



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:07 AM EDT

PDB ID : 9ENH / pdb_00009enh
Title : L-amino acid oxidase 4 (HcLAAO4) from the fungus Hebeloma cylindrosporum
Authors : Gilzer, D.; Koopmeiners, S.; Fischer von Mollard, G.; Niemann, H.H.
Deposited on : 2024-03-13
Resolution : 2.30 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

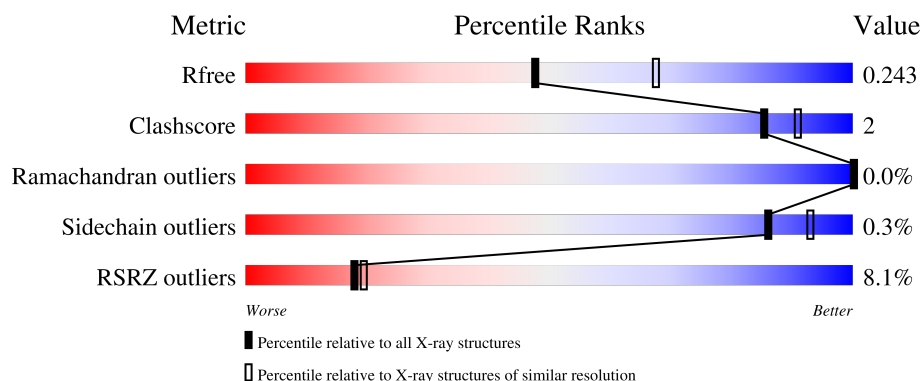
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	562	5% 91% 5%
1	B	562	2% 90% 5% 5%
1	C	562	4% 89% 5% 6%
1	D	562	19% 86% 6% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33682 atoms, of which 16412 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.

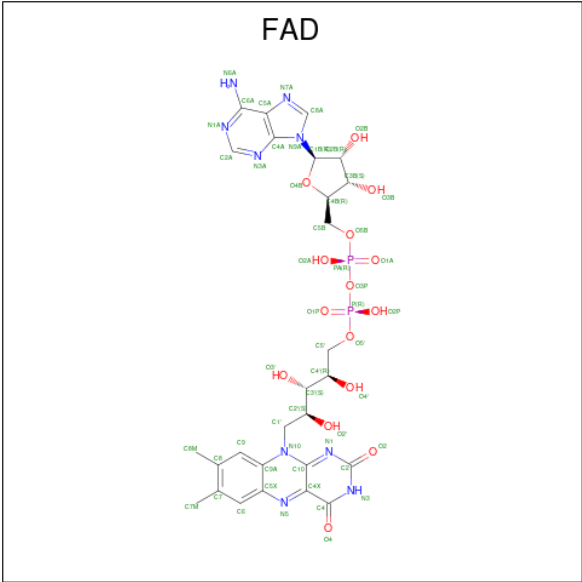
- Molecule 1 is a protein called L-amino acid oxidase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	544	Total	C	H	N	O	S	0	3	0
			8436	2759	4150	718	797	12			
1	B	532	Total	C	H	N	O	S	0	3	0
			8304	2718	4086	708	781	11			
1	C	531	Total	C	H	N	O	S	0	3	0
			8275	2709	4070	705	780	11			
1	D	520	Total	C	H	N	O	S	0	1	0
			8078	2646	3974	688	759	11			

There are 8 discrepancies between the modelled and reference sequences:

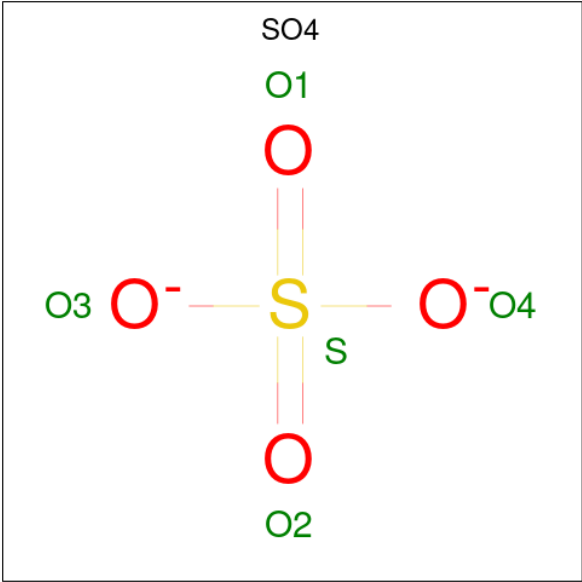
Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ALA	LYS	engineered mutation	UNP S4S6Z0
A	475	ALA	LYS	engineered mutation	UNP S4S6Z0
B	474	ALA	LYS	engineered mutation	UNP S4S6Z0
B	475	ALA	LYS	engineered mutation	UNP S4S6Z0
C	474	ALA	LYS	engineered mutation	UNP S4S6Z0
C	475	ALA	LYS	engineered mutation	UNP S4S6Z0
D	474	ALA	LYS	engineered mutation	UNP S4S6Z0
D	475	ALA	LYS	engineered mutation	UNP S4S6Z0

- 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 84	C 27	H 31	N 9	O 15	P 2	0	0
2	B	1	Total 84	C 27	H 31	N 9	O 15	P 2	0	0
2	C	1	Total 84	C 27	H 31	N 9	O 15	P 2	0	0
2	D	1	Total 84	C 27	H 31	N 9	O 15	P 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



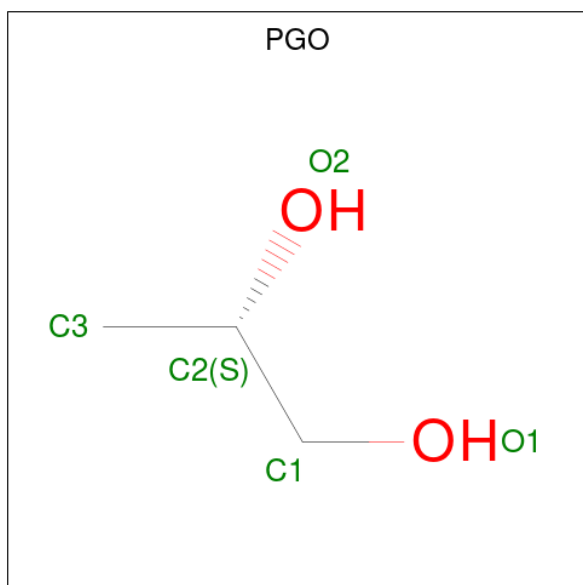
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0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

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

- Molecule 4 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			13	3	8	2		

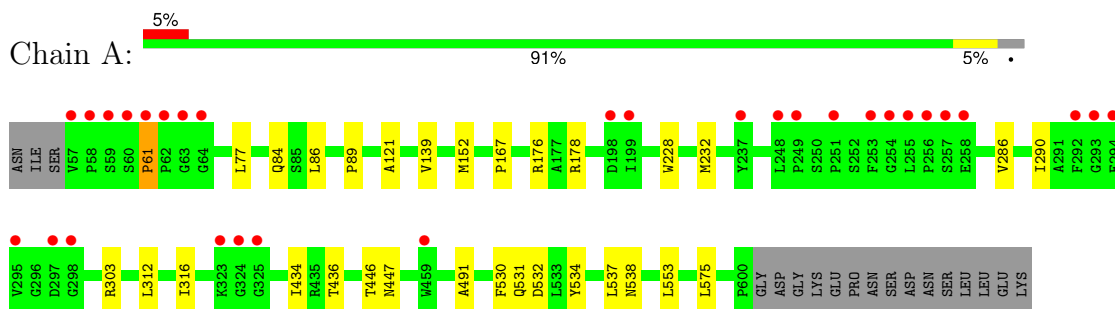
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	B	22	Total	O	0	0
			22	22		
5	C	44	Total	O	0	0
			44	44		
5	D	27	Total	O	0	0
			27	27		

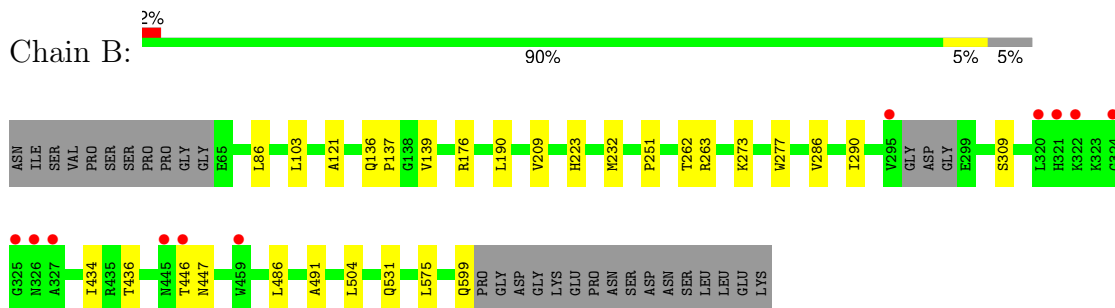
3 Residue-property plots

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.

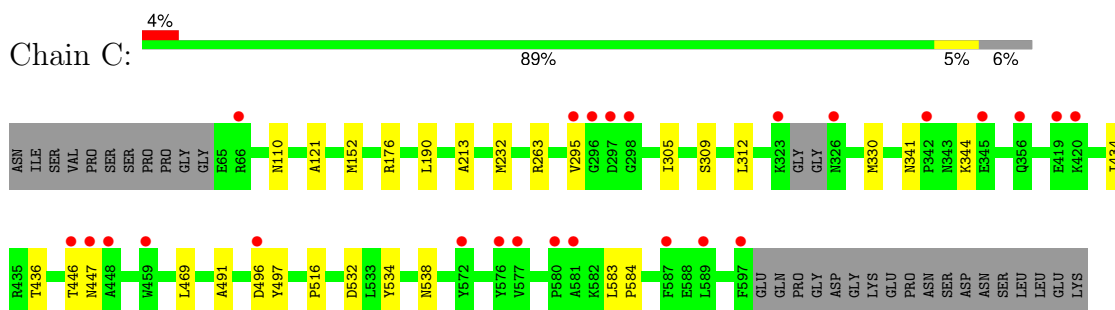
- Molecule 1: L-amino acid oxidase 4



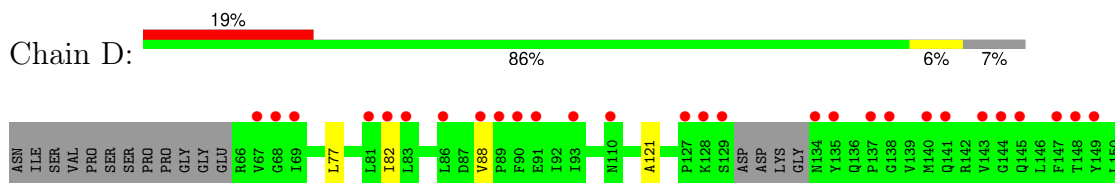
- Molecule 1: L-amino acid oxidase 4

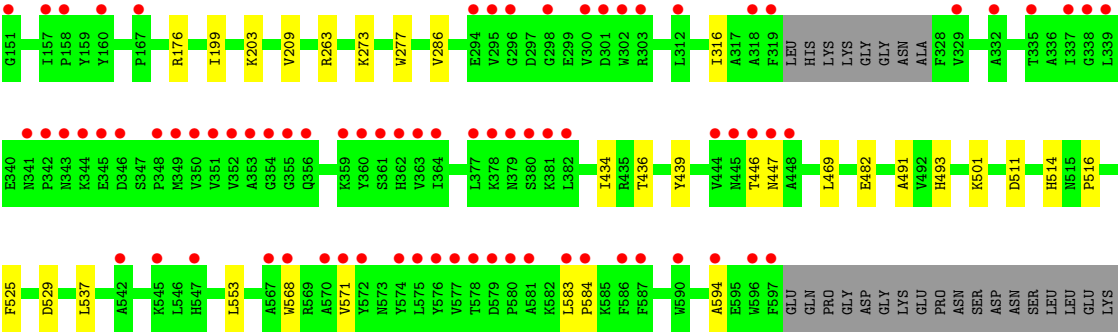


- Molecule 1: L-amino acid oxidase 4



- Molecule 1: L-amino acid oxidase 4





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	156.64Å 158.28Å 217.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.56 – 2.30 49.56 – 2.30	Depositor EDS
% Data completeness (in resolution range)	70.5 (49.56-2.30) 70.5 (49.56-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.211 , 0.246 0.210 , 0.243	Depositor DCC
R_{free} test set	4217 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33682	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: SO4, FAD, PGO

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	0.09	0/4421	0.25	0/6016
1	B	0.09	0/4349	0.25	0/5914
1	C	0.09	0/4335	0.25	0/5896
1	D	0.09	0/4225	0.26	0/5747
All	All	0.09	0/17330	0.25	0/23573

There are no bond length outliers.

There are no bond angle outliers.

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	4286	4150	4150	21	0
1	B	4218	4086	4086	18	0
1	C	4205	4070	4073	18	0
1	D	4104	3974	3974	23	0
2	A	53	31	31	1	0
2	B	53	31	31	0	0
2	C	53	31	31	1	0
2	D	53	31	31	1	0
3	A	40	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	40	0	0	1	0
3	C	20	0	0	0	0
3	D	20	0	0	0	0
4	A	5	8	8	0	0
5	A	27	0	0	1	0
5	B	22	0	0	0	0
5	C	44	0	0	0	0
5	D	27	0	0	0	0
All	All	17270	16412	16415	74	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 (74) 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:C:496[A]:ASP:OD1	1:C:497:TYR:N	2.27	0.66
1:C:516:PRO:HB3	1:D:469:LEU:HD23	1.83	0.60
1:D:209:VAL:HG13	1:D:286:VAL:HG22	1.83	0.60
1:B:176:ARG:NH1	1:B:491:ALA:O	2.35	0.59
1:C:341:ASN:ND2	1:C:344:LYS:HG3	2.18	0.59
1:A:167:PRO:O	1:A:178:ARG:NH1	2.36	0.58
1:B:103:LEU:HD12	1:B:309:SER:HB3	1.85	0.57
1:B:103:LEU:HD13	1:B:121:ALA:HB3	1.87	0.56
1:A:86:LEU:CD1	1:A:575:LEU:HD11	2.37	0.55
1:C:176:ARG:NH1	1:C:491:ALA:O	2.40	0.54
1:A:152:MET:HE1	1:A:312:LEU:HD12	1.89	0.54
1:A:303:ARG:NH2	5:A:801:HOH:O	2.41	0.54
1:A:176:ARG:NH1	1:A:491:ALA:O	2.41	0.53
1:C:213:ALA:HB1	1:C:295:VAL:HG21	1.90	0.53
1:B:232:MET:O	1:B:531:GLN:NE2	2.43	0.52
1:C:232:MET:HA	1:C:232:MET:HE2	1.92	0.51
1:D:537:LEU:CB	1:D:553:LEU:HD11	2.40	0.51
1:A:232:MET:HE1	1:A:530:PHE:HB3	1.92	0.51
1:A:532:ASP:OD1	1:B:263:ARG:NE	2.43	0.50
1:A:152:MET:HE1	1:A:312:LEU:CD1	2.41	0.50
1:C:534:TYR:O	1:C:538:ASN:ND2	2.45	0.49
1:C:532:ASP:OD1	1:D:263:ARG:NE	2.46	0.48
1:B:86:LEU:CD1	1:B:575:LEU:HD11	2.43	0.48
1:A:232:MET:HE1	1:A:530:PHE:CB	2.43	0.48
1:C:446:THR:HG22	1:C:447:ASN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:511:ASP:OD2	1:D:514[A]:HIS:ND1	2.44	0.47
1:A:232:MET:HE2	1:A:531:GLN:HA	1.97	0.47
1:A:446:THR:HG22	1:A:447:ASN:N	2.29	0.47
1:D:439:TYR:OH	1:D:493:HIS:NE2	2.41	0.47
1:B:273:LYS:HD3	1:B:277:TRP:CD2	2.50	0.47
1:B:486:LEU:HD11	1:B:504:LEU:HD13	1.97	0.46
1:C:152:MET:HE1	1:C:312:LEU:HD12	1.98	0.46
1:A:534:TYR:O	1:A:538:ASN:ND2	2.48	0.46
1:D:446:THR:HG22	1:D:447:ASN:N	2.30	0.46
1:A:121:ALA:HA	2:A:701:FAD:C4X	2.46	0.46
1:D:176:ARG:NH1	1:D:491:ALA:O	2.49	0.46
1:B:446:THR:HG22	1:B:447:ASN:N	2.31	0.46
1:D:121:ALA:HA	2:D:701:FAD:C4X	2.47	0.45
1:B:139:VAL:HG21	1:B:290:ILE:HG22	1.98	0.45
1:D:537:LEU:HB3	1:D:553:LEU:HD11	1.98	0.45
1:C:190:LEU:O	1:C:263:ARG:NH1	2.44	0.44
1:A:434:ILE:O	1:A:436:THR:N	2.46	0.44
1:B:273:LYS:HD3	1:B:277:TRP:CE2	2.52	0.44
1:A:537:LEU:CB	1:A:553:LEU:HD11	2.47	0.44
1:A:61:PRO:HA	1:A:89:PRO:HG2	2.00	0.44
1:B:223:HIS:ND1	3:B:703:SO4:O3	2.42	0.44
1:C:121:ALA:HA	2:C:701:FAD:C4X	2.48	0.44
1:A:228:TRP:O	1:A:232:MET:HG2	2.18	0.44
1:C:305:ILE:HD12	1:C:309:SER:HA	2.00	0.44
1:C:469:LEU:HD23	1:D:516:PRO:HB3	2.00	0.43
1:D:583:LEU:N	1:D:584:PRO:HD2	2.33	0.43
1:D:199:ILE:HG23	1:D:203:LYS:HD2	2.01	0.43
1:D:82:ILE:HG21	1:D:571:VAL:HG11	2.00	0.43
1:B:434:ILE:O	1:B:436:THR:N	2.44	0.43
1:C:152:MET:HE1	1:C:312:LEU:CD1	2.49	0.43
1:C:583:LEU:N	1:C:584:PRO:HD2	2.33	0.43
1:A:139:VAL:HG21	1:A:290:ILE:HG22	2.00	0.42
1:D:568:TRP:CE3	1:D:594:ALA:HB2	2.54	0.42
1:D:77:LEU:HB3	1:D:316:ILE:HG21	2.02	0.42
1:D:82:ILE:CG2	1:D:571:VAL:HG11	2.50	0.42
1:D:434:ILE:O	1:D:436:THR:N	2.52	0.42
1:D:525:PHE:HB3	1:D:529:ASP:HB2	2.01	0.42
1:C:434:ILE:O	1:C:436:THR:N	2.47	0.42
1:B:251:PRO:HG2	1:C:330:MET:HE2	2.00	0.42
1:D:537:LEU:HB2	1:D:553:LEU:HD11	2.01	0.42
1:A:531:GLN:OE1	1:B:262:THR:OG1	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:482:GLU:OE2	1:D:501:LYS:NZ	2.50	0.41
1:A:537:LEU:HB2	1:A:553:LEU:HD11	2.03	0.41
1:A:77:LEU:HB3	1:A:316:ILE:HG21	2.02	0.41
1:D:273:LYS:HD3	1:D:277:TRP:CE2	2.55	0.41
1:B:190:LEU:O	1:B:263:ARG:NH1	2.47	0.41
1:B:136:GLN:HB3	1:B:137:PRO:HD2	2.03	0.41
1:B:209:VAL:HG13	1:B:286:VAL:HG22	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	545/562 (97%)	524 (96%)	20 (4%)	1 (0%)	43	55
1	B	531/562 (94%)	514 (97%)	17 (3%)	0	100	100
1	C	530/562 (94%)	511 (96%)	19 (4%)	0	100	100
1	D	515/562 (92%)	498 (97%)	17 (3%)	0	100	100
All	All	2121/2248 (94%)	2047 (96%)	73 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	61	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	454/467 (97%)	452 (100%)	2 (0%)	84	92
1	B	446/467 (96%)	445 (100%)	1 (0%)	87	94
1	C	445/467 (95%)	444 (100%)	1 (0%)	87	94
1	D	434/467 (93%)	433 (100%)	1 (0%)	87	94
All	All	1779/1868 (95%)	1774 (100%)	5 (0%)	86	93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	286	VAL
1	B	599	GLN
1	C	110	ASN
1	D	88	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	394	GLN
1	A	427	GLN
1	B	153	HIS
1	B	461	ASN
1	B	488	ASN
1	B	515	ASN
1	B	538	ASN
1	C	153	HIS
1	C	341	ASN
1	C	394	GLN
1	C	461	ASN
1	C	531	GLN
1	D	153	HIS
1	D	170	GLN

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](#)

29 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	$\# Z > 2$
3	SO4	A	706	-	4,4,4	0.68	0	6,6,6	0.08	0
3	SO4	C	703	-	4,4,4	0.67	0	6,6,6	0.08	0
3	SO4	A	704	-	4,4,4	0.67	0	6,6,6	0.07	0
2	FAD	B	701	-	58,58,58	1.30	3 (5%)	85,89,89	0.83	2 (2%)
3	SO4	D	703	-	4,4,4	0.67	0	6,6,6	0.09	0
3	SO4	A	705	-	4,4,4	0.68	0	6,6,6	0.08	0
3	SO4	A	703	-	4,4,4	0.67	0	6,6,6	0.09	0
3	SO4	B	709	-	4,4,4	0.67	0	6,6,6	0.08	0
4	PGO	A	710	-	4,4,4	0.60	0	4,4,4	0.97	0
3	SO4	D	702	-	4,4,4	0.68	0	6,6,6	0.07	0
2	FAD	C	701	-	58,58,58	1.27	3 (5%)	85,89,89	0.83	2 (2%)
3	SO4	A	702	-	4,4,4	0.68	0	6,6,6	0.09	0
3	SO4	C	705	-	4,4,4	0.67	0	6,6,6	0.08	0
3	SO4	B	704	-	4,4,4	0.67	0	6,6,6	0.09	0
3	SO4	A	709	-	4,4,4	0.67	0	6,6,6	0.08	0
3	SO4	B	702	-	4,4,4	0.68	0	6,6,6	0.07	0
2	FAD	A	701	-	58,58,58	1.28	3 (5%)	85,89,89	0.84	2 (2%)
3	SO4	A	707	-	4,4,4	0.68	0	6,6,6	0.10	0
3	SO4	B	706	-	4,4,4	0.67	0	6,6,6	0.08	0
3	SO4	A	708	-	4,4,4	0.67	0	6,6,6	0.09	0
3	SO4	B	705	-	4,4,4	0.68	0	6,6,6	0.08	0
3	SO4	D	704	-	4,4,4	0.68	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	703	-	4,4,4	0.67	0	6,6,6	0.07	0
2	FAD	D	701	-	58,58,58	1.25	3 (5%)	85,89,89	0.83	2 (2%)
3	SO4	B	708	-	4,4,4	0.68	0	6,6,6	0.08	0
3	SO4	B	707	-	4,4,4	0.68	0	6,6,6	0.08	0
3	SO4	C	702	-	4,4,4	0.67	0	6,6,6	0.09	0
3	SO4	C	704	-	4,4,4	0.68	0	6,6,6	0.07	0
3	SO4	D	705	-	4,4,4	0.68	0	6,6,6	0.08	0

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
4	PGO	A	710	-	-	0/2/2/2	-
2	FAD	D	701	-	-	2/34/50/50	0/6/6/6
2	FAD	A	701	-	-	1/34/50/50	0/6/6/6
2	FAD	B	701	-	-	2/34/50/50	0/6/6/6
2	FAD	C	701	-	-	2/34/50/50	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	P-O3P	6.46	1.66	1.59
2	A	701	FAD	P-O3P	6.33	1.66	1.59
2	C	701	FAD	P-O3P	6.31	1.66	1.59
2	D	701	FAD	P-O3P	6.05	1.66	1.59
2	B	701	FAD	PA-O3P	3.90	1.63	1.59
2	A	701	FAD	PA-O3P	3.81	1.63	1.59
2	C	701	FAD	PA-O3P	3.78	1.63	1.59
2	D	701	FAD	PA-O3P	3.56	1.63	1.59
2	C	701	FAD	C5X-N5	-2.37	1.35	1.39
2	D	701	FAD	C5X-N5	-2.36	1.35	1.39
2	B	701	FAD	C5X-N5	-2.34	1.35	1.39
2	A	701	FAD	C5X-N5	-2.33	1.35	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	FAD	O2P-P-O1P	2.27	123.00	112.44
2	D	701	FAD	O2P-P-O1P	2.26	122.95	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FAD	O2P-P-O1P	2.26	122.94	112.44
2	C	701	FAD	O2P-P-O1P	2.24	122.88	112.44
2	C	701	FAD	C5'-C4'-C3'	-2.21	108.05	112.22
2	B	701	FAD	O2A-PA-O1A	2.08	122.14	112.44
2	A	701	FAD	O2A-PA-O1A	2.03	121.91	112.44
2	D	701	FAD	O2A-PA-O1A	2.03	121.87	112.44

There are no chirality outliers.

All (7) torsion outliers are listed below:

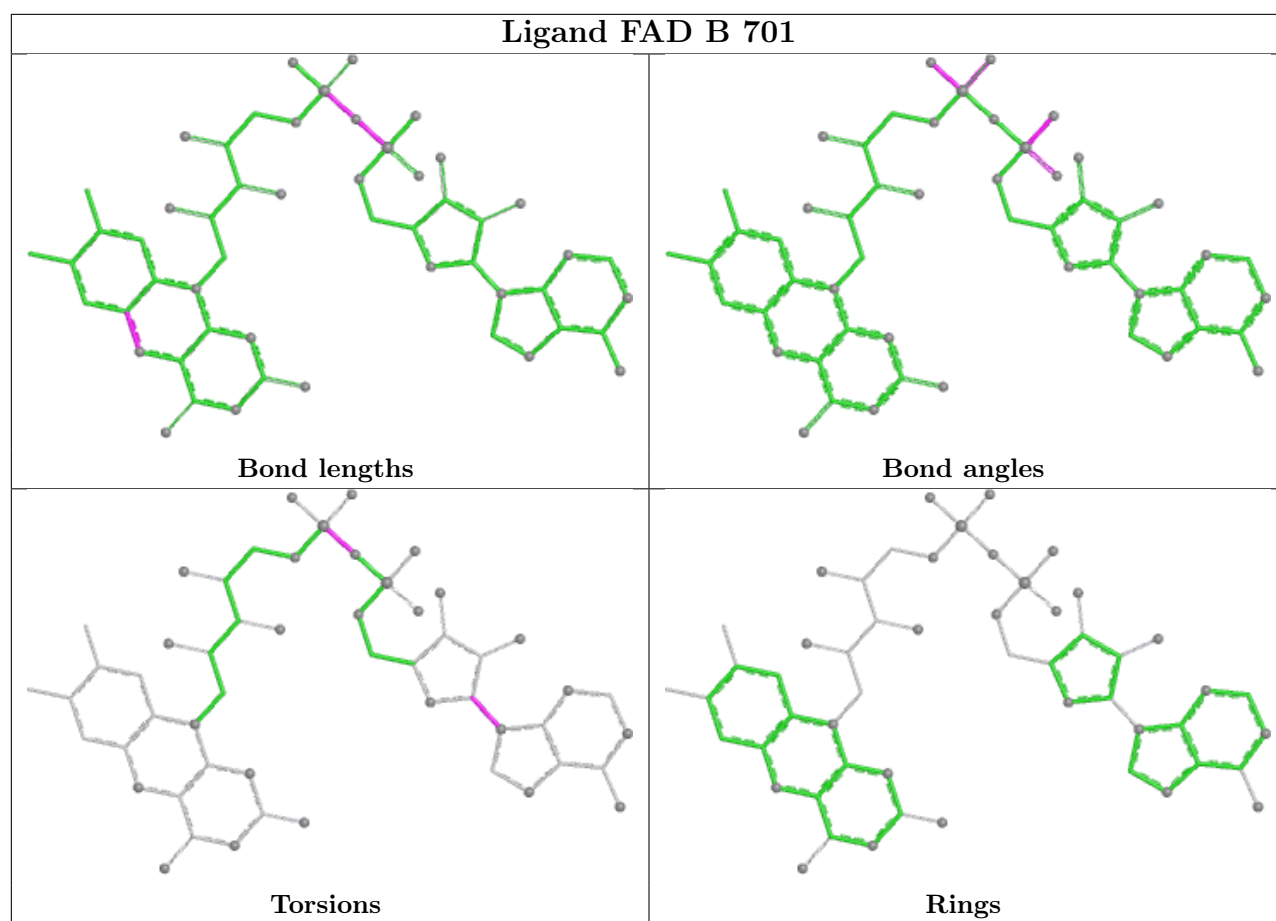
Mol	Chain	Res	Type	Atoms
2	D	701	FAD	PA-O3P-P-O5'
2	B	701	FAD	PA-O3P-P-O5'
2	C	701	FAD	PA-O3P-P-O5'
2	A	701	FAD	C2B-C1B-N9A-C8A
2	B	701	FAD	C2B-C1B-N9A-C8A
2	C	701	FAD	C2B-C1B-N9A-C8A
2	D	701	FAD	C2B-C1B-N9A-C8A

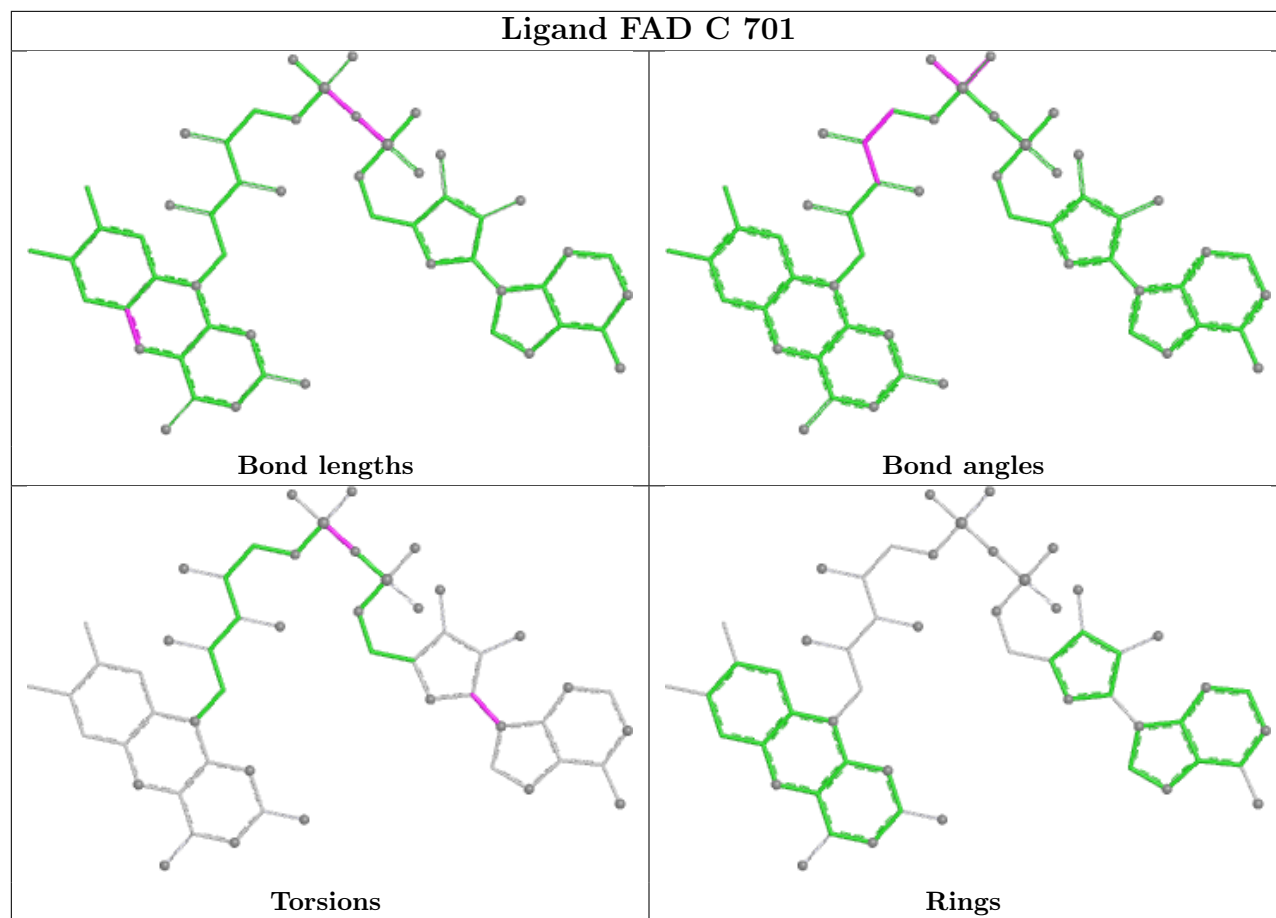
There are no ring outliers.

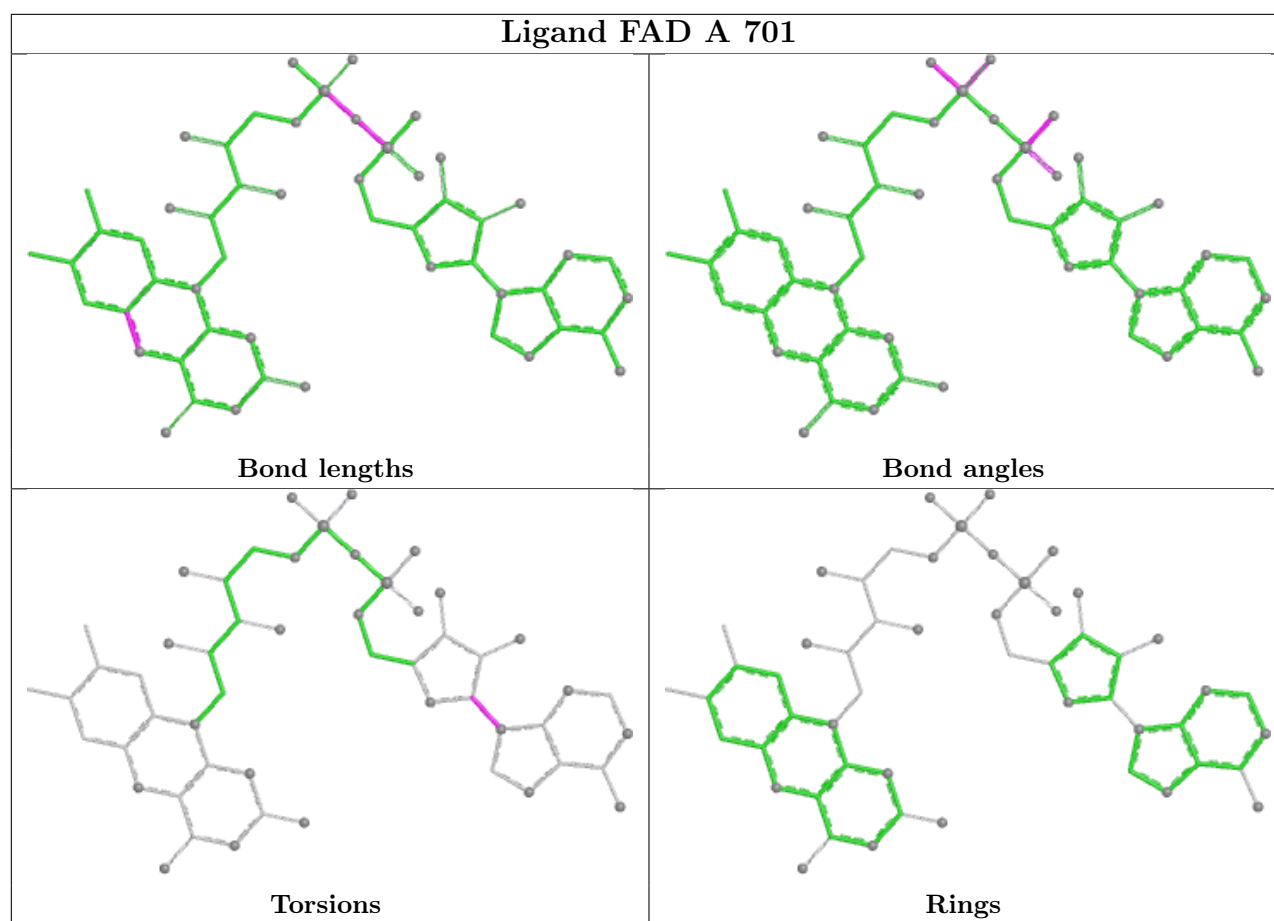
4 monomers are involved in 4 short contacts:

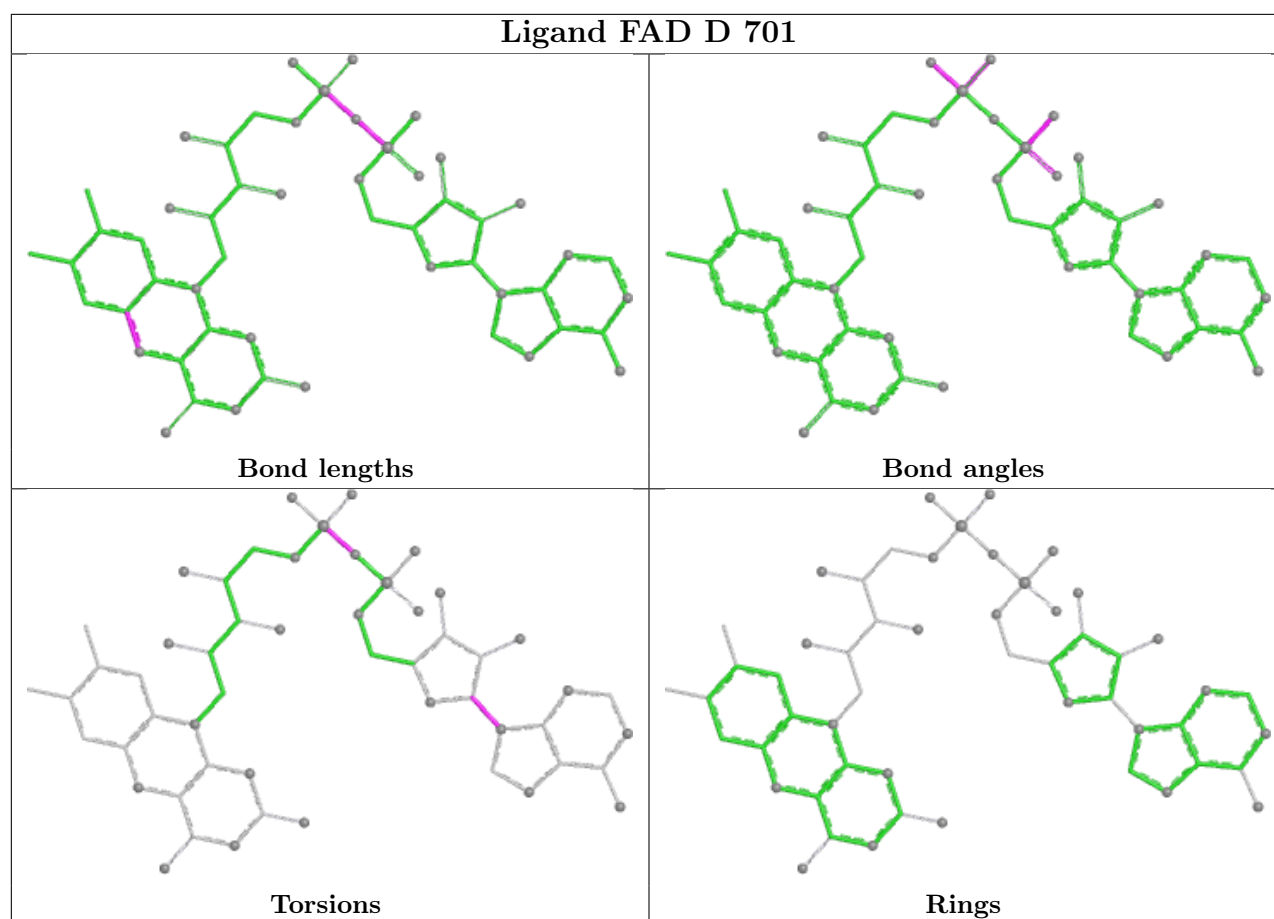
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	FAD	1	0
2	A	701	FAD	1	0
3	B	703	SO4	1	0
2	D	701	FAD	1	0

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

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	544/562 (96%)	0.34	30 (5%)	30	32	24, 52, 91, 133	3 (0%)
1	B	532/562 (94%)	0.30	11 (2%)	63	65	26, 53, 81, 133	3 (0%)
1	C	531/562 (94%)	0.33	25 (4%)	36	38	22, 55, 90, 122	3 (0%)
1	D	520/562 (92%)	0.94	106 (20%)	3	3	26, 65, 108, 141	1 (0%)
All	All	2127/2248 (94%)	0.48	172 (8%)	18	19	22, 55, 96, 141	10 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	576	TYR	6.4
1	A	257	SER	6.2
1	A	256	PRO	6.1
1	D	90	PHE	5.7
1	A	62	PRO	5.7
1	D	571	VAL	5.3
1	B	321[A]	HIS	5.1
1	D	129	SER	5.1
1	A	63	GLY	4.9
1	D	319	PHE	4.7
1	A	295	VAL	4.7
1	D	89	PRO	4.5
1	D	135	TYR	4.5
1	A	58	PRO	4.5
1	D	134	ASN	4.5
1	D	338	GLY	4.2
1	D	350	VAL	4.2
1	B	295	VAL	4.1
1	A	57	VAL	4.1
1	D	575	LEU	4.0
1	D	446	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	324	GLY	4.0
1	D	578	THR	3.9
1	D	137	PRO	3.9
1	D	88	VAL	3.9
1	D	339	LEU	3.8
1	A	61	PRO	3.8
1	D	351	VAL	3.7
1	D	360	TYR	3.7
1	D	342	PRO	3.7
1	D	67	VAL	3.6
1	D	574	TYR	3.6
1	D	542	ALA	3.6
1	D	296	GLY	3.5
1	D	362	HIS	3.5
1	D	572	TYR	3.5
1	D	318	ALA	3.4
1	D	332	ALA	3.4
1	D	141	GLN	3.4
1	D	68	GLY	3.4
1	D	579	ASP	3.4
1	C	576	TYR	3.4
1	D	148	THR	3.4
1	D	143	VAL	3.4
1	D	568	TRP	3.3
1	B	324	GLY	3.2
1	B	326	ASN	3.2
1	D	447	ASN	3.2
1	D	590	TRP	3.2
1	A	325	GLY	3.2
1	D	151	GLY	3.2
1	D	570	ALA	3.1
1	D	145	GLN	3.1
1	D	82	ILE	3.1
1	D	352	VAL	3.1
1	D	597	PHE	3.1
1	A	323	LYS	3.0
1	A	258	GLU	3.0
1	D	329	VAL	3.0
1	D	356	GLN	3.0
1	C	326	ASN	3.0
1	D	380	SER	3.0
1	D	577	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	361	SER	2.9
1	D	91	GLU	2.9
1	A	255	LEU	2.8
1	D	583	LEU	2.8
1	D	596	TRP	2.8
1	D	381	LYS	2.8
1	A	248	LEU	2.8
1	D	83	LEU	2.8
1	D	448	ALA	2.8
1	B	459[A]	TRP	2.8
1	A	60	SER	2.8
1	D	144	GLY	2.8
1	C	446	THR	2.8
1	D	378	LYS	2.8
1	D	581	ALA	2.8
1	A	459[A]	TRP	2.7
1	B	325	GLY	2.7
1	C	580	PRO	2.7
1	C	597	PHE	2.7
1	D	586	PHE	2.7
1	D	444	VAL	2.7
1	A	64	GLY	2.7
1	D	298	GLY	2.7
1	D	93	ILE	2.7
1	D	138	GLY	2.7
1	A	249	PRO	2.7
1	B	446	THR	2.6
1	C	345	GLU	2.6
1	D	364	ILE	2.6
1	D	580	PRO	2.6
1	D	359	LYS	2.6
1	D	295	VAL	2.6
1	D	348	PRO	2.6
1	D	341	ASN	2.6
1	A	293	GLY	2.6
1	C	572	TYR	2.6
1	D	545	LYS	2.6
1	D	301	ASP	2.5
1	C	298	GLY	2.5
1	B	445	ASN	2.5
1	D	158	PRO	2.5
1	C	295	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	448	ALA	2.5
1	D	363	VAL	2.5
1	D	379	ASN	2.5
1	D	147	PHE	2.4
1	D	587	PHE	2.4
1	D	149	TYR	2.4
1	D	343	ASN	2.4
1	D	160	TYR	2.4
1	A	198	ASP	2.4
1	D	69	ILE	2.4
1	D	382	LEU	2.4
1	C	419	GLU	2.4
1	D	445	ASN	2.4
1	D	353	ALA	2.4
1	D	355	GLY	2.4
1	C	66	ARG	2.4
1	D	294	GLU	2.4
1	D	128	LYS	2.3
1	D	344	LYS	2.3
1	A	253	PHE	2.3
1	C	356	GLN	2.3
1	C	296	GLY	2.3
1	A	59	SER	2.3
1	A	251	PRO	2.3
1	D	167	PRO	2.3
1	A	298	GLY	2.3
1	D	302	TRP	2.3
1	D	157	ILE	2.3
1	C	577	VAL	2.3
1	D	300	VAL	2.3
1	D	127	PRO	2.3
1	C	589	LEU	2.2
1	C	342	PRO	2.2
1	D	584	PRO	2.2
1	D	349	MET	2.2
1	C	587	PHE	2.2
1	D	140	MET	2.2
1	A	199	ILE	2.2
1	D	337	ILE	2.2
1	A	292	PHE	2.2
1	C	496[A]	ASP	2.2
1	C	420	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	594	ALA	2.2
1	C	459[A]	TRP	2.2
1	D	81	LEU	2.2
1	B	320	LEU	2.1
1	D	345	GLU	2.1
1	B	327	ALA	2.1
1	D	86	LEU	2.1
1	A	294	GLU	2.1
1	A	297	ASP	2.1
1	D	110	ASN	2.1
1	A	254	GLY	2.1
1	D	354	GLY	2.1
1	D	335	THR	2.1
1	C	581	ALA	2.1
1	B	322	LYS	2.1
1	D	567	ALA	2.1
1	D	377	LEU	2.1
1	C	297	ASP	2.1
1	C	447	ASN	2.1
1	D	547	HIS	2.1
1	C	323	LYS	2.0
1	D	312	LEU	2.0
1	A	237	TYR	2.0
1	D	346	ASP	2.0
1	D	303	ARG	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

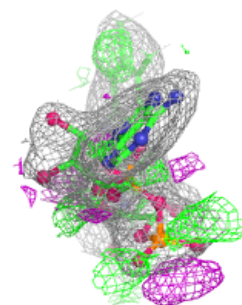
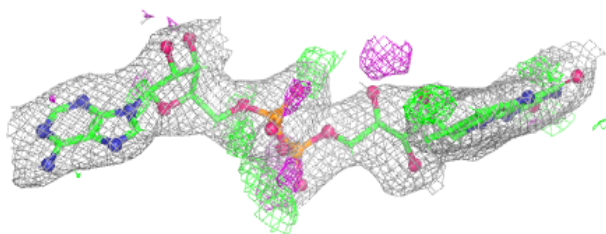
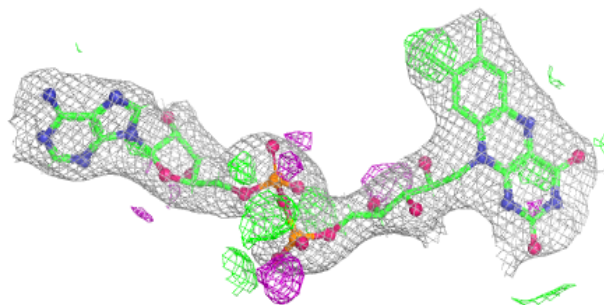
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	705	5/5	0.36	0.21	62,63,85,92	5
3	SO4	B	709	5/5	0.54	0.14	73,78,81,90	5
3	SO4	B	707	5/5	0.61	0.11	76,77,84,87	5
3	SO4	B	706	5/5	0.75	0.09	74,75,77,83	5
3	SO4	D	704	5/5	0.75	0.13	65,71,74,79	5
3	SO4	B	708	5/5	0.75	0.20	36,48,55,67	5
3	SO4	C	704	5/5	0.76	0.10	67,77,87,87	5
3	SO4	D	703	5/5	0.78	0.12	67,76,88,97	0
3	SO4	A	705	5/5	0.79	0.10	63,64,71,78	0
3	SO4	B	704	5/5	0.80	0.13	54,59,71,71	0
3	SO4	A	702	5/5	0.80	0.11	63,64,72,72	0
3	SO4	C	705	5/5	0.80	0.17	59,61,64,76	5
4	PGO	A	710	5/5	0.82	0.19	40,52,66,68	0
3	SO4	B	705	5/5	0.83	0.13	62,64,77,81	5
3	SO4	A	708	5/5	0.85	0.13	60,63,74,77	5
3	SO4	B	702	5/5	0.85	0.12	60,62,69,72	5
3	SO4	C	702	5/5	0.85	0.12	62,65,70,74	5
3	SO4	D	702	5/5	0.86	0.13	48,55,71,72	5
3	SO4	A	709	5/5	0.87	0.12	60,65,70,71	5
3	SO4	A	707	5/5	0.88	0.18	45,47,53,70	5
3	SO4	A	706	5/5	0.88	0.15	49,50,65,66	5
3	SO4	A	704	5/5	0.89	0.09	69,72,73,74	0
3	SO4	B	703	5/5	0.90	0.12	49,58,63,75	0
2	FAD	D	701	53/53	0.92	0.11	34,47,59,71	0
2	FAD	B	701	53/53	0.93	0.09	28,37,47,56	0
2	FAD	A	701	53/53	0.94	0.08	28,37,47,52	0
3	SO4	C	703	5/5	0.94	0.09	53,55,59,60	5
3	SO4	A	703	5/5	0.94	0.08	37,40,44,45	5
2	FAD	C	701	53/53	0.96	0.07	25,34,41,47	0

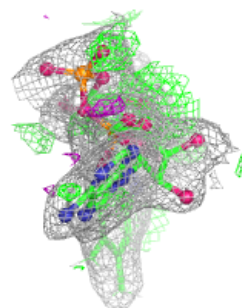
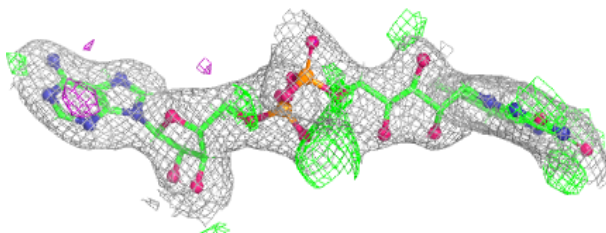
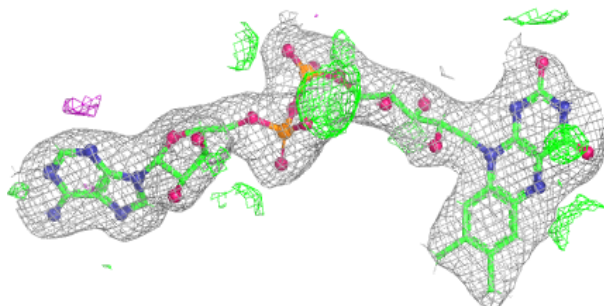
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

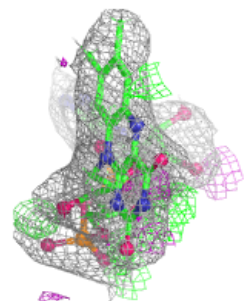
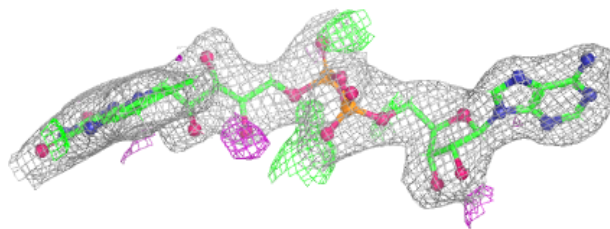
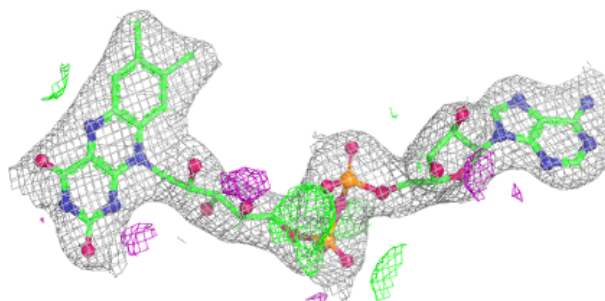
**Electron density around FAD B 701:**

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

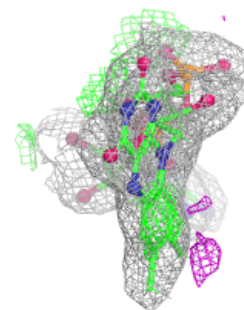
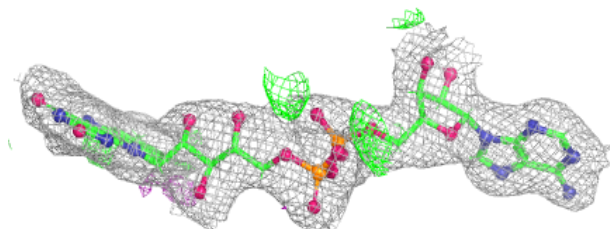
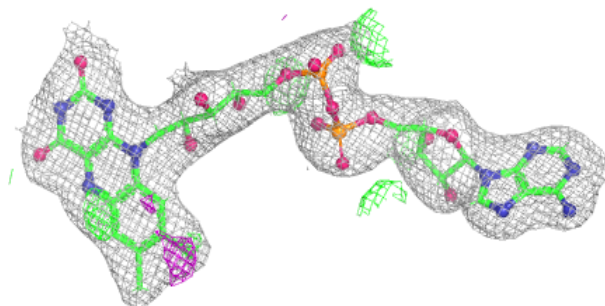


Electron density around FAD A 701:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.