Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 07:16 PM EDT

PDB ID	:	6H3G
Title	:	Alcohol oxidase from Phanerochaete chrysosporium
Authors	:	Nguyen, Q.-T.; Romero, E.; Dijkman, W.P.; de Vasconcellos, S.P.; Binda, C.; Mattevi, A.; Fraaije, M.W.
Deposited on	:	2018-07-18
Resolution	:	2.60 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:

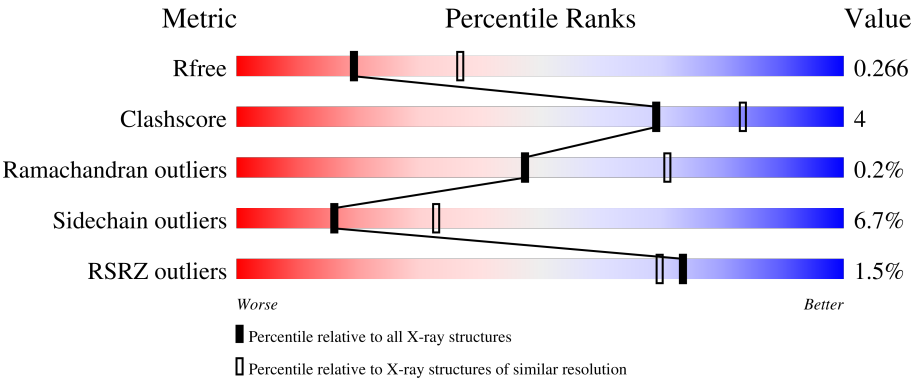
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	651	85% 13%
1	B	651	86% 11%
1	C	651	83% 13%
1	D	651	86% 10%
1	E	651	5% 85% 12%

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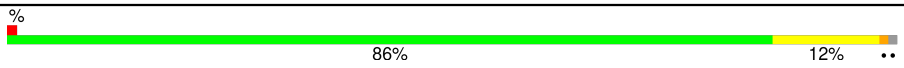
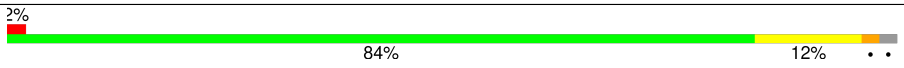
Mol	Chain	Length	Quality of chain
1	F	651	
1	G	651	
1	H	651	

2 Entry composition (i)

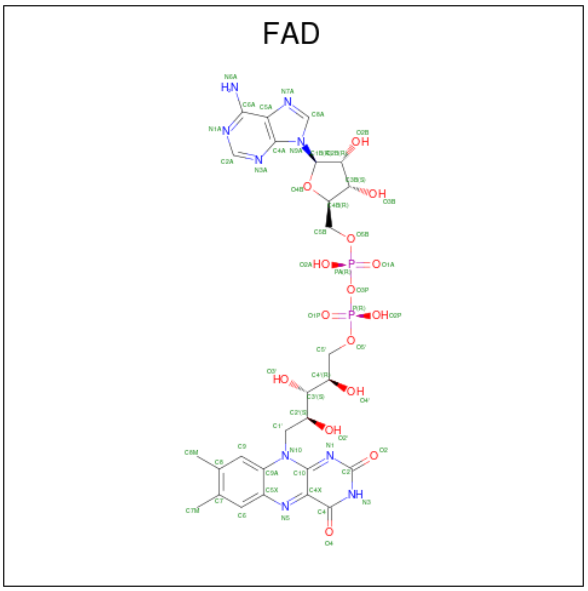
There are 4 unique types of molecules in this entry. The entry contains 41161 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alcohol oxidase.

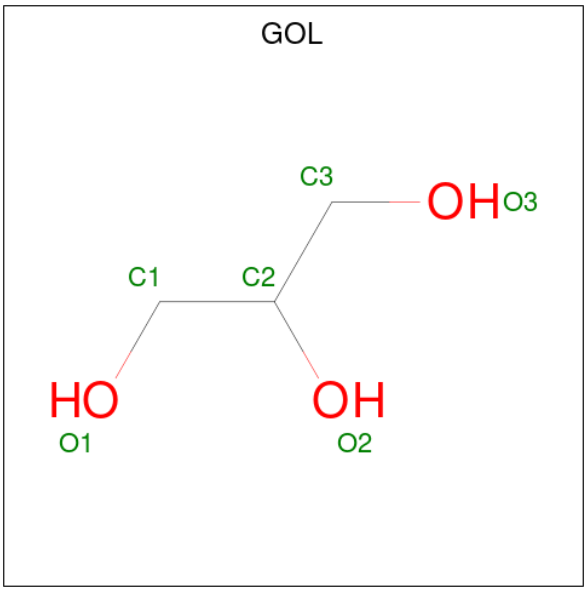
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	S	0	1	0
			5052	3178	893	956	25			
1	B	642	Total	C	N	O	S	0	0	0
			5036	3169	889	953	25			
1	C	636	Total	C	N	O	S	0	1	0
			5003	3147	884	947	25			
1	D	636	Total	C	N	O	S	0	0	0
			4992	3141	880	946	25			
1	E	637	Total	C	N	O	S	0	0	0
			4999	3146	881	947	25			
1	F	646	Total	C	N	O	S	0	1	0
			5074	3190	900	959	25			
1	G	635	Total	C	N	O	S	0	0	0
			4985	3136	879	945	25			
1	H	636	Total	C	N	O	S	0	0	0
			4992	3141	880	946	25			

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	43	Total O 43 43	0	0
4	B	101	Total O 101 101	0	0
4	C	72	Total O 72 72	0	0
4	D	85	Total O 85 85	0	0
4	E	45	Total O 45 45	0	0
4	F	66	Total O 66 66	0	0
4	G	73	Total O 73 73	0	0

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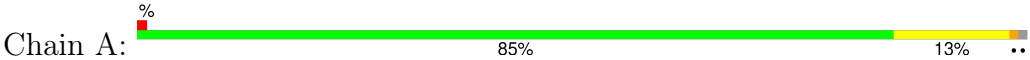
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	89	Total	O	0	0
			89	89		

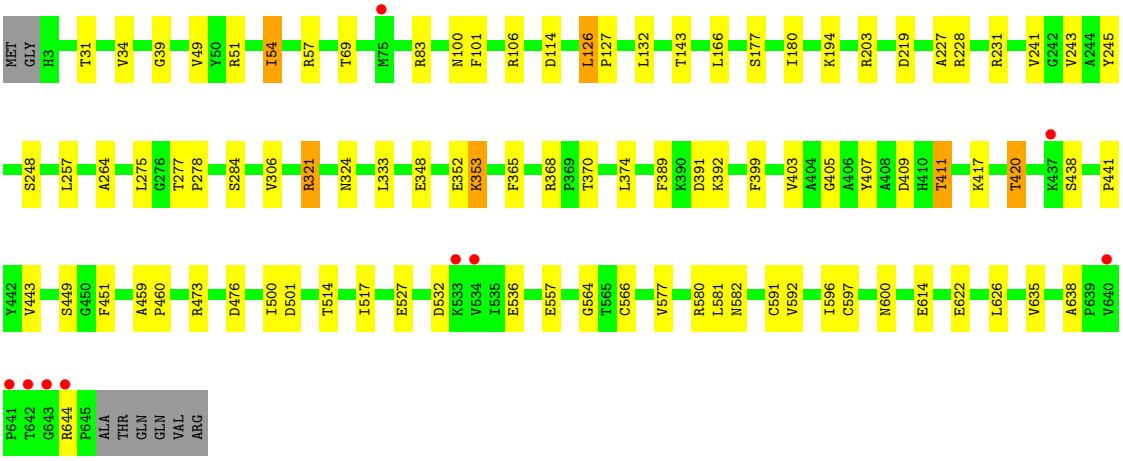
3 Residue-property plots (i)

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: Alcohol oxidase

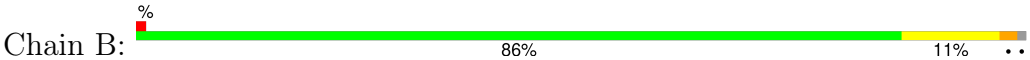
Chain A:

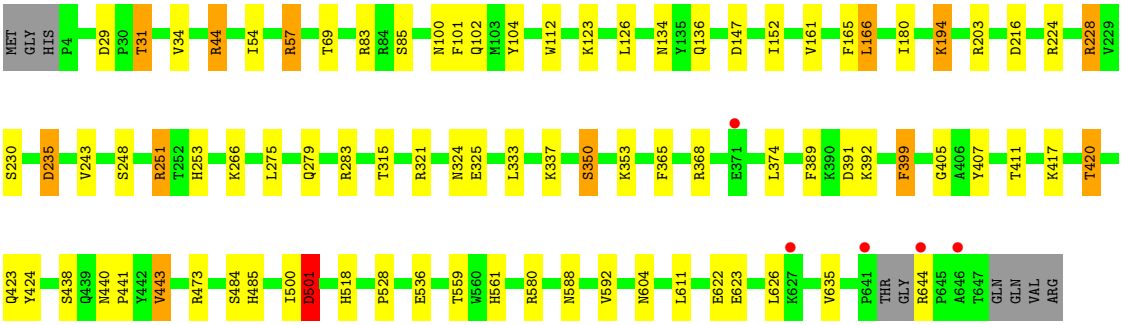




• Molecule 1: Alcohol oxidase

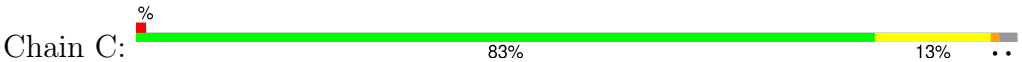
Chain B:

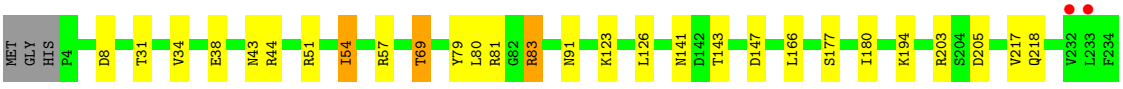


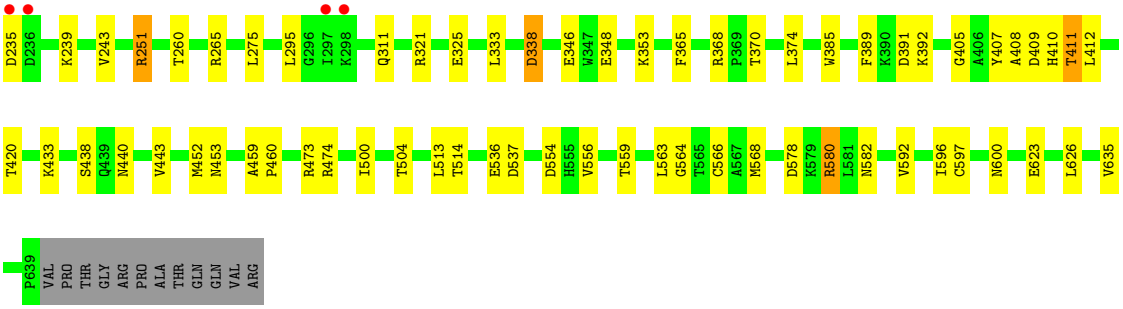


• Molecule 1: Alcohol oxidase

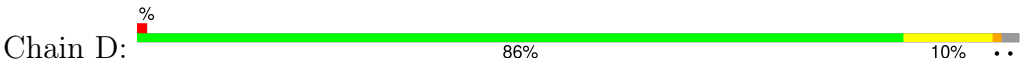
Chain C:

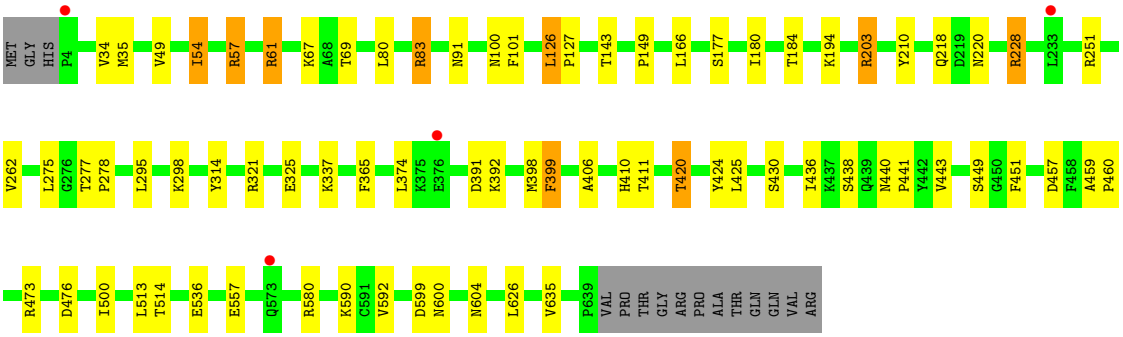




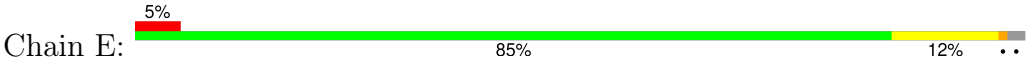


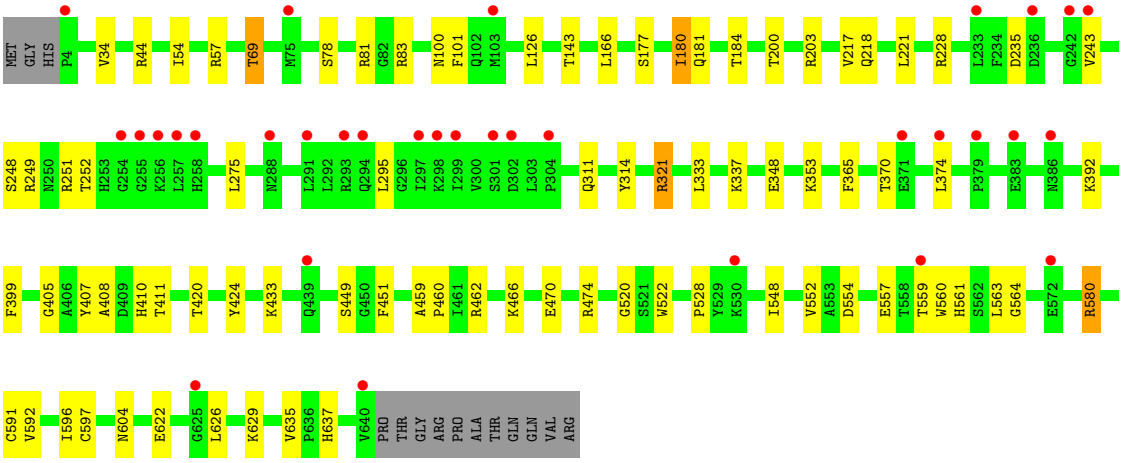
• Molecule 1: Alcohol oxidase



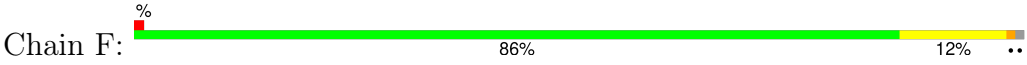


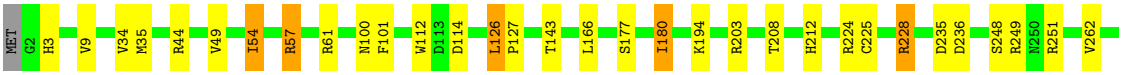
• Molecule 1: Alcohol oxidase

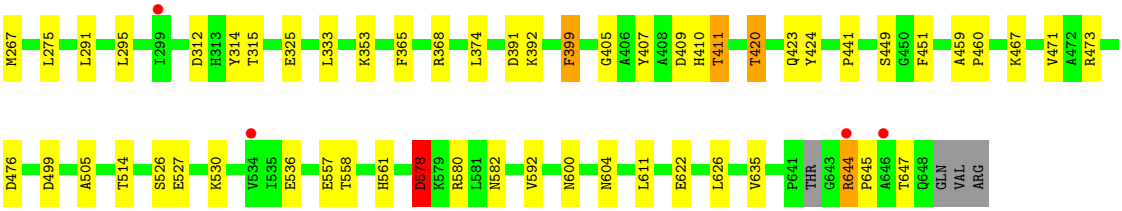




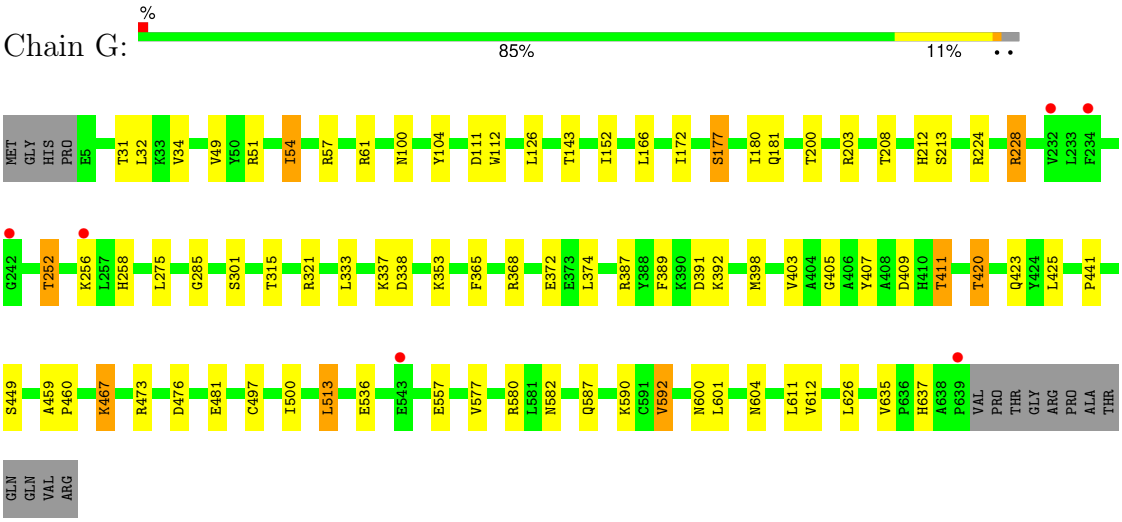
• Molecule 1: Alcohol oxidase



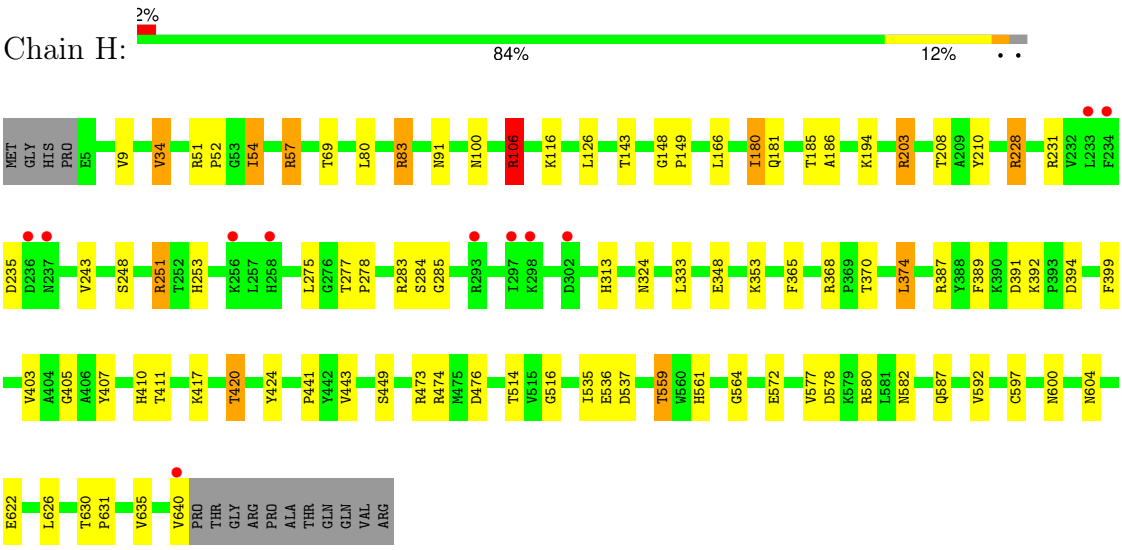




• Molecule 1: Alcohol oxidase



• Molecule 1: Alcohol oxidase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	112.67Å 204.04Å 116.52Å 90.00° 105.02° 90.00°	Depositor
Resolution (Å)	49.32 – 2.60 49.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.32-2.60) 97.7 (49.27-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.193 , 0.264 0.199 , 0.266	Depositor DCC
R_{free} test set	7538 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	41161	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 2.46% 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, GOL

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	0.38	0/5178	0.61	0/7031
1	B	0.40	0/5160	0.63	0/7004
1	C	0.39	0/5126	0.63	0/6956
1	D	0.39	0/5115	0.62	0/6942
1	E	0.39	0/5122	0.60	0/6952
1	F	0.40	0/5199	0.62	0/7056
1	G	0.39	0/5107	0.62	0/6931
1	H	0.40	0/5114	0.64	0/6941
All	All	0.39	0/41121	0.62	0/55813

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
1	E	0	2
1	H	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	ARG	Sidechain
1	B	321	ARG	Sidechain
1	B	500	ILE	Peptide
1	C	203	ARG	Sidechain
1	E	321	ARG	Sidechain
1	E	462	ARG	Sidechain
1	H	106	ARG	Sidechain

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	5052	0	4923	40	0
1	B	5036	0	4912	37	0
1	C	5003	0	4877	37	0
1	D	4992	0	4865	38	0
1	E	4999	0	4874	32	0
1	F	5074	0	4944	47	0
1	G	4985	0	4857	36	0
1	H	4992	0	4866	50	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
2	C	53	0	31	1	0
2	D	53	0	31	3	0
2	E	53	0	31	2	0
2	F	53	0	31	3	0
2	G	53	0	31	2	0
2	H	53	0	31	1	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
3	H	12	0	16	2	0
4	A	43	0	0	0	0
4	B	101	0	0	3	0
4	C	72	0	0	2	0
4	D	85	0	0	1	0
4	E	45	0	0	3	0
4	F	66	0	0	1	0
4	G	73	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	89	0	0	3	0
All	All	41161	0	39406	297	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 4.

All (297) 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:228:ARG:NH1	1:A:441:PRO:O	1.92	1.02
1:D:580:ARG:O	1:D:590:LYS:NZ	2.00	0.94
1:D:410:HIS:ND1	1:H:514:THR:HG21	1.86	0.89
1:F:61[B]:ARG:HH11	1:F:61[B]:ARG:CG	1.95	0.79
1:H:580:ARG:NH2	1:H:622:GLU:OE1	2.14	0.79
1:E:81:ARG:NH1	1:E:554:ASP:OD2	2.20	0.74
1:H:368:ARG:NH2	1:H:389:PHE:O	2.24	0.71
1:A:405:GLY:O	1:A:420:THR:HG22	1.91	0.70
1:D:228:ARG:NH1	1:D:441:PRO:O	2.24	0.70
1:E:100:ASN:O	1:E:203:ARG:NH2	2.25	0.69
1:B:473:ARG:NH2	1:B:536:GLU:O	2.26	0.69
1:C:568:MET:O	4:C:801:HOH:O	2.12	0.68
1:H:283:ARG:NH2	4:H:801:HOH:O	2.25	0.67
1:C:368:ARG:NH2	1:C:389:PHE:O	2.28	0.67
1:C:514:THR:HG21	1:F:410:HIS:ND1	2.09	0.67
1:F:473:ARG:NH2	1:F:536:GLU:O	2.27	0.66
1:B:407:TYR:H	1:B:420:THR:HG21	1.59	0.66
1:F:100:ASN:O	1:F:203:ARG:NH2	2.28	0.66
1:H:228:ARG:NH1	1:H:441:PRO:O	2.29	0.65
1:E:101:PHE:HB2	2:E:701:FAD:O4	1.98	0.64
1:G:473:ARG:NH2	1:G:536:GLU:O	2.32	0.63
1:H:100:ASN:O	1:H:203:ARG:NH2	2.33	0.62
1:C:38:GLU:OE1	2:C:701:FAD:O2B	2.10	0.61
1:F:61[B]:ARG:HH11	1:F:61[B]:ARG:HG2	1.66	0.61
1:G:228:ARG:NH1	1:G:441:PRO:O	2.34	0.61
1:D:399:PHE:CD1	1:D:424:TYR:CD2	2.89	0.60
1:F:101:PHE:HB2	2:F:701:FAD:O4	2.02	0.60
1:A:473:ARG:NH2	1:A:536:GLU:O	2.33	0.60
1:C:8:ASP:OD1	1:C:265:ARG:NH1	2.34	0.59
1:E:399:PHE:CG	1:E:424:TYR:CE2	2.90	0.59
1:F:604:ASN:HB3	2:F:701:FAD:C2	2.32	0.59
1:A:514[B]:THR:HG23	1:A:517:ILE:HD12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ASP:OD1	1:A:411:THR:HB	2.02	0.59
1:E:203:ARG:NH1	4:E:801:HOH:O	2.36	0.58
1:E:217:VAL:HG23	1:E:218:GLN:HG3	1.84	0.58
1:F:312:ASP:OD2	1:F:558:THR:OG1	2.19	0.58
1:F:407:TYR:H	1:F:420:THR:HG21	1.67	0.58
1:D:101:PHE:HB2	2:D:701:FAD:O4	2.04	0.58
1:E:314:TYR:O	1:E:424:TYR:HA	2.04	0.58
1:C:409:ASP:OD1	1:C:411:THR:HB	2.04	0.58
1:A:438:SER:HB3	1:A:443:VAL:HG21	1.86	0.58
1:D:399:PHE:CD1	1:D:424:TYR:CE2	2.91	0.57
1:A:514[A]:THR:HG21	1:E:410:HIS:HB2	1.85	0.57
1:D:430:SER:HB2	1:D:457:ASP:OD2	2.05	0.57
1:A:39:GLY:O	1:A:248:SER:OG	2.22	0.57
1:C:338:ASP:OD1	1:C:338:ASP:N	2.38	0.57
1:B:57:ARG:HD2	4:B:821:HOH:O	2.06	0.56
1:F:61[B]:ARG:HH11	1:F:61[B]:ARG:HG3	1.71	0.56
1:C:141:ASN:OD1	1:C:143:THR:OG1	2.19	0.56
1:A:407:TYR:H	1:A:420:THR:HG21	1.70	0.56
1:C:438:SER:HB3	1:C:443:VAL:HG21	1.86	0.56
1:B:230:SER:O	1:B:283:ARG:HD2	2.05	0.56
1:H:69:THR:HG23	1:H:91:ASN:HB2	1.88	0.55
1:A:403:VAL:HB	1:A:420:THR:HG23	1.89	0.55
1:G:315:THR:HA	1:G:423:GLN:O	2.07	0.55
1:H:407:TYR:H	1:H:420:THR:HG21	1.72	0.55
1:F:100:ASN:HB2	2:F:701:FAD:C5X	2.37	0.55
1:F:580:ARG:HH22	1:F:622:GLU:CD	2.10	0.55
1:G:411:THR:HG21	4:G:806:HOH:O	2.07	0.55
1:E:466:LYS:O	1:E:470:GLU:HG2	2.07	0.55
1:B:161:VAL:HG13	4:B:840:HOH:O	2.06	0.54
1:B:561:HIS:CE1	1:B:604:ASN:HA	2.42	0.54
1:G:100:ASN:O	1:G:203:ARG:NH2	2.40	0.54
1:H:405:GLY:O	1:H:420:THR:HG22	2.06	0.54
1:C:43:ASN:ND2	1:C:205:ASP:OD2	2.40	0.54
1:G:405:GLY:O	1:G:420:THR:HG22	2.06	0.54
1:G:580:ARG:O	1:G:590:LYS:NZ	2.40	0.54
1:H:313:HIS:HB2	1:H:559:THR:HG23	1.88	0.54
1:G:403:VAL:HB	1:G:420:THR:HG23	1.90	0.54
1:F:499:ASP:O	1:F:526:SER:OG	2.21	0.53
1:F:35:MET:CE	1:F:262:VAL:HG21	2.37	0.53
1:B:101:PHE:HB2	2:B:701:FAD:O4	2.07	0.53
1:C:440:ASN:HB3	1:C:443:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ALA:N	1:C:460:PRO:HD2	2.23	0.53
1:G:208:THR:HA	1:G:212:HIS:HB2	1.91	0.53
1:C:473:ARG:NH2	1:C:536:GLU:O	2.41	0.53
1:A:51:ARG:HB2	1:A:54:ILE:HD13	1.91	0.53
1:D:80:LEU:O	1:D:83:ARG:HG2	2.09	0.53
1:C:346:GLU:HB3	4:C:810:HOH:O	2.09	0.52
1:D:149:PRO:HG2	1:D:210:TYR:CE1	2.44	0.52
2:B:701:FAD:O2A	2:B:701:FAD:O4'	2.21	0.52
1:E:311:GLN:HB2	1:E:563:LEU:HD12	1.91	0.52
1:B:251:ARG:NH1	1:D:476:ASP:OD1	2.42	0.51
1:A:368:ARG:NH2	1:A:389:PHE:O	2.43	0.51
1:B:100:ASN:O	1:B:203:ARG:NH2	2.42	0.51
1:F:399:PHE:CD1	1:F:424:TYR:CD2	2.98	0.51
1:H:51:ARG:HB2	1:H:54:ILE:HD13	1.91	0.51
1:A:449:SER:OG	1:A:451:PHE:CD1	2.63	0.51
1:E:459:ALA:N	1:E:460:PRO:HD2	2.25	0.51
1:G:368:ARG:NH2	1:G:389:PHE:O	2.44	0.51
1:A:352:GLU:HG2	1:A:353:LYS:HG2	1.92	0.51
1:A:49:VAL:O	1:A:203:ARG:HD2	2.10	0.50
1:C:578:ASP:OD2	1:C:582:ASN:HB2	2.12	0.50
1:G:557:GLU:HG3	4:G:808:HOH:O	2.11	0.50
1:D:473:ARG:NH2	1:D:536:GLU:O	2.44	0.50
1:A:101:PHE:HB2	2:A:701:FAD:O4	2.11	0.50
1:C:405:GLY:O	1:C:420:THR:HG22	2.11	0.50
1:G:49:VAL:O	1:G:203:ARG:HD2	2.11	0.50
1:E:180:ILE:HG22	1:E:181:GLN:NE2	2.27	0.50
1:F:228:ARG:NH1	1:F:441:PRO:O	2.45	0.50
1:H:578:ASP:OD2	1:H:582:ASN:HB2	2.11	0.50
1:F:112:TRP:CZ2	1:F:611:LEU:HD23	2.47	0.50
1:G:321:ARG:HD3	1:G:500:ILE:HB	1.94	0.50
1:A:635:VAL:HG13	1:A:638:ALA:CB	2.42	0.50
1:B:104:TYR:CE1	1:B:152:ILE:HD13	2.47	0.50
1:H:106:ARG:HH22	1:H:143:THR:HG22	1.76	0.49
1:F:314:TYR:O	1:F:424:TYR:HA	2.12	0.49
1:H:57:ARG:HD2	4:H:825:HOH:O	2.12	0.49
1:D:514:THR:HG21	1:H:410:HIS:ND1	2.28	0.49
1:F:578:ASP:HB3	1:F:580:ARG:H	1.77	0.49
1:H:604:ASN:HB3	2:H:701:FAD:C2	2.42	0.49
1:C:69:THR:HG23	1:C:91:ASN:HB2	1.95	0.49
1:D:410:HIS:H	1:H:514:THR:HG23	1.77	0.49
1:H:561:HIS:CE1	1:H:604:ASN:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:THR:HB	1:A:278:PRO:HD3	1.95	0.49
1:D:126:LEU:HB3	1:D:127:PRO:HD3	1.95	0.49
1:D:406:ALA:HA	1:D:420:THR:HG22	1.95	0.49
1:G:476:ASP:OD1	1:H:251:ARG:NH1	2.46	0.49
1:H:180:ILE:CD1	1:H:185:THR:HG21	2.42	0.49
1:A:476:ASP:OD1	1:C:251:ARG:NH1	2.46	0.48
1:G:604:ASN:HB3	2:G:701:FAD:C2	2.43	0.48
1:B:266:LYS:O	1:B:588:ASN:ND2	2.46	0.48
1:C:385:TRP:CE3	1:C:389:PHE:HB2	2.49	0.48
1:B:368:ARG:NH2	1:B:389:PHE:O	2.47	0.48
1:B:438:SER:HB3	1:B:443:VAL:CG2	2.44	0.48
1:C:81:ARG:NH1	1:C:554:ASP:OD2	2.46	0.47
1:H:564:GLY:HA2	1:H:597:CYS:O	2.14	0.47
1:B:518:HIS:HB3	1:G:61:ARG:NH1	2.30	0.47
1:A:227:ALA:HB1	1:A:245:TYR:CD1	2.50	0.47
1:D:61:ARG:NH1	1:D:61:ARG:HB2	2.30	0.47
1:D:69:THR:HG23	1:D:91:ASN:HB2	1.94	0.47
1:D:438:SER:HB3	1:D:443:VAL:HG21	1.97	0.47
1:G:407:TYR:H	1:G:420:THR:HG21	1.79	0.47
1:A:321:ARG:HD3	1:A:500:ILE:HB	1.97	0.47
1:C:321:ARG:NH1	1:C:500:ILE:HD12	2.29	0.47
1:C:566:CYS:O	1:C:596:ILE:HA	2.14	0.47
1:D:440:ASN:ND2	1:D:441:PRO:HD2	2.30	0.47
1:A:566:CYS:O	1:A:596:ILE:HA	2.14	0.47
1:B:134:ASN:O	1:B:136:GLN:HG3	2.14	0.47
1:C:474:ARG:NH2	1:C:537:ASP:OD1	2.48	0.47
1:E:449:SER:HB3	1:E:451:PHE:CD1	2.50	0.47
1:F:35:MET:HE2	1:F:262:VAL:HG21	1.96	0.47
1:B:580:ARG:NH1	1:B:623:GLU:OE2	2.48	0.47
1:C:79:TYR:CD2	1:C:453:ASN:HA	2.50	0.47
1:F:177:SER:HB3	1:F:180:ILE:CD1	2.45	0.47
1:H:399:PHE:CG	1:H:424:TYR:CE2	3.03	0.47
1:G:104:TYR:CE1	1:G:152:ILE:HD13	2.50	0.47
1:A:580:ARG:HH22	1:A:622:GLU:CD	2.18	0.46
1:D:321:ARG:NH1	1:D:500:ILE:HD12	2.30	0.46
1:D:67:LYS:NZ	4:D:805:HOH:O	2.49	0.46
1:F:409:ASP:OD1	1:F:411:THR:HB	2.15	0.46
1:F:578:ASP:OD2	1:F:582:ASN:HB2	2.16	0.46
1:D:459:ALA:N	1:D:460:PRO:HD2	2.30	0.46
1:F:251:ARG:HG2	1:H:535:ILE:HD12	1.97	0.46
1:E:405:GLY:O	1:E:420:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:644:ARG:HB2	1:F:645:PRO:HD2	1.98	0.46
1:H:577:VAL:HA	1:H:582:ASN:O	2.15	0.46
1:A:577:VAL:HA	1:A:582:ASN:O	2.16	0.46
1:D:277:THR:HB	1:D:278:PRO:HD3	1.98	0.46
1:E:629:LYS:HE2	4:E:839:HOH:O	2.16	0.46
1:B:100:ASN:HB2	2:B:701:FAD:C5X	2.46	0.45
1:F:54:ILE:O	1:F:57:ARG:HG2	2.16	0.45
1:G:32:LEU:HD22	1:G:626:LEU:HD21	1.96	0.45
1:C:51:ARG:HB2	1:C:54:ILE:HD13	1.98	0.45
1:D:49:VAL:O	1:D:203:ARG:HD2	2.17	0.45
1:F:235:ASP:OD1	1:F:236:ASP:N	2.46	0.45
1:B:580:ARG:NH2	1:B:622:GLU:OE1	2.50	0.45
1:E:399:PHE:CD1	1:E:424:TYR:CE2	3.05	0.45
1:G:513:LEU:N	1:G:513:LEU:HD23	2.32	0.45
1:A:132:LEU:HD23	1:A:614:GLU:HG3	1.99	0.45
1:B:399:PHE:CG	1:B:424:TYR:CE2	3.05	0.45
1:G:180:ILE:HG22	1:G:181:GLN:NE2	2.32	0.45
1:H:106:ARG:NH1	1:H:181:GLN:O	2.50	0.45
1:E:580:ARG:HH22	1:E:622:GLU:CD	2.21	0.44
1:G:112:TRP:CZ2	1:G:611:LEU:HD23	2.52	0.44
1:A:100:ASN:HB2	2:A:701:FAD:C5X	2.46	0.44
1:H:374:LEU:HD13	1:H:374:LEU:HA	1.89	0.44
1:B:44:ARG:NH2	1:B:216:ASP:OD1	2.45	0.44
1:G:111:ASP:HB3	1:G:601:LEU:HD23	1.99	0.44
1:G:200:THR:HG21	1:G:637:HIS:O	2.17	0.44
1:C:580:ARG:NH1	1:C:623:GLU:OE2	2.46	0.44
1:D:100:ASN:O	1:D:203:ARG:NH2	2.50	0.44
1:C:311:GLN:HB2	1:C:563:LEU:HD12	1.98	0.44
1:B:484:SER:OG	1:B:485:HIS:ND1	2.45	0.44
1:D:218:GLN:NE2	1:D:220:ASN:OD1	2.48	0.44
1:A:324:ASN:O	1:A:417:LYS:NZ	2.50	0.44
1:C:217:VAL:HG23	1:C:218:GLN:HG3	2.00	0.44
1:D:61:ARG:NH1	1:H:516:GLY:O	2.48	0.44
1:F:314:TYR:CE1	1:F:451:PHE:CD1	3.06	0.44
1:C:235:ASP:HB2	1:C:239:LYS:O	2.18	0.44
1:D:513:LEU:O	1:H:57:ARG:HA	2.18	0.44
1:H:148:GLY:C	3:H:703:GOL:H32	2.38	0.44
1:C:408:ALA:O	1:F:514:THR:OG1	2.34	0.44
1:F:61[B]:ARG:HG2	1:F:61[B]:ARG:NH1	2.33	0.44
1:C:411:THR:HG21	1:F:505:ALA:HB1	1.99	0.43
1:G:100:ASN:HB2	2:G:701:FAD:C5X	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:313:HIS:HB2	1:H:559:THR:CG2	2.48	0.43
1:A:411:THR:O	1:E:321:ARG:NH2	2.51	0.43
1:E:399:PHE:CD1	1:E:424:TYR:CD2	3.06	0.43
1:F:399:PHE:CD1	1:F:424:TYR:CE2	3.06	0.43
1:F:405:GLY:O	1:F:420:THR:HG22	2.18	0.43
1:G:459:ALA:N	1:G:460:PRO:HD2	2.33	0.43
1:A:177:SER:HB3	1:A:180:ILE:CD1	2.48	0.43
1:A:514[B]:THR:HG21	1:E:408:ALA:O	2.18	0.43
1:B:57:ARG:CD	4:B:821:HOH:O	2.65	0.43
1:G:577:VAL:HA	1:G:582:ASN:O	2.18	0.43
1:B:29:ASP:OD1	1:B:31:THR:OG1	2.37	0.43
1:D:177:SER:HB3	1:D:180:ILE:CD1	2.48	0.43
1:D:399:PHE:CG	1:D:424:TYR:CE2	3.06	0.43
1:G:252:THR:HG21	1:G:258:HIS:HB2	2.00	0.43
1:A:100:ASN:N	1:A:203:ARG:NH2	2.67	0.43
1:B:405:GLY:O	1:B:420:THR:HG22	2.19	0.43
1:E:69:THR:HG22	4:E:835:HOH:O	2.18	0.43
1:A:126:LEU:N	1:A:127:PRO:HD2	2.34	0.43
1:A:459:ALA:N	1:A:460:PRO:HD2	2.33	0.43
1:C:564:GLY:HA2	1:C:597:CYS:O	2.19	0.43
1:D:100:ASN:HB2	2:D:701:FAD:C5X	2.48	0.43
1:B:102:GLN:O	1:B:194:LYS:HA	2.19	0.43
1:H:559:THR:O	1:H:559:THR:OG1	2.34	0.43
1:A:564:GLY:HA2	1:A:597:CYS:O	2.19	0.43
1:A:241:VAL:O	1:A:264:ALA:N	2.47	0.42
1:C:80:LEU:HB3	1:C:83:ARG:HG3	2.01	0.42
1:E:560:TRP:CE3	2:E:701:FAD:C6	3.02	0.42
1:B:501:ASP:OD2	1:B:528:PRO:HA	2.19	0.42
1:E:34:VAL:HG22	1:E:221:LEU:HD13	2.01	0.42
1:F:126:LEU:N	1:F:127:PRO:CD	2.82	0.42
1:D:35:MET:CE	1:D:262:VAL:HG21	2.50	0.42
1:D:604:ASN:HB3	2:D:701:FAD:C2	2.48	0.42
1:F:9:VAL:HA	1:F:267:MET:O	2.19	0.42
1:F:203:ARG:NH1	4:F:802:HOH:O	2.51	0.42
1:G:398:MET:SD	1:G:425:LEU:HA	2.58	0.42
1:H:149:PRO:N	3:H:703:GOL:H32	2.34	0.42
1:H:231:ARG:HB2	1:H:284:SER:HA	2.00	0.42
1:F:459:ALA:N	1:F:460:PRO:HD2	2.35	0.42
1:H:324:ASN:O	1:H:417:LYS:NZ	2.52	0.42
1:B:440:ASN:OD1	1:B:441:PRO:HD2	2.19	0.42
1:H:277:THR:HB	1:H:278:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:ILE:HD12	1:D:438:SER:O	2.19	0.42
1:G:172:ILE:HD12	1:G:467:LYS:HD2	2.02	0.42
1:G:177:SER:HB3	1:G:180:ILE:CD1	2.48	0.42
1:C:452:MET:HE3	1:C:556:VAL:HG21	2.02	0.42
1:D:61:ARG:HB2	1:D:61:ARG:HH11	1.84	0.42
1:G:481:GLU:OE1	1:G:497:CYS:HA	2.19	0.42
1:H:640:VAL:HG22	4:H:855:HOH:O	2.18	0.42
1:A:348:GLU:HG3	1:B:350:SER:OG	2.19	0.42
1:B:279:GLN:HB3	1:B:283:ARG:NH2	2.34	0.42
1:C:407:TYR:H	1:C:420:THR:HG21	1.85	0.42
1:E:249:ARG:NH1	1:F:476:ASP:OD2	2.52	0.42
1:H:180:ILE:HG22	1:H:181:GLN:NE2	2.35	0.42
1:H:403:VAL:HB	1:H:420:THR:HG23	2.02	0.42
1:D:398:MET:SD	1:D:425:LEU:HA	2.60	0.42
1:B:112:TRP:CZ2	1:B:611:LEU:HD23	2.54	0.42
1:F:315:THR:HA	1:F:423:GLN:O	2.20	0.42
1:E:200:THR:HG21	1:E:637:HIS:O	2.20	0.41
1:E:591:CYS:O	1:E:596:ILE:HG21	2.20	0.41
1:F:224:ARG:NH1	1:F:225:CYS:O	2.53	0.41
1:H:149:PRO:HG2	1:H:210:TYR:CZ	2.55	0.41
1:A:219:ASP:OD1	1:A:219:ASP:C	2.59	0.41
1:B:315:THR:HA	1:B:423:GLN:O	2.20	0.41
1:H:106:ARG:HH12	1:H:143:THR:HG22	1.85	0.41
1:B:166:LEU:HD12	1:B:166:LEU:HA	1.97	0.41
1:H:399:PHE:CD1	1:H:424:TYR:CD2	3.08	0.41
1:B:324:ASN:O	1:B:417:LYS:NZ	2.52	0.41
1:C:410:HIS:HB2	1:F:514:THR:HG21	2.02	0.41
1:C:500:ILE:HD11	1:C:504:THR:HG22	2.02	0.41
1:B:438:SER:HB3	1:B:443:VAL:HG21	2.02	0.41
1:D:314:TYR:CE1	1:D:451:PHE:CD1	3.09	0.41
1:F:249:ARG:NH1	1:H:476:ASP:OD2	2.53	0.41
1:F:208:THR:HA	1:F:212:HIS:HB2	2.03	0.41
1:G:51:ARG:HB2	1:G:54:ILE:HD13	2.03	0.41
1:H:630:THR:HA	1:H:631:PRO:HA	1.95	0.41
1:E:561:HIS:CE1	1:E:604:ASN:HA	2.56	0.41
1:E:177:SER:HB3	1:E:180:ILE:CD1	2.51	0.41
1:F:561:HIS:CE1	1:F:604:ASN:HA	2.56	0.41
1:G:409:ASP:OD1	1:G:411:THR:HB	2.21	0.41
1:H:9:VAL:O	1:H:34:VAL:HA	2.19	0.41
1:H:51:ARG:HA	1:H:52:PRO:HD3	1.97	0.41
1:B:165:PHE:CD1	1:B:165:PHE:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ILE:O	1:D:57:ARG:CG	2.69	0.41
1:E:564:GLY:HA2	1:E:597:CYS:O	2.21	0.41
1:H:80:LEU:O	1:H:83:ARG:HG2	2.20	0.41
1:A:581:LEU:HB3	1:A:591:CYS:O	2.21	0.40
1:E:407:TYR:H	1:E:420:THR:HG21	1.86	0.40
1:E:520:GLY:HA3	1:E:522:TRP:NE1	2.36	0.40
1:F:251:ARG:CG	1:H:535:ILE:HD12	2.51	0.40
1:E:548:ILE:O	1:E:552:VAL:HG23	2.21	0.40
1:B:399:PHE:CD1	1:B:424:TYR:CD2	3.09	0.40
1:F:49:VAL:O	1:F:203:ARG:HD2	2.21	0.40
1:F:467:LYS:O	1:F:471:VAL:HG23	2.22	0.40
1:H:186:ALA:HB2	1:H:394:ASP:C	2.42	0.40
1:H:473:ARG:NH2	1:H:536:GLU:O	2.55	0.40
1:H:580:ARG:HH22	1:H:622:GLU:CD	2.23	0.40
1:A:449:SER:OG	1:A:451:PHE:CG	2.74	0.40
1:G:403:VAL:HB	1:G:420:THR:CG2	2.50	0.40
1:A:231:ARG:HB2	1:A:284:SER:HA	2.01	0.40
1:B:228:ARG:NH1	1:B:441:PRO:O	2.54	0.40
1:G:592:VAL:HG23	1:G:612:VAL:HG12	2.03	0.40

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	642/651 (99%)	606 (94%)	35 (6%)	1 (0%)	47 71
1	B	638/651 (98%)	603 (94%)	32 (5%)	3 (0%)	29 52
1	C	635/651 (98%)	593 (93%)	41 (6%)	1 (0%)	47 71
1	D	634/651 (97%)	598 (94%)	36 (6%)	0	100 100
1	E	635/651 (98%)	598 (94%)	36 (6%)	1 (0%)	47 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	643/651 (99%)	605 (94%)	37 (6%)	1 (0%)	47 71
1	G	633/651 (97%)	588 (93%)	44 (7%)	1 (0%)	47 71
1	H	634/651 (97%)	597 (94%)	34 (5%)	3 (0%)	29 52
All	All	5094/5208 (98%)	4788 (94%)	295 (6%)	11 (0%)	47 71

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	501	ASP
1	B	235	ASP
1	F	578	ASP
1	H	449	SER
1	B	253	HIS
1	E	528	PRO
1	A	306	VAL
1	C	123	LYS
1	H	253	HIS
1	H	285	GLY
1	G	285	GLY

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	543/548 (99%)	510 (94%)	33 (6%)	18 38
1	B	541/548 (99%)	501 (93%)	40 (7%)	13 28
1	C	537/548 (98%)	499 (93%)	38 (7%)	14 29
1	D	536/548 (98%)	504 (94%)	32 (6%)	19 39
1	E	537/548 (98%)	501 (93%)	36 (7%)	16 33
1	F	544/548 (99%)	506 (93%)	38 (7%)	15 30
1	G	535/548 (98%)	501 (94%)	34 (6%)	17 35
1	H	536/548 (98%)	497 (93%)	39 (7%)	14 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4309/4384 (98%)	4019 (93%)	290 (7%)	16 33

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	34	VAL
1	A	54	ILE
1	A	57	ARG
1	A	69	THR
1	A	83	ARG
1	A	106	ARG
1	A	114	ASP
1	A	126	LEU
1	A	143	THR
1	A	166	LEU
1	A	194	LYS
1	A	243	VAL
1	A	257	LEU
1	A	275	LEU
1	A	333	LEU
1	A	353	LYS
1	A	365	PHE
1	A	370	THR
1	A	374	LEU
1	A	391	ASP
1	A	392	LYS
1	A	399	PHE
1	A	411	THR
1	A	420	THR
1	A	501	ASP
1	A	527	GLU
1	A	532	ASP
1	A	557	GLU
1	A	592	VAL
1	A	600	ASN
1	A	626	LEU
1	A	644	ARG
1	B	31	THR
1	B	34	VAL
1	B	44	ARG
1	B	54	ILE

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Mol	Chain	Res	Type
1	B	57	ARG
1	B	69	THR
1	B	83	ARG
1	B	85	SER
1	B	123	LYS
1	B	126	LEU
1	B	147	ASP
1	B	166	LEU
1	B	180	ILE
1	B	194	LYS
1	B	224	ARG
1	B	228	ARG
1	B	235	ASP
1	B	243	VAL
1	B	248	SER
1	B	251	ARG
1	B	275	LEU
1	B	325	GLU
1	B	333	LEU
1	B	337	LYS
1	B	350	SER
1	B	353	LYS
1	B	365	PHE
1	B	374	LEU
1	B	391	ASP
1	B	392	LYS
1	B	399	PHE
1	B	411	THR
1	B	420	THR
1	B	443	VAL
1	B	501	ASP
1	B	559	THR
1	B	592	VAL
1	B	626	LEU
1	B	635	VAL
1	B	644	ARG
1	C	31	THR
1	C	34	VAL
1	C	44	ARG
1	C	54	ILE
1	C	57	ARG
1	C	69	THR

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Mol	Chain	Res	Type
1	C	83	ARG
1	C	126	LEU
1	C	147	ASP
1	C	166	LEU
1	C	177	SER
1	C	180	ILE
1	C	194	LYS
1	C	243	VAL
1	C	251	ARG
1	C	260	THR
1	C	275	LEU
1	C	295	LEU
1	C	325	GLU
1	C	333	LEU
1	C	338	ASP
1	C	348	GLU
1	C	353	LYS
1	C	365	PHE
1	C	370	THR
1	C	374	LEU
1	C	391	ASP
1	C	392	LYS
1	C	411	THR
1	C	412	LEU
1	C	433	LYS
1	C	513	LEU
1	C	559	THR
1	C	580	ARG
1	C	592	VAL
1	C	600	ASN
1	C	626	LEU
1	C	635	VAL
1	D	34	VAL
1	D	54	ILE
1	D	57	ARG
1	D	61	ARG
1	D	83	ARG
1	D	126	LEU
1	D	143	THR
1	D	166	LEU
1	D	184	THR
1	D	194	LYS

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Mol	Chain	Res	Type
1	D	203	ARG
1	D	228	ARG
1	D	251	ARG
1	D	275	LEU
1	D	295	LEU
1	D	298	LYS
1	D	325	GLU
1	D	337	LYS
1	D	365	PHE
1	D	374	LEU
1	D	391	ASP
1	D	392	LYS
1	D	399	PHE
1	D	411	THR
1	D	420	THR
1	D	449	SER
1	D	557	GLU
1	D	592	VAL
1	D	599	ASP
1	D	600	ASN
1	D	626	LEU
1	D	635	VAL
1	E	44	ARG
1	E	54	ILE
1	E	57	ARG
1	E	69	THR
1	E	78	SER
1	E	83	ARG
1	E	126	LEU
1	E	143	THR
1	E	166	LEU
1	E	180	ILE
1	E	184	THR
1	E	228	ARG
1	E	235	ASP
1	E	243	VAL
1	E	248	SER
1	E	251	ARG
1	E	252	THR
1	E	275	LEU
1	E	295	LEU
1	E	333	LEU

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Mol	Chain	Res	Type
1	E	337	LYS
1	E	348	GLU
1	E	353	LYS
1	E	365	PHE
1	E	370	THR
1	E	374	LEU
1	E	392	LYS
1	E	411	THR
1	E	433	LYS
1	E	474	ARG
1	E	557	GLU
1	E	559	THR
1	E	580	ARG
1	E	592	VAL
1	E	626	LEU
1	E	635	VAL
1	F	3	HIS
1	F	34	VAL
1	F	44	ARG
1	F	54	ILE
1	F	57	ARG
1	F	114	ASP
1	F	126	LEU
1	F	143	THR
1	F	166	LEU
1	F	180	ILE
1	F	194	LYS
1	F	228	ARG
1	F	248	SER
1	F	275	LEU
1	F	291	LEU
1	F	295	LEU
1	F	325	GLU
1	F	333	LEU
1	F	353	LYS
1	F	365	PHE
1	F	368	ARG
1	F	374	LEU
1	F	391	ASP
1	F	392	LYS
1	F	399	PHE
1	F	411	THR

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Mol	Chain	Res	Type
1	F	420	THR
1	F	449	SER
1	F	527	GLU
1	F	530	LYS
1	F	557	GLU
1	F	578	ASP
1	F	592	VAL
1	F	600	ASN
1	F	626	LEU
1	F	635	VAL
1	F	644	ARG
1	F	647	THR
1	G	31	THR
1	G	34	VAL
1	G	54	ILE
1	G	57	ARG
1	G	126	LEU
1	G	143	THR
1	G	166	LEU
1	G	177	SER
1	G	213	SER
1	G	224	ARG
1	G	228	ARG
1	G	252	THR
1	G	256	LYS
1	G	275	LEU
1	G	301	SER
1	G	333	LEU
1	G	337	LYS
1	G	338	ASP
1	G	353	LYS
1	G	365	PHE
1	G	372	GLU
1	G	374	LEU
1	G	387	ARG
1	G	391	ASP
1	G	392	LYS
1	G	411	THR
1	G	420	THR
1	G	449	SER
1	G	467	LYS
1	G	513	LEU

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Mol	Chain	Res	Type
1	G	587	GLN
1	G	592	VAL
1	G	600	ASN
1	G	635	VAL
1	H	34	VAL
1	H	54	ILE
1	H	57	ARG
1	H	83	ARG
1	H	106	ARG
1	H	116	LYS
1	H	126	LEU
1	H	166	LEU
1	H	180	ILE
1	H	194	LYS
1	H	203	ARG
1	H	208	THR
1	H	228	ARG
1	H	235	ASP
1	H	243	VAL
1	H	248	SER
1	H	251	ARG
1	H	275	LEU
1	H	333	LEU
1	H	348	GLU
1	H	353	LYS
1	H	365	PHE
1	H	370	THR
1	H	374	LEU
1	H	387	ARG
1	H	391	ASP
1	H	392	LYS
1	H	411	THR
1	H	420	THR
1	H	443	VAL
1	H	474	ARG
1	H	537	ASP
1	H	559	THR
1	H	572	GLU
1	H	587	GLN
1	H	592	VAL
1	H	600	ASN
1	H	626	LEU

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Mol	Chain	Res	Type
1	H	635	VAL

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

Mol	Chain	Res	Type
1	A	218	GLN
1	B	157	GLN
1	B	279	GLN
1	C	440	ASN
1	C	600	ASN
1	D	157	GLN
1	D	531	HIS
1	D	573	GLN
1	E	157	GLN
1	E	423	GLN
1	E	524	GLN
1	H	531	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

13 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	-	54,58,58	1.38	6 (11%)	71,89,89	1.42	9 (12%)
2	FAD	D	701	-	54,58,58	1.47	4 (7%)	71,89,89	1.29	6 (8%)
2	FAD	H	701	-	54,58,58	1.53	6 (11%)	71,89,89	1.30	9 (12%)
2	FAD	G	701	-	54,58,58	1.38	3 (5%)	71,89,89	1.41	10 (14%)
2	FAD	B	701	-	54,58,58	1.56	6 (11%)	71,89,89	1.25	7 (9%)
3	GOL	H	703	-	5,5,5	0.72	0	5,5,5	1.20	1 (20%)
2	FAD	E	701	-	54,58,58	1.44	5 (9%)	71,89,89	1.45	12 (16%)
3	GOL	H	702	-	5,5,5	0.42	0	5,5,5	0.51	0
3	GOL	D	702	-	5,5,5	0.45	0	5,5,5	0.36	0
3	GOL	C	702	-	5,5,5	0.32	0	5,5,5	0.35	0
2	FAD	C	701	-	54,58,58	1.41	5 (9%)	71,89,89	1.40	10 (14%)
3	GOL	B	702	-	5,5,5	0.77	0	5,5,5	0.62	0
2	FAD	F	701	-	54,58,58	1.36	4 (7%)	71,89,89	1.31	11 (15%)

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	-	-	8/30/50/50	0/6/6/6
2	FAD	D	701	-	-	5/30/50/50	0/6/6/6
2	FAD	H	701	-	-	8/30/50/50	0/6/6/6
2	FAD	G	701	-	-	8/30/50/50	0/6/6/6
2	FAD	B	701	-	-	5/30/50/50	0/6/6/6
3	GOL	H	703	-	-	2/4/4/4	-
2	FAD	E	701	-	-	6/30/50/50	0/6/6/6
3	GOL	H	702	-	-	2/4/4/4	-
3	GOL	D	702	-	-	2/4/4/4	-
3	GOL	C	702	-	-	0/4/4/4	-
2	FAD	C	701	-	-	6/30/50/50	0/6/6/6
3	GOL	B	702	-	-	2/4/4/4	-
2	FAD	F	701	-	-	4/30/50/50	0/6/6/6

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	FAD	C9A-C5X	6.41	1.51	1.41
2	B	701	FAD	C9A-C5X	6.32	1.51	1.41
2	H	701	FAD	C9A-C5X	6.24	1.51	1.41
2	G	701	FAD	C9A-C5X	6.19	1.51	1.41
2	D	701	FAD	C9A-C5X	6.10	1.51	1.41
2	E	701	FAD	C9A-C5X	6.01	1.50	1.41
2	F	701	FAD	C9A-C5X	5.42	1.49	1.41
2	A	701	FAD	C9A-C5X	5.23	1.49	1.41
2	B	701	FAD	P-O3P	4.87	1.64	1.59
2	D	701	FAD	P-O3P	4.54	1.64	1.59
2	G	701	FAD	C8-C7	4.21	1.51	1.40
2	H	701	FAD	P-O3P	3.98	1.63	1.59
2	A	701	FAD	P-O3P	3.97	1.63	1.59
2	H	701	FAD	C8-C7	3.82	1.50	1.40
2	C	701	FAD	C8-C7	3.81	1.50	1.40
2	E	701	FAD	C8-C7	3.77	1.50	1.40
2	D	701	FAD	C8-C7	3.71	1.49	1.40
2	A	701	FAD	C8-C7	3.68	1.49	1.40
2	B	701	FAD	PA-O3P	3.61	1.63	1.59
2	F	701	FAD	C8-C7	3.55	1.49	1.40
2	E	701	FAD	P-O3P	3.49	1.63	1.59
2	B	701	FAD	C8-C7	3.48	1.49	1.40
2	D	701	FAD	PA-O3P	3.21	1.63	1.59
2	F	701	FAD	PA-O3P	3.14	1.62	1.59
2	H	701	FAD	PA-O3P	3.07	1.62	1.59
2	F	701	FAD	P-O3P	3.06	1.62	1.59
2	A	701	FAD	PA-O3P	2.95	1.62	1.59
2	H	701	FAD	C2A-N3A	2.70	1.36	1.32
2	E	701	FAD	PA-O3P	2.60	1.62	1.59
2	H	701	FAD	C4X-N5	2.33	1.35	1.30
2	C	701	FAD	C4X-N5	2.31	1.35	1.30
2	B	701	FAD	C4X-N5	2.27	1.35	1.30
2	G	701	FAD	C4X-N5	2.19	1.35	1.30
2	E	701	FAD	C10-N10	2.12	1.41	1.37
2	C	701	FAD	C10-N10	2.11	1.41	1.37
2	B	701	FAD	C4-N3	-2.11	1.34	1.38
2	A	701	FAD	C2A-N3A	2.08	1.35	1.32
2	C	701	FAD	P-O3P	2.04	1.61	1.59
2	A	701	FAD	C4-N3	-2.02	1.35	1.38

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	701	FAD	N3A-C2A-N1A	-4.87	122.07	128.67
2	C	701	FAD	N3A-C2A-N1A	-4.86	122.08	128.67
2	D	701	FAD	N3A-C2A-N1A	-4.83	122.12	128.67
2	A	701	FAD	N3A-C2A-N1A	-4.74	122.24	128.67
2	E	701	FAD	N3A-C2A-N1A	-4.70	122.29	128.67
2	A	701	FAD	C4'-C3'-C2'	-4.37	106.29	113.57
2	F	701	FAD	N3A-C2A-N1A	-4.37	122.74	128.67
2	B	701	FAD	N3A-C2A-N1A	-4.25	122.90	128.67
2	C	701	FAD	C4-C4X-N5	3.85	123.53	118.21
2	H	701	FAD	N3A-C2A-N1A	-3.78	123.54	128.67
2	H	701	FAD	C4'-C3'-C2'	-3.66	107.47	113.57
2	G	701	FAD	C4-C4X-N5	3.59	123.17	118.21
2	B	701	FAD	C4-C4X-N5	3.53	123.08	118.21
2	G	701	FAD	C1B-N9A-C4A	-3.42	120.64	126.64
2	E	701	FAD	C4'-C3'-C2'	-3.41	107.89	113.57
2	A	701	FAD	C4-C4X-N5	3.24	122.69	118.21
2	E	701	FAD	O4B-C1B-N9A	3.23	113.03	108.75
2	D	701	FAD	C1B-N9A-C4A	-3.23	120.97	126.64
2	B	701	FAD	C4A-C5A-N7A	-3.17	105.99	109.34
2	E	701	FAD	C1B-N9A-C4A	-3.15	121.10	126.64
2	F	701	FAD	C4-C4X-N5	3.12	122.52	118.21
2	E	701	FAD	C4-C4X-N5	3.08	122.46	118.21
2	C	701	FAD	C9A-C5X-N5	-3.06	119.21	122.45
2	D	701	FAD	O4-C4-C4X	-2.98	118.66	126.53
2	H	701	FAD	C4-C4X-N5	2.94	122.27	118.21
2	F	701	FAD	C4A-C5A-N7A	-2.92	106.25	109.34
2	D	701	FAD	C4'-C3'-C2'	-2.89	108.77	113.57
2	G	701	FAD	C4'-C3'-C2'	-2.88	108.77	113.57
2	A	701	FAD	C4A-C5A-N7A	-2.83	106.34	109.34
2	G	701	FAD	C4A-C5A-N7A	-2.79	106.39	109.34
2	D	701	FAD	C4A-C5A-N7A	-2.76	106.42	109.34
2	D	701	FAD	O2A-PA-O3P	2.74	114.69	107.27
2	C	701	FAD	O2A-PA-O3P	2.71	114.59	107.27
2	F	701	FAD	C1B-N9A-C4A	-2.68	121.93	126.64
2	E	701	FAD	C4A-C5A-N7A	-2.64	106.55	109.34
2	A	701	FAD	O2A-PA-O3P	2.58	114.24	107.27
2	C	701	FAD	C4X-C10-N10	2.57	120.17	116.48
2	H	701	FAD	C4A-C5A-N7A	-2.54	106.65	109.34
2	C	701	FAD	C9-C9A-N10	-2.45	118.56	121.85
2	C	701	FAD	C1B-N9A-C4A	-2.44	122.35	126.64
2	F	701	FAD	C4X-C10-N1	-2.43	118.64	124.59
2	H	701	FAD	O4-C4-C4X	-2.41	120.16	126.53
2	E	701	FAD	C4X-C10-N1	-2.41	118.68	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	703	GOL	O3-C3-C2	2.38	121.11	110.38
2	E	701	FAD	C9A-C5X-N5	-2.38	119.93	122.45
2	G	701	FAD	C9A-C5X-N5	-2.35	119.96	122.45
2	E	701	FAD	C10-N1-C2	2.35	121.93	116.85
2	H	701	FAD	C4X-C4-N3	2.34	119.22	113.25
2	E	701	FAD	O4-C4-C4X	-2.34	120.36	126.53
2	A	701	FAD	O4-C4-C4X	-2.33	120.38	126.53
2	C	701	FAD	C9A-N10-C10	-2.32	117.22	120.75
2	G	701	FAD	C10-C4X-N5	-2.29	120.14	124.81
2	A	701	FAD	C4X-C4-N3	2.28	119.06	113.25
2	F	701	FAD	O4-C4-C4X	-2.28	120.53	126.53
2	F	701	FAD	C4X-C4-N3	2.22	118.89	113.25
2	F	701	FAD	C10-N1-C2	2.21	121.64	116.85
2	H	701	FAD	C10-N1-C2	2.21	121.63	116.85
2	C	701	FAD	C10-C4X-N5	-2.19	120.33	124.81
2	E	701	FAD	C4X-C4-N3	2.18	118.80	113.25
2	G	701	FAD	C4X-C10-N1	-2.17	119.27	124.59
2	A	701	FAD	C4X-C10-N1	-2.17	119.28	124.59
2	E	701	FAD	C9A-N10-C10	-2.15	117.47	120.75
2	B	701	FAD	C9A-C5X-N5	-2.15	120.17	122.45
2	B	701	FAD	C4'-C3'-C2'	-2.14	110.00	113.57
2	F	701	FAD	O2A-PA-O3P	2.14	113.07	107.27
2	C	701	FAD	C4X-C10-N1	-2.12	119.38	124.59
2	B	701	FAD	C4X-C10-N10	2.12	119.52	116.48
2	A	701	FAD	C4-N3-C2	-2.11	121.89	125.64
2	G	701	FAD	O4-C4-C4X	-2.09	121.01	126.53
2	G	701	FAD	C4X-C10-N10	2.08	119.46	116.48
2	H	701	FAD	C4X-C10-N1	-2.07	119.52	124.59
2	H	701	FAD	O3'-C3'-C2'	2.06	113.60	108.93
2	F	701	FAD	C10-C4X-N5	-2.05	120.61	124.81
2	B	701	FAD	C4X-C4-N3	2.05	118.48	113.25
2	F	701	FAD	C4-N3-C2	-2.04	122.02	125.64

There are no chirality outliers.

All (58) 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	B	701	FAD	N10-C1'-C2'-O2'
2	C	701	FAD	N10-C1'-C2'-O2'
2	D	701	FAD	N10-C1'-C2'-O2'

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Mol	Chain	Res	Type	Atoms
2	E	701	FAD	N10-C1'-C2'-O2'
2	E	701	FAD	N10-C1'-C2'-C3'
2	F	701	FAD	N10-C1'-C2'-O2'
2	G	701	FAD	N10-C1'-C2'-O2'
2	G	701	FAD	N10-C1'-C2'-C3'
2	H	701	FAD	N10-C1'-C2'-O2'
3	D	702	GOL	O1-C1-C2-C3
3	H	703	GOL	C1-C2-C3-O3
3	B	702	GOL	O1-C1-C2-O2
3	B	702	GOL	O1-C1-C2-C3
3	H	702	GOL	O1-C1-C2-C3
3	D	702	GOL	O1-C1-C2-O2
3	H	703	GOL	O2-C2-C3-O3
2	H	701	FAD	O4'-C4'-C5'-O5'
2	E	701	FAD	O4B-C4B-C5B-O5B
2	H	701	FAD	P-O3P-PA-O1A
2	H	701	FAD	PA-O3P-P-O1P
3	H	702	GOL	O1-C1-C2-O2
2	A	701	FAD	PA-O3P-P-O5'
2	C	701	FAD	PA-O3P-P-O5'
2	D	701	FAD	PA-O3P-P-O5'
2	E	701	FAD	PA-O3P-P-O5'
2	F	701	FAD	PA-O3P-P-O5'
2	G	701	FAD	PA-O3P-P-O5'
2	H	701	FAD	PA-O3P-P-O5'
2	A	701	FAD	P-O3P-PA-O2A
2	E	701	FAD	O4'-C4'-C5'-O5'
2	G	701	FAD	O4'-C4'-C5'-O5'
2	B	701	FAD	N10-C1'-C2'-C3'
2	H	701	FAD	N10-C1'-C2'-C3'
2	A	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5'-O5'-P-O1P
2	C	701	FAD	C5'-O5'-P-O1P
2	H	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	P-O3P-PA-O1A
2	D	701	FAD	P-O3P-PA-O2A
2	D	701	FAD	PA-O3P-P-O1P
2	G	701	FAD	P-O3P-PA-O2A
2	E	701	FAD	C3B-C4B-C5B-O5B
2	A	701	FAD	O4'-C4'-C5'-O5'
2	F	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	P-O3P-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	G	701	FAD	P-O3P-PA-O1A
2	G	701	FAD	PA-O3P-P-O1P
2	B	701	FAD	PA-O3P-P-O5'
2	C	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	P-O3P-PA-O1A
2	A	701	FAD	PA-O3P-P-O1P
2	C	701	FAD	P-O3P-PA-O2A
2	D	701	FAD	P-O3P-PA-O1A
2	H	701	FAD	P-O3P-PA-O2A
2	G	701	FAD	O4B-C4B-C5B-O5B
2	B	701	FAD	O3'-C3'-C4'-C5'

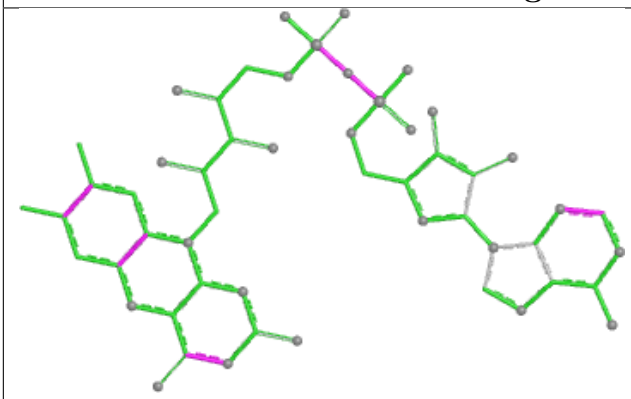
There are no ring outliers.

9 monomers are involved in 19 short contacts:

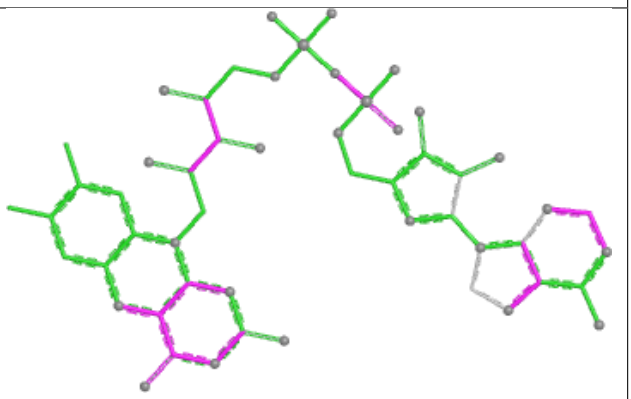
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	FAD	2	0
2	D	701	FAD	3	0
2	H	701	FAD	1	0
2	G	701	FAD	2	0
2	B	701	FAD	3	0
3	H	703	GOL	2	0
2	E	701	FAD	2	0
2	C	701	FAD	1	0
2	F	701	FAD	3	0

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 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.

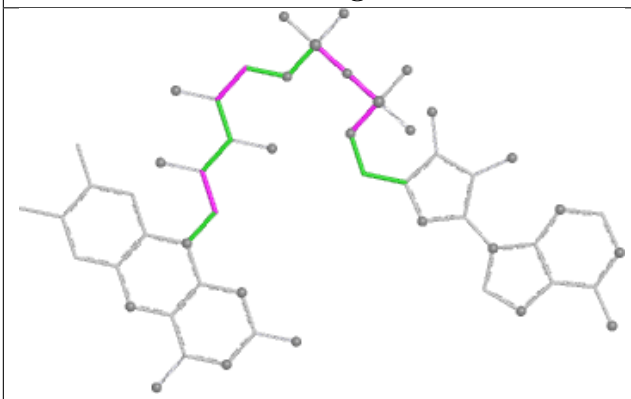
Ligand FAD A 701



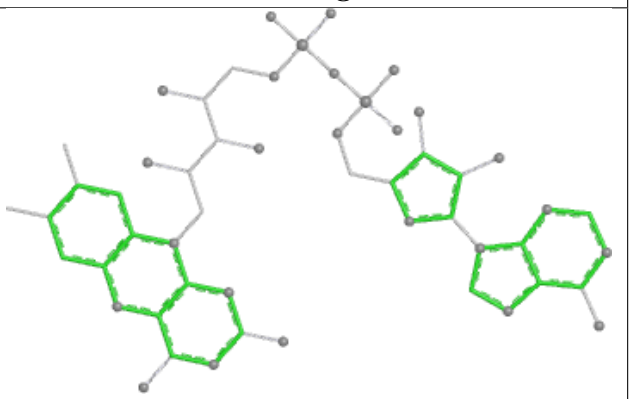
Bond lengths



Bond angles

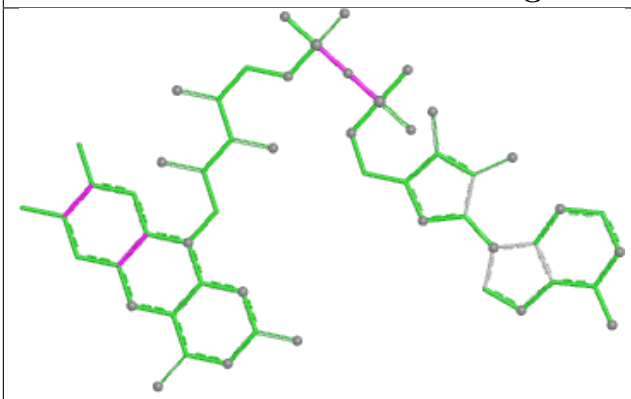


Torsions

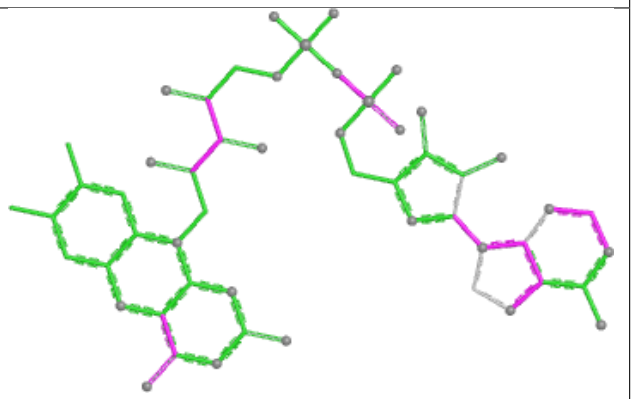


Rings

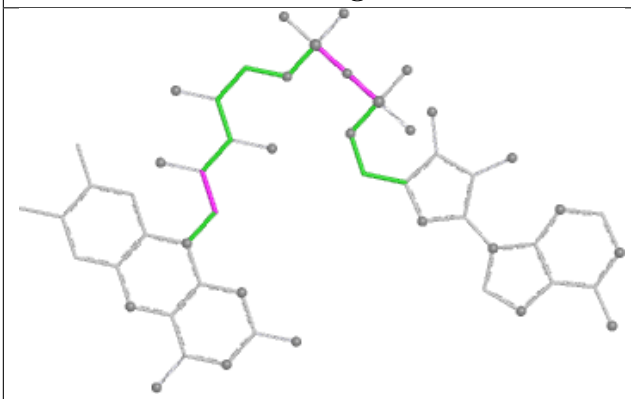
Ligand FAD D 701



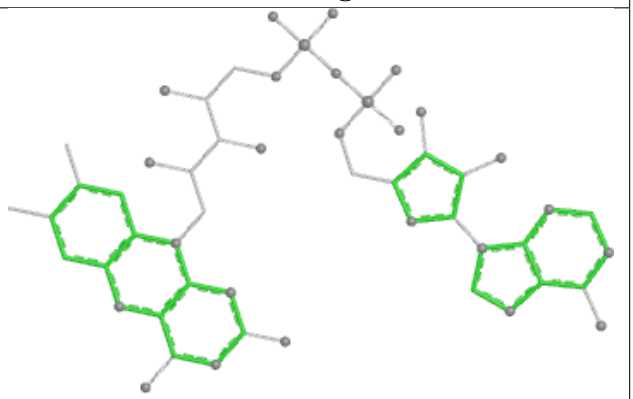
Bond lengths



Bond angles

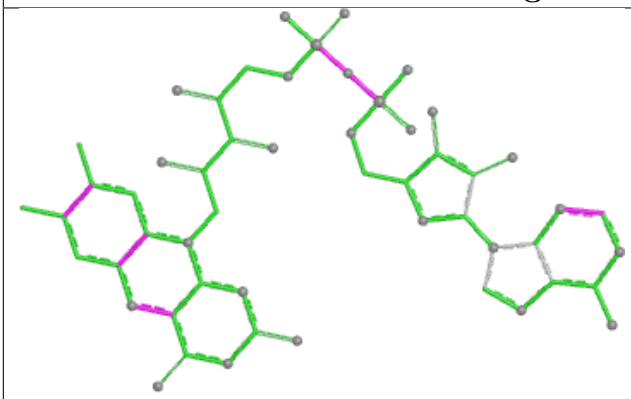


Torsions

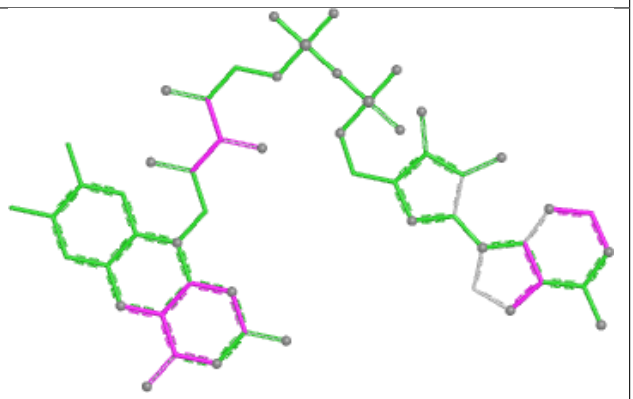


Rings

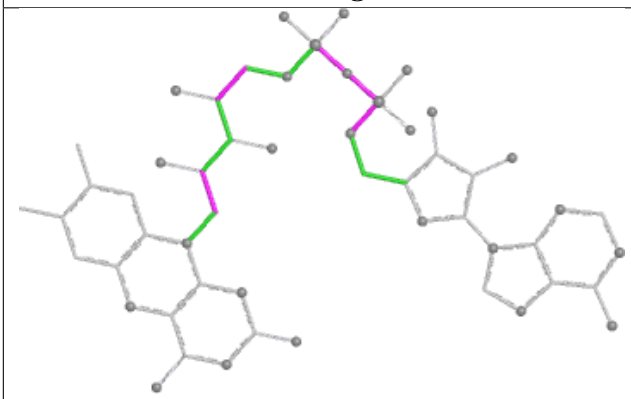
Ligand FAD H 701



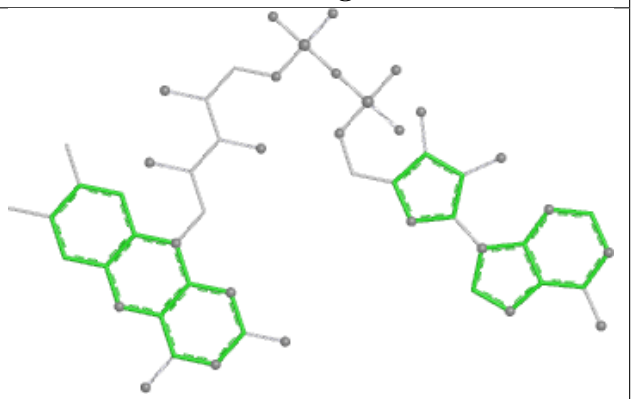
Bond lengths



Bond angles

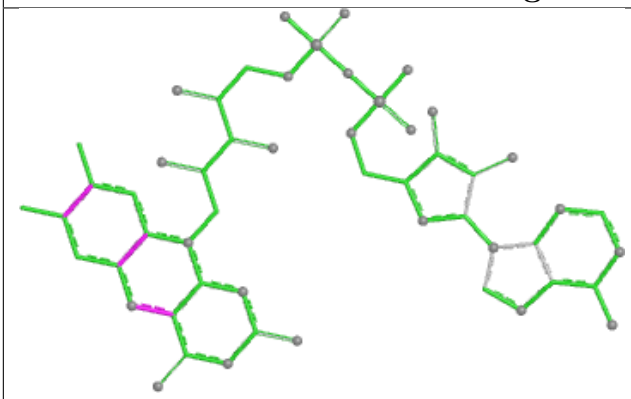


Torsions

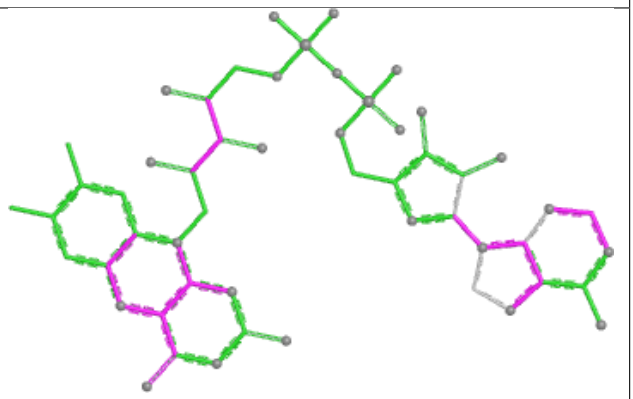


Rings

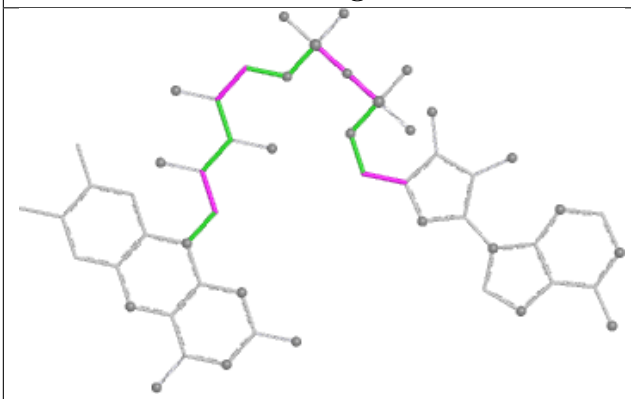
Ligand FAD G 701



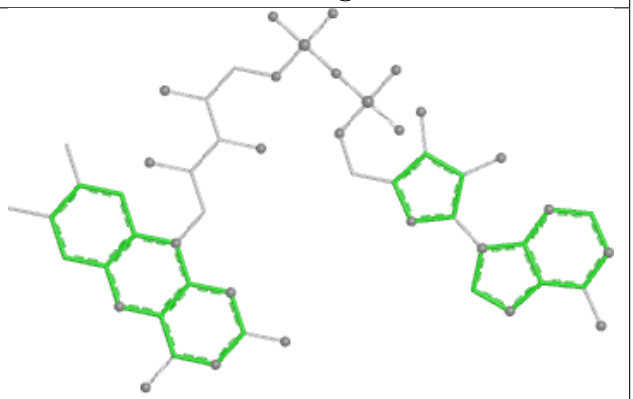
Bond lengths



Bond angles

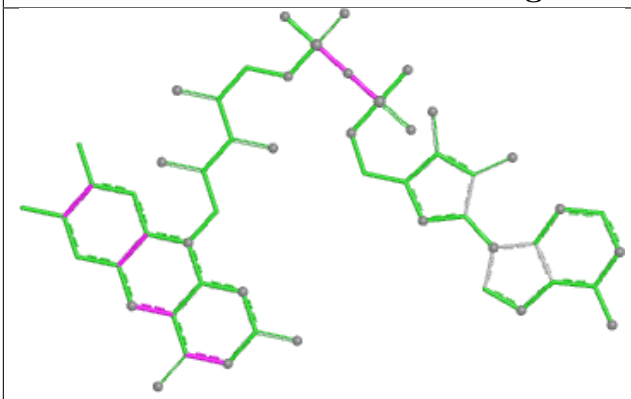


Torsions

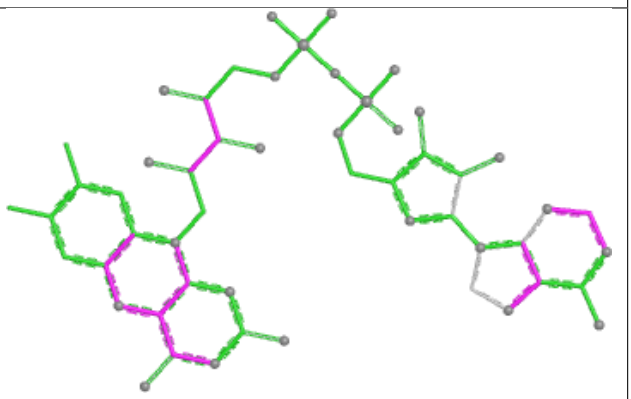


Rings

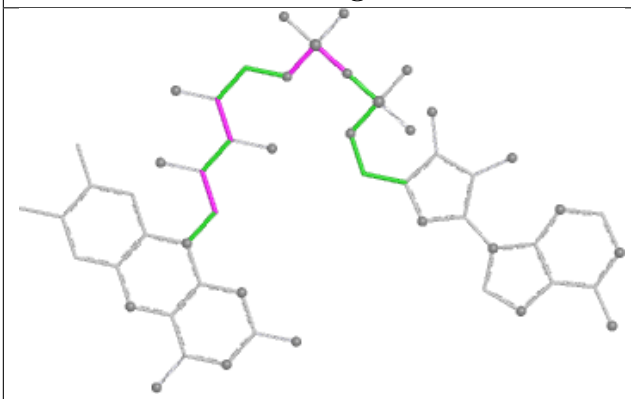
Ligand FAD B 701



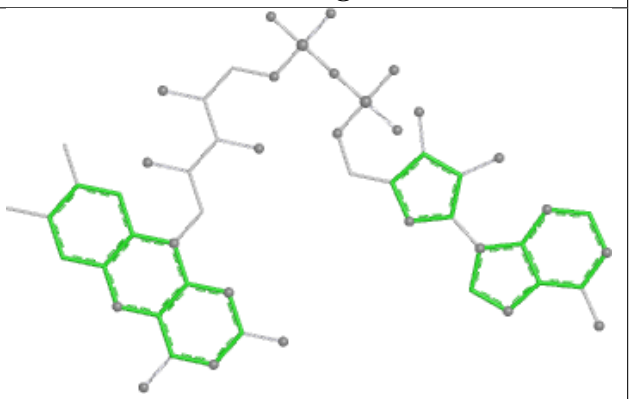
Bond lengths



Bond angles

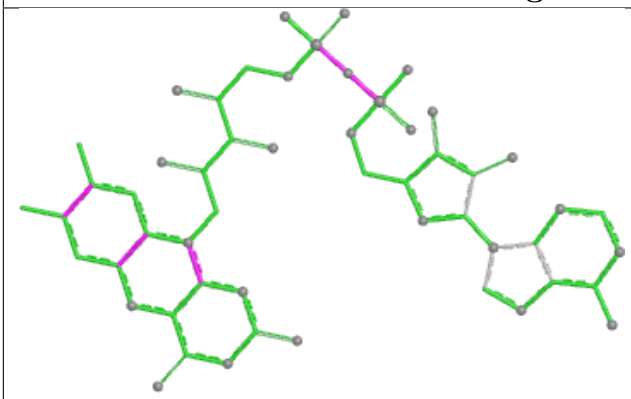


Torsions

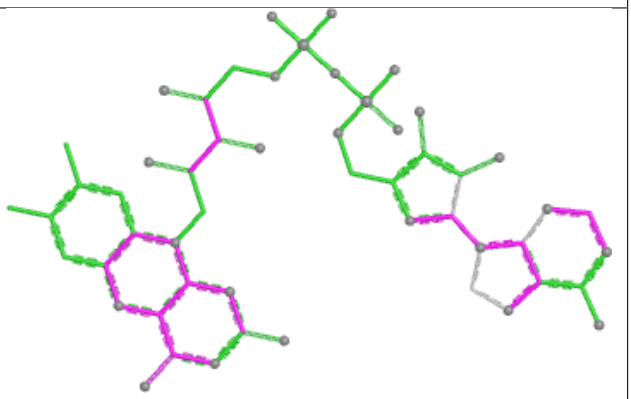


Rings

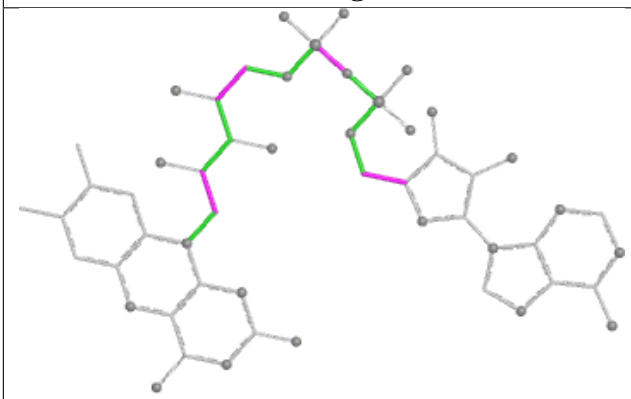
Ligand FAD E 701



Bond lengths



Bond angles



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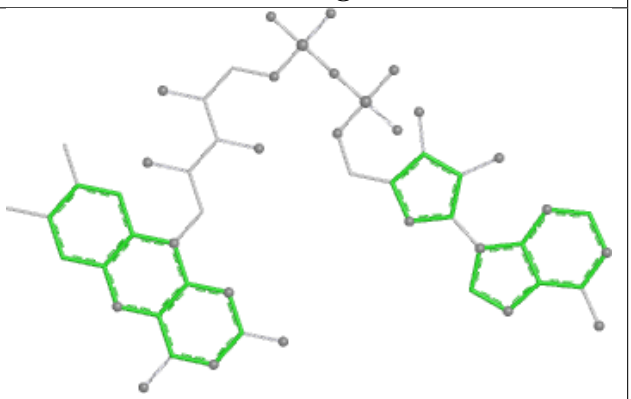
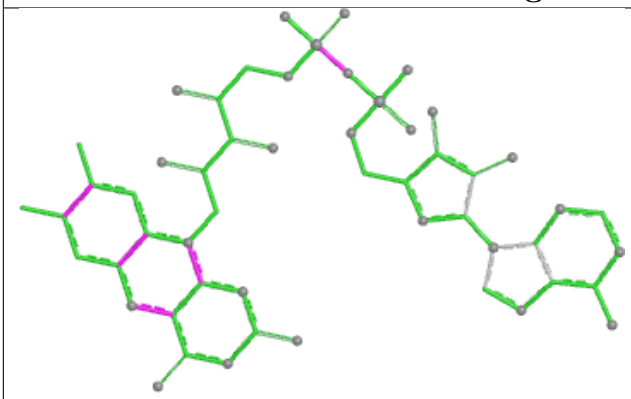
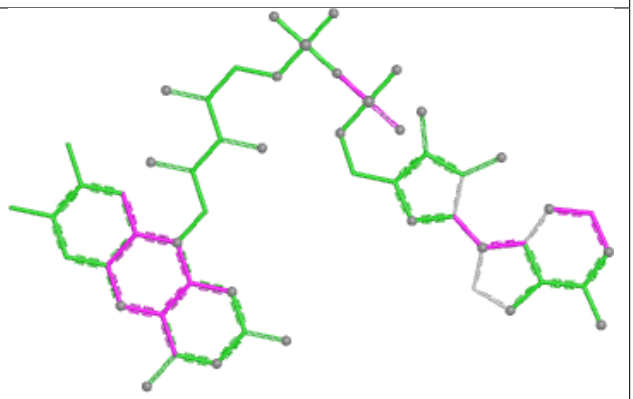


Rings

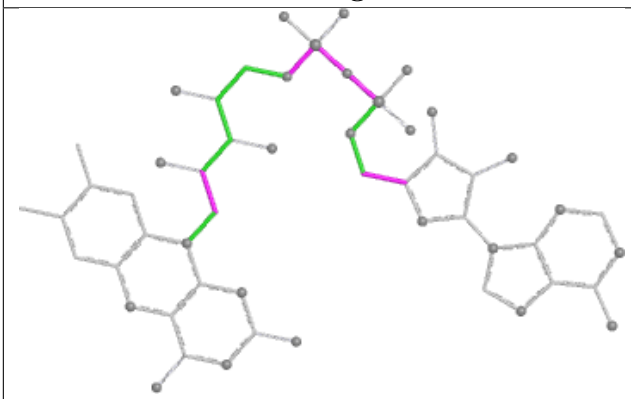
Ligand FAD C 701



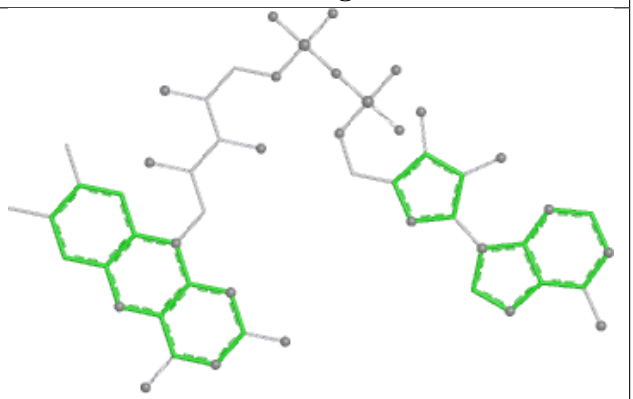
Bond lengths



Bond angles

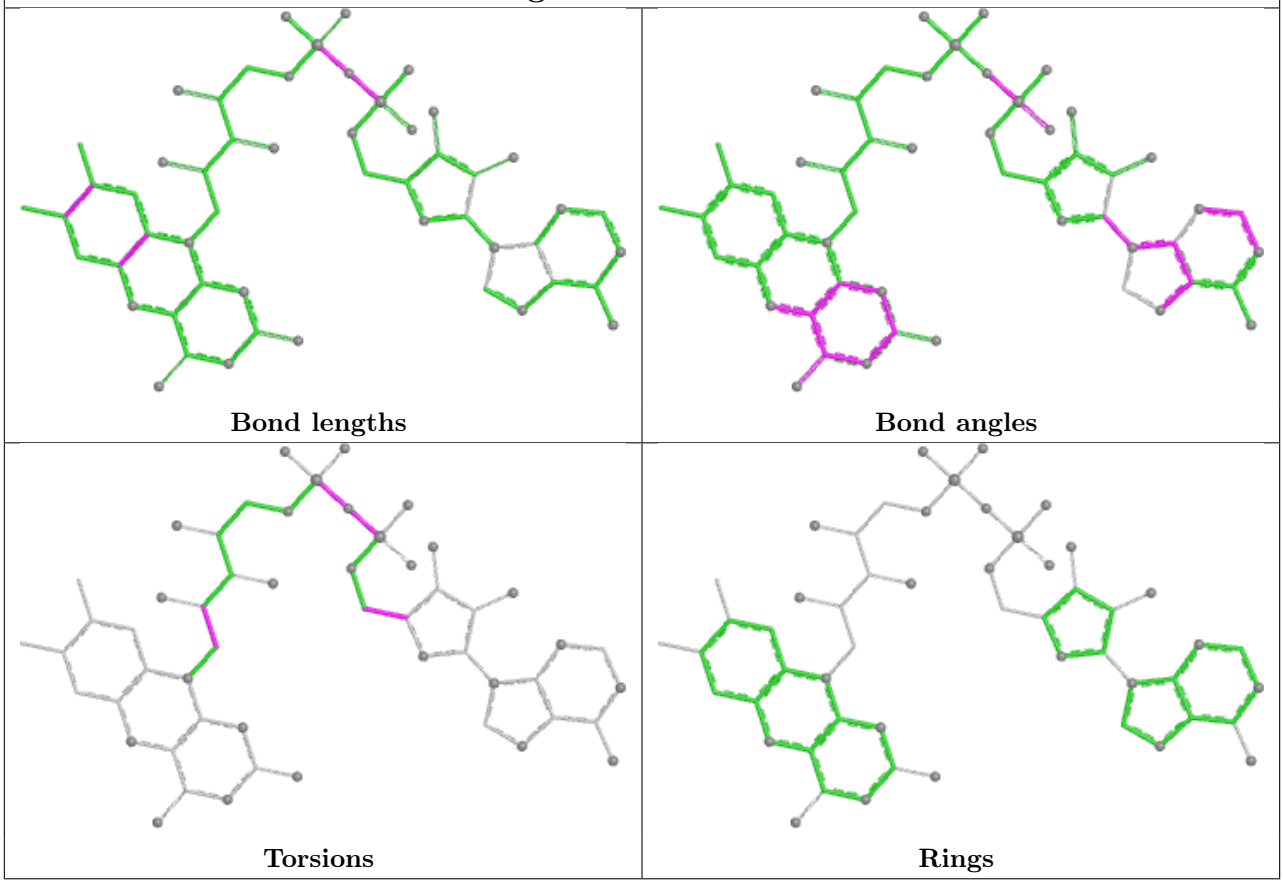


Torsions



Rings

Ligand FAD F 701



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	643/651 (98%)	-0.32	9 (1%)	75	71	40, 60, 83, 124	0
1	B	642/651 (98%)	-0.30	5 (0%)	86	84	35, 50, 74, 107	0
1	C	636/651 (97%)	-0.27	6 (0%)	84	82	37, 57, 79, 95	0
1	D	636/651 (97%)	-0.44	4 (0%)	89	88	29, 51, 77, 99	1 (0%)
1	E	637/651 (97%)	0.12	33 (5%)	27	21	45, 69, 92, 112	0
1	F	646/651 (99%)	-0.36	4 (0%)	89	88	36, 54, 78, 120	0
1	G	635/651 (97%)	-0.28	6 (0%)	84	82	37, 58, 90, 114	0
1	H	636/651 (97%)	-0.31	11 (1%)	70	66	36, 52, 79, 108	0
All	All	5111/5208 (98%)	-0.27	78 (1%)	73	70	29, 56, 84, 124	1 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	299	ILE	4.3
1	E	298	LYS	4.0
1	E	236	ASP	4.0
1	G	242	GLY	3.7
1	E	297	ILE	3.7
1	B	641	PRO	3.6
1	A	643	GLY	3.6
1	B	646	ALA	3.3
1	G	639	PRO	3.3
1	E	255	GLY	3.3
1	C	233	LEU	3.3
1	H	237	ASN	3.2
1	A	644	ARG	3.1
1	H	233	LEU	3.0
1	E	379	PRO	3.0
1	C	236	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	298	LYS	3.0
1	A	533	LYS	2.9
1	B	644	ARG	2.9
1	F	644	ARG	2.9
1	E	625	GLY	2.9
1	D	4	PRO	2.8
1	H	298	LYS	2.8
1	E	301	SER	2.7
1	E	640	VAL	2.7
1	E	4	PRO	2.7
1	H	297	ILE	2.7
1	G	232	VAL	2.7
1	D	233	LEU	2.6
1	H	293	ARG	2.6
1	E	374	LEU	2.6
1	E	103	MET	2.6
1	A	640	VAL	2.6
1	B	627	LYS	2.5
1	H	640	VAL	2.5
1	H	256	LYS	2.5
1	D	573	GLN	2.4
1	E	243	VAL	2.4
1	E	383	GLU	2.4
1	C	235	ASP	2.4
1	H	236	ASP	2.4
1	E	288	ASN	2.4
1	A	534	VAL	2.4
1	A	75	MET	2.3
1	A	641	PRO	2.3
1	E	256	LYS	2.3
1	F	534	VAL	2.3
1	G	234	PHE	2.3
1	H	234	PHE	2.3
1	E	233	LEU	2.3
1	E	257	LEU	2.3
1	F	646	ALA	2.3
1	E	559	THR	2.3
1	B	371	GLU	2.2
1	A	642	THR	2.2
1	H	258	HIS	2.2
1	E	371	GLU	2.2
1	E	304	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	254	GLY	2.2
1	E	386	ASN	2.2
1	E	293	ARG	2.1
1	A	437	LYS	2.1
1	E	530	LYS	2.1
1	E	572	GLU	2.1
1	E	294	GLN	2.1
1	G	256	LYS	2.1
1	H	302	ASP	2.1
1	F	299	ILE	2.1
1	E	258	HIS	2.1
1	C	232	VAL	2.1
1	E	302	ASP	2.1
1	E	291	LEU	2.0
1	C	297	ILE	2.0
1	E	75	MET	2.0
1	E	242	GLY	2.0
1	D	376	GLU	2.0
1	G	543	GLU	2.0
1	E	439	GLN	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	GOL	B	702	6/6	0.81	0.22	59,63,65,66	0
3	GOL	H	703	6/6	0.83	0.21	56,57,60,63	0
3	GOL	H	702	6/6	0.86	0.21	61,65,68,68	0

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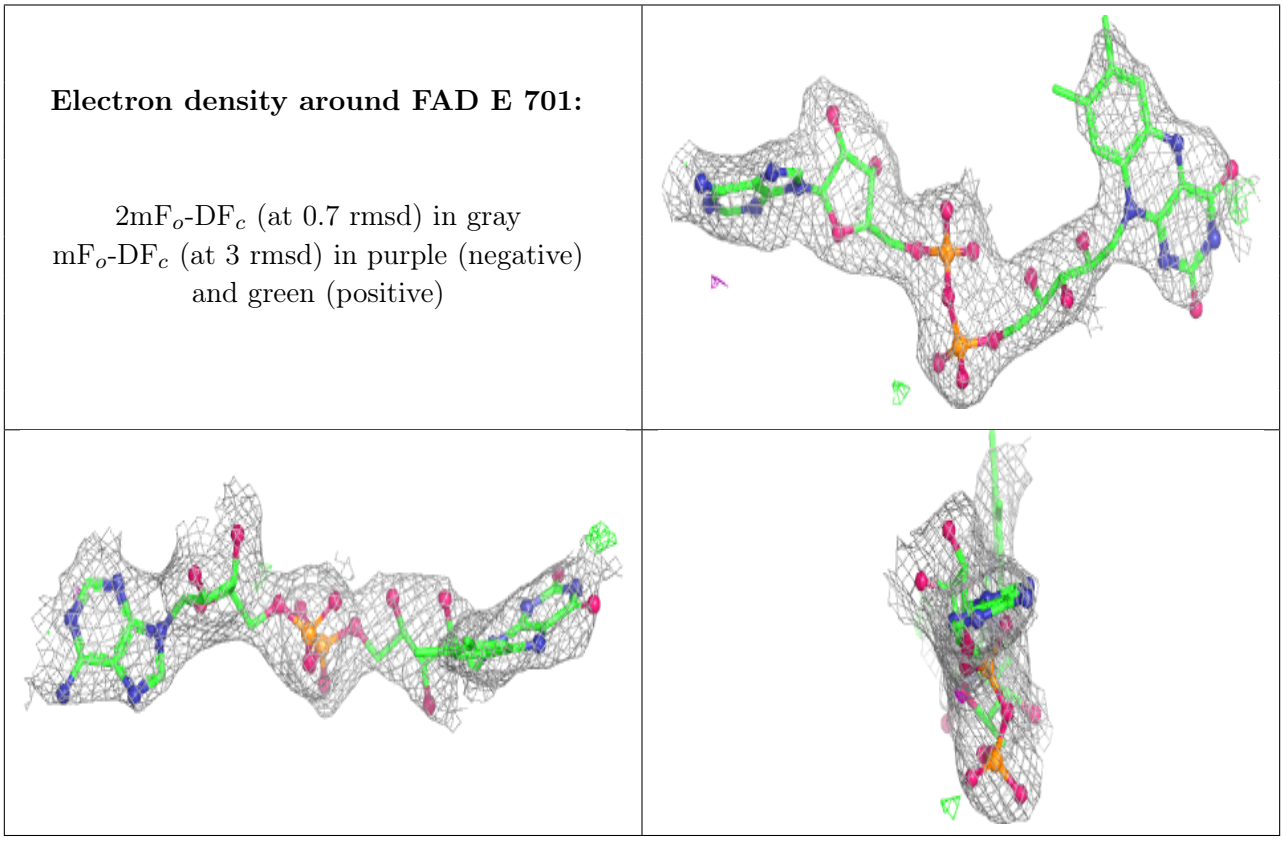
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	D	702	6/6	0.89	0.17	55,63,64,67	0
3	GOL	C	702	6/6	0.90	0.17	65,66,67,68	0
2	FAD	E	701	53/53	0.92	0.21	68,76,102,108	0
2	FAD	G	701	53/53	0.94	0.14	51,78,86,87	0
2	FAD	D	701	53/53	0.94	0.17	49,68,88,90	0
2	FAD	H	701	53/53	0.96	0.19	41,66,96,102	0
2	FAD	C	701	53/53	0.96	0.17	51,70,82,86	0
2	FAD	A	701	53/53	0.96	0.13	44,70,81,85	0
2	FAD	F	701	53/53	0.97	0.16	38,64,87,91	0
2	FAD	B	701	53/53	0.97	0.14	44,53,81,87	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.

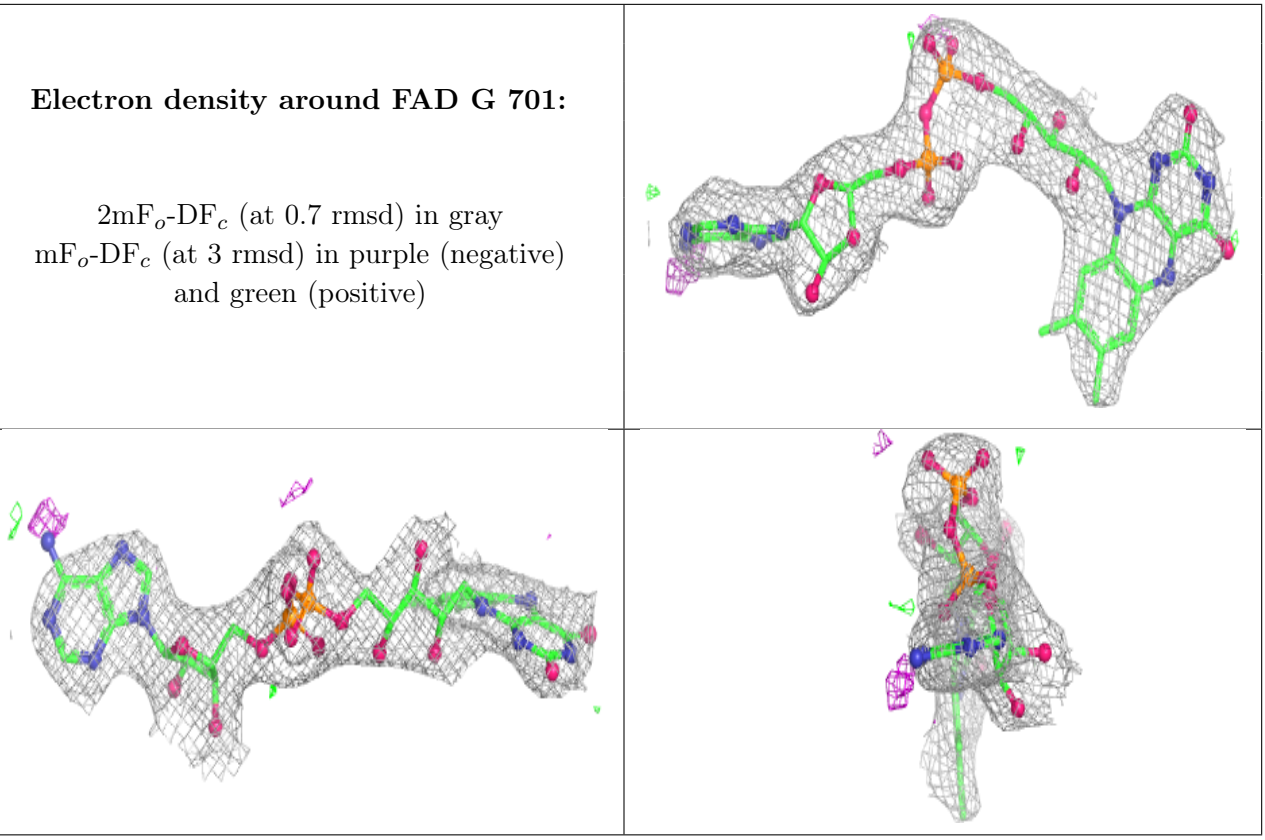
Electron density around FAD E 701:

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



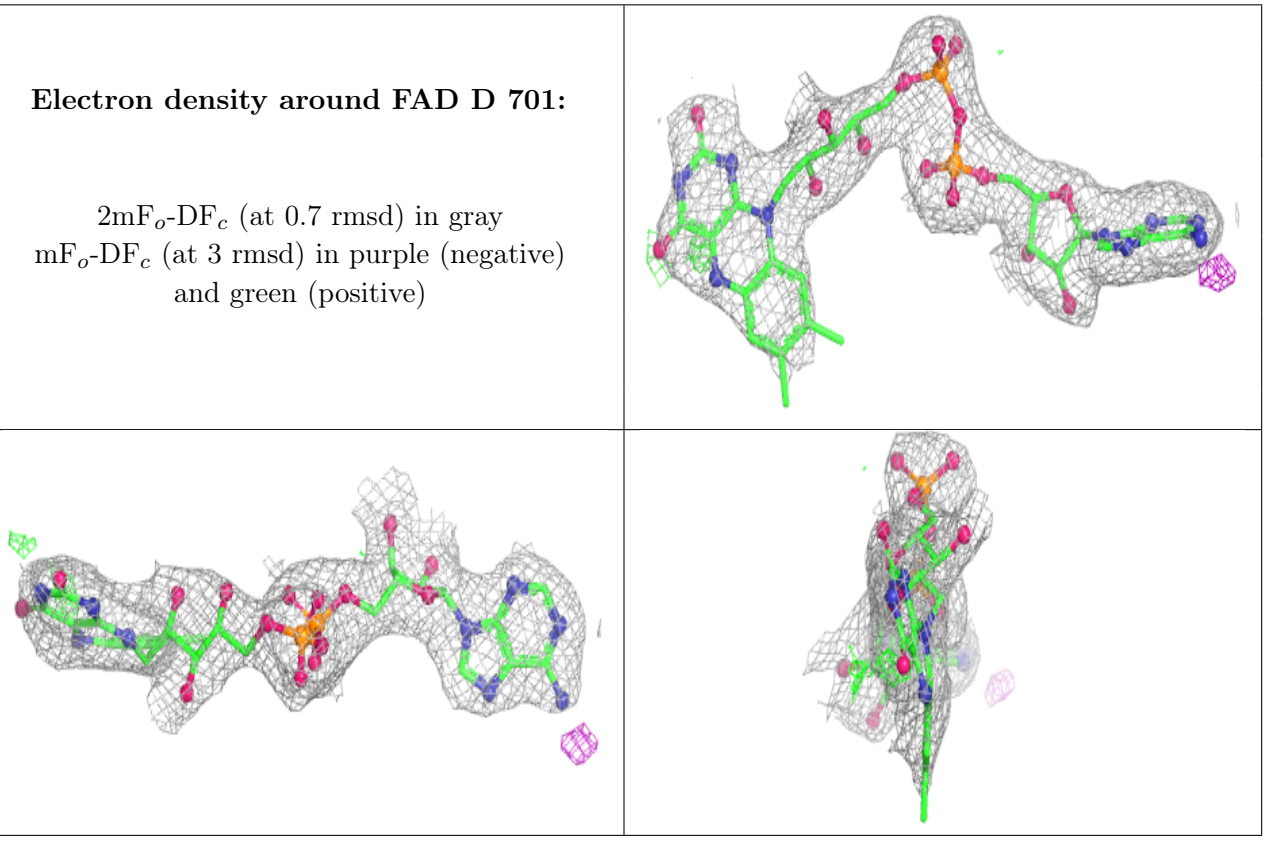
Electron density around FAD G 701:

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



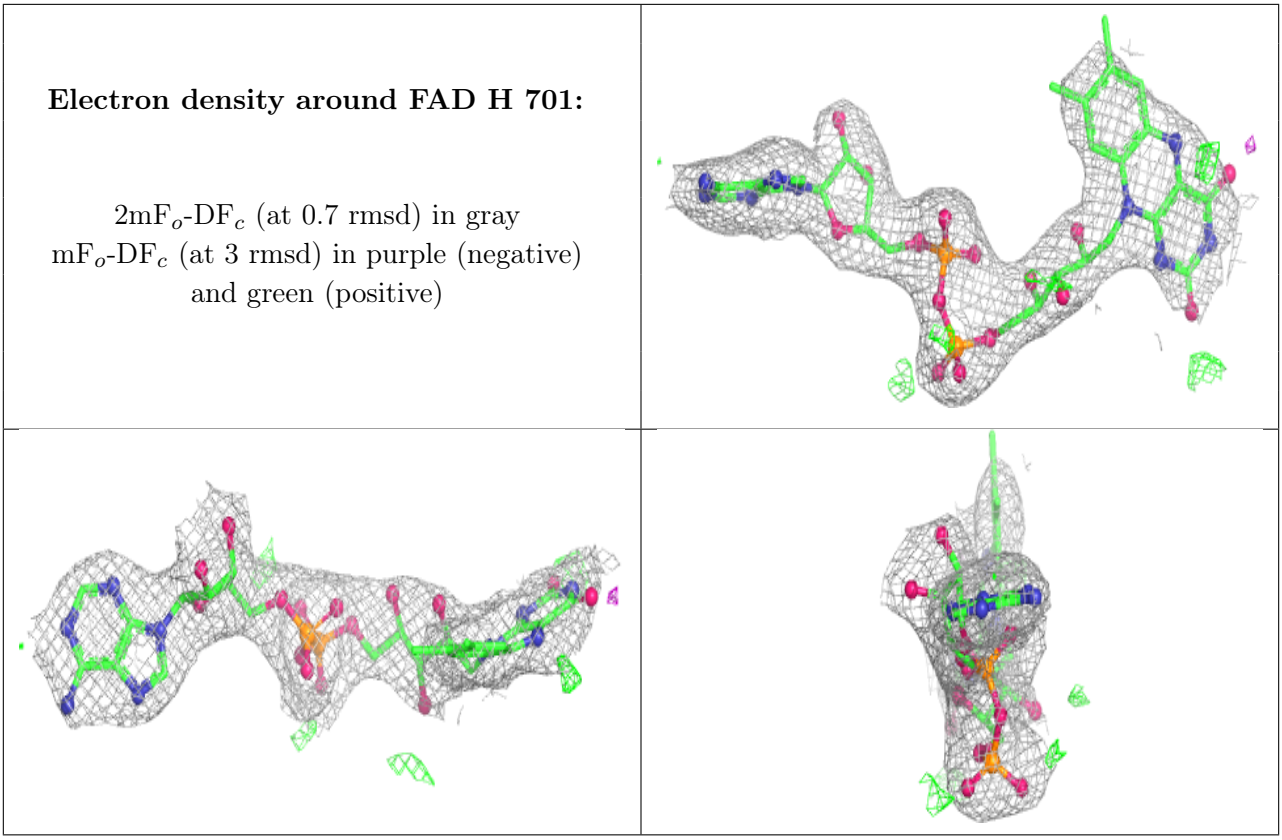
Electron density around FAD D 701:

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



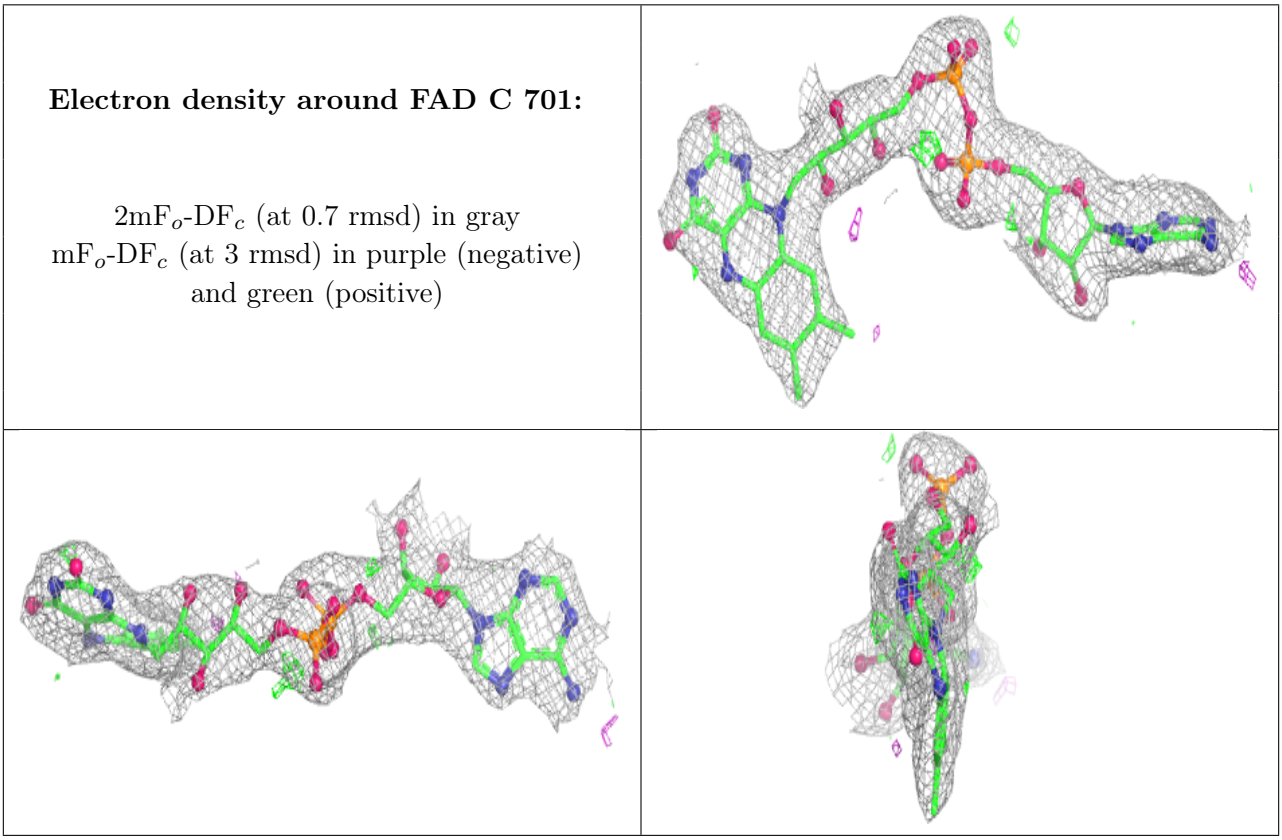
Electron density around FAD H 701:

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



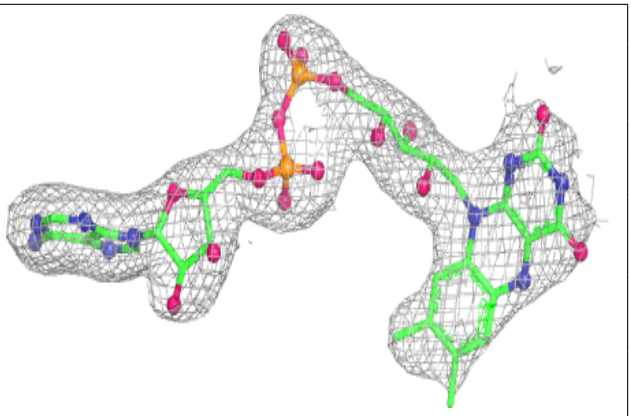
Electron density around FAD C 701:

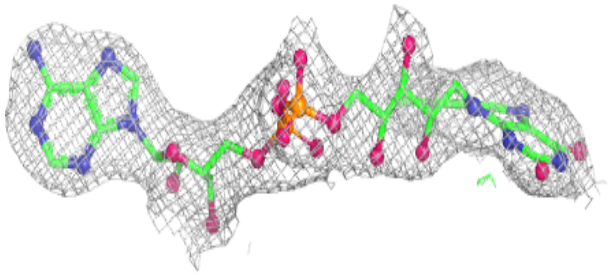
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

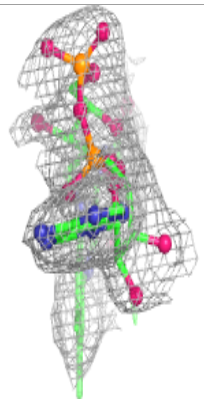


Electron density around FAD A 701:

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

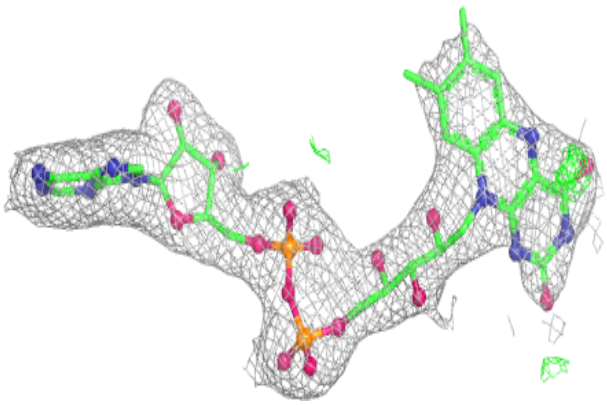


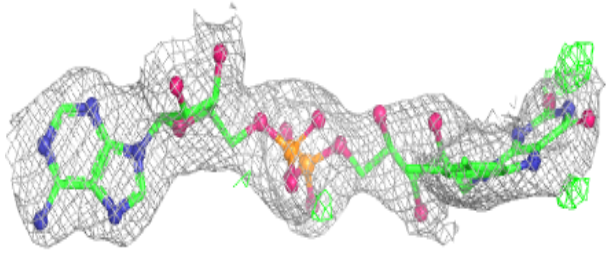


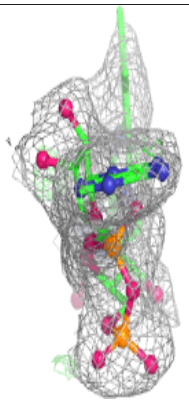


Electron density around FAD F 701:

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

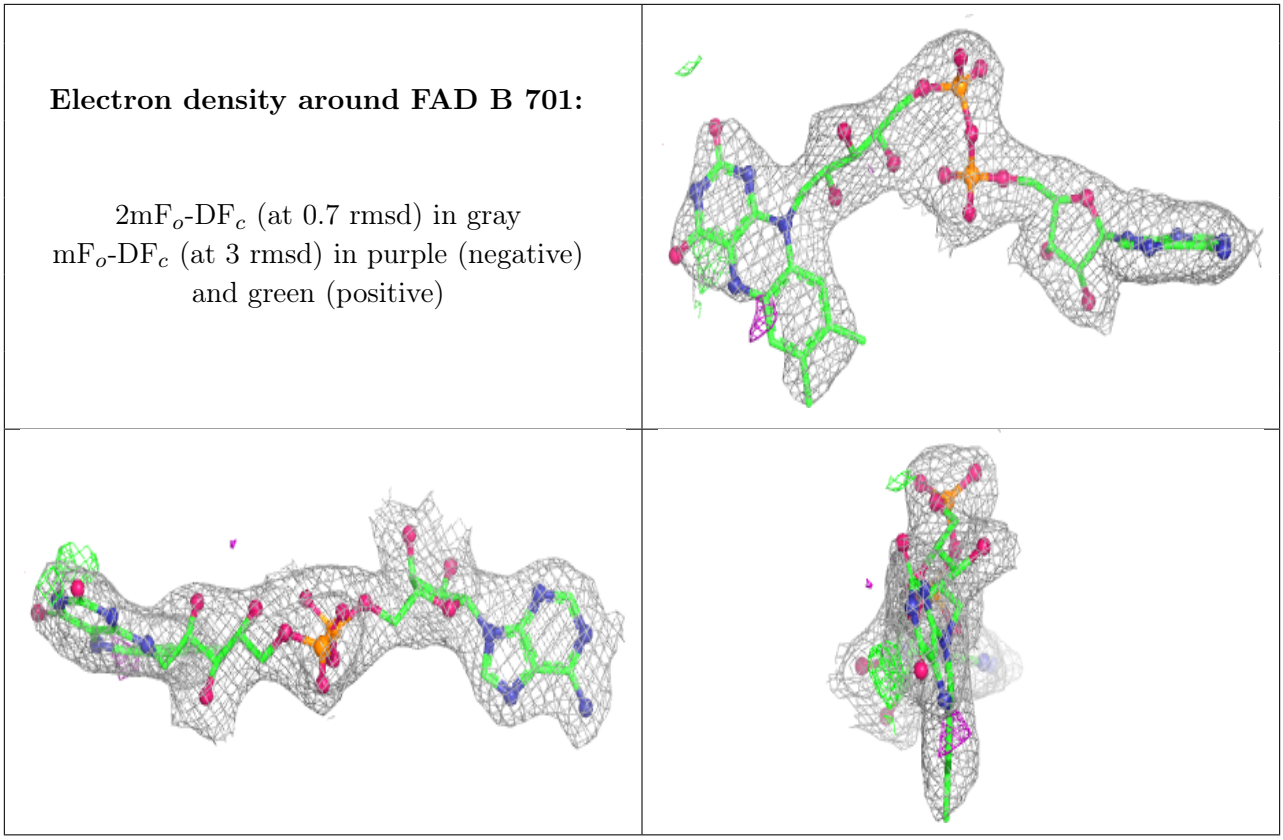






Electron density around FAD B 701:

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



6.5 Other polymers (i)

There are no such residues in this entry.