



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:23 PM UTC

PDB ID : 8UY1 / pdb_00008uy1
Title : Methylenetetrahydrofolate reductase from Chaetomium thermophilum DSM 1495, Active (R) State
Authors : Yamada, K.; Mendoza, J.; Koutmos, M.
Deposited on : 2023-11-12
Resolution : 3.49 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

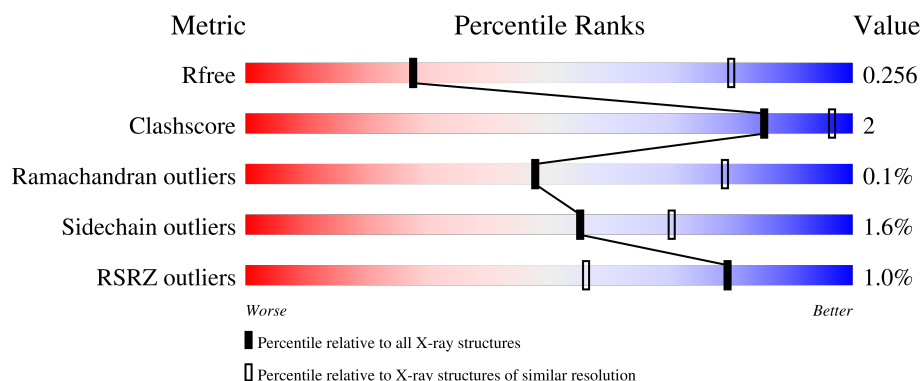
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	617	87% 8% • •
1	B	617	84% 8% • 7%
1	C	617	87% 10% • •
1	D	617	85% 9% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19297 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 Methylenetetrahydrofolate reductase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	592	Total	C	N	O	S	0	0	0
			4769	3028	836	877	28			
1	A	598	Total	C	N	O	S	0	0	0
			4826	3064	847	887	28			
1	B	575	Total	C	N	O	S	0	0	0
			4657	2966	813	851	27			
1	C	598	Total	C	N	O	S	0	0	0
			4829	3066	848	887	28			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP G0S5U9
D	-1	ASN	-	expression tag	UNP G0S5U9
D	0	ALA	-	expression tag	UNP G0S5U9
D	21	GLN	GLU	engineered mutation	UNP G0S5U9
D	393	MET	LEU	engineered mutation	UNP G0S5U9
D	516	PHE	VAL	engineered mutation	UNP G0S5U9
A	-2	SER	-	expression tag	UNP G0S5U9
A	-1	ASN	-	expression tag	UNP G0S5U9
A	0	ALA	-	expression tag	UNP G0S5U9
A	21	GLN	GLU	engineered mutation	UNP G0S5U9
A	393	MET	LEU	engineered mutation	UNP G0S5U9
A	516	PHE	VAL	engineered mutation	UNP G0S5U9
B	-2	SER	-	expression tag	UNP G0S5U9
B	-1	ASN	-	expression tag	UNP G0S5U9
B	0	ALA	-	expression tag	UNP G0S5U9
B	21	GLN	GLU	engineered mutation	UNP G0S5U9
B	393	MET	LEU	engineered mutation	UNP G0S5U9
B	516	PHE	VAL	engineered mutation	UNP G0S5U9
C	-2	SER	-	expression tag	UNP G0S5U9
C	-1	ASN	-	expression tag	UNP G0S5U9
C	0	ALA	-	expression tag	UNP G0S5U9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	GLN	GLU	engineered mutation	UNP G0S5U9
C	393	MET	LEU	engineered mutation	UNP G0S5U9
C	516	PHE	VAL	engineered mutation	UNP G0S5U9

- # FAD

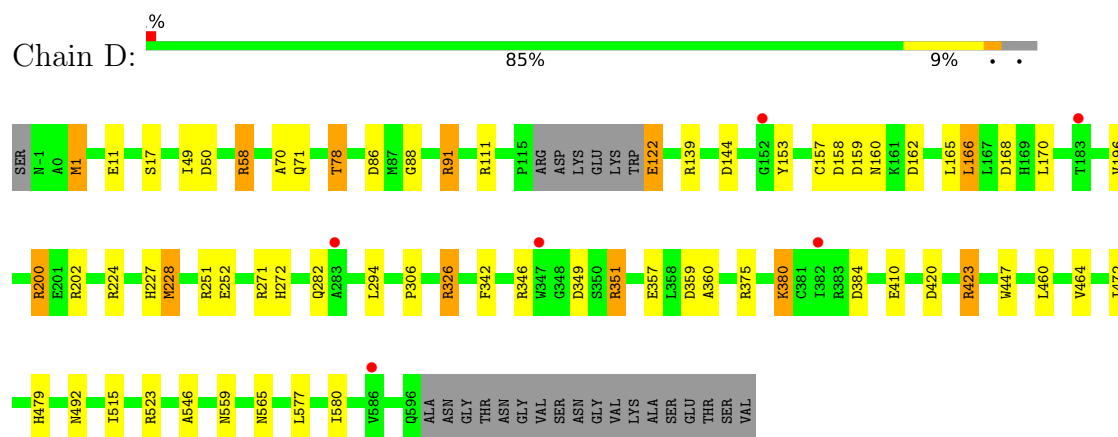
- Molecule 3 is water.

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

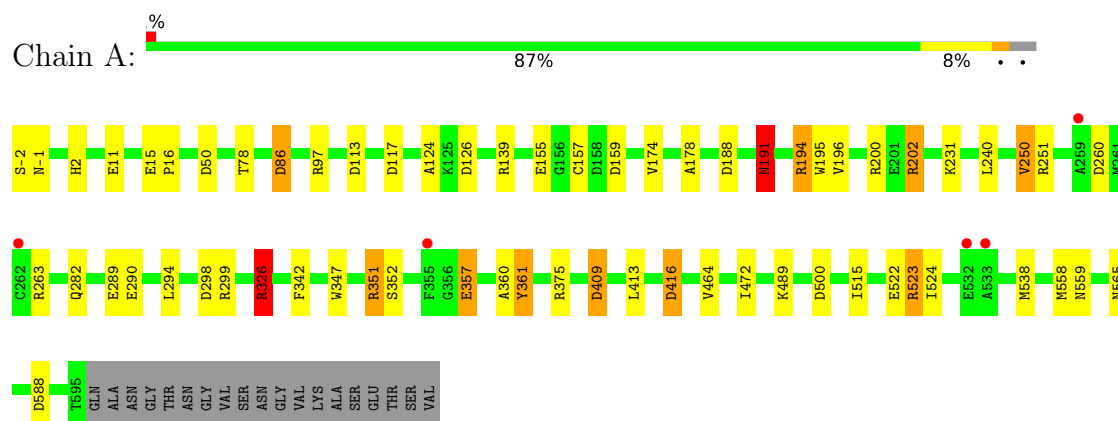
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

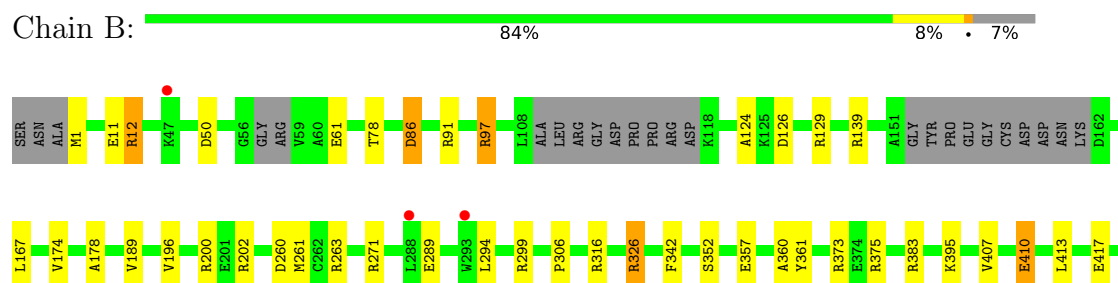
- Molecule 1: Methylenetetrahydrofolate reductase-like protein



- Molecule 1: Methylenetetrahydrofolate reductase-like protein

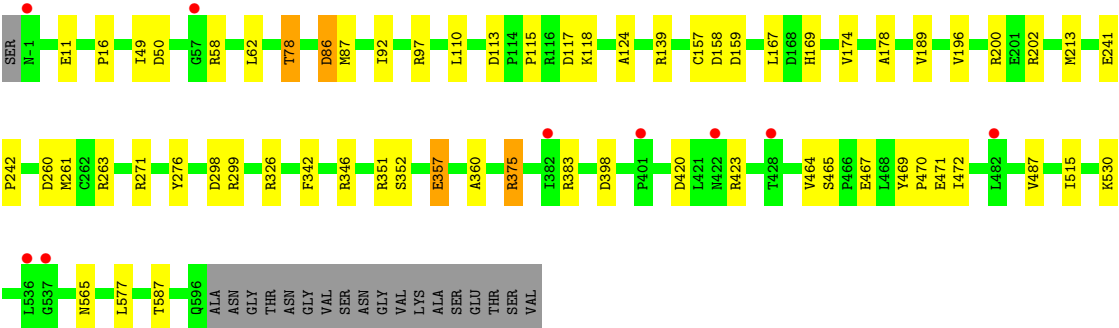
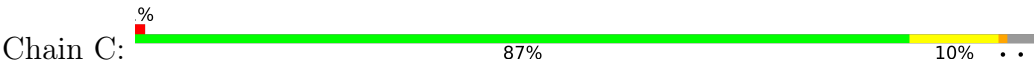


- Molecule 1: Methylenetetrahydrofolate reductase-like protein





● Molecule 1: Methylene tetrahydrofolate reductase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.97Å 151.38Å 188.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.04 – 3.49 52.04 – 3.49	Depositor EDS
% Data completeness (in resolution range)	99.4 (52.04-3.49) 99.4 (52.04-3.49)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.216 , 0.256 0.219 , 0.256	Depositor DCC
R_{free} test set	2182 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	131.2	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 163.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19297	wwPDB-VP
Average B, all atoms (Å ²)	159.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.77	1/4953 (0.0%)	1.29	24/6713 (0.4%)
1	B	0.78	2/4777 (0.0%)	1.28	18/6470 (0.3%)
1	C	0.77	3/4956 (0.1%)	1.26	16/6717 (0.2%)
1	D	0.76	1/4893 (0.0%)	1.29	23/6632 (0.3%)
All	All	0.77	7/19579 (0.0%)	1.28	81/26532 (0.3%)

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	8
1	B	0	8
1	C	0	5
1	D	0	10
All	All	0	31

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	326	ARG	NE-CZ	6.68	1.40	1.33
1	B	326	ARG	NE-CZ	6.47	1.40	1.33
1	A	352	SER	CA-CB	-5.88	1.45	1.53
1	C	326	ARG	NE-CZ	5.46	1.39	1.33
1	B	352	SER	CA-CB	-5.42	1.45	1.53
1	C	352	SER	CA-CB	-5.04	1.46	1.53
1	C	169	HIS	CG-CD2	-5.03	1.30	1.35

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ASP	CA-CB-CG	9.12	121.72	112.60
1	A	11	GLU	CB-CG-CD	9.09	128.05	112.60
1	D	1	MET	CG-SD-CE	9.08	120.88	100.90
1	B	126	ASP	CB-CA-C	8.84	124.44	111.89
1	D	11	GLU	CB-CG-CD	8.65	127.31	112.60
1	C	298	ASP	CA-CB-CG	8.59	121.19	112.60
1	A	361	TYR	N-CA-CB	8.41	124.71	110.49
1	B	11	GLU	CB-CG-CD	8.26	126.64	112.60
1	B	126	ASP	CA-CB-CG	8.25	120.85	112.60
1	A	342	PHE	CA-CB-CG	-7.65	106.15	113.80
1	B	61	GLU	CB-CG-CD	7.56	125.45	112.60
1	C	159	ASP	CA-CB-CG	7.55	120.16	112.60
1	D	228	MET	CG-SD-CE	7.31	116.99	100.90
1	A	326	ARG	NE-CZ-NH2	7.15	125.63	119.20
1	A	159	ASP	CA-CB-CG	7.11	119.71	112.60
1	D	342	PHE	CA-CB-CG	-7.01	106.79	113.80
1	C	11	GLU	CB-CG-CD	6.95	124.41	112.60
1	C	342	PHE	CA-CB-CG	-6.94	106.86	113.80
1	C	50	ASP	CA-CB-CG	6.91	119.51	112.60
1	B	1	MET	CG-SD-CE	6.70	115.65	100.90
1	A	50	ASP	CA-CB-CG	6.63	119.23	112.60
1	C	326	ARG	CD-NE-CZ	6.63	133.68	124.40
1	A	231	LYS	CB-CA-C	6.55	121.03	110.29
1	D	86	ASP	CA-CB-CG	6.48	119.08	112.60
1	D	227	HIS	CA-CB-CG	-6.45	107.35	113.80
1	D	159	ASP	CA-CB-CG	6.45	119.05	112.60
1	A	126	ASP	CA-CB-CG	6.44	119.04	112.60
1	B	50	ASP	CA-CB-CG	6.35	118.95	112.60
1	B	342	PHE	CA-CB-CG	-6.30	107.50	113.80
1	D	410	GLU	CB-CG-CD	6.22	123.18	112.60
1	A	117	ASP	CA-CB-CG	6.20	118.80	112.60
1	C	357	GLU	CB-CG-CD	6.17	123.09	112.60
1	C	117	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	86	ASP	CA-CB-CG	6.13	118.73	112.60
1	D	50	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	361	TYR	CB-CA-C	6.12	119.66	109.38
1	D	158	ASP	CA-CB-CG	6.11	118.71	112.60
1	D	227	HIS	CB-CG-CD2	-6.07	123.31	131.20
1	B	410	GLU	CB-CG-CD	6.05	122.89	112.60
1	B	299	ARG	CB-CG-CD	6.04	125.20	111.30
1	A	326	ARG	CD-NE-CZ	6.01	132.82	124.40
1	A	357	GLU	CB-CG-CD	5.97	122.75	112.60
1	D	122	GLU	CB-CA-C	5.95	121.40	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	326	ARG	CD-NE-CZ	5.92	132.69	124.40
1	B	86	ASP	CA-CB-CG	5.91	118.51	112.60
1	A	588	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	298	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	326	ARG	CD-NE-CZ	5.84	132.57	124.40
1	D	351	ARG	CD-NE-CZ	5.78	132.49	124.40
1	A	500	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	565	ASN	CA-CB-CG	5.74	118.34	112.60
1	C	78	THR	CA-CB-OG1	-5.73	101.01	109.60
1	A	78	THR	CA-CB-OG1	-5.71	101.03	109.60
1	B	78	THR	CA-CB-OG1	-5.63	101.16	109.60
1	A	409	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	545	ASP	CA-CB-CG	5.58	118.17	112.60
1	D	78	THR	CA-CB-OG1	-5.49	101.37	109.60
1	C	158	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	191	ASN	CA-CB-CG	5.44	118.04	112.60
1	C	565	ASN	CA-CB-CG	5.44	118.04	112.60
1	C	351	ARG	CD-NE-CZ	5.42	131.98	124.40
1	D	559	ASN	CA-CB-CG	-5.38	107.22	112.60
1	A	126	ASP	CB-CA-C	5.37	119.05	111.86
1	D	1	MET	CA-C-O	-5.37	114.03	120.10
1	D	227	HIS	CB-CG-ND1	5.31	130.66	122.70
1	C	169	HIS	CG-CD2-NE2	5.30	112.50	107.20
1	C	113	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	413	LEU	CB-CG-CD2	5.29	126.59	110.70
1	D	162	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	559	ASN	CA-CB-CG	-5.25	107.35	112.60
1	B	565	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	416	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	565	ASN	CA-CB-CG	5.19	117.79	112.60
1	D	144	ASP	CA-CB-CG	5.14	117.74	112.60
1	D	11	GLU	CB-CA-C	5.12	120.10	110.63
1	B	588	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	417	GLU	CB-CG-CD	5.05	121.19	112.60
1	C	86	ASP	CA-CB-CG	5.04	117.64	112.60
1	B	516	PHE	CA-CB-CG	5.02	118.82	113.80
1	C	471	GLU	CB-CG-CD	5.01	121.12	112.60
1	D	546	ALA	CA-C-O	-5.01	115.16	121.02

There are no chirality outliers.

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	ARG	Sidechain
1	A	194	ARG	Sidechain
1	A	202	ARG	Sidechain
1	A	299	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	375	ARG	Sidechain
1	A	523	ARG	Sidechain
1	A	97	ARG	Sidechain
1	B	12	ARG	Sidechain
1	B	129	ARG	Sidechain
1	B	271	ARG	Sidechain
1	B	316	ARG	Sidechain
1	B	375	ARG	Sidechain
1	B	523	ARG	Sidechain
1	B	91	ARG	Sidechain
1	B	97	ARG	Sidechain
1	C	139	ARG	Sidechain
1	C	271	ARG	Sidechain
1	C	346	ARG	Sidechain
1	C	375	ARG	Sidechain
1	C	97	ARG	Sidechain
1	D	139	ARG	Sidechain
1	D	200	ARG	Sidechain
1	D	271	ARG	Sidechain
1	D	346	ARG	Sidechain
1	D	351	ARG	Sidechain
1	D	375	ARG	Sidechain
1	D	423	ARG	Sidechain
1	D	523	ARG	Sidechain
1	D	58	ARG	Sidechain
1	D	91	ARG	Sidechain

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	4826	0	4695	22	0
1	B	4657	0	4541	16	0
1	C	4829	0	4698	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4769	0	4638	23	0
2	A	53	0	31	0	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0
2	D	53	0	31	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
All	All	19297	0	18696	85	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 2.

All (85) 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:240:LEU:HD22	1:A:250:VAL:HG22	1.72	0.71
1:A:155:GLU:HG2	1:A:191:ASN:HD21	1.57	0.70
1:D:168:ASP:OD1	1:D:202:ARG:NH1	2.25	0.69
1:A:522:GLU:OE2	1:A:524:ILE:HD12	1.92	0.68
1:D:111:ARG:NH2	1:D:122:GLU:OE1	2.27	0.67
1:A:515:ILE:HG21	1:B:515:ILE:HG21	1.80	0.63
1:B:420:ASP:OD1	1:B:423:ARG:NH2	2.34	0.61
1:A:251:ARG:NH1	1:A:282:GLN:OE1	2.35	0.60
1:D:160:ASN:HB3	1:D:166:LEU:HD11	1.86	0.57
1:B:289:GLU:HG3	1:B:294:LEU:HD12	1.88	0.56
2:B:701:FAD:H3'	2:B:701:FAD:N1	2.20	0.56
1:C:16:PRO:HG3	1:C:299:ARG:HH21	1.71	0.56
1:A:464:VAL:HG21	1:A:472:ILE:HD12	1.88	0.55
1:B:357:GLU:HB2	1:B:360:ALA:HB3	1.89	0.54
1:D:160:ASN:ND2	2:D:701:FAD:O3B	2.41	0.54
1:C:420:ASP:OD1	1:C:423:ARG:NH2	2.43	0.52
1:D:196:VAL:O	1:D:200:ARG:HG2	2.11	0.51
1:C:58:ARG:NH2	1:C:62:LEU:HD11	2.24	0.51
1:C:86:ASP:HA	1:C:124:ALA:HB2	1.92	0.51
1:D:464:VAL:HG21	1:D:472:ILE:HD12	1.92	0.51
1:A:196:VAL:O	1:A:200:ARG:HG2	2.11	0.50
1:C:469:TYR:N	1:C:470:PRO:HD2	2.26	0.50
1:B:167:LEU:HB3	1:B:202:ARG:HD2	1.94	0.49
1:D:153:TYR:OH	2:D:701:FAD:H5'2	2.12	0.49
1:C:115:PRO:HD2	1:C:118:LYS:HB2	1.94	0.49
1:B:196:VAL:O	1:B:200:ARG:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LYS:HE3	1:A:538:MET:HE3	1.95	0.48
1:C:58:ARG:HH21	1:C:62:LEU:HD11	1.78	0.48
1:A:538:MET:HE2	1:A:558:MET:HB2	1.94	0.48
1:A:188:ASP:CG	1:A:191:ASN:HB3	2.38	0.48
1:B:373:ARG:HG2	1:B:544:TYR:CE1	2.48	0.48
1:C:375:ARG:NH2	1:C:398:ASP:HB2	2.28	0.48
1:D:251:ARG:HH22	1:D:282:GLN:HG2	1.80	0.47
1:C:196:VAL:O	1:C:200:ARG:HG2	2.13	0.47
1:D:492:ASN:OD1	1:A:523:ARG:NH2	2.47	0.47
1:D:515:ILE:HG21	1:C:515:ILE:HG21	1.96	0.47
1:B:383:ARG:HH11	1:B:383:ARG:HG3	1.80	0.47
1:A:260:ASP:OD1	1:A:263:ARG:NH1	2.48	0.46
1:C:260:ASP:OD1	1:C:263:ARG:NH1	2.47	0.46
1:D:460:LEU:HB3	1:D:577:LEU:HD21	1.98	0.46
1:A:347:TRP:CE2	1:A:351:ARG:HD3	2.51	0.46
1:C:464:VAL:HG21	1:C:472:ILE:HD12	1.98	0.46
1:D:420:ASP:HA	1:D:423:ARG:HG2	1.98	0.45
1:C:87:MET:HE2	1:C:92:ILE:HD13	1.99	0.45
1:B:260:ASP:OD1	1:B:263:ARG:NH1	2.48	0.45
1:D:479:HIS:CE1	1:D:580:ILE:HG21	2.52	0.45
1:A:86:ASP:HA	1:A:124:ALA:HB2	1.98	0.45
1:C:487:VAL:HG21	1:C:530:LYS:HD3	1.99	0.45
1:D:357:GLU:HB2	1:D:360:ALA:HB3	1.99	0.44
1:C:357:GLU:HG2	1:C:360:ALA:HB3	1.99	0.44
1:D:70:ALA:HB3	1:D:78:THR:HG21	2.00	0.44
1:C:167:LEU:HB3	1:C:202:ARG:HD2	1.99	0.43
1:C:213:MET:HE2	1:C:276:TYR:HB3	1.99	0.43
1:C:110:LEU:HD13	2:C:701:FAD:C10	2.48	0.43
1:C:110:LEU:HD13	2:C:701:FAD:C4X	2.49	0.43
1:C:420:ASP:HA	1:C:423:ARG:HG2	1.99	0.43
1:B:413:LEU:CD1	1:B:444:VAL:HG11	2.49	0.43
1:D:71:GLN:HE21	1:D:78:THR:H	1.67	0.43
1:C:241:GLU:HB3	1:C:242:PRO:HD3	2.01	0.42
1:B:566:ILE:HG21	1:B:577:LEU:HD21	2.00	0.42
1:A:194:ARG:HH21	1:A:195:TRP:HB2	1.84	0.42
1:C:49:ILE:CG1	1:C:78:THR:HG22	2.49	0.42
1:C:465:SER:OG	1:C:467:GLU:OE1	2.36	0.42
1:D:88:GLY:H	1:D:91:ARG:HD3	1.85	0.41
1:A:464:VAL:HG21	1:A:472:ILE:CD1	2.49	0.41
1:C:49:ILE:HD11	1:C:78:THR:HG22	2.02	0.41
1:C:189:VAL:HG22	1:C:261:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:HH22	1:A:290:GLU:HG3	1.86	0.41
1:B:86:ASP:HA	1:B:124:ALA:HB2	2.03	0.41
1:A:15:GLU:HB3	1:A:16:PRO:HD2	2.03	0.41
1:B:306:PRO:HD3	1:B:447:TRP:CD2	2.56	0.41
1:D:17:SER:OG	1:D:272:HIS:ND1	2.45	0.41
1:D:49:ILE:CG1	1:D:78:THR:HG22	2.51	0.41
1:A:174:VAL:HA	1:A:178:ALA:HB3	2.03	0.41
1:A:289:GLU:HG3	1:A:294:LEU:HD12	2.03	0.41
1:B:395:LYS:HG2	1:B:407:VAL:CG1	2.50	0.41
1:B:174:VAL:HA	1:B:178:ALA:HB3	2.03	0.41
1:D:380:LYS:HG2	1:D:384:ASP:OD2	2.22	0.40
1:C:174:VAL:HA	1:C:178:ALA:HB3	2.03	0.40
1:D:306:PRO:HD3	1:D:447:TRP:CD2	2.56	0.40
1:A:-2:SER:O	1:A:-1:ASN:C	2.64	0.40
1:D:224:ARG:O	1:D:228:MET:HG2	2.21	0.40
1:D:251:ARG:HH22	1:D:282:GLN:CG	2.34	0.40
1:A:191:ASN:OD1	1:A:191:ASN:C	2.64	0.40
1:B:189:VAL:HG22	1:B:261:MET:SD	2.62	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	596/617 (97%)	576 (97%)	17 (3%)	3 (0%)	24	57
1	B	567/617 (92%)	551 (97%)	16 (3%)	0	100	100
1	C	596/617 (97%)	576 (97%)	20 (3%)	0	100	100
1	D	588/617 (95%)	569 (97%)	19 (3%)	0	100	100
All	All	2347/2468 (95%)	2272 (97%)	72 (3%)	3 (0%)	48	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	HIS
1	A	361	TYR
1	A	360	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/523 (97%)	500 (98%)	9 (2%)	51	69
1	B	492/523 (94%)	484 (98%)	8 (2%)	55	70
1	C	509/523 (97%)	505 (99%)	4 (1%)	73	77
1	D	503/523 (96%)	491 (98%)	12 (2%)	43	64
All	All	2013/2092 (96%)	1980 (98%)	33 (2%)	55	70

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1	MET
1	D	58	ARG
1	D	157	CYS
1	D	165	LEU
1	D	166	LEU
1	D	170	LEU
1	D	252	GLU
1	D	294	LEU
1	D	326	ARG
1	D	349	ASP
1	D	359	ASP
1	D	380	LYS
1	A	157	CYS
1	A	191	ASN
1	A	202	ARG
1	A	250	VAL
1	A	326	ARG
1	A	351	ARG
1	A	357	GLU

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Mol	Chain	Res	Type
1	A	409	ASP
1	A	416	ASP
1	B	12	ARG
1	B	97	ARG
1	B	139	ARG
1	B	326	ARG
1	B	410	GLU
1	B	423	ARG
1	B	577	LEU
1	B	595	THR
1	C	157	CYS
1	C	383	ARG
1	C	577	LEU
1	C	587	THR

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

Mol	Chain	Res	Type
1	D	29	GLN
1	D	71	GLN
1	D	160	ASN
1	A	-1	ASN
1	A	29	GLN
1	A	160	ASN
1	A	169	HIS
1	A	292	ASN
1	A	559	ASN
1	B	43	ASN
1	C	145	HIS
1	C	169	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	A	701	-	58,58,58	0.68	1 (1%)	85,89,89	0.94	4 (4%)
2	FAD	D	701	-	58,58,58	0.82	2 (3%)	85,89,89	0.88	1 (1%)
2	FAD	B	701	-	58,58,58	1.27	2 (3%)	85,89,89	1.30	9 (10%)
2	FAD	C	701	-	58,58,58	0.94	2 (3%)	85,89,89	1.19	7 (8%)

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	701	-	-	4/34/50/50	0/6/6/6
2	FAD	D	701	-	-	13/34/50/50	0/6/6/6
2	FAD	B	701	-	-	14/34/50/50	0/6/6/6
2	FAD	C	701	-	-	18/34/50/50	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	P-O3P	5.94	1.65	1.59
2	B	701	FAD	PA-O3P	4.93	1.64	1.59
2	C	701	FAD	P-O3P	3.57	1.63	1.59
2	C	701	FAD	PA-O3P	2.98	1.62	1.59
2	D	701	FAD	C8-C7	2.08	1.45	1.40
2	A	701	FAD	C8-C7	2.07	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	FAD	PA-O3P	2.01	1.61	1.59

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FAD	O5'-C5'-C4'	5.52	124.10	109.36
2	B	701	FAD	C1'-C2'-C3'	4.48	121.80	109.66
2	C	701	FAD	O2A-PA-O3P	3.88	117.75	107.27
2	B	701	FAD	C4'-C3'-C2'	3.75	119.80	113.57
2	C	701	FAD	C5'-C4'-C3'	3.52	118.87	112.22
2	C	701	FAD	C2'-C1'-N10	3.32	125.87	110.20
2	A	701	FAD	C5'-C4'-C3'	3.15	118.17	112.22
2	B	701	FAD	O2A-PA-O3P	3.04	115.49	107.27
2	B	701	FAD	C9-C9A-N10	2.89	125.74	121.85
2	A	701	FAD	O4'-C4'-C3'	-2.61	103.14	109.25
2	D	701	FAD	C4'-C3'-C2'	-2.37	109.62	113.57
2	B	701	FAD	C2B-C1B-N9A	2.37	119.19	113.30
2	A	701	FAD	O5'-C5'-C4'	2.35	115.64	109.36
2	C	701	FAD	C9-C9A-N10	2.34	125.01	121.85
2	B	701	FAD	P-O5'-C5'	2.28	134.42	121.35
2	C	701	FAD	C1'-C2'-C3'	2.23	115.71	109.66
2	C	701	FAD	O4'-C4'-C3'	-2.23	104.03	109.25
2	B	701	FAD	C5'-C4'-C3'	2.16	116.29	112.22
2	C	701	FAD	O5'-C5'-C4'	2.09	114.94	109.36
2	A	701	FAD	O5'-P-O1P	2.04	117.00	108.94
2	B	701	FAD	C1'-N10-C9A	2.00	124.53	120.63

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5B-O5B-PA-O2A
2	B	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	N10-C1'-C2'-O2'
2	B	701	FAD	N10-C1'-C2'-C3'
2	B	701	FAD	C3'-C4'-C5'-O5'
2	B	701	FAD	O4'-C4'-C5'-O5'
2	B	701	FAD	C4'-C5'-O5'-P
2	B	701	FAD	C5'-O5'-P-O1P
2	B	701	FAD	C5'-O5'-P-O2P
2	B	701	FAD	C5'-O5'-P-O3P

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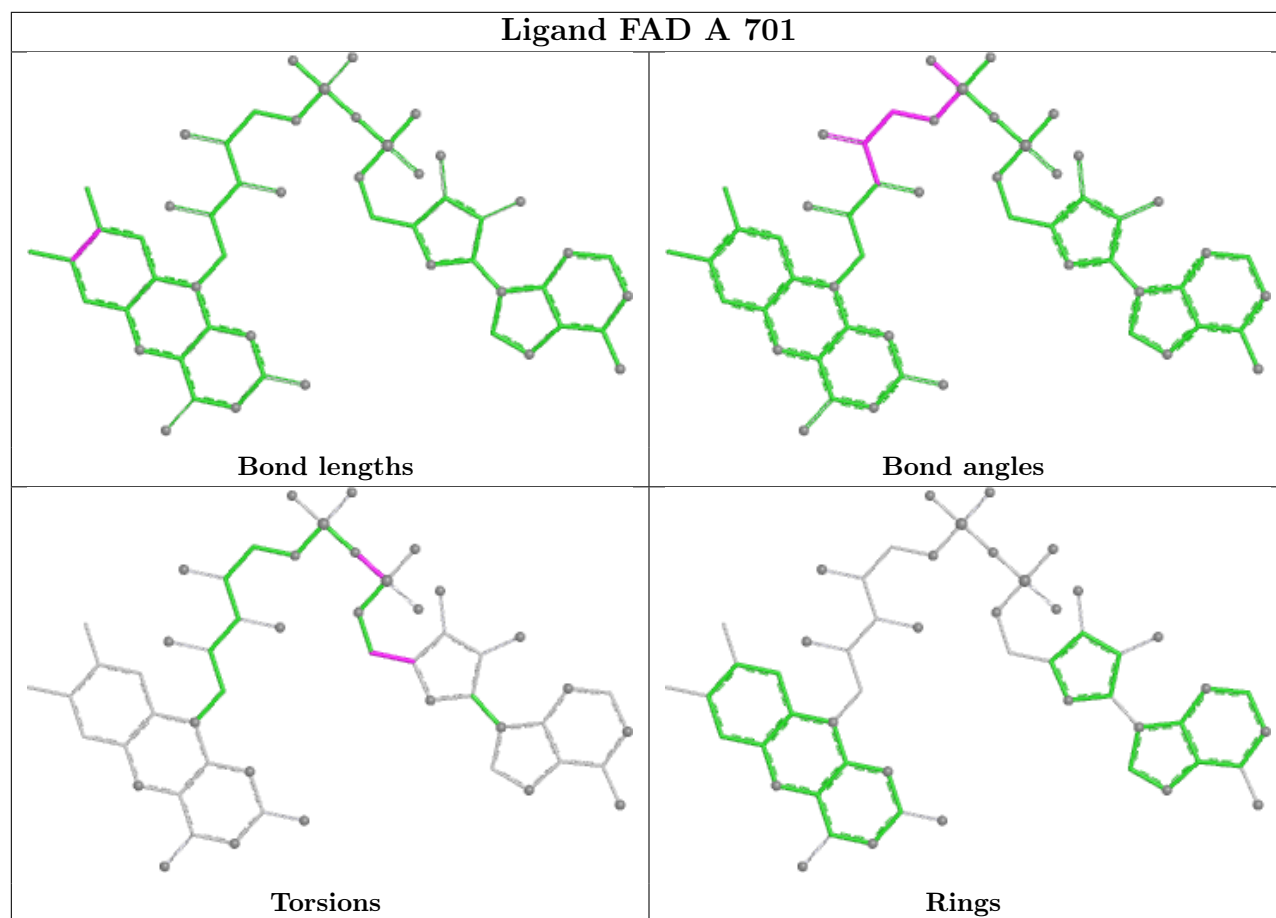
Mol	Chain	Res	Type	Atoms
2	C	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	C5B-O5B-PA-O3P
2	C	701	FAD	C2B-C1B-N9A-C8A
2	C	701	FAD	N10-C1'-C2'-O2'
2	C	701	FAD	C2'-C3'-C4'-O4'
2	C	701	FAD	C2'-C3'-C4'-C5'
2	C	701	FAD	O3'-C3'-C4'-O4'
2	C	701	FAD	O3'-C3'-C4'-C5'
2	D	701	FAD	O3'-C3'-C4'-C5'
2	D	701	FAD	C2'-C3'-C4'-C5'
2	D	701	FAD	C2'-C3'-C4'-O4'
2	C	701	FAD	C2B-C1B-N9A-C4A
2	D	701	FAD	O3'-C3'-C4'-O4'
2	A	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	C4B-C5B-O5B-PA
2	A	701	FAD	C3B-C4B-C5B-O5B
2	D	701	FAD	P-O3P-PA-O5B
2	D	701	FAD	PA-O3P-P-O5'
2	B	701	FAD	P-O3P-PA-O5B
2	D	701	FAD	C5'-O5'-P-O1P
2	C	701	FAD	C2'-C1'-N10-C10
2	C	701	FAD	C5'-O5'-P-O1P
2	D	701	FAD	C4'-C5'-O5'-P
2	C	701	FAD	C4'-C5'-O5'-P
2	C	701	FAD	C3'-C4'-C5'-O5'
2	D	701	FAD	C2B-C1B-N9A-C4A
2	D	701	FAD	C2B-C1B-N9A-C8A
2	A	701	FAD	P-O3P-PA-O1A
2	C	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	C3B-C4B-C5B-O5B
2	C	701	FAD	O2'-C2'-C3'-C4'
2	A	701	FAD	P-O3P-PA-O2A
2	B	701	FAD	P-O3P-PA-O2A
2	C	701	FAD	PA-O3P-P-O1P
2	C	701	FAD	PA-O3P-P-O2P
2	D	701	FAD	O4B-C1B-N9A-C8A
2	B	701	FAD	C2B-C1B-N9A-C4A
2	D	701	FAD	O4B-C4B-C5B-O5B

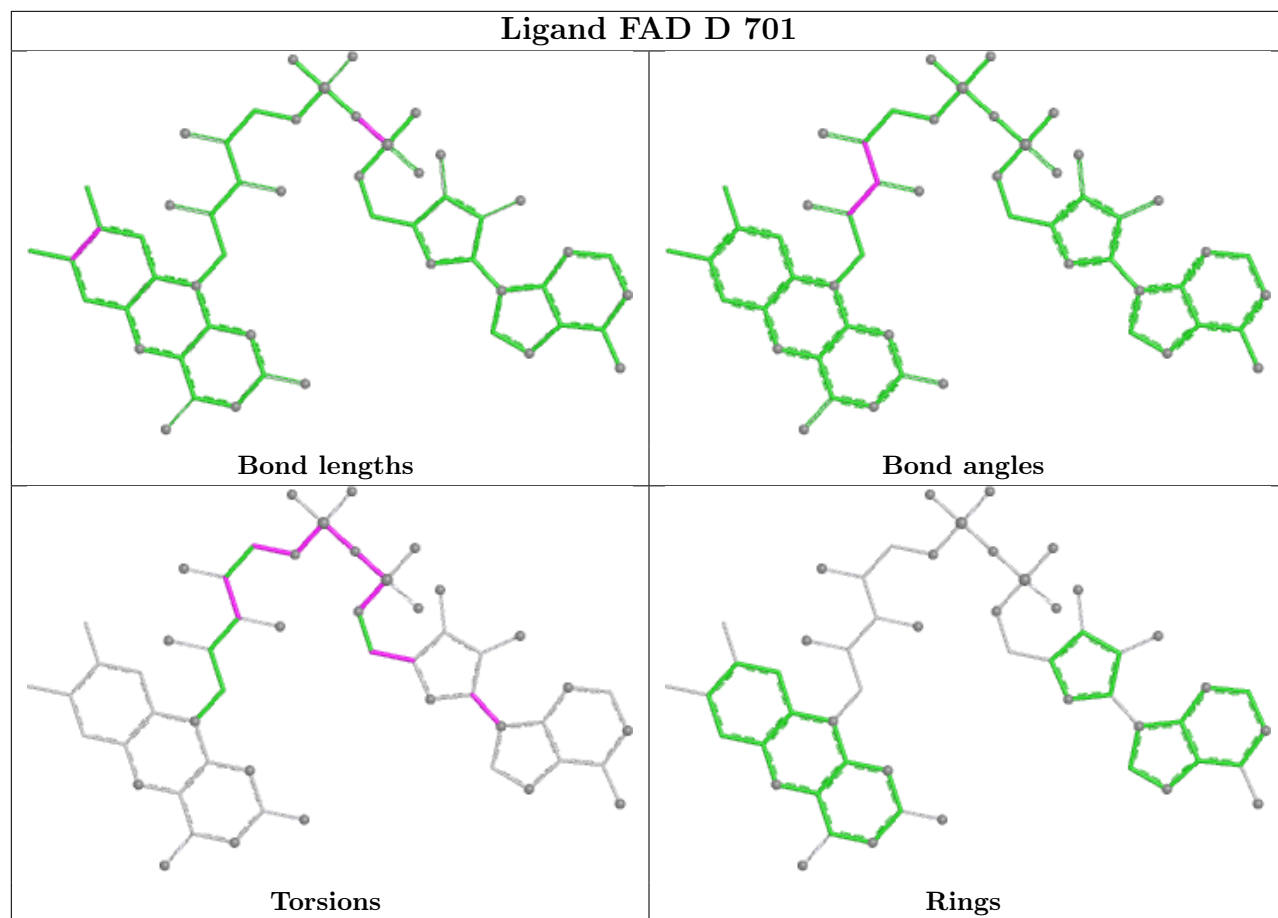
There are no ring outliers.

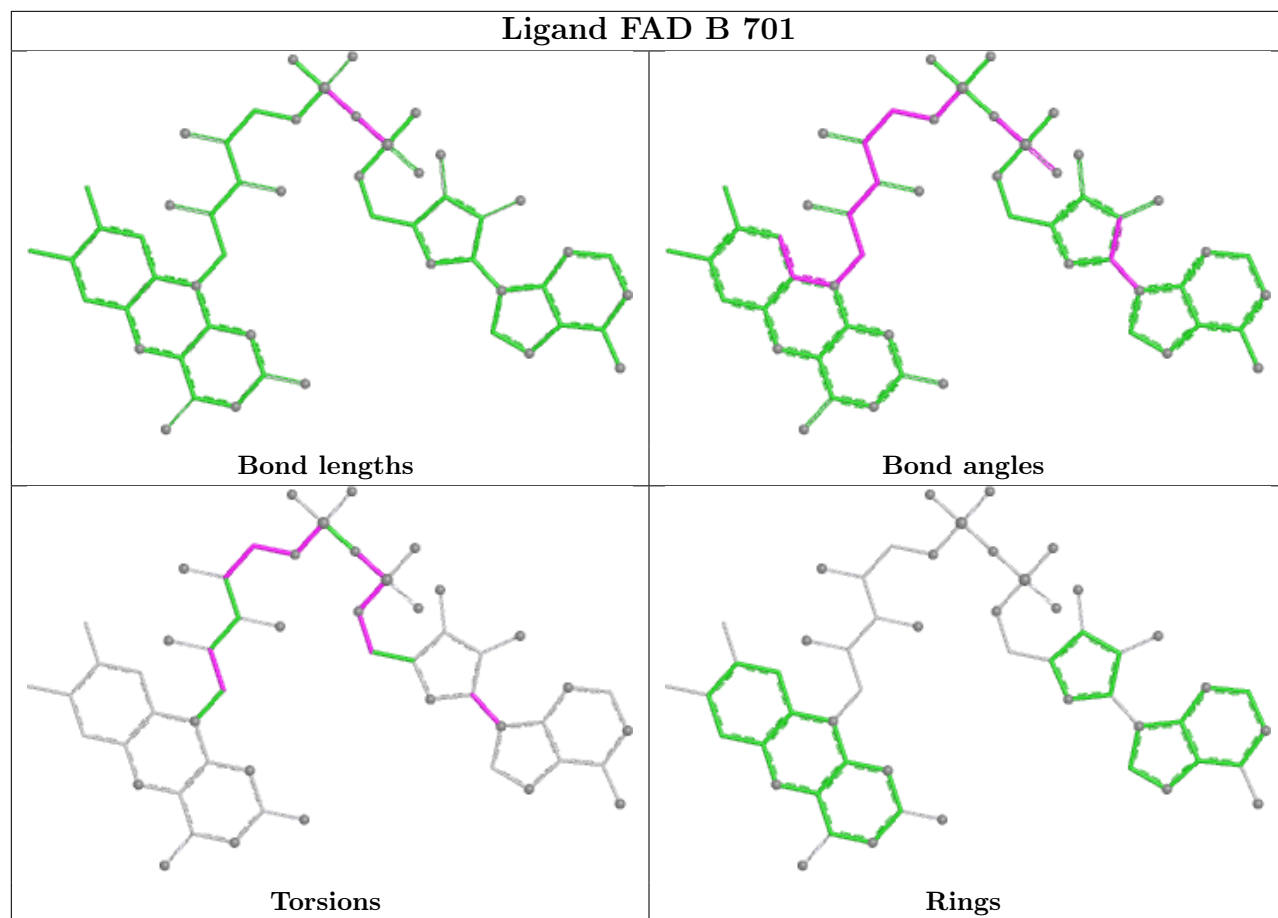
3 monomers are involved in 5 short contacts:

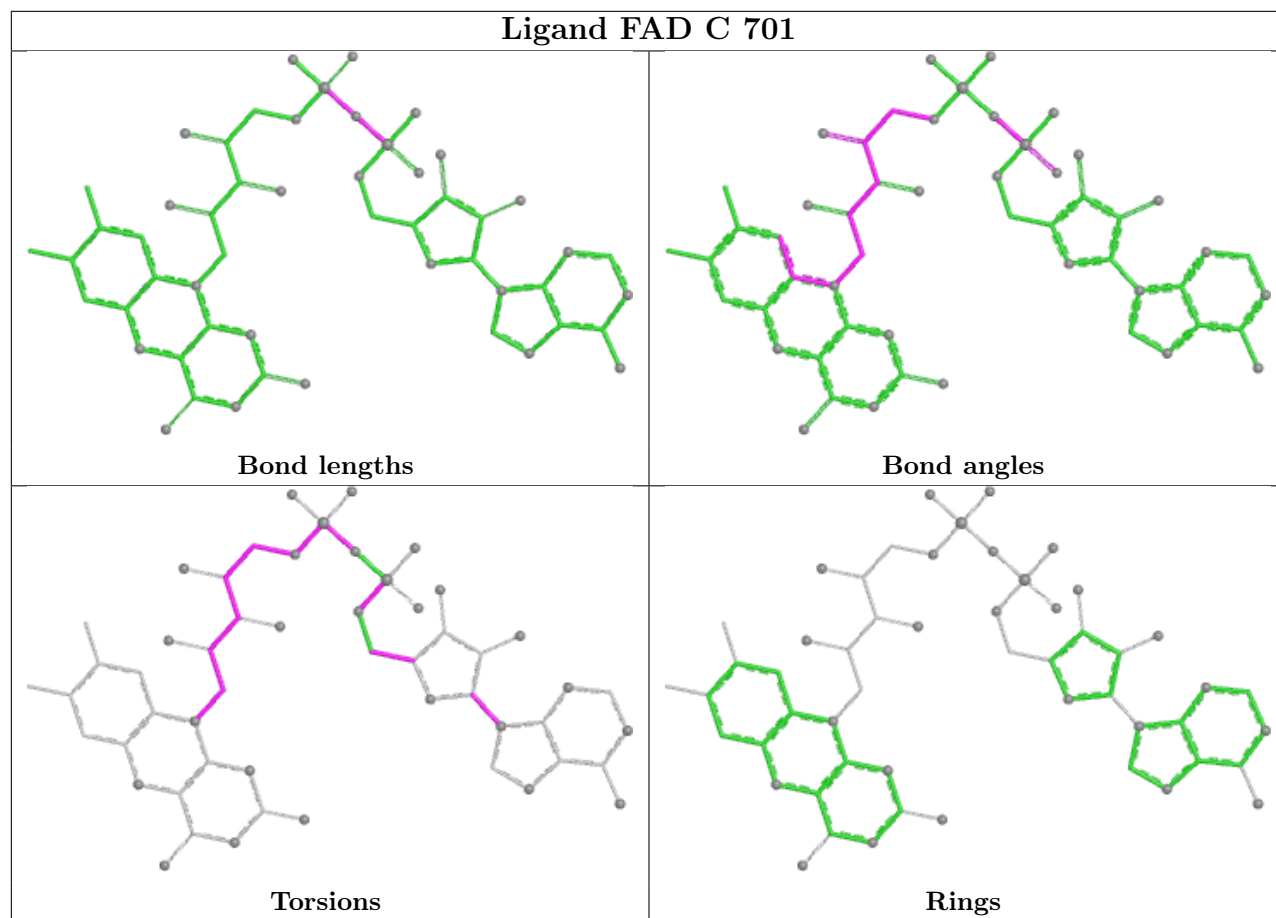
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	FAD	2	0
2	B	701	FAD	1	0
2	C	701	FAD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	598/617 (96%)	-0.43	5 (0%) 82 60	91, 132, 201, 237	0
1	B	575/617 (93%)	-0.52	3 (0%) 87 68	83, 150, 264, 299	0
1	C	598/617 (96%)	-0.44	9 (1%) 72 47	87, 168, 244, 301	0
1	D	592/617 (95%)	-0.44	6 (1%) 79 56	108, 155, 214, 278	0
All	All	2363/2468 (95%)	-0.46	23 (0%) 79 56	83, 152, 236, 301	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	536	LEU	5.1
1	C	401	PRO	3.5
1	A	355	PHE	3.2
1	A	532	GLU	2.7
1	D	183	THR	2.7
1	C	537	GLY	2.7
1	B	293	TRP	2.6
1	B	288	LEU	2.6
1	A	533	ALA	2.6
1	C	-1	ASN	2.5
1	C	382	ILE	2.5
1	D	382	ILE	2.5
1	A	262	CYS	2.4
1	D	283	ALA	2.4
1	C	428	THR	2.4
1	D	152	GLY	2.3
1	D	586	VAL	2.3
1	C	482	LEU	2.3
1	D	347	TRP	2.3
1	B	47	LYS	2.2
1	C	422	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	57	GLY	2.0
1	A	259	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

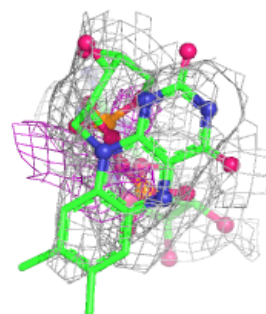
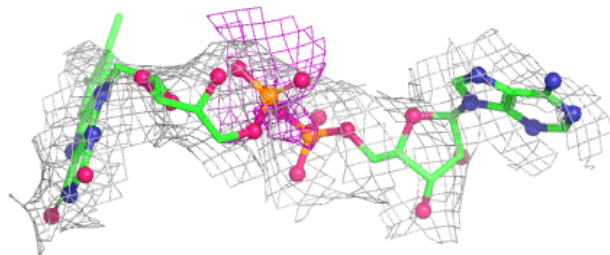
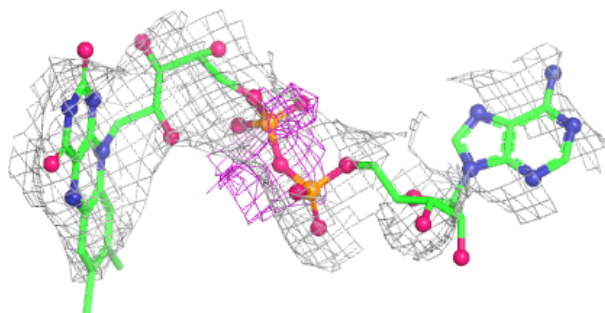
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	B	701	53/53	0.65	0.09	174,211,241,250	0
2	FAD	C	701	53/53	0.83	0.07	156,200,254,259	0
2	FAD	D	701	53/53	0.91	0.07	142,175,193,194	0
2	FAD	A	701	53/53	0.92	0.05	104,141,161,195	0

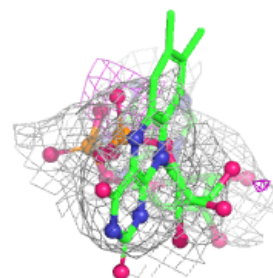
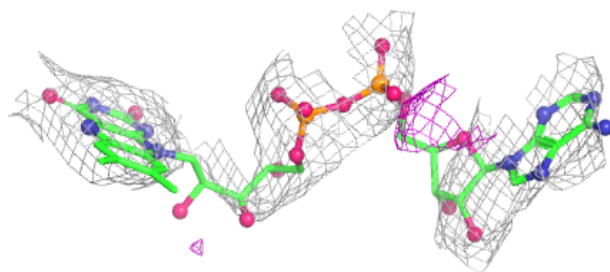
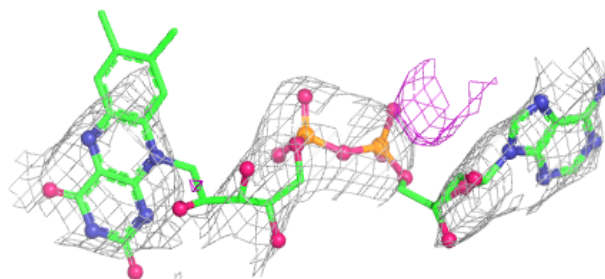
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 701:

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

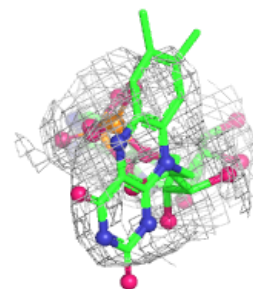
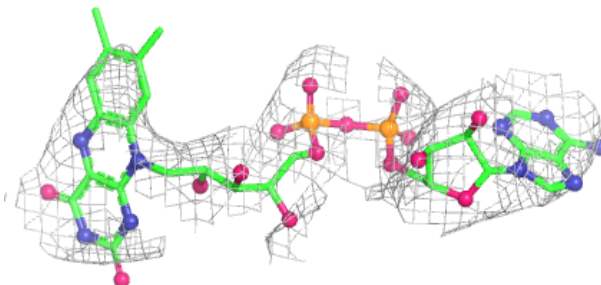
**Electron density around FAD C 701:**

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

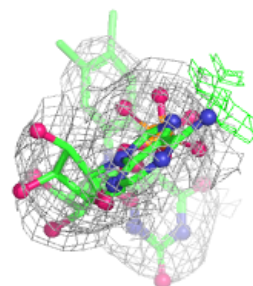
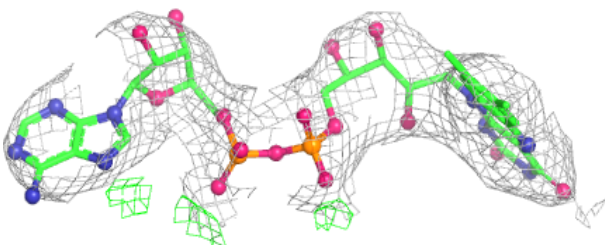
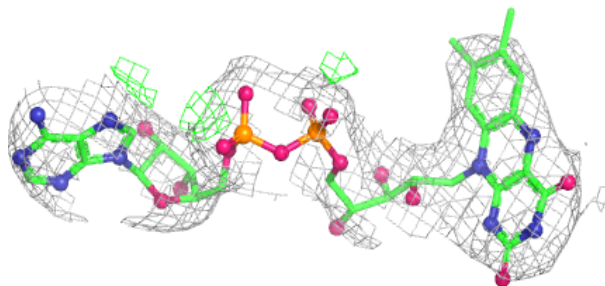


Electron density around FAD D 701:

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

**Electron density around FAD A 701:**

$2mF_o-DF_c$ (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.