Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2024 – 02:48 pm BST

PDB ID	:	9ENH
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 (i) 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 (i)) were used in the production of this report:

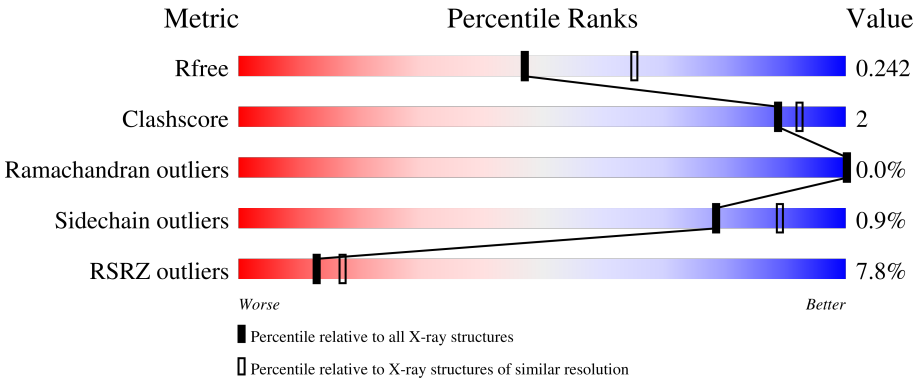
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 <=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	4% 91% 5% .
1	B	562	3% 90% 5% 5%
1	C	562	7% 89% 5% 6%
1	D	562	15% 86% 7% 7%

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
3	SO4	D	705	-	-	-	X

2 Entry composition (i)

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.

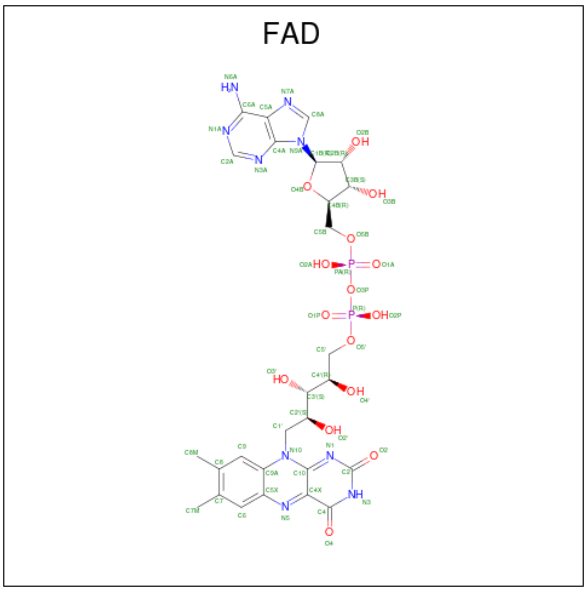
- Molecule 1 is a protein called L-amino acid oxidase 4.

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:

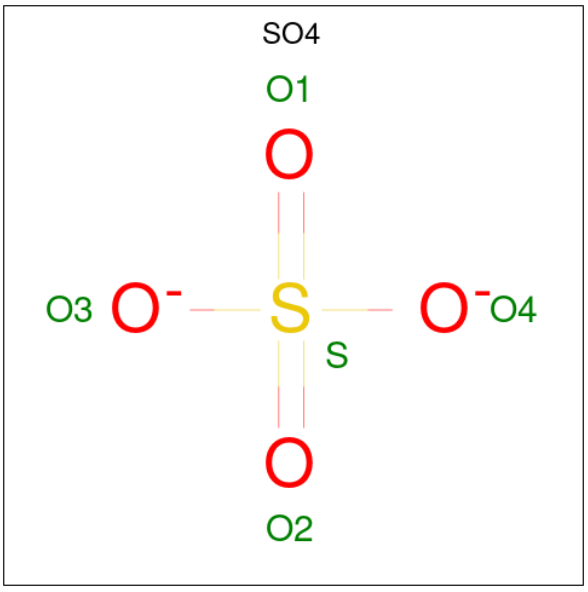
Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ALA	LYS	engineered mutation	UNP S4S6Z0
A	475	ALA	LYS	engineered mutation	UNP S4S6Z0
B	474	ALA	LYS	engineered mutation	UNP S4S6Z0
B	475	ALA	LYS	engineered mutation	UNP S4S6Z0
C	474	ALA	LYS	engineered mutation	UNP S4S6Z0
C	475	ALA	LYS	engineered mutation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

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: 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	H	N	O	P	0	0
			84	27	31	9	15	2		
2	B	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	C	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		
2	D	1	Total	C	H	N	O	P	0	0
			84	27	31	9	15	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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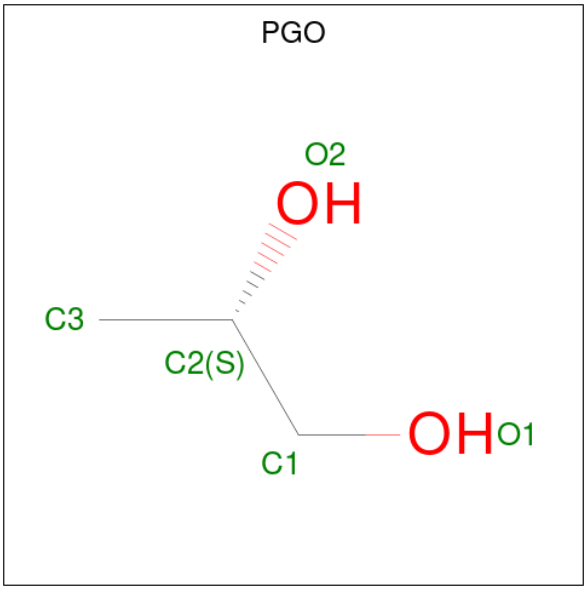
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



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

- Molecule 5 is water.

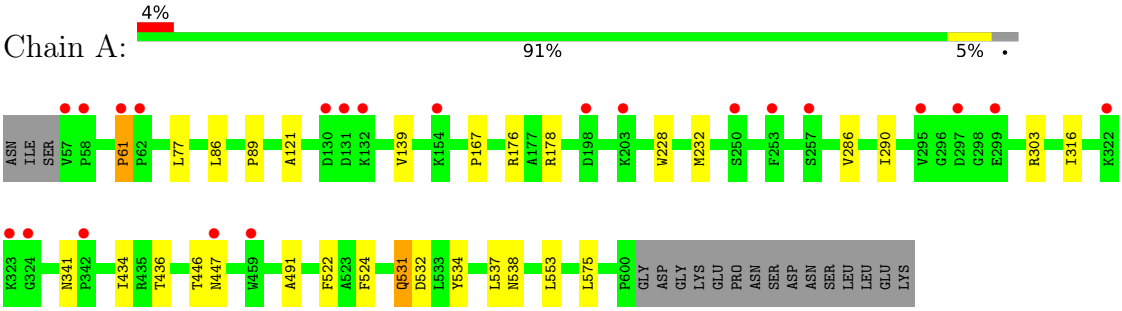
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	27	Total O 27 27	0	0
5	B	22	Total O 22 22	0	0
5	C	44	Total O 44 44	0	0
5	D	27	Total O 27 27	0	0

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.

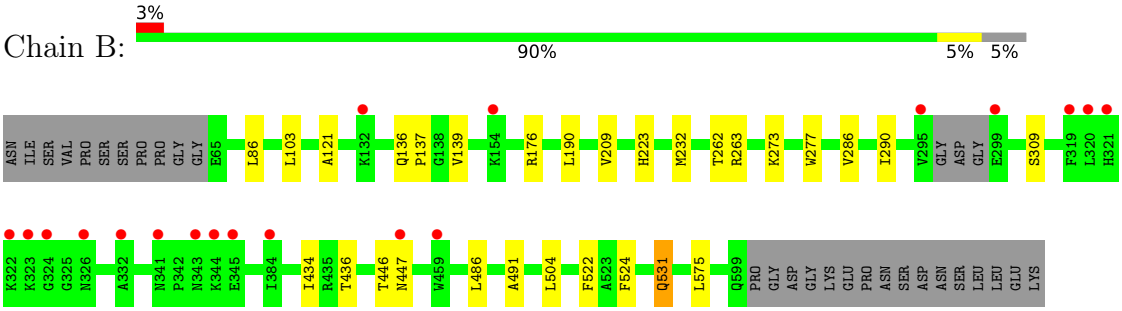
• Molecule 1: L-amino acid oxidase 4

Chain A:



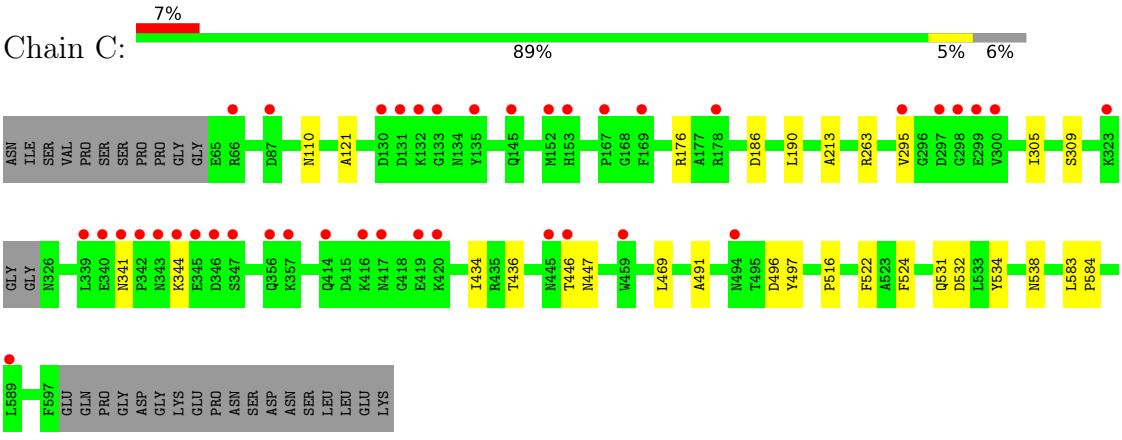
• Molecule 1: L-amino acid oxidase 4

Chain B:



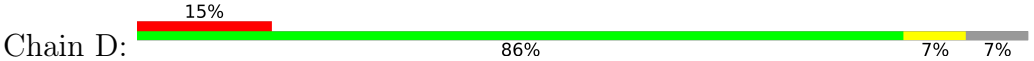
• Molecule 1: L-amino acid oxidase 4

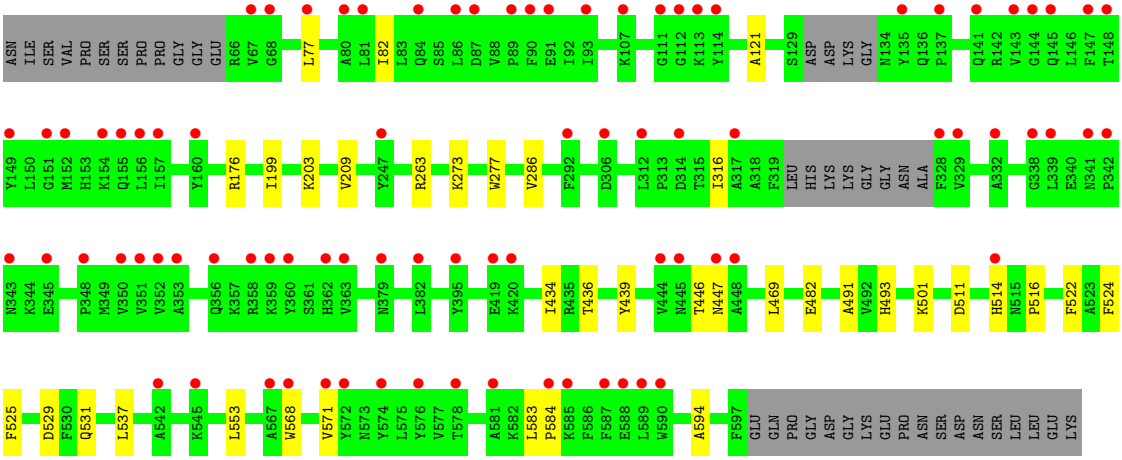
Chain C:



• Molecule 1: L-amino acid oxidase 4

Chain D:




ASN ILE SER VAL PRO SER SER PRO PRO GLY GLY GLU R66 V67 G68 L77 A80 L81 I82 L83 Q84 S85 L86 D87 V88 P89 F90 E91 I92 I93 K107 G111 G112 K113 Y114 A121 S129 ASP ASP LYS GLY N134 Y135 Q136 P137 Q141 R142 V143 G144 Q145 L146 F147 T148
Y149 L150 G151 M152 H153 K154 Q155 L156 I157 Y160 R176 I199 K203 V209 Y247 R263 K273 W277 V286 F292 D306 L312 P313 D314 T315 I316 A317 A318 F319 LEU HIS LYS LYS GLY GLY ASN ALA F328 V329 A332 G338 L339 E340 N341 P342
N343 K344 E345 P348 M349 V350 V351 V352 A353 Q356 K357 R358 K359 Y360 S361 H362 V363 N379 L382 Y396 E419 K420 I434 R435 T436 Y439 V444 N445 T446 N447 A448 L469 E482 A491 V492 H493 K501 D511 H514 N515 P516 F522 A523 F524
F525 D529 F530 Q531 L537 A542 K545 L553 A567 W568 V571 Y572 N573 Y574 L575 Y576 V577 T578 A581 K582 L583 P584 K585 F586 F587 E588 L589 W590 A594 F597 GLU GLN PRO GLY ASP GLY LYS GLU PRO ASN SER ASP ASN SER LEU LEU GLU LYS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.77 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.211 , 0.246 0.208 , 0.242	Depositor DCC
R_{free} test set	4217 reflections (5.01%)	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 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, SO4, 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	0.25	0/4421	0.46	0/6016
1	B	0.25	0/4349	0.46	0/5914
1	C	0.25	0/4335	0.47	0/5896
1	D	0.25	0/4225	0.47	0/5747
All	All	0.25	0/17330	0.47	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

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	16	0
1	B	4218	4086	4086	17	0
1	C	4205	4070	4073	14	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	65	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 (65) 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: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:D:537:LEU:CB	1:D:553:LEU:HD11	2.40	0.51
1:A:532:ASP:OD1	1:B:263:ARG:NE	2.43	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:C:446:THR:HG22	1:C:447:ASN:N	2.28	0.48
1:D:511:ASP:OD2	1:D:514[A]:HIS:ND1	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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%)	47 58
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%)	449 (99%)	5 (1%)	73 86
1	B	446/467 (96%)	443 (99%)	3 (1%)	84 92
1	C	445/467 (95%)	440 (99%)	5 (1%)	73 86
1	D	434/467 (93%)	431 (99%)	3 (1%)	84 92
All	All	1779/1868 (95%)	1763 (99%)	16 (1%)	78 89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	VAL
1	A	341	ASN
1	A	522	PHE
1	A	524	PHE
1	A	531	GLN
1	B	522	PHE
1	B	524	PHE
1	B	531	GLN
1	C	110	ASN
1	C	186	ASP
1	C	522	PHE
1	C	524	PHE
1	C	531	GLN
1	D	522	PHE
1	D	524	PHE
1	D	531	GLN

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

Mol	Chain	Res	Type
1	C	341	ASN
1	C	531	GLN

5.3.3 RNA (i)

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 monosaccharides 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	B	709	-	4,4,4	0.60	0	6,6,6	0.05	0
3	SO4	B	708	-	4,4,4	0.61	0	6,6,6	0.05	0
3	SO4	D	704	-	4,4,4	0.60	0	6,6,6	0.06	0
3	SO4	B	707	-	4,4,4	0.60	0	6,6,6	0.05	0
3	SO4	D	702	-	4,4,4	0.60	0	6,6,6	0.04	0
3	SO4	A	703	-	4,4,4	0.60	0	6,6,6	0.06	0
3	SO4	B	704	-	4,4,4	0.60	0	6,6,6	0.08	0
3	SO4	B	703	-	4,4,4	0.60	0	6,6,6	0.05	0
3	SO4	D	705	-	4,4,4	0.61	0	6,6,6	0.05	0
3	SO4	B	705	-	4,4,4	0.60	0	6,6,6	0.05	0
3	SO4	A	705	-	4,4,4	0.60	0	6,6,6	0.05	0
2	FAD	A	701	-	53,58,58	0.92	2 (3%)	68,89,89	0.94	1 (1%)
3	SO4	C	704	-	4,4,4	0.60	0	6,6,6	0.05	0
2	FAD	B	701	-	53,58,58	0.93	2 (3%)	68,89,89	0.94	3 (4%)
3	SO4	A	704	-	4,4,4	0.60	0	6,6,6	0.04	0
3	SO4	A	706	-	4,4,4	0.60	0	6,6,6	0.06	0
3	SO4	A	709	-	4,4,4	0.60	0	6,6,6	0.05	0
4	PGO	A	710	-	3,4,4	0.28	0	1,4,4	0.59	0
3	SO4	C	703	-	4,4,4	0.60	0	6,6,6	0.05	0
3	SO4	D	703	-	4,4,4	0.59	0	6,6,6	0.06	0
3	SO4	A	708	-	4,4,4	0.60	0	6,6,6	0.06	0
3	SO4	C	702	-	4,4,4	0.60	0	6,6,6	0.06	0
3	SO4	A	702	-	4,4,4	0.60	0	6,6,6	0.06	0
3	SO4	C	705	-	4,4,4	0.59	0	6,6,6	0.05	0
3	SO4	B	706	-	4,4,4	0.60	0	6,6,6	0.05	0
2	FAD	C	701	-	53,58,58	0.93	2 (3%)	68,89,89	0.94	2 (2%)
3	SO4	B	702	-	4,4,4	0.60	0	6,6,6	0.05	0
2	FAD	D	701	-	53,58,58	0.94	2 (3%)	68,89,89	0.94	1 (1%)
3	SO4	A	707	-	4,4,4	0.61	0	6,6,6	0.07	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
2	FAD	A	701	-	-	1/30/50/50	0/6/6/6
2	FAD	B	701	-	-	2/30/50/50	0/6/6/6
2	FAD	C	701	-	-	2/30/50/50	0/6/6/6
2	FAD	D	701	-	-	2/30/50/50	0/6/6/6
4	PGO	A	710	-	-	0/2/2/2	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	FAD	C8A-N7A	-2.45	1.30	1.34
2	C	701	FAD	C8A-N7A	-2.43	1.30	1.34
2	A	701	FAD	C8A-N7A	-2.38	1.30	1.34
2	B	701	FAD	C8A-N7A	-2.37	1.30	1.34
2	C	701	FAD	C5X-N5	-2.27	1.35	1.39
2	D	701	FAD	C5X-N5	-2.26	1.35	1.39
2	B	701	FAD	C5X-N5	-2.25	1.35	1.39
2	A	701	FAD	C5X-N5	-2.24	1.35	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	FAD	O2P-P-O1P	2.18	123.00	112.24
2	D	701	FAD	O2P-P-O1P	2.17	122.95	112.24
2	B	701	FAD	O2P-P-O1P	2.16	122.94	112.24
2	C	701	FAD	C5'-C4'-C3'	-2.15	108.05	112.20
2	C	701	FAD	O2P-P-O1P	2.15	122.88	112.24
2	B	701	FAD	C5A-C6A-N6A	2.06	123.48	120.35
2	B	701	FAD	O2A-PA-O1A	2.00	122.14	112.24

There are no chirality outliers.

All (7) torsion outliers are listed below:

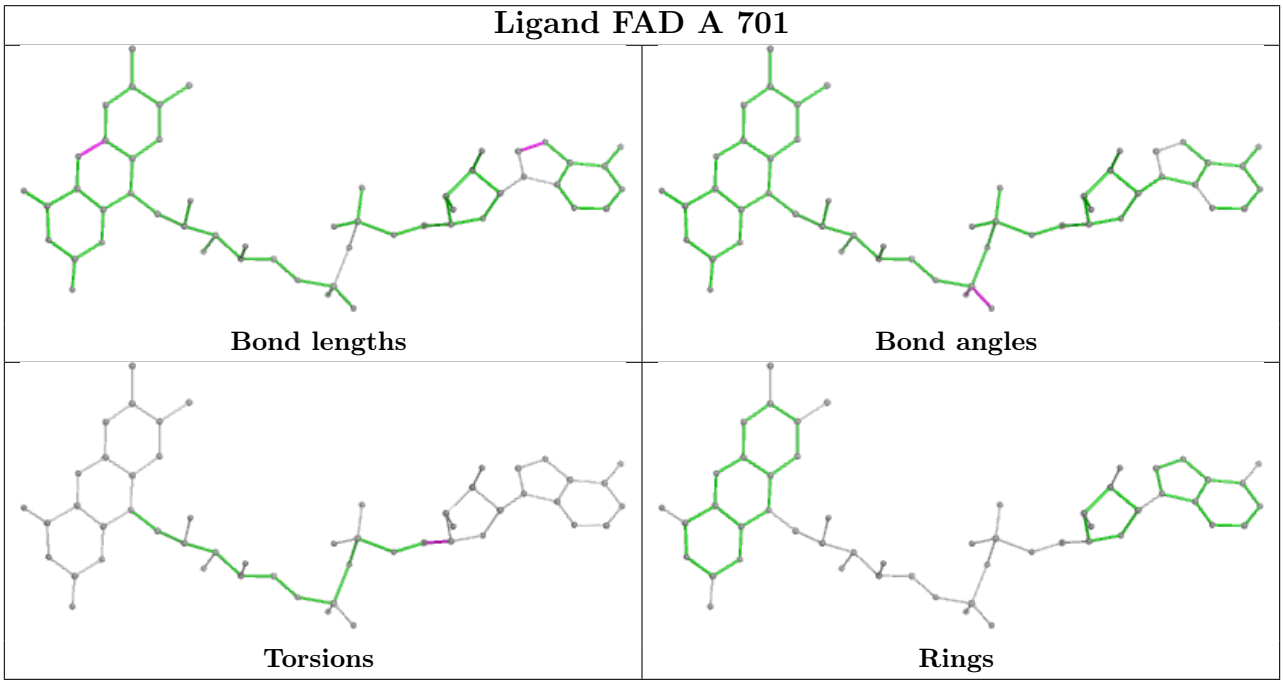
Mol	Chain	Res	Type	Atoms
2	D	701	FAD	PA-O3P-P-O5'
2	B	701	FAD	PA-O3P-P-O5'
2	C	701	FAD	PA-O3P-P-O5'
2	A	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	O4B-C4B-C5B-O5B
2	C	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

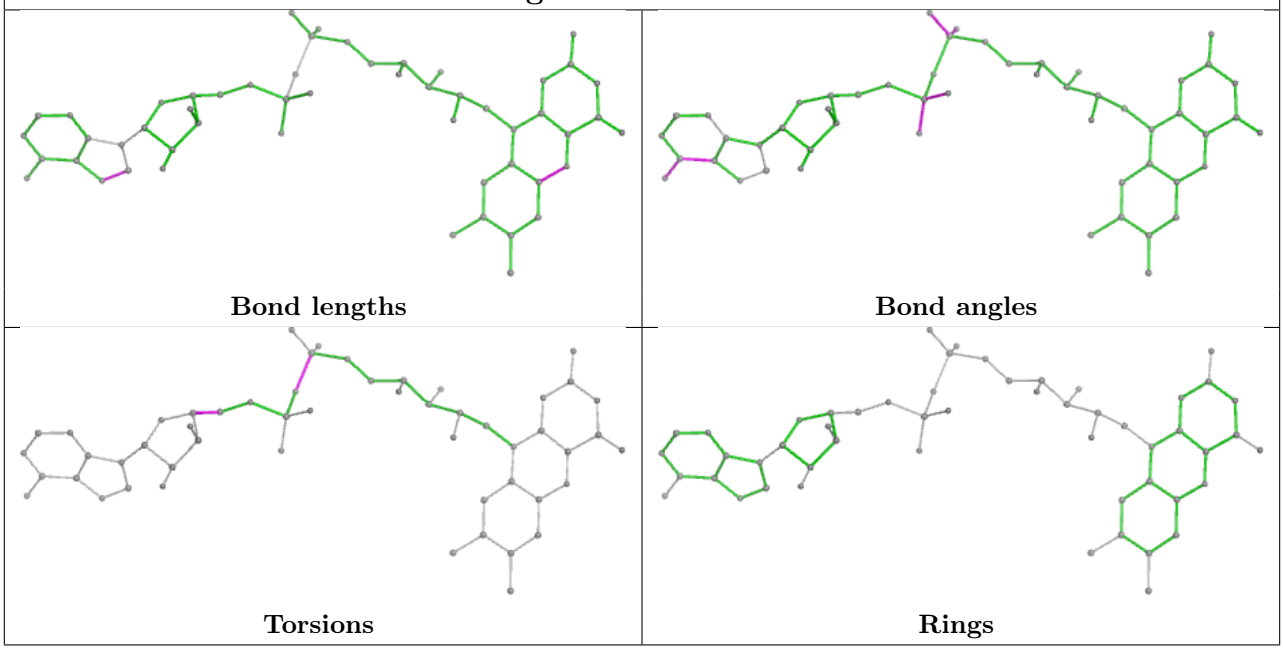
4 monomers are involved in 4 short contacts:

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

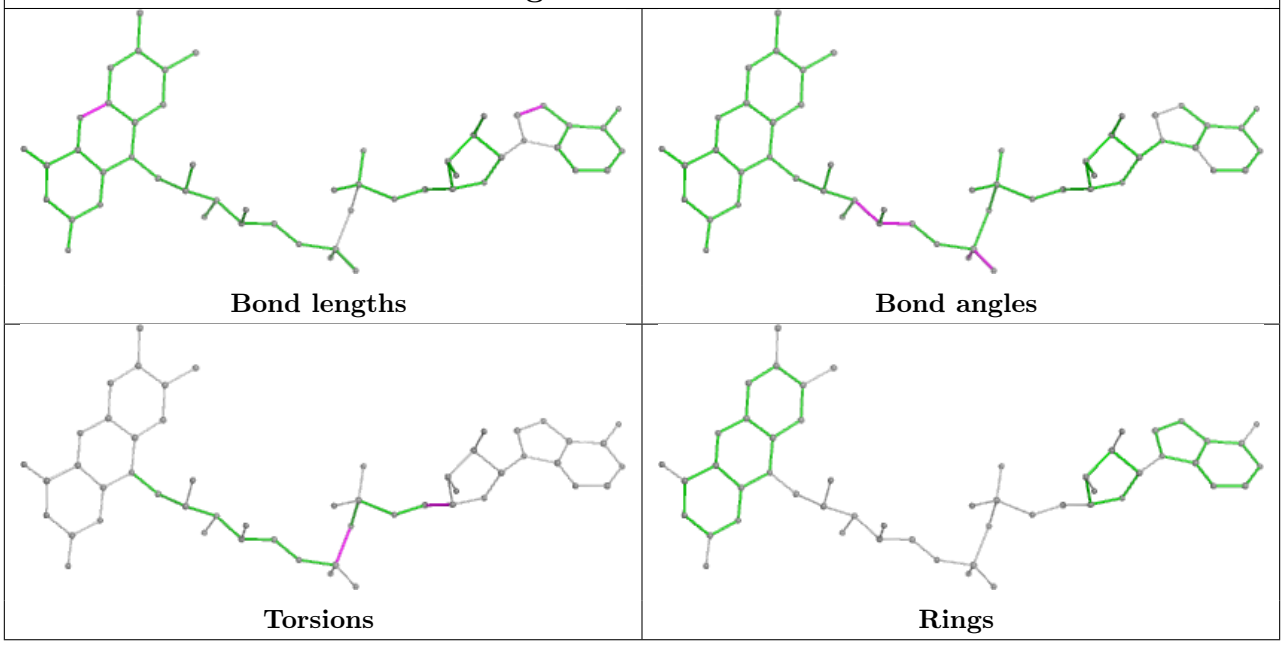
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

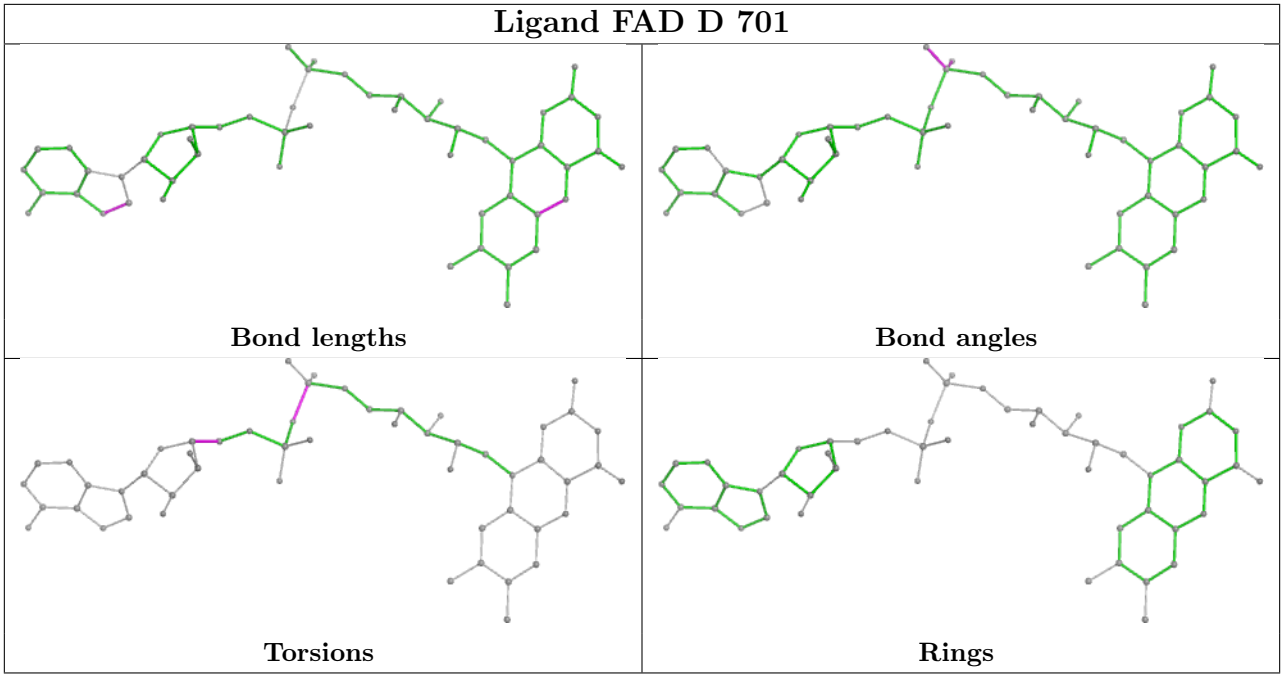


Ligand FAD B 701



Ligand FAD C 701





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, 95^{th} 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%)	0.50	22 (4%)	38	45	33, 48, 83, 121	0
1	B	532/562 (94%)	0.37	19 (3%)	42	49	34, 49, 73, 122	0
1	C	531/562 (94%)	0.54	40 (7%)	14	19	26, 50, 81, 113	0
1	D	520/562 (92%)	0.94	85 (16%)	1	2	29, 60, 100, 130	0
All	All	2127/2248 (94%)	0.59	166 (7%)	13	17	26, 51, 88, 130	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	90	PHE	6.6
1	A	257	SER	6.0
1	C	345	GLU	5.8
1	A	299	GLU	5.7
1	D	329	VAL	5.6
1	D	447	ASN	5.6
1	D	351	VAL	5.6
1	D	576	TYR	5.2
1	D	68	GLY	5.2
1	C	343	ASN	5.0
1	D	444	VAL	5.0
1	C	589	LEU	4.9
1	D	571	VAL	4.9
1	A	62	PRO	4.9
1	C	297	ASP	4.7
1	A	58	PRO	4.7
1	D	113	LYS	4.7
1	D	135	TYR	4.6
1	A	61	PRO	4.6
1	C	131	ASP	4.5
1	C	344	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	137	PRO	4.5
1	D	342	PRO	4.4
1	C	133	GLY	4.3
1	D	356	GLN	4.3
1	B	344	LYS	4.0
1	C	132	LYS	4.0
1	D	574	TYR	4.0
1	D	157	ILE	3.9
1	C	342	PRO	3.9
1	D	339	LEU	3.9
1	D	338	GLY	3.9
1	B	295	VAL	3.8
1	C	323	LYS	3.8
1	D	345	GLU	3.7
1	D	89	PRO	3.7
1	C	417	ASN	3.7
1	A	342	PRO	3.6
1	D	317	ALA	3.6
1	D	379	ASN	3.6
1	D	332	ALA	3.6
1	A	57	VAL	3.6
1	A	198	ASP	3.6
1	D	445	ASN	3.5
1	B	299	GLU	3.5
1	C	445	ASN	3.4
1	D	154	LYS	3.4
1	D	81	LEU	3.4
1	C	419	GLU	3.4
1	D	588	GLU	3.3
1	A	323	LYS	3.3
1	A	253	PHE	3.3
1	C	420	LYS	3.3
1	D	578	THR	3.3
1	D	114	TYR	3.2
1	C	66	ARG	3.2
1	D	86	LEU	3.2
1	B	459[A]	TRP	3.2
1	C	341	ASN	3.2
1	C	167	PRO	3.1
1	D	353	ALA	3.1
1	B	321[A]	HIS	3.1
1	D	147	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	326	ASN	3.1
1	D	572	TYR	3.1
1	A	297	ASP	3.1
1	C	153	HIS	3.0
1	D	584	PRO	3.0
1	D	341	ASN	3.0
1	B	320	LEU	3.0
1	A	132	LYS	3.0
1	D	587	PHE	3.0
1	A	131	ASP	3.0
1	C	300	VAL	3.0
1	C	356	GLN	3.0
1	D	107	LYS	3.0
1	D	84	GLN	2.9
1	C	494	ASN	2.9
1	A	459[A]	TRP	2.9
1	B	132	LYS	2.9
1	C	416	LYS	2.9
1	B	343	ASN	2.8
1	A	250	SER	2.8
1	C	446	THR	2.8
1	D	314	ASP	2.8
1	D	93	ILE	2.8
1	D	156	LEU	2.8
1	D	350	VAL	2.7
1	A	203	LYS	2.7
1	B	154	LYS	2.7
1	A	447	ASN	2.7
1	D	143	VAL	2.7
1	D	545	LYS	2.7
1	D	360	TYR	2.7
1	C	87	ASP	2.7
1	D	362	HIS	2.7
1	D	568	TRP	2.7
1	D	160	TYR	2.7
1	D	306	ASP	2.6
1	D	420	LYS	2.6
1	C	169	PHE	2.6
1	D	112	GLY	2.6
1	C	346	ASP	2.6
1	C	414	GLN	2.6
1	D	358	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	324	GLY	2.6
1	C	298	GLY	2.6
1	C	135	TYR	2.6
1	D	67	VAL	2.6
1	D	111	GLY	2.6
1	D	155	GLN	2.6
1	A	154	LYS	2.6
1	D	312	LEU	2.6
1	A	322	LYS	2.6
1	D	359	LYS	2.6
1	C	130	ASP	2.5
1	D	419	GLU	2.5
1	D	141	GLN	2.5
1	D	292	PHE	2.5
1	D	363	VAL	2.5
1	D	145	GLN	2.5
1	B	447	ASN	2.4
1	C	459[A]	TRP	2.4
1	C	339	LEU	2.3
1	D	382	LEU	2.3
1	D	328	PHE	2.3
1	B	323	LYS	2.3
1	A	130	ASP	2.3
1	D	589	LEU	2.3
1	D	395	TYR	2.3
1	C	152	MET	2.3
1	D	152	MET	2.3
1	A	295	VAL	2.3
1	C	295	VAL	2.3
1	D	581	ALA	2.3
1	B	345	GLU	2.2
1	D	514[A]	HIS	2.2
1	C	145	GLN	2.2
1	D	542	ALA	2.2
1	C	340	GLU	2.2
1	D	91	GLU	2.2
1	C	357	LYS	2.2
1	A	324	GLY	2.2
1	B	341	ASN	2.2
1	D	567	ALA	2.2
1	B	384	ILE	2.2
1	D	590	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	299	GLU	2.2
1	B	322	LYS	2.1
1	D	151	GLY	2.2
1	D	87	ASP	2.1
1	D	585	LYS	2.1
1	D	352	VAL	2.1
1	D	448	ALA	2.1
1	D	343	ASN	2.1
1	D	144	GLY	2.1
1	D	149	TYR	2.1
1	B	319	PHE	2.1
1	B	332	ALA	2.1
1	D	80	ALA	2.1
1	D	247	TYR	2.1
1	D	348	PRO	2.0
1	D	77	LEU	2.0
1	C	178	ARG	2.0
1	C	347	SER	2.0
1	D	148	THR	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 monosaccharides 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, 95^{th} 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	SO4	D	705	5/5	0.50	0.41	62,63,85,92	5
3	SO4	B	708	5/5	0.74	0.33	36,48,55,67	5
3	SO4	B	709	5/5	0.77	0.31	73,78,81,90	5
3	SO4	A	707	5/5	0.85	0.23	45,47,53,70	5

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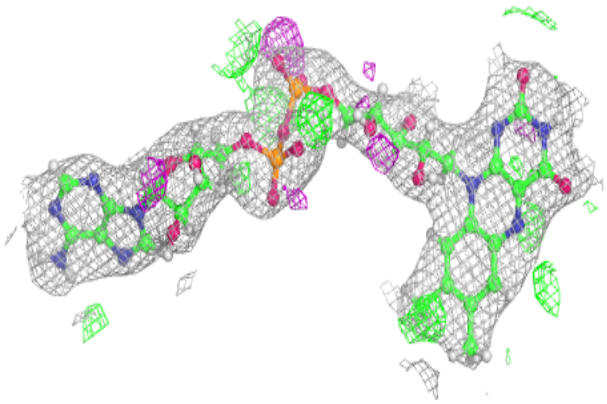
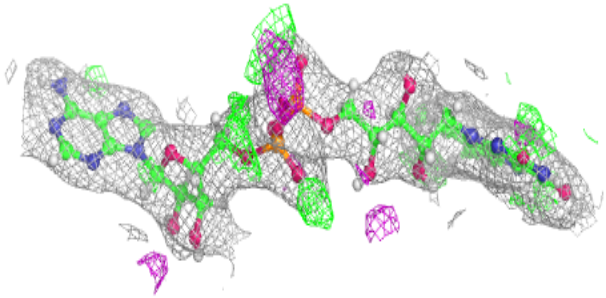
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PGO	A	710	5/5	0.86	0.22	40,52,66,68	0
3	SO4	B	704	5/5	0.87	0.15	54,59,71,71	0
3	SO4	B	706	5/5	0.87	0.30	74,75,77,83	5
3	SO4	D	704	5/5	0.88	0.23	65,71,74,79	5
3	SO4	A	709	5/5	0.89	0.26	60,65,70,71	5
3	SO4	C	704	5/5	0.89	0.19	67,77,87,87	5
3	SO4	C	705	5/5	0.89	0.25	59,61,64,76	5
3	SO4	A	708	5/5	0.90	0.26	60,63,74,77	5
3	SO4	B	707	5/5	0.91	0.24	76,77,84,87	5
3	SO4	A	706	5/5	0.91	0.17	49,50,65,66	5
3	SO4	D	702	5/5	0.92	0.12	48,55,71,72	5
3	SO4	B	705	5/5	0.92	0.15	62,64,77,81	5
3	SO4	B	703	5/5	0.93	0.18	49,58,63,75	0
3	SO4	A	702	5/5	0.93	0.12	63,64,72,72	0
3	SO4	A	705	5/5	0.93	0.11	63,64,71,78	0
3	SO4	C	702	5/5	0.93	0.17	62,65,70,74	5
3	SO4	B	702	5/5	0.93	0.14	60,62,69,72	5
3	SO4	D	703	5/5	0.94	0.12	67,76,88,97	0
2	FAD	D	701	53/53	0.94	0.17	34,47,59,71	0
2	FAD	B	701	53/53	0.95	0.15	28,37,47,56	0
2	FAD	A	701	53/53	0.95	0.17	28,37,47,52	0
3	SO4	C	703	5/5	0.96	0.12	53,55,59,60	5
3	SO4	A	704	5/5	0.96	0.09	69,72,73,74	0
3	SO4	A	703	5/5	0.97	0.18	37,40,44,45	5
2	FAD	C	701	53/53	0.97	0.15	25,34,41,47	0

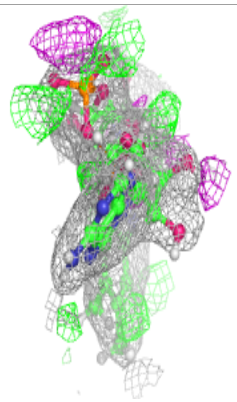
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

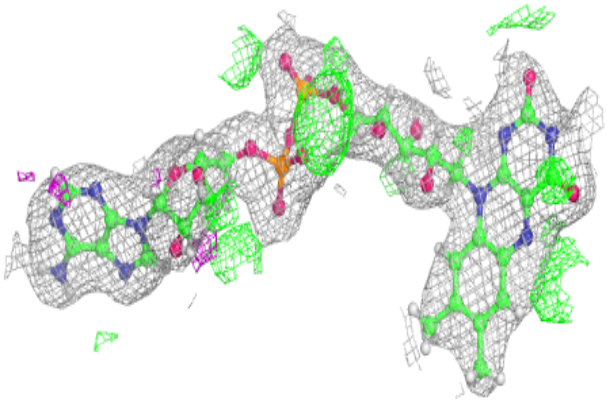


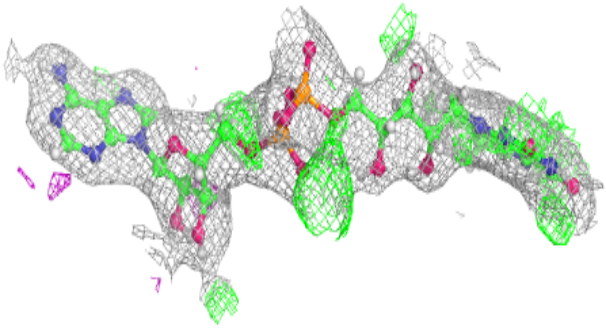


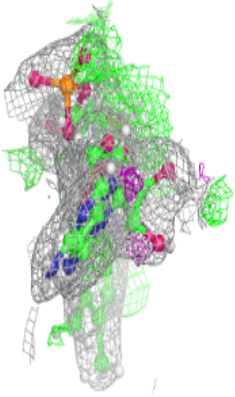


Electron density around FAD B 701:

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

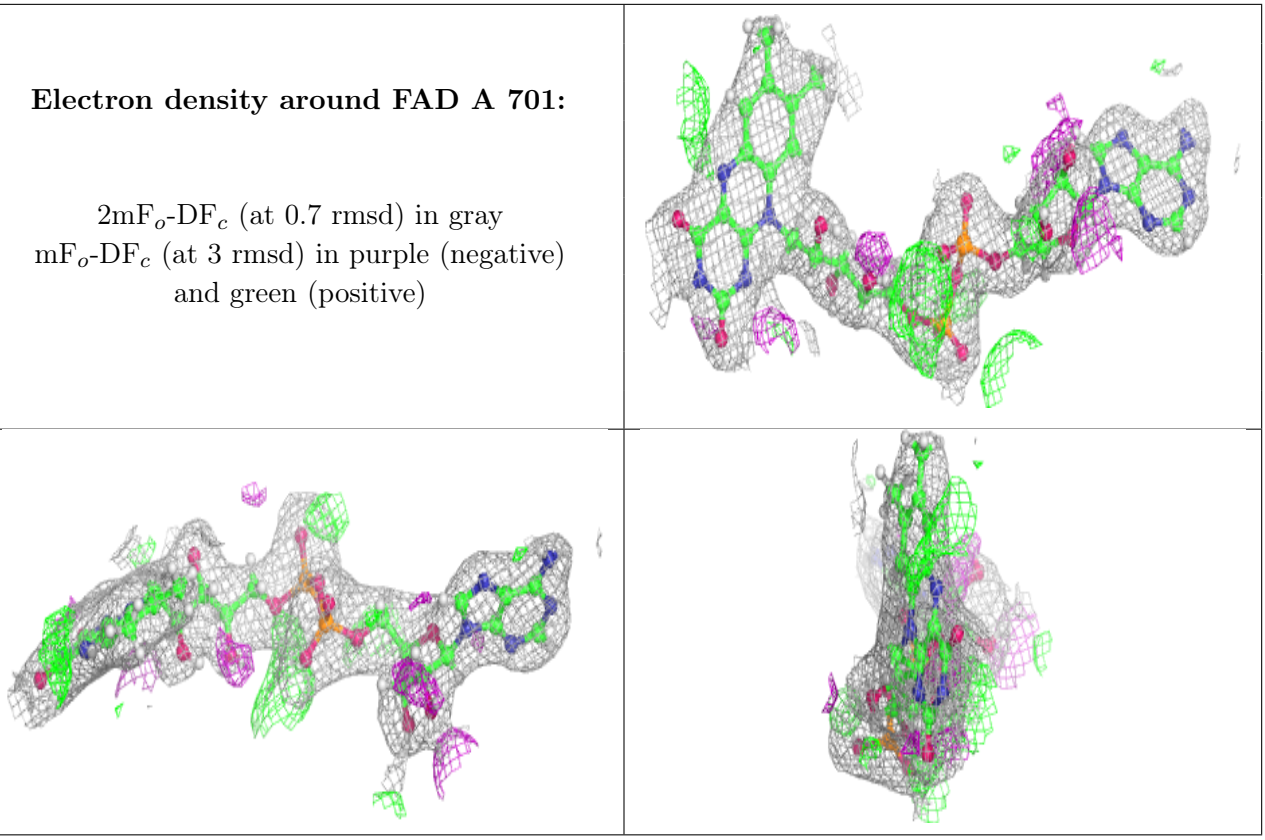






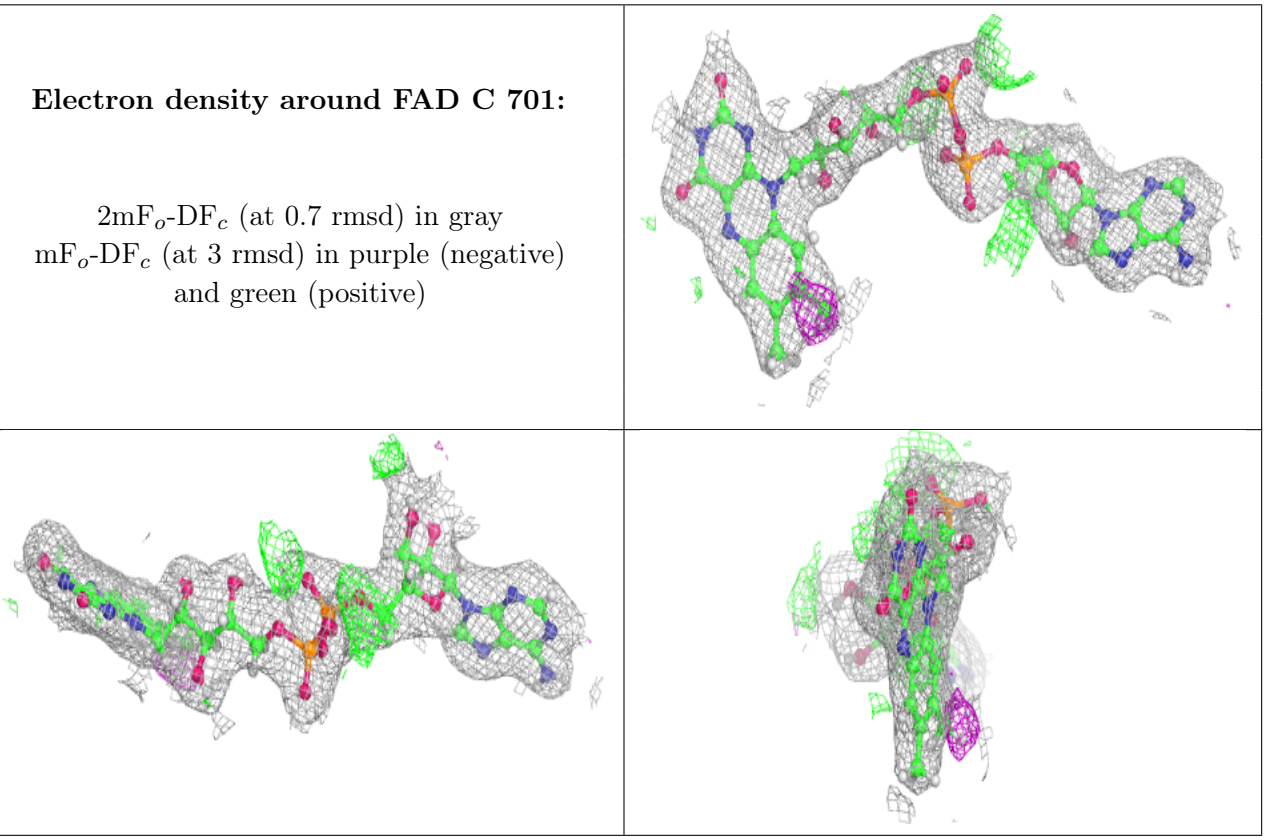
Electron density around FAD A 701:

$2mF_o$-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.