



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:17 PM UTC

PDB ID : 7Q86 / pdb_00007q86
Title : Crystal structure of human peroxisomal acyl-Co-A oxidase 1a, FAD-bound-form
Authors : Sonani, R.R.; Blat, A.; Dubin, G.
Deposited on : 2021-11-10
Resolution : 2.09 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

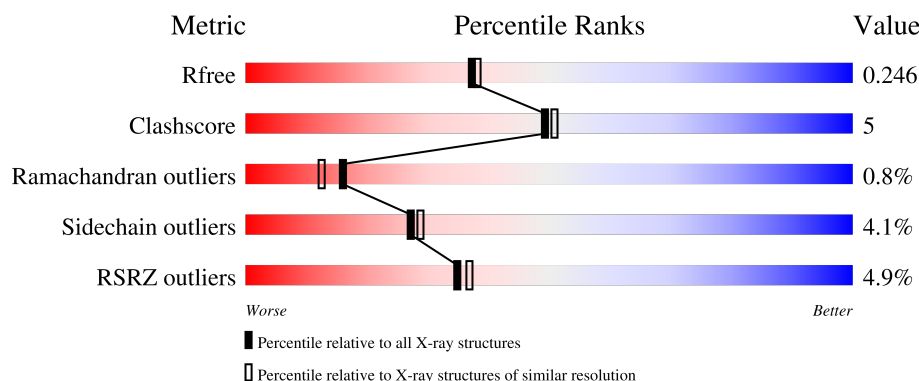
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	667	
1	B	667	

2 Entry composition [i](#)

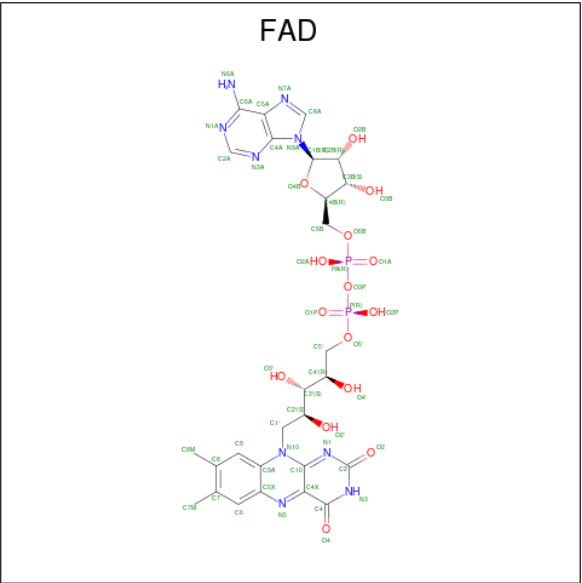
There are 3 unique types of molecules in this entry. The entry contains 10219 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Isoform 2 of Peroxisomal acyl-coenzyme A oxidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	0	0	0
			4877	3107	846	895	29			
1	B	607	Total	C	N	O	S	0	0	0
			4841	3086	839	887	29			

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



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

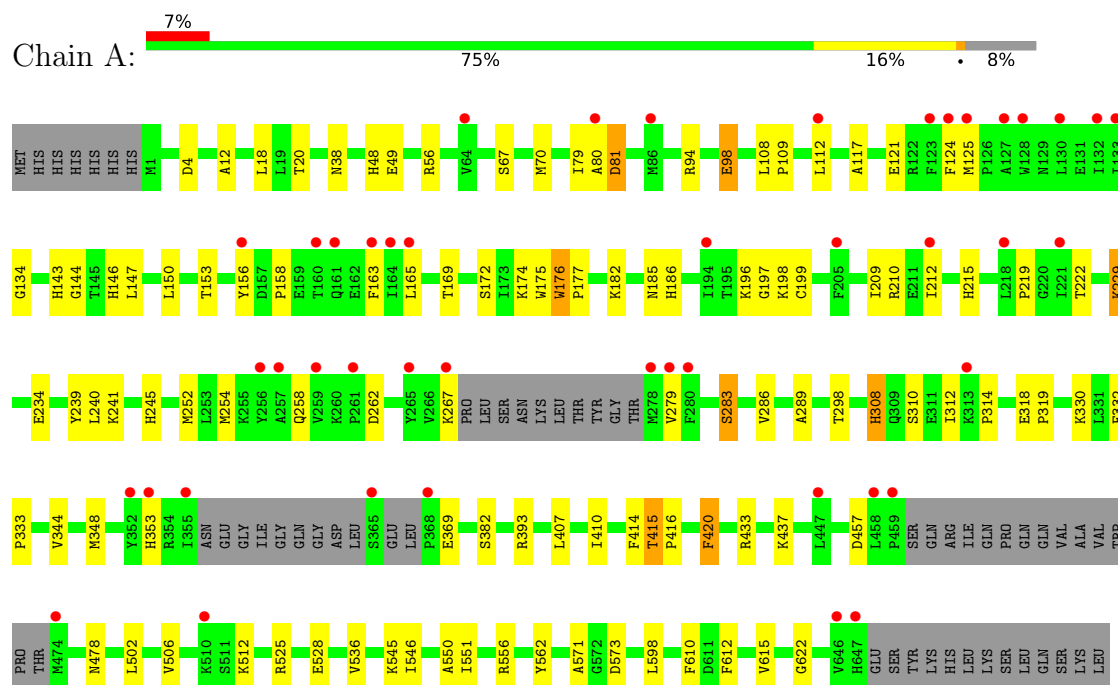
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	188	Total 188	O 188	0	0
3	B	207	Total 207	O 207	0	0

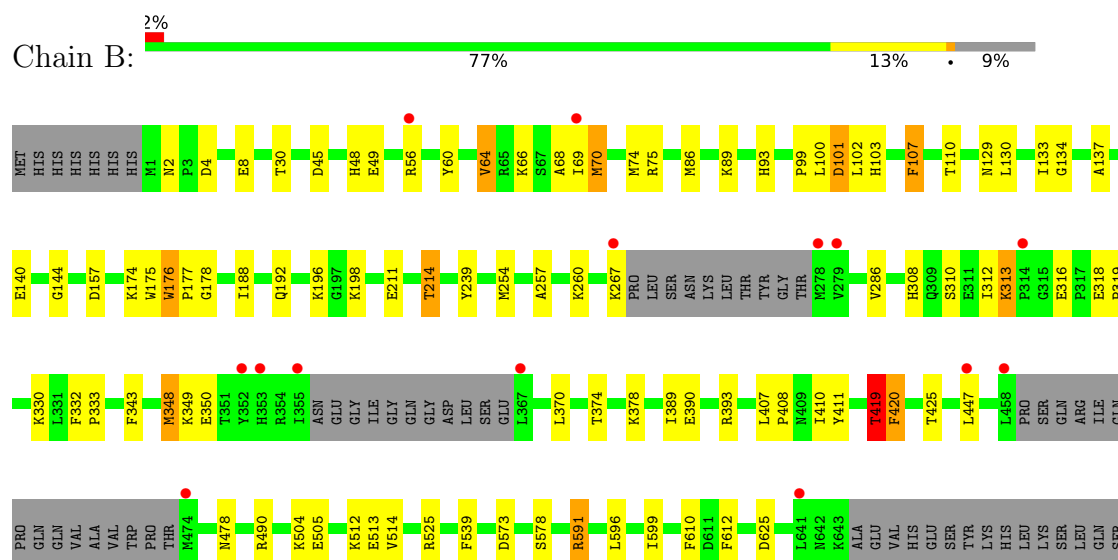
3 Residue-property plots

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

- Molecule 1: Isoform 2 of Peroxisomal acyl-coenzyme A oxidase 1



- Molecule 1: Isoform 2 of Peroxisomal acyl-coenzyme A oxidase 1



LYS
LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.96Å 124.06Å 142.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.84 – 2.09 47.84 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.84-2.09) 99.9 (47.84-2.09)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.187 , 0.240 0.199 , 0.246	Depositor DCC
R_{free} test set	4055 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10219	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.18	5/4970 (0.1%)	1.48	22/6720 (0.3%)
1	B	1.20	9/4933 (0.2%)	1.47	13/6671 (0.2%)
All	All	1.19	14/9903 (0.1%)	1.48	35/13391 (0.3%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	622	GLY	C-O	8.89	1.30	1.24
1	B	505	GLU	C-O	-6.65	1.16	1.24
1	B	93	HIS	CE1-NE2	6.65	1.39	1.32
1	B	425	THR	C-O	6.45	1.31	1.24
1	B	343	PHE	C-O	6.03	1.31	1.24
1	A	562	TYR	C-O	5.79	1.30	1.24
1	B	330	LYS	C-O	5.59	1.30	1.24
1	B	196	LYS	C-O	5.27	1.29	1.24
1	B	30	THR	C-O	5.26	1.30	1.24
1	B	192	GLN	C-O	5.19	1.30	1.24
1	B	107	PHE	C-O	5.14	1.29	1.24
1	A	143	HIS	CE1-NE2	5.12	1.37	1.32
1	A	20	THR	C-O	5.11	1.30	1.24
1	A	209	ILE	N-CA	5.05	1.50	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	420	PHE	CA-CB-CG	8.10	121.90	113.80
1	A	571	ALA	CA-C-N	6.50	127.20	119.98
1	A	571	ALA	C-N-CA	6.50	127.20	119.98
1	B	101	ASP	CA-CB-CG	-6.45	106.15	112.60
1	B	625	ASP	CA-CB-CG	6.28	118.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	573	ASP	CA-CB-CG	6.17	118.77	112.60
1	B	68	ALA	CA-C-O	-6.09	114.62	120.90
1	B	539	PHE	CA-CB-CG	5.90	119.70	113.80
1	A	289	ALA	N-CA-C	-5.70	104.98	111.14
1	A	457	ASP	CA-CB-CG	5.70	118.30	112.60
1	A	98	GLU	CB-CA-C	5.69	117.75	110.13
1	A	433	ARG	N-CA-CB	5.69	118.26	110.01
1	A	420	PHE	CA-CB-CG	5.56	119.36	113.80
1	B	378	LYS	N-CA-C	-5.54	105.15	111.07
1	B	410	ILE	CA-C-O	-5.52	115.21	120.95
1	A	12	ALA	CA-C-O	-5.47	115.75	121.55
1	A	550	ALA	CA-C-N	5.41	127.49	120.56
1	A	550	ALA	C-N-CA	5.41	127.49	120.56
1	A	410	ILE	N-CA-C	-5.33	105.30	110.42
1	A	308	HIS	CA-C-O	-5.28	114.94	120.80
1	B	93	HIS	CB-CA-C	5.25	118.78	109.65
1	A	546	ILE	CA-C-N	5.13	127.61	120.63
1	A	546	ILE	C-N-CA	5.13	127.61	120.63
1	B	419	THR	CB-CA-C	5.13	117.30	109.34
1	B	389	ILE	N-CA-C	-5.13	105.39	110.62
1	A	433	ARG	N-CA-C	-5.11	105.60	111.07
1	A	415	THR	CA-CB-OG1	-5.09	101.96	109.60
1	A	283	SER	CA-C-N	5.06	127.06	120.28
1	A	283	SER	C-N-CA	5.06	127.06	120.28
1	B	596	LEU	N-CA-C	-5.05	105.77	111.28
1	A	457	ASP	CB-CA-C	5.04	118.00	111.50
1	A	536	VAL	CA-C-N	5.04	127.34	120.54
1	A	536	VAL	C-N-CA	5.04	127.34	120.54
1	B	514	VAL	N-CA-C	-5.03	105.64	110.72
1	A	298	THR	N-CA-C	-5.02	105.70	111.07

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	4877	0	4859	64	0
1	B	4841	0	4831	44	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	188	0	0	7	0
3	B	207	0	0	2	0
All	All	10219	0	9752	106	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 5.

All (106) 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:156:TYR:CE2	1:A:158:PRO:HA	1.93	1.03
1:A:156:TYR:CE2	1:A:158:PRO:CA	2.58	0.86
1:A:108:LEU:HD22	1:A:124:PHE:CE1	2.16	0.79
1:A:112:LEU:HD21	1:A:124:PHE:CZ	2.21	0.76
1:A:156:TYR:CZ	1:A:158:PRO:HA	2.25	0.71
1:A:156:TYR:HE2	1:A:158:PRO:HA	1.54	0.70
1:A:112:LEU:HD21	1:A:124:PHE:CE2	2.28	0.68
1:A:222:THR:HB	1:A:241:LYS:HB3	1.76	0.67
1:A:156:TYR:HE2	1:A:158:PRO:CA	2.07	0.67
1:B:103:HIS:HD2	1:B:134:GLY:H	1.44	0.65
1:B:103:HIS:CD2	1:B:134:GLY:H	2.14	0.65
1:B:478:ASN:HD21	1:B:591:ARG:HD3	1.62	0.65
1:B:4:ASP:OD2	1:B:308:HIS:HE1	1.81	0.64
1:A:48:HIS:HD2	1:A:49:GLU:O	1.85	0.60
1:A:108:LEU:CD2	1:A:124:PHE:CD1	2.85	0.60
1:B:102:LEU:HD12	1:B:178:GLY:O	2.02	0.59
1:B:286:VAL:HB	1:B:348:MET:HE1	1.86	0.58
1:A:344:VAL:O	1:A:348:MET:HG2	2.05	0.57
1:B:267:LYS:O	1:B:267:LYS:HG3	2.03	0.57
1:A:330:LYS:NZ	3:A:803:HOH:O	2.38	0.57
1:A:234:GLU:HG3	3:A:877:HOH:O	2.05	0.56
1:A:108:LEU:HD22	1:A:124:PHE:CD1	2.42	0.55
1:A:94:ARG:HD3	1:A:615:VAL:HG22	1.88	0.55
1:B:308:HIS:HD2	1:B:318:GLU:O	1.90	0.54
1:B:254:MET:HA	1:B:257:ALA:O	2.06	0.54
1:B:478:ASN:ND2	1:B:591:ARG:HD3	2.22	0.54
1:B:175:TRP:O	1:B:176:TRP:HB2	2.06	0.54
1:A:175:TRP:C	1:A:177:PRO:HD3	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HB2	1:A:109:PRO:HD3	1.90	0.53
1:A:108:LEU:HD23	1:A:124:PHE:CD1	2.44	0.53
1:A:254:MET:HB3	1:A:258:GLN:HG3	1.91	0.53
1:B:4:ASP:O	1:B:8:GLU:HG2	2.08	0.53
1:B:313:LYS:HD3	1:B:316:GLU:OE1	2.09	0.53
1:B:312:ILE:HG13	1:B:319:PRO:HG3	1.90	0.52
1:A:117:ALA:O	1:A:121:GLU:HG3	2.09	0.52
1:A:4:ASP:OD2	1:A:308:HIS:HE1	1.92	0.52
1:A:414:PHE:C	1:A:416:PRO:HD2	2.35	0.51
1:A:393:ARG:HA	1:A:407:LEU:HD13	1.93	0.51
3:A:973:HOH:O	1:B:525:ARG:HD2	2.11	0.50
1:B:107:PHE:CG	1:B:134:GLY:HA3	2.47	0.50
1:A:18:LEU:HB2	1:A:551:ILE:HD11	1.94	0.50
1:A:415:THR:N	1:A:416:PRO:HD2	2.26	0.50
1:A:308:HIS:HD2	1:A:318:GLU:O	1.95	0.49
1:A:330:LYS:HE2	3:A:803:HOH:O	2.13	0.49
1:B:175:TRP:C	1:B:177:PRO:HD3	2.38	0.48
1:B:60:TYR:O	1:B:64:VAL:HG22	2.12	0.48
1:B:140:GLU:HG2	1:B:174:LYS:HD3	1.94	0.48
1:A:169:THR:O	1:A:172:SER:OG	2.28	0.48
1:A:382:SER:HB3	3:A:944:HOH:O	2.14	0.48
1:A:525:ARG:NH2	1:A:573:ASP:OD2	2.37	0.48
1:B:157:ASP:OD1	1:B:157:ASP:C	2.56	0.48
1:A:156:TYR:CE2	1:A:158:PRO:N	2.82	0.48
1:A:108:LEU:CD2	1:A:124:PHE:CE1	2.93	0.47
1:B:512:LYS:HG3	3:B:943:HOH:O	2.14	0.47
1:A:134:GLY:HA2	1:A:186:HIS:O	2.14	0.47
1:B:393:ARG:HA	1:B:407:LEU:HD13	1.96	0.47
1:A:478:ASN:O	1:A:556:ARG:NH2	2.49	0.46
1:A:153:THR:O	1:A:165:LEU:HA	2.16	0.46
1:A:332:PHE:N	1:A:333:PRO:CD	2.78	0.46
1:A:174:LYS:HB2	1:A:240:LEU:HB3	1.97	0.46
1:A:286:VAL:HG21	1:A:348:MET:HE2	1.98	0.46
1:A:219:PRO:O	1:A:245:HIS:HD2	1.99	0.45
1:A:176:TRP:O	1:A:177:PRO:C	2.59	0.45
1:A:283:SER:HA	1:A:348:MET:CE	2.47	0.45
1:B:174:LYS:O	1:B:239:TYR:HA	2.17	0.45
1:A:80:ALA:O	1:A:81:ASP:CB	2.65	0.45
1:B:390:GLU:HG2	1:B:411:TYR:CD1	2.52	0.45
1:B:176:TRP:O	1:B:177:PRO:C	2.59	0.45
1:A:156:TYR:HE2	1:A:158:PRO:CB	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LYS:O	1:B:70:MET:HB3	2.17	0.44
1:A:174:LYS:O	1:A:239:TYR:HA	2.17	0.44
3:A:892:HOH:O	1:B:419:THR:HB	2.17	0.44
1:B:370:LEU:O	1:B:374:THR:HG23	2.17	0.44
1:A:330:LYS:CE	3:A:803:HOH:O	2.65	0.44
1:B:267:LYS:O	1:B:267:LYS:CG	2.65	0.44
1:A:415:THR:N	1:A:416:PRO:CD	2.80	0.43
1:A:175:TRP:O	1:A:176:TRP:HB2	2.16	0.43
1:A:176:TRP:N	1:A:177:PRO:CD	2.81	0.43
1:A:182:LYS:O	1:A:215:HIS:HE1	2.00	0.43
1:A:80:ALA:O	1:A:81:ASP:HB3	2.17	0.43
1:B:211:GLU:HB3	1:B:214:THR:OG1	2.18	0.43
1:A:38:ASN:HD22	1:A:38:ASN:HA	1.72	0.43
1:A:219:PRO:O	1:A:245:HIS:CD2	2.72	0.43
1:B:45:ASP:HB3	1:B:69:ILE:HG21	2.00	0.43
1:B:110:THR:HG21	1:B:188:ILE:HD13	2.01	0.43
1:B:348:MET:HE2	1:B:348:MET:HB2	1.62	0.43
1:B:490:ARG:HH11	1:B:490:ARG:HD3	1.72	0.43
1:A:146:HIS:HD2	3:B:974:HOH:O	2.02	0.42
1:B:48:HIS:HD2	1:B:49:GLU:O	2.03	0.42
1:A:229:LYS:HE3	1:A:229:LYS:HB2	1.80	0.42
1:A:314:PRO:HD3	1:B:513:GLU:CD	2.45	0.42
1:B:332:PHE:N	1:B:333:PRO:CD	2.82	0.42
1:A:502:LEU:O	1:A:506:VAL:HG23	2.20	0.41
1:B:64:VAL:HA	1:B:99:PRO:HG2	2.00	0.41
1:B:610:PHE:HB3	1:B:612:PHE:CE2	2.55	0.41
1:A:310:SER:O	1:A:319:PRO:HD2	2.20	0.41
1:A:163:PHE:CE2	1:A:252:MET:HB2	2.55	0.41
1:B:137:ALA:HA	1:B:177:PRO:HG2	2.02	0.41
1:A:108:LEU:HD23	1:A:124:PHE:HD1	1.84	0.41
1:A:147:LEU:O	1:A:150:LEU:HG	2.20	0.41
1:A:185:ASN:HA	1:A:210:ARG:HB2	2.03	0.41
1:B:478:ASN:ND2	1:B:591:ARG:HH11	2.17	0.41
1:B:129:ASN:O	1:B:130:LEU:HB2	2.20	0.40
1:A:146:HIS:CG	1:B:310:SER:HA	2.56	0.40
1:B:100:LEU:O	1:B:101:ASP:C	2.64	0.40
1:A:610:PHE:HB3	1:A:612:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	601/667 (90%)	576 (96%)	18 (3%)	7 (1%)	10	7
1	B	597/667 (90%)	581 (97%)	14 (2%)	2 (0%)	36	36
All	All	1198/1334 (90%)	1157 (97%)	32 (3%)	9 (1%)	16	12

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	TRP
1	B	176	TRP
1	A	197	GLY
1	A	279	VAL
1	A	81	ASP
1	A	196	LYS
1	A	312	ILE
1	B	144	GLY
1	A	144	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	526/576 (91%)	507 (96%)	19 (4%)	31	34
1	B	522/576 (91%)	498 (95%)	24 (5%)	24	25
All	All	1048/1152 (91%)	1005 (96%)	43 (4%)	27	29

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	67	SER
1	A	70	MET
1	A	79	ILE
1	A	98	GLU
1	A	125	MET
1	A	198	LYS
1	A	212	ILE
1	A	229	LYS
1	A	262	ASP
1	A	267	LYS
1	A	353	HIS
1	A	369	GLU
1	A	420	PHE
1	A	437	LYS
1	A	512	LYS
1	A	528	GLU
1	A	545	LYS
1	A	598	LEU
1	B	2	ASN
1	B	56	ARG
1	B	64	VAL
1	B	70	MET
1	B	74	MET
1	B	75	ARG
1	B	86	MET
1	B	89	LYS
1	B	133	ILE
1	B	198	LYS
1	B	214	THR
1	B	260	LYS
1	B	313	LYS
1	B	348	MET
1	B	349	LYS
1	B	350	GLU
1	B	408	PRO
1	B	419	THR
1	B	420	PHE
1	B	447	LEU
1	B	504	LYS
1	B	578	SER
1	B	591	ARG

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Mol	Chain	Res	Type
1	B	599	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	42	ASN
1	A	48	HIS
1	A	90	ASN
1	A	103	HIS
1	A	215	HIS
1	A	245	HIS
1	A	308	HIS
1	A	371	HIS
1	A	503	GLN
1	A	547	GLN
1	A	590	GLN
1	A	613	GLN
1	A	627	ASN
1	B	21	HIS
1	B	38	ASN
1	B	47	GLN
1	B	48	HIS
1	B	90	ASN
1	B	103	HIS
1	B	138	GLN
1	B	146	HIS
1	B	203	HIS
1	B	308	HIS
1	B	441	GLN
1	B	478	ASN
1	B	552	GLN
1	B	576	GLN
1	B	613	GLN
1	B	627	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	CSO	B	199	1	3,6,7	1.15	0	1,6,8	0.10	0
1	CSO	A	199	1	3,6,7	1.38	1 (33%)	1,6,8	0.10	0
1	CSO	B	449	1	3,6,7	0.61	0	1,6,8	0.26	0
1	CSO	A	449	1	3,6,7	0.81	0	1,6,8	1.27	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
1	CSO	B	199	1	-	0/1/5/7	-
1	CSO	A	199	1	-	0/1/5/7	-
1	CSO	B	449	1	-	0/1/5/7	-
1	CSO	A	449	1	-	1/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	CSO	O-C	2.32	1.28	1.20

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	449	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	B	701	-	58,58,58	1.15	4 (6%)	85,89,89	0.88	3 (3%)
2	FAD	A	701	-	58,58,58	0.65	0	85,89,89	0.78	2 (2%)

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	B	701	-	-	2/34/50/50	0/6/6/6
2	FAD	A	701	-	-	1/34/50/50	0/6/6/6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	FAD	C9-C8	-5.13	1.32	1.39
2	B	701	FAD	PA-O3P	3.02	1.62	1.59
2	B	701	FAD	P-O3P	2.49	1.62	1.59
2	B	701	FAD	O2-C2	2.23	1.28	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FAD	O3B-C3B-C4B	2.83	119.20	111.08
2	A	701	FAD	O5'-C5'-C4'	2.77	116.77	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	FAD	O3B-C3B-C2B	-2.71	103.14	111.82
2	A	701	FAD	C4-N3-C2	-2.33	121.50	125.64
2	B	701	FAD	O3'-C3'-C2'	-2.13	104.08	108.93

There are no chirality outliers.

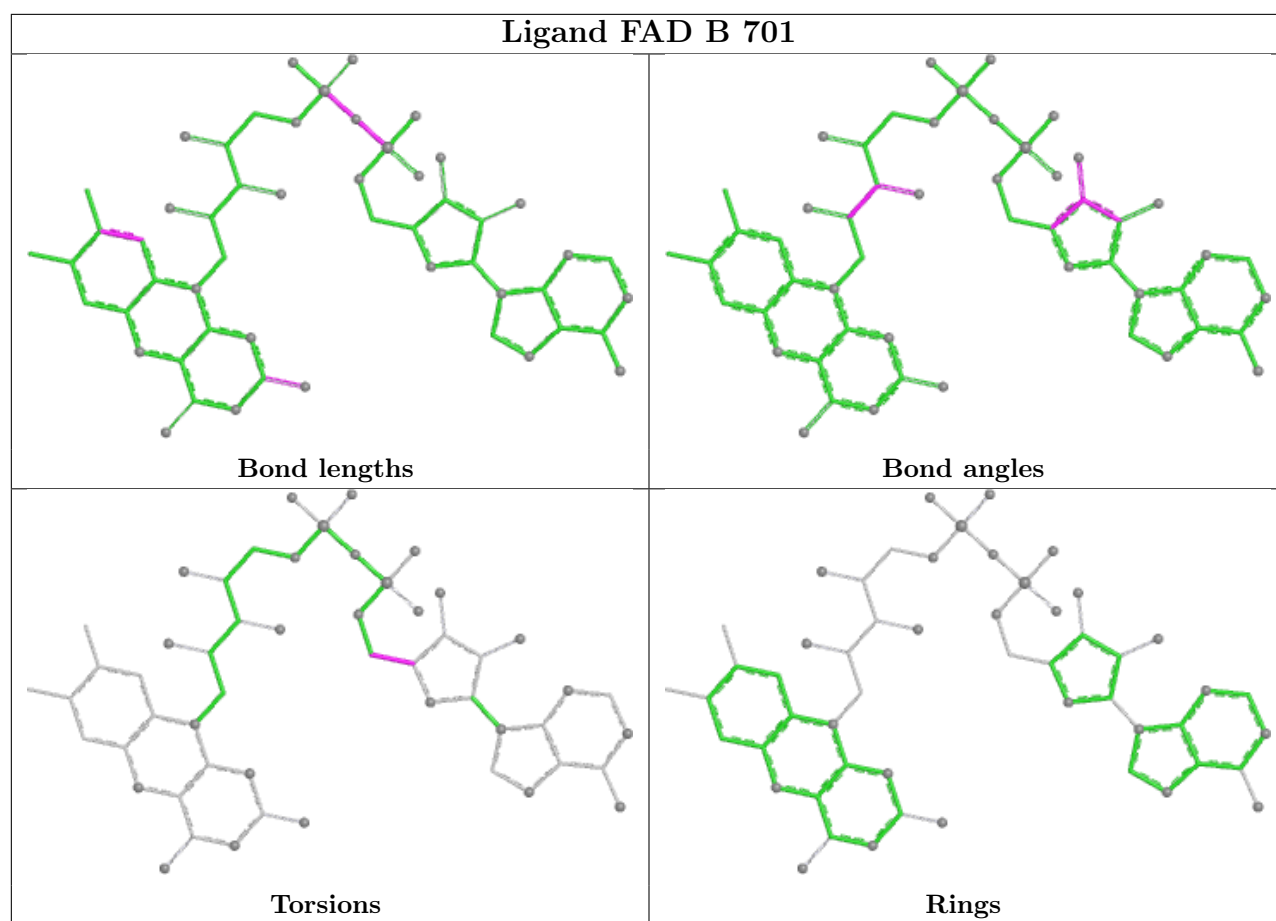
All (3) torsion outliers are listed below:

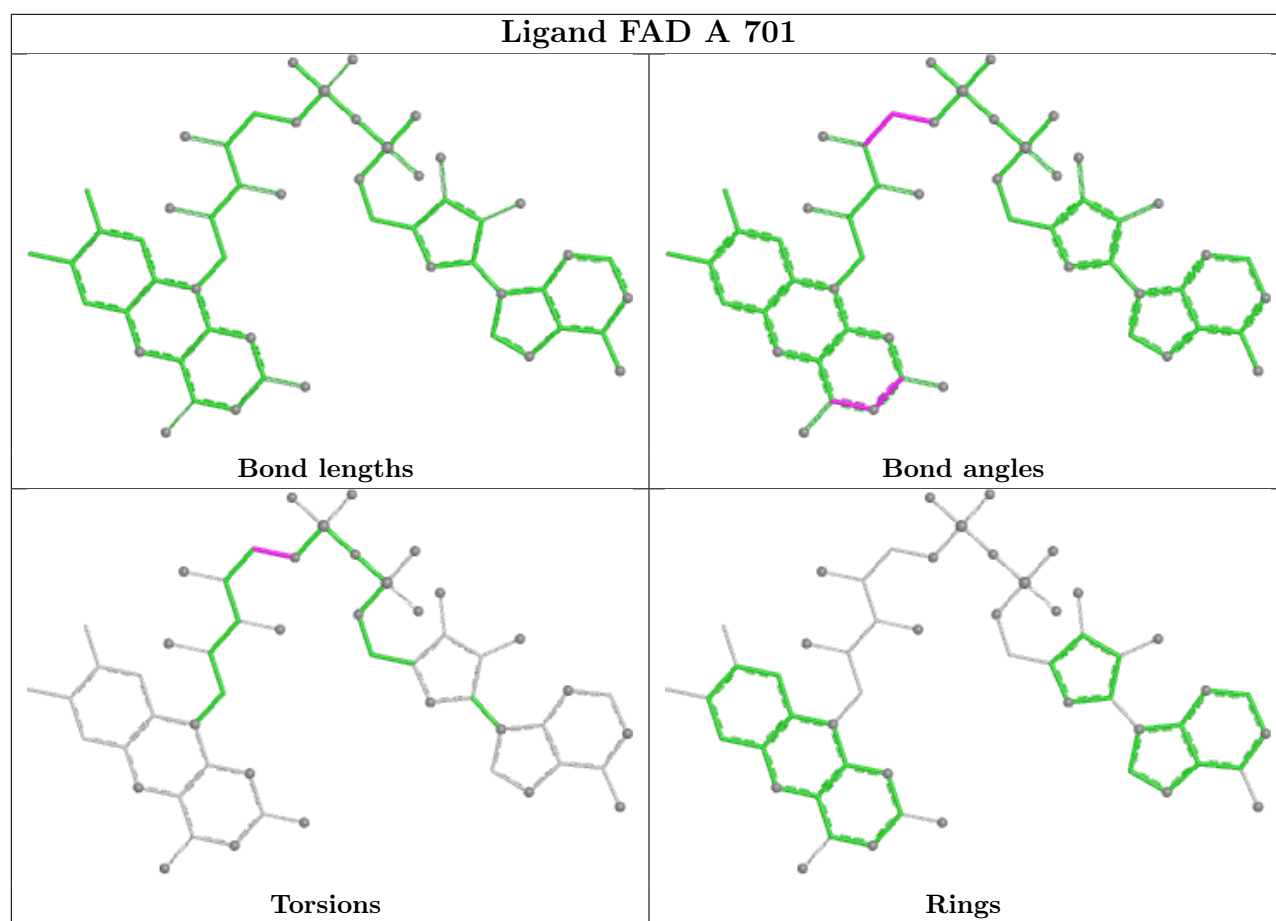
Mol	Chain	Res	Type	Atoms
2	B	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	C4'-C5'-O5'-P
2	B	701	FAD	C3B-C4B-C5B-O5B

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	610/667 (91%)	0.40	45 (7%)	20 22	22, 48, 101, 135	0
1	B	605/667 (90%)	0.04	14 (2%)	61 64	21, 41, 73, 133	0
All	All	1215/1334 (91%)	0.22	59 (4%)	35 37	21, 43, 93, 135	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	TRP	5.7
1	A	124	PHE	5.6
1	A	279	VAL	5.2
1	A	368	PRO	4.3
1	B	367	LEU	4.1
1	A	278	MET	4.1
1	A	127	ALA	3.9
1	B	352	TYR	3.8
1	A	646	VAL	3.8
1	A	355	ILE	3.7
1	B	355	ILE	3.6
1	A	267	LYS	3.5
1	B	278	MET	3.5
1	A	365	SER	3.4
1	A	256	TYR	3.4
1	A	459	PRO	3.2
1	A	259	VAL	3.2
1	A	458	LEU	3.1
1	A	125	MET	3.1
1	A	352	TYR	3.0
1	B	458	LEU	2.9
1	B	279	VAL	2.9
1	B	641	LEU	2.8
1	A	156	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	261	PRO	2.8
1	A	164	ILE	2.7
1	A	163	PHE	2.7
1	A	447	LEU	2.7
1	B	447	LEU	2.6
1	A	194	ILE	2.6
1	A	221	ILE	2.6
1	A	474	MET	2.6
1	A	257	ALA	2.6
1	A	80	ALA	2.4
1	A	218	LEU	2.4
1	A	123	PHE	2.3
1	A	265	TYR	2.3
1	A	112	LEU	2.3
1	B	353	HIS	2.3
1	A	205	PHE	2.3
1	A	647	HIS	2.2
1	B	69	ILE	2.2
1	A	64	VAL	2.2
1	B	267	LYS	2.2
1	A	353	HIS	2.2
1	A	212	ILE	2.2
1	B	314	PRO	2.2
1	B	474	MET	2.2
1	A	130	LEU	2.2
1	A	86	MET	2.2
1	A	160	THR	2.2
1	A	133	ILE	2.1
1	B	56	ARG	2.1
1	A	132	ILE	2.1
1	A	165	LEU	2.0
1	A	280	PHE	2.0
1	A	161	GLN	2.0
1	A	313	LYS	2.0
1	A	510	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	CSO	B	449	7/8	0.82	0.10	63,65,78,82	0
1	CSO	A	199	7/8	0.86	0.29	20,20,20,20	0
1	CSO	A	449	7/8	0.87	0.09	62,68,77,88	0
1	CSO	B	199	7/8	0.92	0.17	20,20,20,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

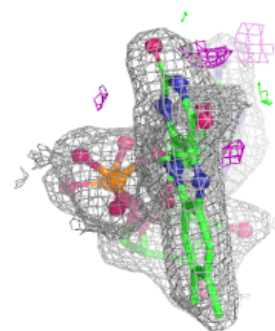
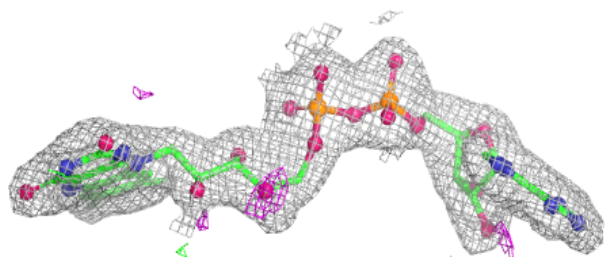
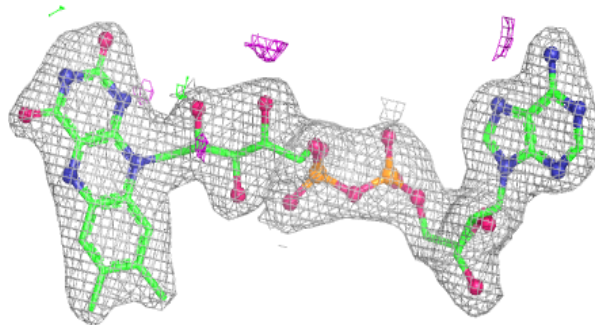
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	A	701	53/53	0.97	0.06	35,42,49,51	0
2	FAD	B	701	53/53	0.98	0.05	22,26,30,33	0

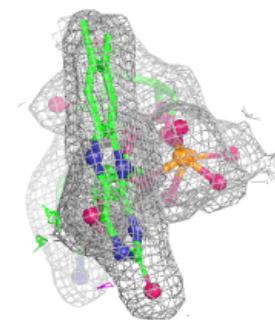
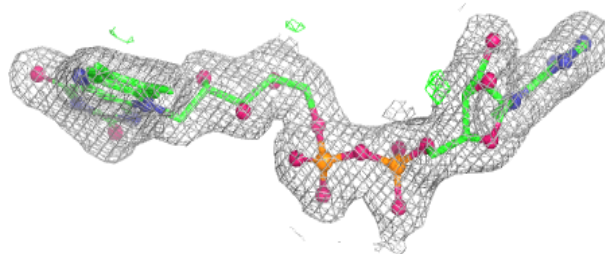
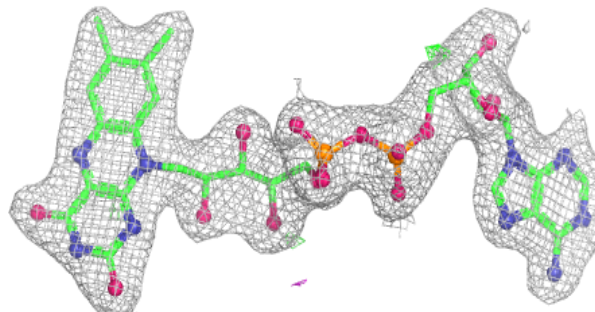
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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 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.