



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:01 PM UTC

PDB ID : 8JZ6 / pdb_00008jz6
Title : Crystal structure of AetF in complex with FAD and NADP+ at 2.66 angstrom
Authors : Li, H.; Dai, L.; Chen, C.-C.; Guo, R.-T.
Deposited on : 2023-07-04
Resolution : 2.66 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

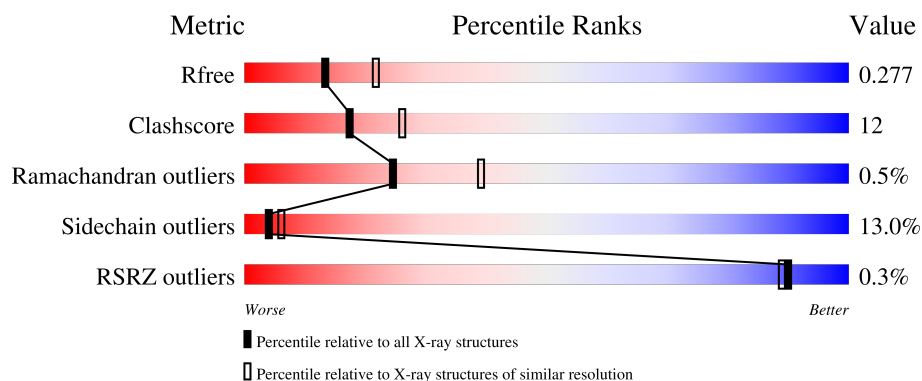
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	679	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5389 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 AetF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	628	5196	3339	879	963	15	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

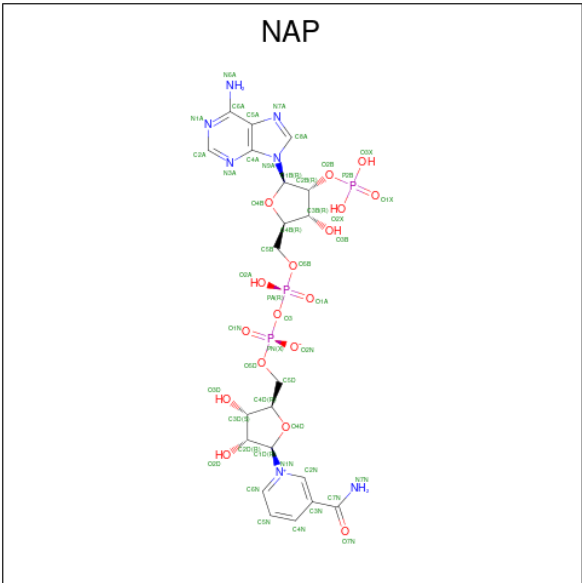
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP A0A861B9Z9
A	-9	ALA	-	expression tag	UNP A0A861B9Z9
A	-8	GLY	-	expression tag	UNP A0A861B9Z9
A	-7	ALA	-	expression tag	UNP A0A861B9Z9
A	-6	GLY	-	expression tag	UNP A0A861B9Z9
A	-5	ALA	-	expression tag	UNP A0A861B9Z9
A	-4	GLY	-	expression tag	UNP A0A861B9Z9
A	-3	ALA	-	expression tag	UNP A0A861B9Z9
A	-2	GLY	-	expression tag	UNP A0A861B9Z9
A	-1	ALA	-	expression tag	UNP A0A861B9Z9
A	0	GLY	-	expression tag	UNP A0A861B9Z9

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

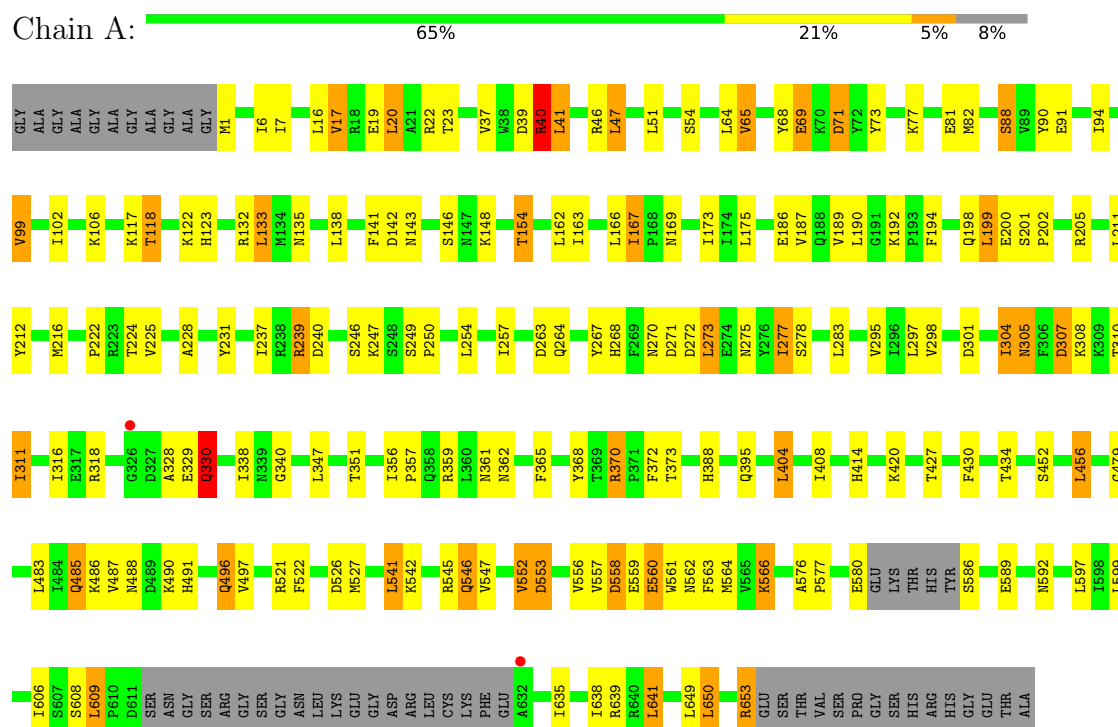
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total 92	O 92	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: AetF



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.08Å 75.47Å 143.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.56 – 2.66 24.56 – 2.66	Depositor EDS
% Data completeness (in resolution range)	95.6 (24.56-2.66) 96.7 (24.56-2.66)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.191 , 0.273 0.194 , 0.277	Depositor DCC
R_{free} test set	971 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.926	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5389	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.03	0/5330	1.50	10/7220 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	434	THR	N-CA-C	-6.35	104.28	111.14
1	A	586	SER	CA-C-N	6.21	128.89	120.38
1	A	586	SER	C-N-CA	6.21	128.89	120.38
1	A	71	ASP	CA-CB-CG	6.11	118.71	112.60
1	A	99	VAL	N-CA-CB	5.71	116.95	110.72
1	A	330	GLN	CB-CA-C	5.29	117.22	110.13
1	A	88	SER	CA-C-N	5.19	127.84	120.53
1	A	88	SER	C-N-CA	5.19	127.84	120.53
1	A	558	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	73	TYR	CB-CA-C	5.03	115.86	110.08

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5196	0	5061	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	31	1	0
3	A	48	0	25	3	0
4	A	92	0	0	7	0
All	All	5389	0	5117	130	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 12.

All (130) 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:562:ASN:O	1:A:566:LYS:HD2	1.64	0.97
1:A:305:ASN:OD1	1:A:308:LYS:HB3	1.81	0.80
1:A:270:ASN:ND2	1:A:271:ASP:OD1	2.18	0.76
1:A:118:THR:HG23	4:A:879:HOH:O	1.85	0.75
1:A:222:PRO:HA	1:A:231:TYR:CZ	2.21	0.75
1:A:237:ILE:HG23	1:A:297:LEU:HD11	1.68	0.74
1:A:304:ILE:HG22	1:A:311:ILE:HA	1.68	0.73
1:A:162:LEU:CD2	1:A:166:LEU:HD11	2.19	0.72
1:A:546:GLN:HE21	1:A:546:GLN:HA	1.53	0.71
1:A:118:THR:CG2	4:A:879:HOH:O	2.37	0.70
1:A:521:ARG:HD3	1:A:522:PHE:O	1.93	0.69
1:A:173:ILE:HB	1:A:295:VAL:HG22	1.76	0.67
1:A:304:ILE:HB	1:A:310:THR:O	1.96	0.66
1:A:304:ILE:HG21	1:A:311:ILE:HD12	1.76	0.66
3:A:702:NAP:N3A	3:A:702:NAP:H3B	2.11	0.66
1:A:553:ASP:O	1:A:556:VAL:HG23	1.97	0.65
1:A:485:GLN:HE21	1:A:485:GLN:HA	1.61	0.65
1:A:304:ILE:CG2	1:A:311:ILE:HA	2.27	0.64
1:A:222:PRO:HA	1:A:231:TYR:CE1	2.37	0.60
1:A:19:GLU:HB3	1:A:388:HIS:CD2	2.36	0.60
1:A:542:LYS:NZ	4:A:802:HOH:O	2.36	0.59
1:A:561:TRP:HA	1:A:564:MET:HG3	1.87	0.57
1:A:318:ARG:HH21	1:A:560:GLU:CG	2.19	0.56
1:A:305:ASN:HD22	1:A:305:ASN:N	2.03	0.56
1:A:307:ASP:N	1:A:307:ASP:OD1	2.39	0.55
1:A:328:ALA:O	1:A:330:GLN:N	2.38	0.55
1:A:162:LEU:O	1:A:162:LEU:HD23	2.07	0.55
1:A:305:ASN:O	1:A:305:ASN:ND2	2.38	0.55
1:A:560:GLU:O	1:A:564:MET:HG3	2.06	0.55
1:A:69:GLU:O	1:A:490:LYS:HE3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD12	1:A:497:VAL:HG22	1.89	0.54
1:A:496:GLN:H	1:A:496:GLN:CD	2.16	0.54
1:A:559:GLU:HG3	1:A:563:PHE:CE2	2.43	0.54
1:A:198:GLN:NE2	1:A:491:HIS:NE2	2.56	0.53
1:A:301:ASP:O	1:A:301:ASP:OD1	2.27	0.53
1:A:46:ARG:HD2	1:A:141:PHE:CZ	2.43	0.53
1:A:77:LYS:O	1:A:81:GLU:HG3	2.09	0.53
1:A:318:ARG:HH21	1:A:560:GLU:HG2	1.74	0.53
1:A:365:PHE:HB3	1:A:368:TYR:HD2	1.72	0.53
1:A:275:ASN:O	1:A:278:SER:HB3	2.08	0.53
1:A:365:PHE:HB3	1:A:368:TYR:CD2	2.44	0.53
1:A:186:GLU:OE1	1:A:268:HIS:NE2	2.42	0.52
1:A:545:ARG:NE	1:A:552:VAL:HG21	2.25	0.51
1:A:330:GLN:NE2	1:A:330:GLN:HA	2.25	0.50
1:A:305:ASN:OD1	1:A:308:LYS:CB	2.58	0.50
1:A:162:LEU:O	1:A:166:LEU:HG	2.12	0.50
1:A:541:LEU:O	1:A:545:ARG:HG3	2.11	0.49
1:A:40:ARG:HG3	4:A:878:HOH:O	2.12	0.49
1:A:257:ILE:HD12	1:A:257:ILE:N	2.27	0.49
1:A:132:ARG:O	1:A:135:ASN:HB2	2.13	0.49
1:A:249:SER:HA	1:A:250:PRO:C	2.37	0.49
1:A:46:ARG:CG	1:A:141:PHE:CE1	2.96	0.49
1:A:304:ILE:CG2	1:A:311:ILE:HD12	2.43	0.48
1:A:653:ARG:C	1:A:653:ARG:HE	2.21	0.48
1:A:239:ARG:NH2	3:A:702:NAP:O3X	2.46	0.48
1:A:370:ARG:O	1:A:427:THR:HA	2.14	0.48
1:A:167:ILE:HD11	1:A:173:ILE:HG13	1.96	0.48
1:A:521:ARG:HD3	1:A:521:ARG:C	2.39	0.48
1:A:237:ILE:CG2	1:A:297:LEU:HD11	2.39	0.48
1:A:263:ASP:OD2	1:A:521:ARG:NH2	2.47	0.48
1:A:51:LEU:HG	2:A:701:FAD:O4	2.14	0.48
1:A:338:ILE:C	1:A:340:GLY:N	2.70	0.47
1:A:212:TYR:CE2	1:A:216:MET:HG3	2.49	0.47
1:A:46:ARG:CD	1:A:141:PHE:CZ	2.98	0.47
1:A:133:LEU:HD22	1:A:328:ALA:HB2	1.95	0.47
1:A:606:ILE:O	1:A:609:LEU:HB2	2.15	0.47
1:A:638:ILE:HA	1:A:641:LEU:HD22	1.95	0.47
1:A:359:ARG:NH1	4:A:807:HOH:O	2.47	0.46
1:A:37:VAL:O	1:A:40:ARG:HB2	2.15	0.46
1:A:522:PHE:CE1	1:A:526:ASP:HA	2.50	0.46
1:A:123:HIS:HA	1:A:362:ASN:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:SER:HB3	1:A:497:VAL:CG1	2.45	0.46
1:A:237:ILE:HG23	1:A:297:LEU:CD1	2.43	0.46
1:A:456:LEU:HD13	1:A:606:ILE:HD13	1.97	0.46
1:A:7:ILE:CD1	1:A:102:ILE:HD11	2.45	0.46
1:A:491:HIS:O	1:A:496:GLN:OE1	2.34	0.45
1:A:82:MET:HE3	1:A:82:MET:HB3	1.90	0.45
1:A:202:PRO:O	1:A:205:ARG:HG2	2.15	0.45
1:A:167:ILE:HD11	1:A:173:ILE:CG1	2.47	0.45
1:A:141:PHE:N	1:A:141:PHE:CD1	2.84	0.45
1:A:338:ILE:C	1:A:340:GLY:H	2.25	0.45
1:A:452:SER:O	1:A:606:ILE:HD11	2.16	0.45
1:A:576:ALA:N	1:A:577:PRO:CD	2.80	0.45
1:A:154:THR:HG23	3:A:702:NAP:O3B	2.17	0.44
1:A:305:ASN:CG	1:A:308:LYS:HB3	2.41	0.44
1:A:372:PHE:CD2	1:A:373:THR:HG23	2.52	0.44
1:A:557:VAL:O	1:A:557:VAL:HG12	2.17	0.44
1:A:163:ILE:O	1:A:167:ILE:HD13	2.17	0.44
1:A:650:LEU:HD12	1:A:650:LEU:HA	1.85	0.44
1:A:106:LYS:HA	1:A:361:ASN:ND2	2.33	0.44
1:A:46:ARG:HG3	1:A:141:PHE:CE1	2.53	0.44
1:A:65:VAL:HG22	1:A:479:GLY:C	2.43	0.43
1:A:201:SER:HB3	1:A:497:VAL:HG11	2.00	0.43
1:A:225:VAL:HG12	1:A:225:VAL:O	2.18	0.43
1:A:305:ASN:HD22	1:A:305:ASN:H	1.63	0.43
1:A:264:GLN:O	1:A:268:HIS:HD2	2.02	0.43
1:A:91:GLU:HA	1:A:94:ILE:HD12	2.01	0.43
1:A:430:PHE:C	1:A:430:PHE:CD1	2.96	0.43
1:A:270:ASN:HD21	1:A:271:ASP:CG	2.27	0.42
1:A:305:ASN:ND2	1:A:305:ASN:H	2.18	0.42
1:A:194:PHE:CD2	1:A:199:LEU:HD11	2.54	0.42
1:A:17:VAL:HG12	1:A:90:TYR:CZ	2.54	0.42
1:A:404:LEU:O	1:A:408:ILE:HG13	2.20	0.42
1:A:20:LEU:HD12	1:A:20:LEU:HA	1.79	0.42
1:A:162:LEU:HD23	1:A:166:LEU:CD1	2.49	0.42
1:A:357:PRO:HG2	4:A:820:HOH:O	2.20	0.42
1:A:162:LEU:HD23	1:A:162:LEU:C	2.44	0.42
1:A:246:SER:OG	1:A:414:HIS:O	2.38	0.42
1:A:589:GLU:N	1:A:589:GLU:CD	2.78	0.42
1:A:211:LEU:C	1:A:211:LEU:HD13	2.45	0.41
1:A:641:LEU:HD12	1:A:641:LEU:HA	1.89	0.41
1:A:173:ILE:CB	1:A:295:VAL:HG22	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:THR:HG22	1:A:231:TYR:OH	2.20	0.41
1:A:305:ASN:N	1:A:305:ASN:ND2	2.68	0.41
1:A:68:TYR:O	1:A:69:GLU:OE1	2.39	0.41
1:A:228:ALA:O	1:A:527:MET:HG2	2.21	0.41
1:A:487:VAL:O	1:A:488:ASN:C	2.62	0.41
1:A:20:LEU:CD1	1:A:388:HIS:HD2	2.34	0.41
1:A:200:GLU:O	1:A:201:SER:C	2.63	0.41
1:A:270:ASN:ND2	1:A:271:ASP:CG	2.78	0.41
1:A:273:LEU:O	1:A:277:ILE:HG13	2.21	0.41
1:A:23:THR:HG21	1:A:388:HIS:CE1	2.56	0.40
1:A:37:VAL:O	1:A:41:LEU:HD22	2.21	0.40
1:A:169:ASN:HA	1:A:552:VAL:HG11	2.03	0.40
1:A:187:VAL:HG12	1:A:189:VAL:HG23	2.02	0.40
1:A:41:LEU:HB3	1:A:47:LEU:HD13	2.02	0.40
1:A:54:SER:HB2	4:A:875:HOH:O	2.21	0.40
1:A:143:ASN:O	1:A:143:ASN:OD1	2.39	0.40
1:A:190:LEU:H	1:A:190:LEU:HD23	1.87	0.40
1:A:351:THR:HA	1:A:356:ILE:O	2.21	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	622/679 (92%)	576 (93%)	43 (7%)	3 (0%)	24	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	272	ASP
1	A	329	GLU
1	A	40	ARG

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	570/603 (94%)	496 (87%)	74 (13%)	4 6

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	6	ILE
1	A	16	LEU
1	A	17	VAL
1	A	20	LEU
1	A	22	ARG
1	A	39	ASP
1	A	40	ARG
1	A	41	LEU
1	A	47	LEU
1	A	64	LEU
1	A	65	VAL
1	A	69	GLU
1	A	71	ASP
1	A	88	SER
1	A	99	VAL
1	A	117	LYS
1	A	118	THR
1	A	122	LYS
1	A	133	LEU
1	A	138	LEU
1	A	142	ASP
1	A	146	SER
1	A	148	LYS
1	A	154	THR
1	A	167	ILE
1	A	175	LEU
1	A	192	LYS
1	A	199	LEU
1	A	239	ARG

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Mol	Chain	Res	Type
1	A	240	ASP
1	A	247	LYS
1	A	254	LEU
1	A	267	TYR
1	A	273	LEU
1	A	277	ILE
1	A	283	LEU
1	A	298	VAL
1	A	304	ILE
1	A	305	ASN
1	A	307	ASP
1	A	311	ILE
1	A	316	ILE
1	A	330	GLN
1	A	347	LEU
1	A	370	ARG
1	A	395	GLN
1	A	404	LEU
1	A	420	LYS
1	A	456	LEU
1	A	483	LEU
1	A	485	GLN
1	A	486	LYS
1	A	496	GLN
1	A	541	LEU
1	A	546	GLN
1	A	547	VAL
1	A	552	VAL
1	A	553	ASP
1	A	558	ASP
1	A	560	GLU
1	A	566	LYS
1	A	580	GLU
1	A	592	ASN
1	A	597	LEU
1	A	599	LEU
1	A	608	SER
1	A	609	LEU
1	A	635	ILE
1	A	639	ARG
1	A	641	LEU
1	A	649	LEU

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Mol	Chain	Res	Type
1	A	650	LEU
1	A	653	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN
1	A	171	ASN
1	A	264	GLN
1	A	270	ASN
1	A	275	ASN
1	A	305	ASN
1	A	330	GLN
1	A	358	GLN
1	A	361	ASN
1	A	395	GLN
1	A	413	GLN
1	A	426	HIS
1	A	485	GLN
1	A	496	GLN
1	A	546	GLN
1	A	592	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	0.74	2 (3%)	85,89,89	0.92	5 (5%)
3	NAP	A	702	-	50,52,52	1.63	6 (12%)	71,80,80	1.92	13 (18%)

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	-	-	5/34/50/50	0/6/6/6
3	NAP	A	702	-	-	7/35/67/67	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	NAP	PN-O3	5.46	1.65	1.59
3	A	702	NAP	C5A-C4A	5.08	1.48	1.39
3	A	702	NAP	PA-O3	5.03	1.64	1.59
3	A	702	NAP	C5A-C6A	3.82	1.51	1.41
3	A	702	NAP	C8A-N7A	2.70	1.36	1.31
2	A	701	FAD	PA-O3P	2.32	1.62	1.59
3	A	702	NAP	O4D-C1D	2.05	1.43	1.40
2	A	701	FAD	C8A-N9A	-2.04	1.34	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAP	C5A-C4A-N3A	-6.42	117.87	126.72
3	A	702	NAP	N3A-C4A-N9A	5.09	135.82	127.17
3	A	702	NAP	C4A-C5A-N7A	-4.95	104.92	110.58
3	A	702	NAP	C2B-C1B-N9A	-4.57	106.22	113.75
3	A	702	NAP	C2A-N3A-C4A	4.41	122.60	111.83
3	A	702	NAP	C4A-N9A-C8A	4.01	109.95	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NAP	C5A-N7A-C8A	3.98	109.71	103.45
3	A	702	NAP	N3A-C2A-N1A	-3.82	122.81	128.58
3	A	702	NAP	N9A-C8A-N7A	-3.41	109.11	113.94
3	A	702	NAP	C6A-C5A-N7A	3.05	137.98	132.09
3	A	702	NAP	O2B-P2B-O1X	-2.58	100.13	109.33
3	A	702	NAP	C6N-N1N-C2N	-2.51	119.74	121.88
2	A	701	FAD	O5'-P-O1P	2.33	118.15	108.94
3	A	702	NAP	C5N-C4N-C3N	-2.32	118.09	120.36
2	A	701	FAD	O4B-C1B-N9A	-2.25	103.78	108.09
2	A	701	FAD	C4-N3-C2	-2.22	121.70	125.64
2	A	701	FAD	C5'-C4'-C3'	2.22	116.40	112.22
2	A	701	FAD	O4'-C4'-C3'	-2.20	104.10	109.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	N10-C1'-C2'-O2'
2	A	701	FAD	N10-C1'-C2'-C3'
2	A	701	FAD	C5'-O5'-P-O1P
2	A	701	FAD	C5'-O5'-P-O2P
2	A	701	FAD	C5'-O5'-P-O3P
3	A	702	NAP	C3D-C4D-C5D-O5D
3	A	702	NAP	C4D-C5D-O5D-PN
3	A	702	NAP	O4D-C4D-C5D-O5D
3	A	702	NAP	C1B-C2B-O2B-P2B
3	A	702	NAP	PA-O3-PN-O5D
3	A	702	NAP	C3B-C2B-O2B-P2B
3	A	702	NAP	PA-O3-PN-O2N

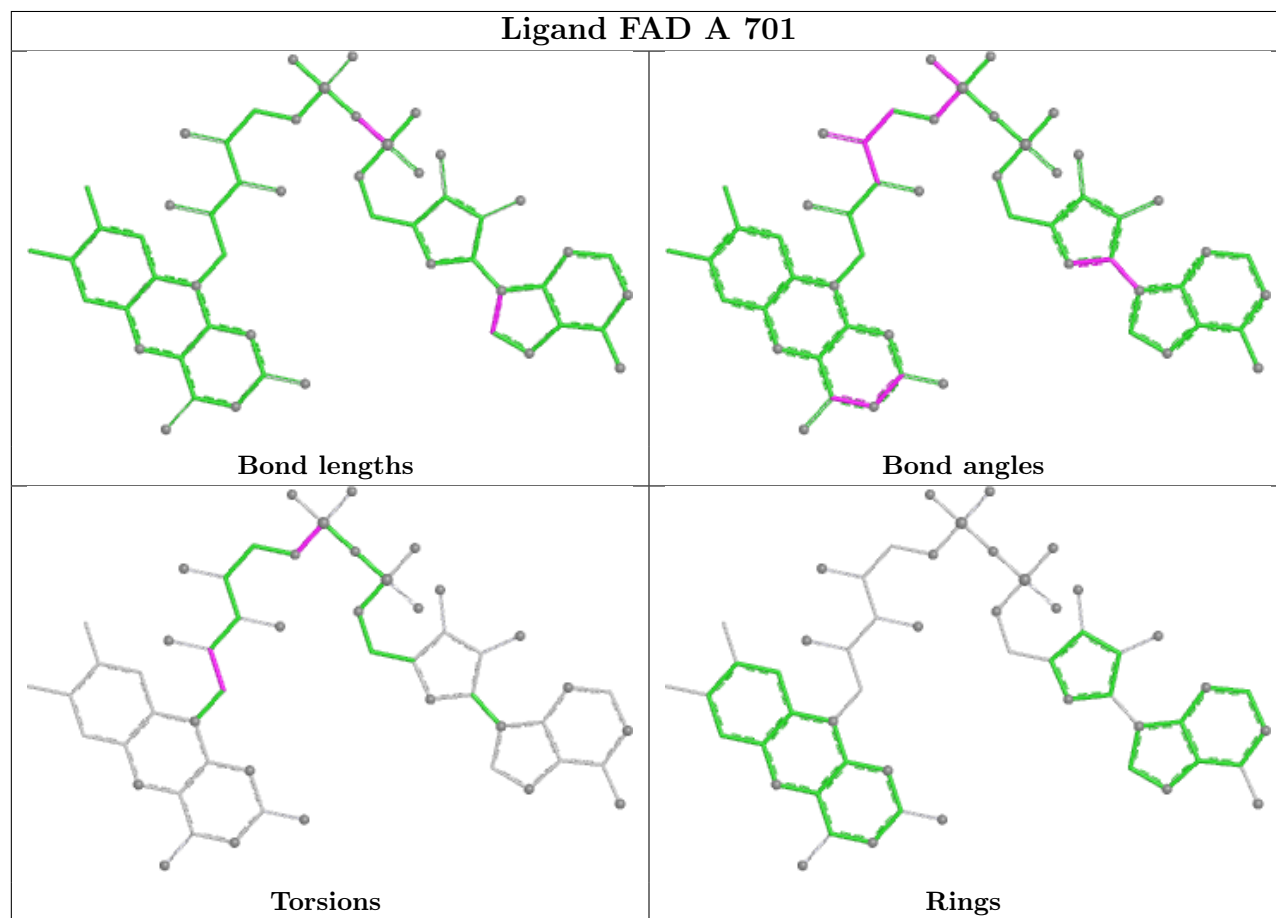
There are no ring outliers.

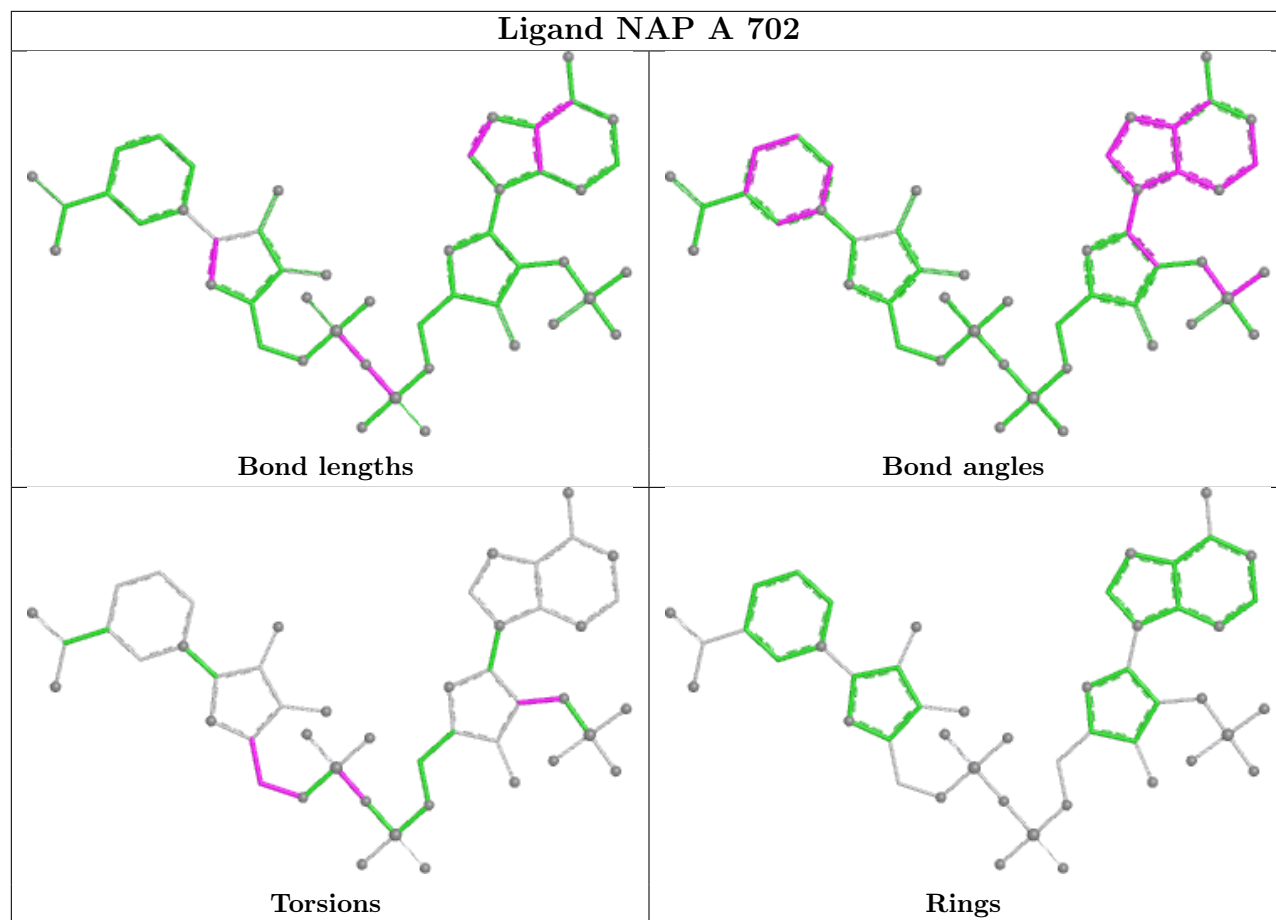
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAD	1	0
3	A	702	NAP	3	0

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

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	628/679 (92%)	-0.34	2 (0%) 90 89	31, 54, 92, 129	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	632	ALA	2.2
1	A	326	GLY	2.1

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.

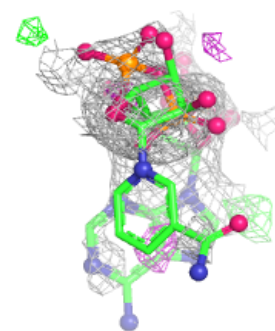
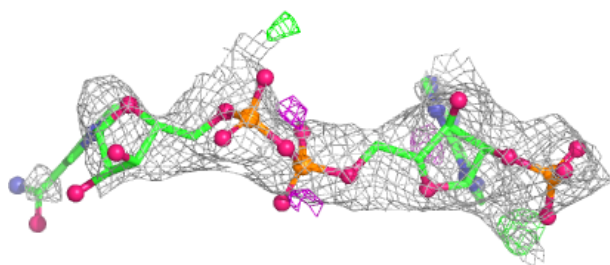
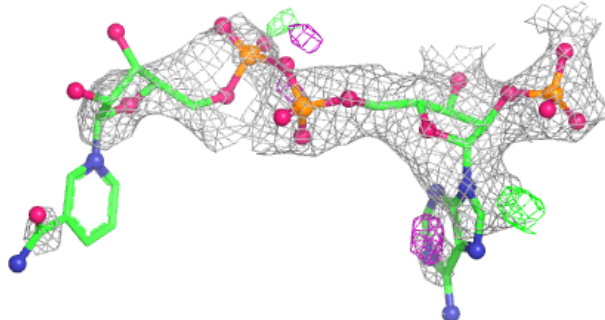
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAP	A	702	48/48	0.77	0.12	94,115,162,169	0
2	FAD	A	701	53/53	0.96	0.07	32,44,77,80	0

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.

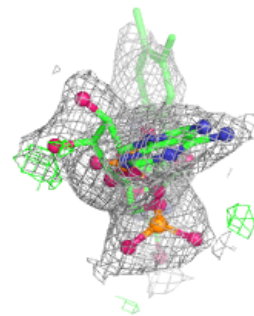
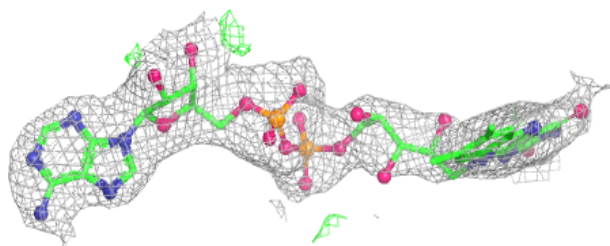
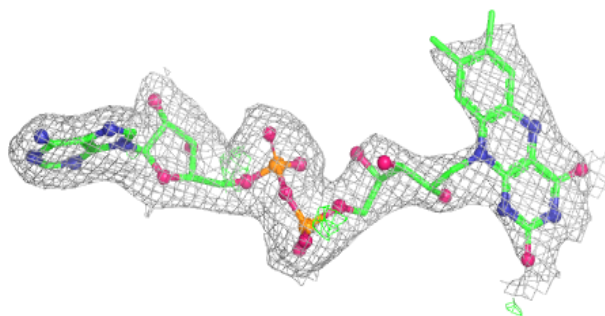
Electron density around NAP A 702:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.