601	FAD	O2B-C2B-C1B	2.69	119.36	110.10
2	A	600	FAD	C10-C4X-N5	-2.62	119.46	124.81
2	A	600	FAD	C4A-N9A-C1B	-2.60	120.55	126.63
2	A	600	FAD	C10-N1-C2	2.59	122.45	116.85
2	B	601	FAD	C10-C4X-N5	-2.54	119.63	124.81
2	B	601	FAD	C8M-C8-C7	-2.53	115.60	120.76
2	B	601	FAD	C7M-C7-C8	-2.52	115.62	120.76
2	B	601	FAD	C5A-C4A-N3A	-2.48	123.30	126.72
2	A	600	FAD	O5B-C5B-C4B	-2.47	100.57	108.99
2	A	600	FAD	C4-C4X-C10	2.40	121.05	116.93
2	B	601	FAD	O5'-C5'-C4'	2.37	115.69	109.36
2	A	600	FAD	C2A-N1A-C6A	2.37	122.62	118.73
2	B	601	FAD	O2A-PA-O1A	2.34	123.33	112.44
2	A	600	FAD	O2'-C2'-C1'	-2.22	101.07	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	O3P-P-O1P	-2.21	104.05	110.70
2	A	600	FAD	C7M-C7-C6	2.19	123.44	119.57
2	B	601	FAD	C2B-C3B-C4B	-2.18	98.40	102.61
2	B	601	FAD	C1B-N9A-C8A	2.14	131.84	127.09
2	B	601	FAD	C5A-C4A-N9A	2.09	108.09	105.81
2	B	601	FAD	PA-O5B-C5B	2.09	133.34	121.35
2	B	601	FAD	O3P-P-O1P	-2.09	104.42	110.70
2	A	600	FAD	C6-C7-C8	-2.04	116.70	119.69

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	600	FAD	C2B
2	A	600	FAD	C4B
2	B	601	FAD	C2B
2	B	601	FAD	C3B
2	B	601	FAD	C4B

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O2A
2	A	600	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	C3B-C4B-C5B-O5B
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	C2B-C1B-N9A-C8A

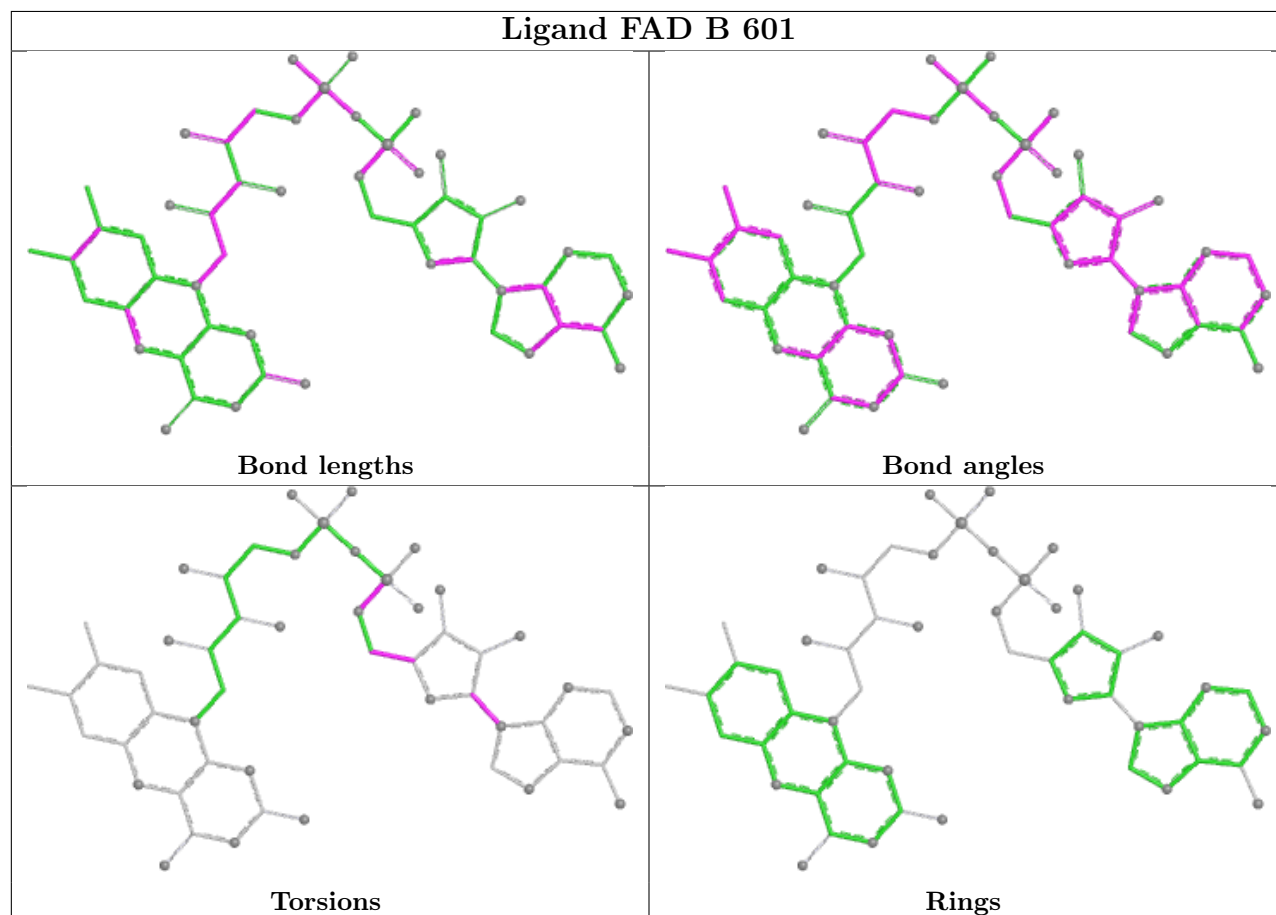
There are no ring outliers.

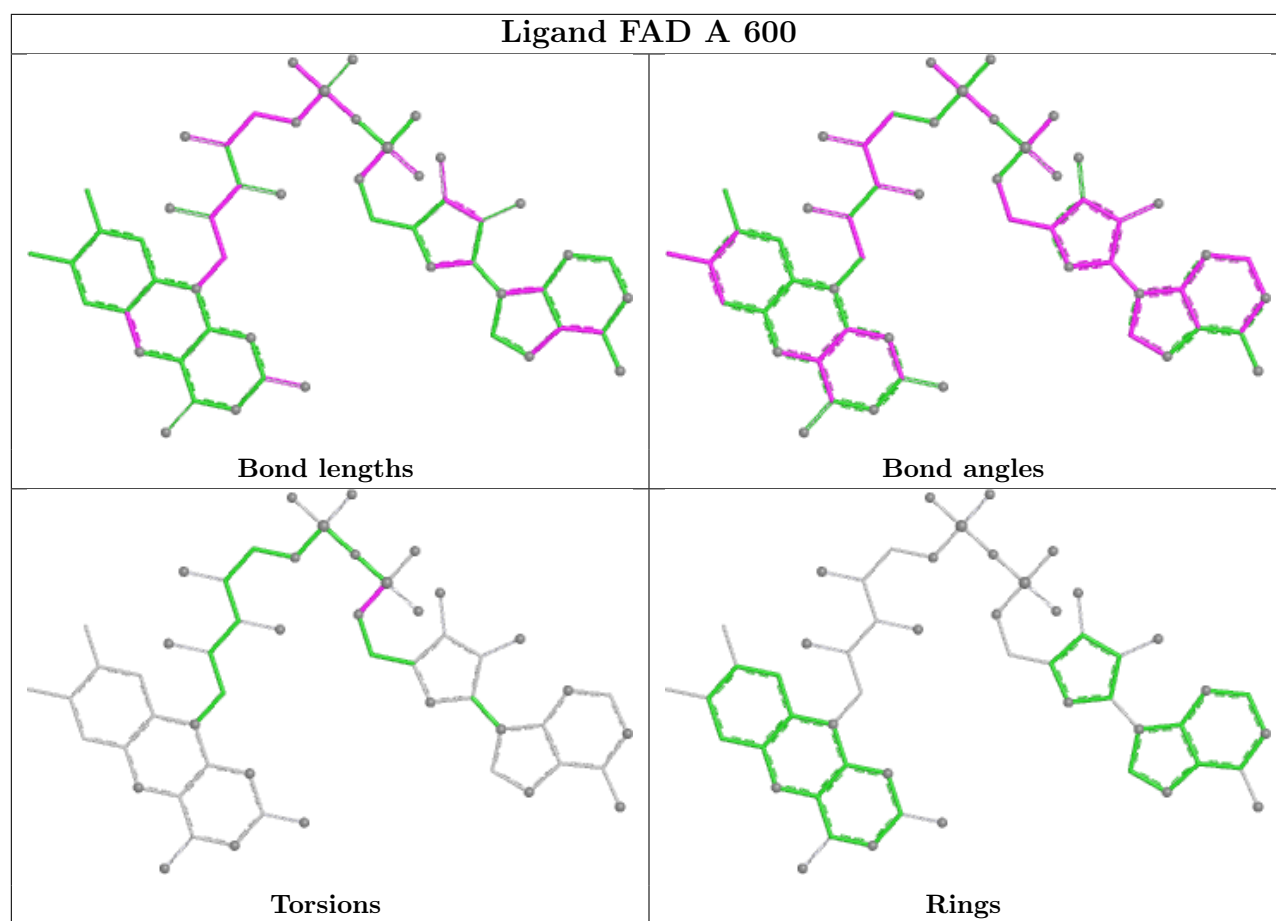
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	1	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.





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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.