



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:05 AM UTC

PDB ID : 1W07 / pdb_00001w07
Title : Arabidopsis thaliana acyl-CoA oxidase 1
Authors : Henriksen, A.; Pedersen, L.
Deposited on : 2004-06-01
Resolution : 2.00 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

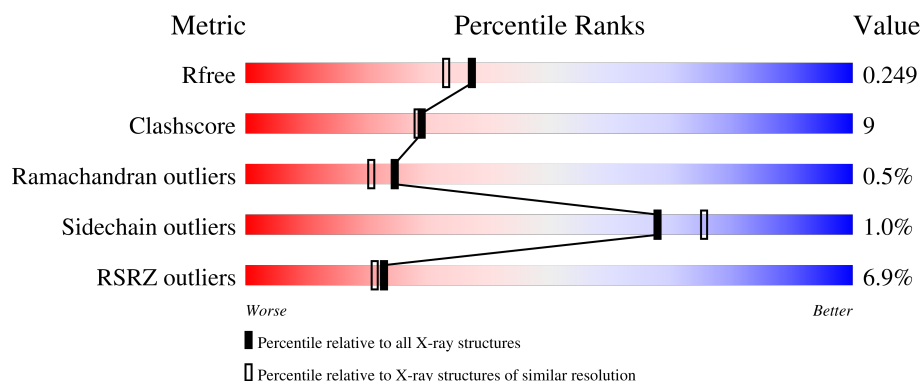
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	659	7% 79% 20% .
1	B	659	6% 79% 20% .

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 11165 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.

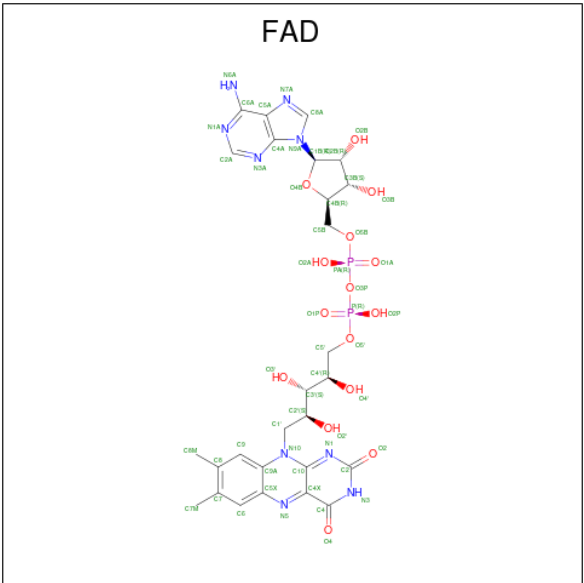
- Molecule 1 is a protein called ACYL-COA OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	655	5136	3255	900	955	26	0	3	0
1	B	658	5166	3276	908	956	26	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	LEU	PHE	engineered mutation	UNP P10725
B	155	LEU	PHE	engineered mutation	UNP P10725

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Pt	0	0
			3	3		
5	B	3	Total	Pt	0	0
			3	3		

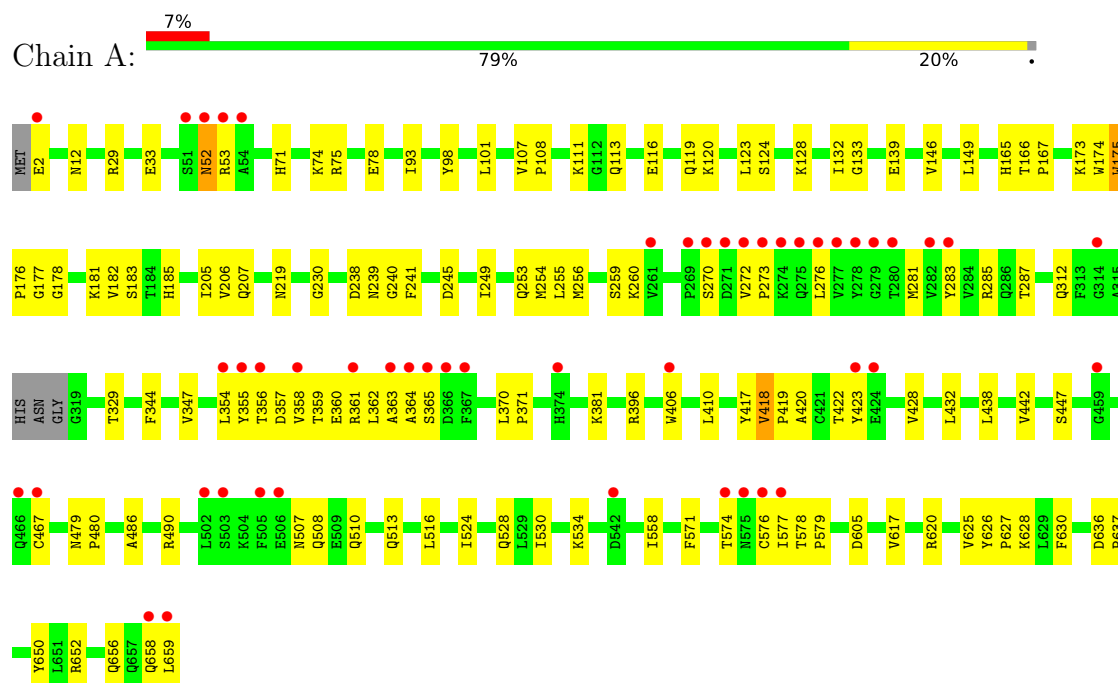
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	363	Total	O	0	0
			363	363		
6	B	385	Total	O	0	0
			385	385		

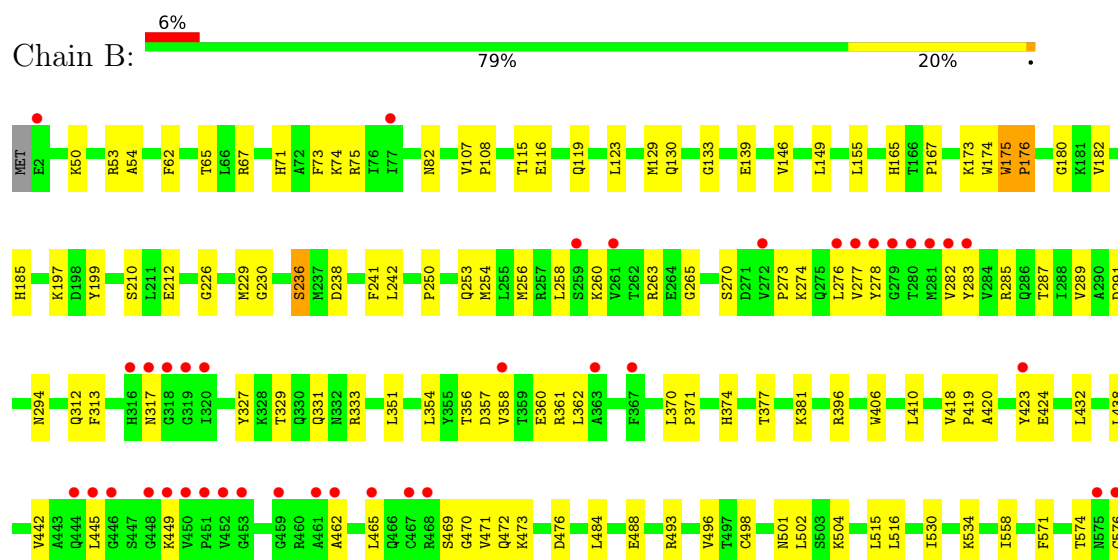
3 Residue-property plots [i](#)

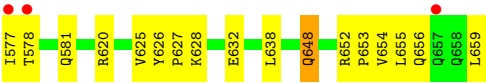
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ACYL-COA OXIDASE



• Molecule 1: ACYL-COA OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.20Å 117.00Å 131.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 2.00 29.59 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.59-2.00) 96.9 (29.59-2.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.249 0.205 , 0.249	Depositor DCC
R_{free} test set	4411 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.7	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	0.94	EDS
Total number of atoms	11165	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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

5.1 Standard geometry

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

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	0.45	0/5243	0.85	13/7109 (0.2%)
1	B	0.44	0/5276	0.84	9/7155 (0.1%)
All	All	0.45	0/10519	0.84	22/14264 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	625	VAL	N-CA-C	9.92	119.77	110.74
1	B	625	VAL	N-CA-C	9.23	119.10	110.42
1	A	576	CYS	N-CA-C	-7.62	103.09	113.30
1	A	240	GLY	N-CA-C	6.53	120.70	111.42
1	A	558	ILE	N-CA-C	-6.46	104.46	110.53
1	A	230	GLY	N-CA-C	6.35	120.17	112.48
1	B	130	GLN	N-CA-C	-6.11	105.67	113.01
1	B	236	SER	N-CA-C	-5.81	106.19	113.28
1	A	93	ILE	N-CA-C	-5.65	103.99	111.05
1	B	230	GLY	N-CA-C	5.49	119.12	112.48
1	B	180	GLY	N-CA-C	5.44	119.22	112.64
1	A	467	CYS	N-CA-C	5.30	117.53	110.53
1	B	576	CYS	N-CA-C	-5.30	106.82	113.28
1	A	239	ASN	CA-C-N	-5.28	117.47	122.17
1	A	239	ASN	C-N-CA	-5.28	117.47	122.17
1	B	182	VAL	N-CA-C	5.28	120.32	109.34
1	A	183	SER	N-CA-C	5.26	118.11	110.42
1	A	166	THR	CA-C-N	5.18	124.63	119.24
1	A	166	THR	C-N-CA	5.18	124.63	119.24
1	A	605	ASP	N-CA-C	-5.09	105.91	111.82
1	B	226	GLY	N-CA-C	5.06	117.19	112.08
1	B	558	ILE	N-CA-C	-5.05	105.79	110.53

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	5136	0	5049	96	0
1	B	5166	0	5098	93	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	363	0	0	8	0
6	B	385	0	0	7	0
All	All	11165	0	10209	180	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 9.

All (180) 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:52:ASN:H	1:A:52:ASN:HD22	1.29	0.80
1:B:578:THR:HG22	1:B:581:GLN:HG3	1.67	0.77
1:B:360:GLU:HG3	6:B:2230:HOH:O	1.85	0.77
1:B:501:ASN:HA	1:B:504:LYS:HE2	1.67	0.75
1:A:174:TRP:O	1:A:175:TRP:HB2	1.87	0.73
1:A:329:THR:HG23	1:B:516:LEU:HB3	1.72	0.72
1:B:258:LEU:HD11	1:B:277:VAL:HG23	1.75	0.69
1:B:648:GLN:NE2	1:B:648:GLN:H	1.91	0.69
1:B:174:TRP:O	1:B:175:TRP:HB2	1.93	0.68
1:A:396:ARG:HA	1:A:410:LEU:HD13	1.76	0.67
1:B:571:PHE:HB3	1:B:577:ILE:HD12	1.76	0.67
1:B:356:THR:O	1:B:360:GLU:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:GLN:O	1:A:659:LEU:HB2	1.94	0.66
1:B:632:GLU:HG2	6:B:2362:HOH:O	1.96	0.66
1:B:258:LEU:HD13	1:B:274:LYS:HA	1.76	0.66
1:A:101:LEU:HD13	1:A:177:GLY:HA3	1.78	0.65
1:A:357:ASP:O	1:A:361:ARG:HG2	1.97	0.65
1:B:107:VAL:HB	1:B:108:PRO:HD3	1.78	0.64
1:A:406:TRP:HZ2	6:A:2227:HOH:O	1.80	0.64
1:A:276:LEU:HA	1:A:362:LEU:HD13	1.82	0.62
1:A:107:VAL:HB	1:A:108:PRO:HD3	1.81	0.62
1:A:579:PRO:HG2	6:A:2301:HOH:O	2.00	0.61
1:B:418:VAL:HG23	1:B:419:PRO:HD3	1.83	0.60
1:A:119:GLN:O	1:A:123:LEU:HB2	2.02	0.60
1:A:116:GLU:O	1:A:120:LYS:HG2	2.02	0.60
1:A:428:VAL:HG21	1:B:333:ARG:NH1	2.18	0.59
1:B:473:LYS:HG2	1:B:476:ASP:OD2	2.04	0.58
1:B:254:MET:O	1:B:256:MET:HG3	2.03	0.57
1:B:146:VAL:O	1:B:149:LEU:HG	2.04	0.57
1:B:370:LEU:HB3	1:B:371:PRO:HD3	1.86	0.57
1:A:181:LYS:HE3	1:B:638:LEU:O	2.04	0.57
1:A:652:ARG:NH1	1:A:656:GLN:HG3	2.21	0.56
1:B:282:VAL:HG13	1:B:377:THR:HG21	1.87	0.56
1:B:465:LEU:HD11	1:B:496:VAL:HG21	1.86	0.56
1:A:256:MET:HB3	1:A:260:LYS:HB3	1.87	0.56
1:B:357:ASP:O	1:B:361:ARG:HG2	2.06	0.56
1:A:507:ASN:HB3	1:A:510:GLN:HB3	1.88	0.55
1:B:277:VAL:HG13	6:B:2106:HOH:O	2.05	0.55
1:B:276:LEU:HD21	1:B:362:LEU:O	2.06	0.55
1:B:498:CYS:O	1:B:502:LEU:HG	2.07	0.55
1:A:516:LEU:HB3	1:B:329:THR:HG23	1.88	0.55
1:A:344:PHE:O	1:A:347:VAL:HG12	2.07	0.54
1:A:513:GLN:HA	1:A:516:LEU:HG	1.88	0.54
1:B:139:GLU:HG3	1:B:149:LEU:HD22	1.90	0.54
1:A:74:LYS:O	1:A:78:GLU:HG3	2.09	0.53
1:A:205:ILE:O	1:A:253:GLN:HG2	2.08	0.53
1:B:358:VAL:O	1:B:362:LEU:HB2	2.08	0.53
1:B:626:TYR:HB2	1:B:627:PRO:HD3	1.90	0.53
1:B:165:HIS:O	1:B:167:PRO:HD3	2.09	0.53
1:A:206:VAL:HG22	1:A:249:ILE:HG21	1.90	0.53
1:A:659:LEU:HB3	1:B:74:LYS:HD3	1.91	0.53
1:B:173:LYS:O	1:B:241:PHE:HA	2.09	0.53
1:A:52:ASN:HD22	1:A:52:ASN:N	1.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:VAL:O	1:A:149:LEU:HG	2.10	0.52
1:A:418:VAL:HG12	1:A:419:PRO:HD3	1.90	0.52
1:A:101:LEU:HD13	1:A:177:GLY:CA	2.40	0.51
1:A:363:ALA:C	1:A:365:SER:H	2.16	0.51
1:B:260:LYS:HE2	1:B:270:SER:HB3	1.92	0.51
1:B:283:TYR:O	1:B:287:THR:HG23	2.11	0.51
1:A:53:ARG:HD2	6:A:2227:HOH:O	2.11	0.51
1:A:626:TYR:HB2	1:A:627:PRO:HD3	1.92	0.51
1:B:273:PRO:HD2	1:B:276:LEU:HD12	1.92	0.51
1:A:101:LEU:CD1	1:A:177:GLY:HA3	2.41	0.51
1:A:370:LEU:HB3	1:A:371:PRO:HD3	1.93	0.51
1:B:54:ALA:HB2	1:B:406:TRP:CE2	2.47	0.50
1:B:71:HIS:O	1:B:75:ARG:HG2	2.11	0.50
1:A:659:LEU:HD13	1:B:74:LYS:NZ	2.27	0.50
1:B:530:ILE:O	1:B:534:LYS:HG2	2.11	0.50
1:A:178:GLY:HA2	1:A:238:ASP:OD1	2.12	0.50
1:B:432:LEU:HD22	1:B:516:LEU:HD22	1.93	0.50
1:B:578:THR:HG22	1:B:581:GLN:CG	2.40	0.50
1:A:174:TRP:C	1:A:176:PRO:HD3	2.36	0.50
1:B:652:ARG:O	1:B:656:GLN:HG3	2.12	0.50
1:B:115:THR:HG22	1:B:116:GLU:N	2.26	0.50
1:B:278:TYR:O	1:B:282:VAL:HG23	2.11	0.50
6:A:2226:HOH:O	1:B:229:MET:HE3	2.11	0.49
1:B:652:ARG:HB3	1:B:653:PRO:HD3	1.94	0.49
1:A:447:SER:HB2	6:A:2241:HOH:O	2.12	0.49
1:A:658:GLN:O	1:A:659:LEU:CB	2.59	0.49
1:A:254:MET:HB3	1:A:256:MET:HE2	1.94	0.48
1:A:524:ILE:O	1:A:528:GLN:HG3	2.13	0.48
1:B:484:LEU:O	1:B:488:GLU:HG3	2.13	0.48
1:B:254:MET:HE2	1:B:256:MET:HG2	1.95	0.48
1:A:530:ILE:O	1:A:534:LYS:HG2	2.14	0.48
1:B:654:VAL:HG22	1:B:659:LEU:HD21	1.96	0.48
1:B:396:ARG:HA	1:B:410:LEU:HD13	1.96	0.48
1:A:479:ASN:C	1:A:479:ASN:HD22	2.22	0.48
1:B:173:LYS:HB2	1:B:242:LEU:HB3	1.96	0.48
1:A:52:ASN:H	1:A:52:ASN:ND2	2.05	0.47
1:A:111:LYS:HG2	1:A:123:LEU:HD11	1.96	0.47
1:A:438:LEU:O	1:A:442:VAL:HG23	2.14	0.47
1:A:29:ARG:O	1:A:33[B]:GLU:HG3	2.15	0.47
1:B:258:LEU:HA	1:B:270:SER:OG	2.14	0.47
1:A:486:ALA:HB1	1:A:577:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:LYS:HD3	1:B:199:TYR:CZ	2.50	0.47
1:B:250:PRO:HD2	1:B:253:GLN:NE2	2.30	0.47
1:A:659:LEU:HD13	1:B:74:LYS:HZ3	1.81	0.46
1:B:312:GLN:O	1:B:313:PHE:HB2	2.16	0.46
1:A:173:LYS:O	1:A:241:PHE:HA	2.15	0.46
1:B:119:GLN:O	1:B:123:LEU:HB2	2.15	0.46
1:A:175:TRP:N	1:A:176:PRO:CD	2.79	0.46
1:A:356:THR:O	1:A:360:GLU:HB2	2.16	0.46
1:B:174:TRP:C	1:B:176:PRO:HD3	2.40	0.46
1:A:219:ASN:HB3	1:A:245:ASP:HB3	1.97	0.46
1:A:381:LYS:HD3	1:A:381:LYS:C	2.41	0.46
1:A:636:ASP:CG	1:A:637:PRO:HD2	2.41	0.46
1:A:53:ARG:HB3	6:A:2227:HOH:O	2.16	0.45
1:A:283:TYR:O	1:A:287:THR:HG23	2.16	0.45
1:B:210:SER:OG	1:B:212:GLU:HG2	2.15	0.45
1:B:260:LYS:HE2	1:B:270:SER:CB	2.46	0.45
1:B:294:ASN:HB3	6:B:2338:HOH:O	2.16	0.45
1:B:493:ARG:HG2	1:B:574:THR:HG22	1.99	0.45
1:A:132:ILE:HG13	1:B:655:LEU:HD21	1.99	0.45
1:A:174:TRP:O	1:A:175:TRP:CB	2.61	0.45
1:B:381:LYS:C	1:B:381:LYS:HD3	2.40	0.45
1:A:508:GLN:NE2	1:A:508:GLN:HA	2.32	0.45
1:A:98:TYR:CG	1:A:182:VAL:HG11	2.51	0.45
1:A:422:THR:HG23	1:A:423:TYR:N	2.32	0.45
1:A:254:MET:HE2	1:A:256:MET:HG2	1.99	0.45
1:A:479:ASN:HD22	1:A:480:PRO:CD	2.29	0.45
1:A:490:ARG:HD2	1:A:571:PHE:CZ	2.51	0.45
1:A:354:LEU:O	1:A:358:VAL:HG23	2.17	0.44
1:B:501:ASN:O	1:B:504:LYS:HG2	2.16	0.44
1:A:119:GLN:HB3	1:A:123:LEU:HD12	1.98	0.44
1:B:175:TRP:N	1:B:176:PRO:CD	2.80	0.44
1:B:354:LEU:O	1:B:358:VAL:HG23	2.18	0.44
1:A:650:TYR:CE2	1:B:67:ARG:HG3	2.53	0.44
1:B:578:THR:CG2	1:B:581:GLN:HG3	2.45	0.44
1:A:260:LYS:HE3	1:A:270:SER:OG	2.17	0.44
1:B:470:GLY:O	1:B:472:GLN:HG3	2.18	0.44
1:A:423:TYR:CD1	1:A:423:TYR:C	2.96	0.44
1:B:438:LEU:O	1:B:442:VAL:HG23	2.18	0.44
1:B:82:ASN:HB2	6:B:2079:HOH:O	2.16	0.44
1:A:71:HIS:O	1:A:75:ARG:HG2	2.18	0.44
1:A:124:SER:O	1:A:128:LYS:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:PHE:CZ	1:B:129:MET:HE2	2.53	0.44
1:A:133:GLY:HA2	1:A:185:HIS:O	2.18	0.43
1:A:256:MET:HA	1:A:259:SER:O	2.18	0.43
1:A:617:VAL:HG13	1:A:628:LYS:HB2	2.00	0.43
1:A:139:GLU:HG3	1:A:149:LEU:HD22	2.01	0.43
1:A:490:ARG:HA	1:A:574:THR:HG21	2.00	0.43
1:B:432:LEU:CD2	1:B:516:LEU:HD22	2.48	0.43
1:B:129:MET:HE3	1:B:129:MET:HB3	1.89	0.43
1:B:133:GLY:HA2	1:B:185:HIS:O	2.19	0.43
1:B:285:ARG:O	1:B:289:VAL:HG23	2.18	0.42
1:A:620:ARG:CD	1:A:628:LYS:HG3	2.50	0.42
1:B:62:PHE:CE1	1:B:238:ASP:HB3	2.54	0.42
1:B:420:ALA:HA	1:B:423:TYR:CZ	2.54	0.42
1:B:53:ARG:HD3	6:B:2179:HOH:O	2.19	0.42
1:B:155:LEU:CD2	1:B:265:GLY:HA2	2.49	0.42
1:A:420:ALA:HA	1:A:423:TYR:CZ	2.55	0.42
1:A:507:ASN:HB3	1:A:510:GLN:CB	2.49	0.42
1:B:327:TYR:O	1:B:331:GLN:HG3	2.20	0.42
1:A:432:LEU:HD22	1:A:516:LEU:HD22	2.02	0.41
1:A:344:PHE:HA	1:A:347:VAL:HG12	2.02	0.41
1:A:355:TYR:O	1:A:359:THR:HG23	2.20	0.41
1:A:370:LEU:N	1:A:371:PRO:CD	2.83	0.41
1:B:289:VAL:HG21	1:B:351:LEU:CD1	2.51	0.41
1:A:578:THR:HB	1:A:579:PRO:HD2	2.01	0.41
1:B:423:TYR:O	1:B:424:GLU:HB2	2.21	0.41
1:B:65:THR:OG1	1:B:236:SER:HB2	2.20	0.41
1:A:185:HIS:NE2	1:A:207:GLN:HG3	2.35	0.41
1:A:167:PRO:HG3	6:A:2132:HOH:O	2.20	0.41
1:A:361:ARG:C	1:A:363:ALA:H	2.29	0.41
1:B:423:TYR:C	1:B:423:TYR:CD1	2.98	0.41
1:A:12:ASN:ND2	6:A:2023:HOH:O	2.53	0.41
1:A:281:MET:O	1:A:285:ARG:HD2	2.21	0.41
1:A:479:ASN:HD22	1:A:480:PRO:N	2.18	0.41
1:B:620:ARG:CD	1:B:628:LYS:HG3	2.51	0.41
1:A:165:HIS:O	1:A:167:PRO:HD3	2.21	0.41
1:A:272:VAL:HA	1:A:273:PRO:HD3	1.90	0.41
1:B:469:SER:OG	1:B:471:VAL:HG23	2.21	0.41
1:B:155:LEU:HD23	1:B:265:GLY:HA2	2.02	0.40
1:B:285:ARG:NH2	6:B:2194:HOH:O	2.51	0.40
1:B:174:TRP:O	1:B:175:TRP:CB	2.66	0.40
1:B:502:LEU:HD23	1:B:515:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:MET:HB3	1:B:256:MET:HE2	2.03	0.40
1:A:113:GLN:HB2	1:A:255:LEU:HD13	2.03	0.40
1:A:417:TYR:C	1:A:419:PRO:HD2	2.47	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	653/659 (99%)	631 (97%)	20 (3%)	2 (0%)	36	35
1	B	659/659 (100%)	623 (94%)	32 (5%)	4 (1%)	21	17
All	All	1312/1318 (100%)	1254 (96%)	52 (4%)	6 (0%)	24	21

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	TRP
1	B	175	TRP
1	B	445	LEU
1	B	449	LYS
1	A	364	ALA
1	B	462	ALA

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	538/550 (98%)	534 (99%)	4 (1%)	76	82
1	B	543/550 (99%)	536 (99%)	7 (1%)	61	68
All	All	1081/1100 (98%)	1070 (99%)	11 (1%)	68	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	312	GLN
1	A	418	VAL
1	A	630	PHE
1	B	50	LYS
1	B	176	PRO
1	B	263	ARG
1	B	291	ASP
1	B	317	ASN
1	B	374	HIS
1	B	648	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	52	ASN
1	A	113	GLN
1	A	147	GLN
1	A	246	HIS
1	A	332	ASN
1	A	374	HIS
1	A	479	ASN
1	A	508	GLN
1	A	553	ASN
1	A	554	ASN
1	A	586	ASN
1	A	615	ASN
1	A	648	GLN
1	B	113	GLN
1	B	137	GLN
1	B	253	GLN
1	B	332	ASN
1	B	444	GLN

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Mol	Chain	Res	Type
1	B	513	GLN
1	B	541	GLN
1	B	551	GLN
1	B	553	ASN
1	B	588	GLN
1	B	595	GLN
1	B	648	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

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	1660	-	58,58,58	1.33	6 (10%)	85,89,89	1.52	14 (16%)
2	FAD	A	1660	-	58,58,58	1.33	5 (8%)	85,89,89	1.51	15 (17%)

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	1660	-	-	10/34/50/50	0/6/6/6
2	FAD	A	1660	-	-	5/34/50/50	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1660	FAD	C4X-N5	4.64	1.40	1.30
2	A	1660	FAD	C4X-N5	4.60	1.40	1.30
2	A	1660	FAD	C2A-N1A	3.71	1.40	1.33
2	B	1660	FAD	C10-N1	3.67	1.40	1.33
2	B	1660	FAD	C2A-N1A	3.60	1.40	1.33
2	A	1660	FAD	C10-N1	3.59	1.40	1.33
2	B	1660	FAD	C5A-N7A	-3.18	1.33	1.39
2	A	1660	FAD	C5A-N7A	-3.05	1.33	1.39
2	B	1660	FAD	C8A-N9A	-2.19	1.33	1.37
2	A	1660	FAD	C8A-N9A	-2.15	1.33	1.37
2	B	1660	FAD	C4A-N9A	-2.10	1.33	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1660	FAD	N3A-C2A-N1A	-5.77	119.85	128.58
2	A	1660	FAD	N3A-C2A-N1A	-5.66	120.01	128.58
2	B	1660	FAD	C2A-N3A-C4A	4.09	121.83	111.83
2	B	1660	FAD	C5A-C4A-N3A	-4.05	121.13	126.72
2	A	1660	FAD	C2A-N3A-C4A	4.02	121.64	111.83
2	A	1660	FAD	C5A-C4A-N3A	-3.96	121.26	126.72
2	A	1660	FAD	C9A-C5X-N5	-3.09	119.17	122.45
2	B	1660	FAD	N9A-C8A-N7A	-3.05	109.60	113.94
2	B	1660	FAD	C4-N3-C2	-3.03	120.27	125.64
2	A	1660	FAD	C4-N3-C2	-2.99	120.33	125.64
2	A	1660	FAD	N9A-C8A-N7A	-2.93	109.78	113.94
2	B	1660	FAD	C9A-C5X-N5	-2.86	119.42	122.45
2	A	1660	FAD	N3A-C4A-N9A	2.83	131.99	127.17
2	B	1660	FAD	C10-C4X-N5	-2.81	119.08	124.81
2	B	1660	FAD	C5A-N7A-C8A	2.80	107.86	103.45
2	B	1660	FAD	C4A-C5A-N7A	-2.80	107.38	110.58
2	A	1660	FAD	C4X-C4-N3	2.71	120.14	113.25
2	B	1660	FAD	C4X-C4-N3	2.67	120.05	113.25
2	A	1660	FAD	C5A-N7A-C8A	2.62	107.57	103.45
2	B	1660	FAD	N3A-C4A-N9A	2.61	131.61	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1660	FAD	C10-C4X-N5	-2.60	119.50	124.81
2	A	1660	FAD	O4-C4-C4X	-2.46	120.04	126.53
2	B	1660	FAD	O4-C4-C4X	-2.35	120.32	126.53
2	A	1660	FAD	C4A-C5A-N7A	-2.35	107.89	110.58
2	B	1660	FAD	C4X-C10-N10	2.34	119.84	116.48
2	A	1660	FAD	C4X-C10-N10	2.21	119.65	116.48
2	A	1660	FAD	C4A-N9A-C8A	2.16	108.00	105.74
2	A	1660	FAD	C5X-C9A-N10	2.08	119.84	117.97
2	B	1660	FAD	C4A-N9A-C8A	2.07	107.91	105.74

There are no chirality outliers.

All (15) torsion outliers are listed below:

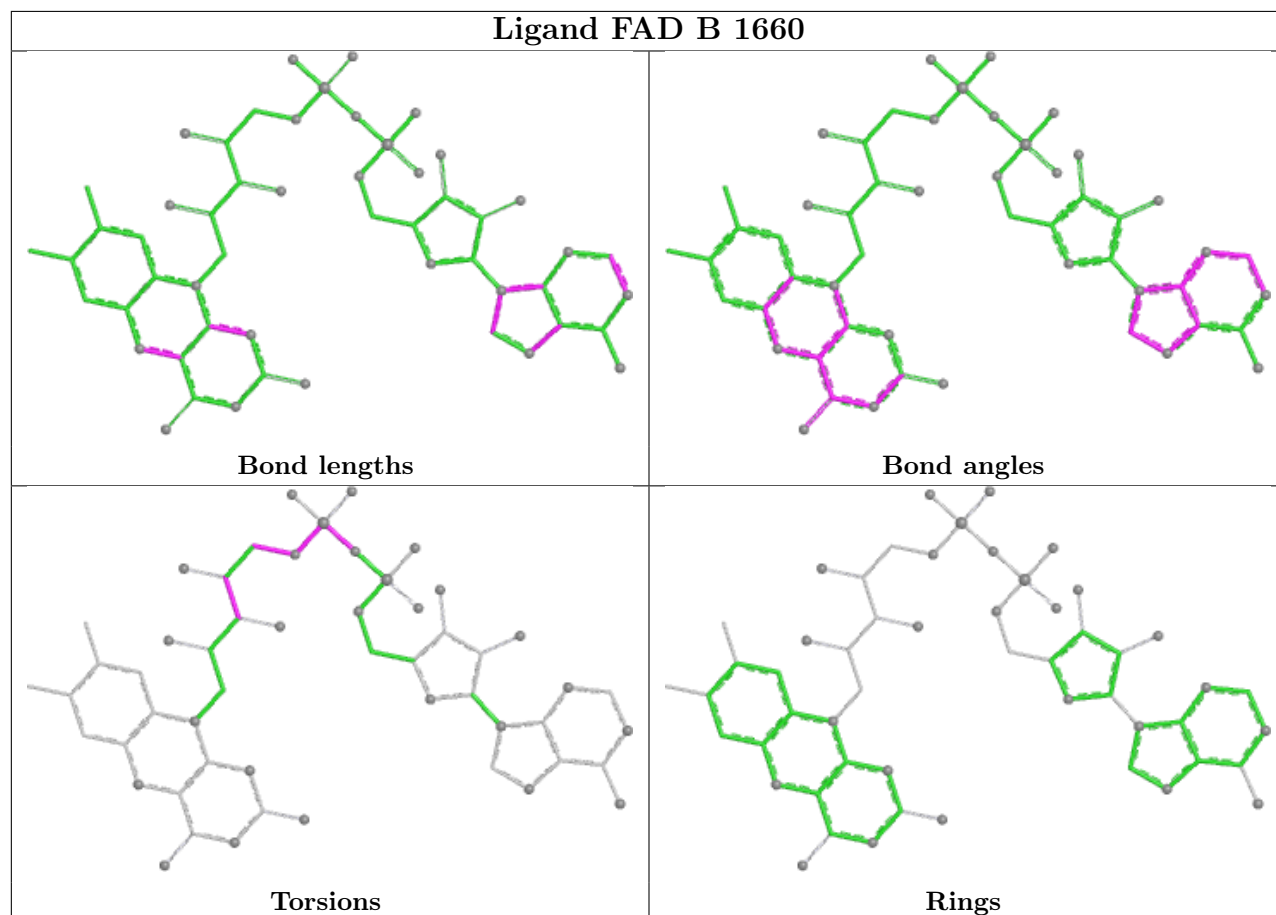
Mol	Chain	Res	Type	Atoms
2	A	1660	FAD	C5'-O5'-P-O1P
2	A	1660	FAD	C5'-O5'-P-O2P
2	A	1660	FAD	C5'-O5'-P-O3P
2	B	1660	FAD	C5'-O5'-P-O1P
2	B	1660	FAD	C5'-O5'-P-O2P
2	B	1660	FAD	C5'-O5'-P-O3P
2	B	1660	FAD	C2'-C3'-C4'-O4'
2	B	1660	FAD	O3'-C3'-C4'-C5'
2	B	1660	FAD	O3'-C3'-C4'-O4'
2	B	1660	FAD	C2'-C3'-C4'-C5'
2	A	1660	FAD	C4'-C5'-O5'-P
2	B	1660	FAD	C4'-C5'-O5'-P
2	A	1660	FAD	PA-O3P-P-O1P
2	B	1660	FAD	PA-O3P-P-O1P
2	B	1660	FAD	PA-O3P-P-O2P

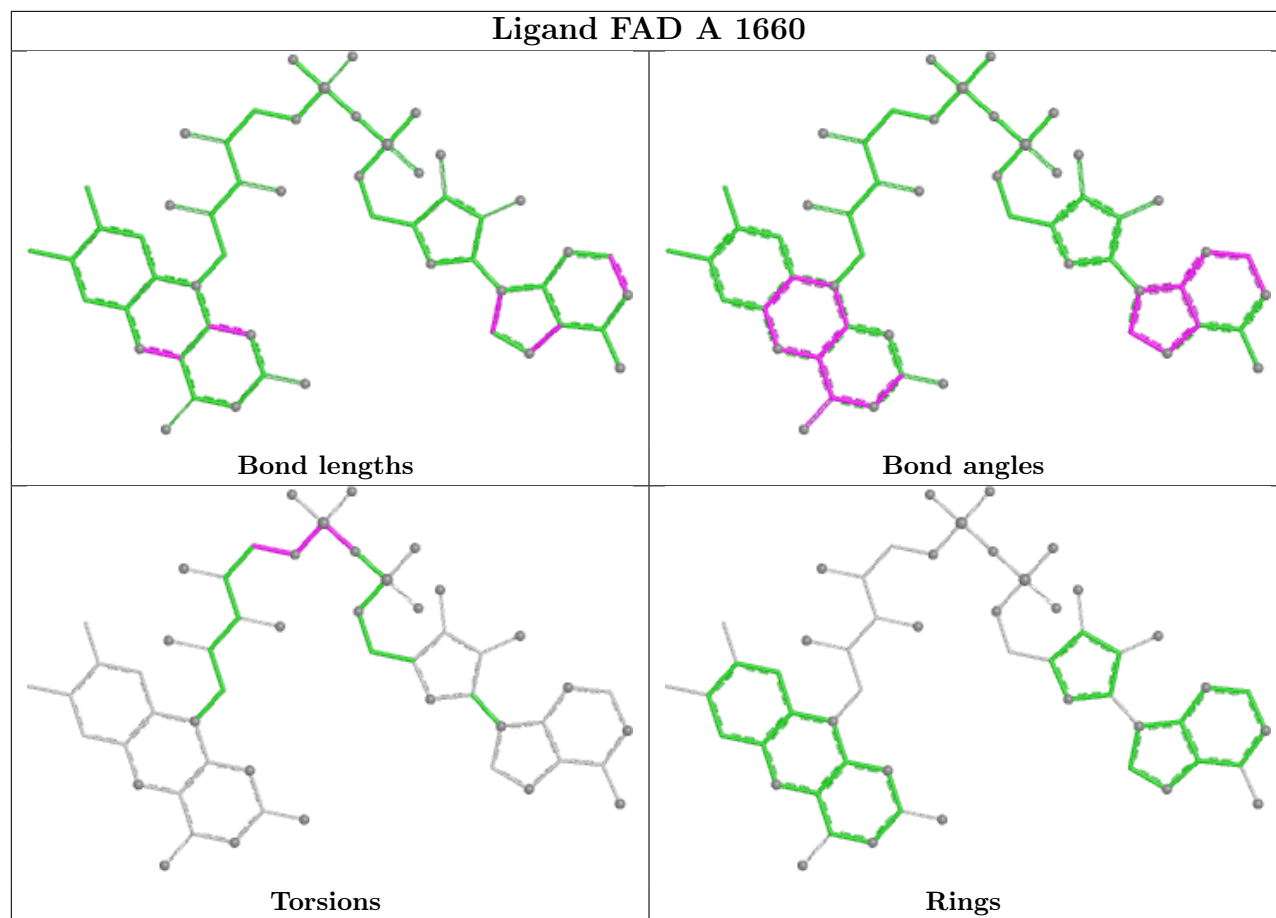
There are no ring outliers.

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	655/659 (99%)	0.19	49 (7%)	20 19	10, 24, 47, 60	3 (0%)
1	B	658/659 (99%)	0.16	42 (6%)	25 24	9, 24, 46, 55	3 (0%)
All	All	1313/1318 (99%)	0.18	91 (6%)	23 21	9, 24, 46, 60	6 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	TYR	5.5
1	A	279	GLY	5.3
1	B	446	GLY	4.9
1	A	356	THR	4.5
1	A	282	VAL	4.5
1	A	576	CYS	4.4
1	A	280	THR	4.3
1	B	423	TYR	4.2
1	A	54	ALA	4.2
1	B	278	TYR	4.1
1	A	277	VAL	4.1
1	B	450	VAL	3.9
1	A	358	VAL	3.8
1	A	273	PRO	3.7
1	A	270	SER	3.7
1	B	452	VAL	3.6
1	A	503	SER	3.6
1	B	276	LEU	3.4
1	A	423	TYR	3.3
1	A	365	SER	3.2
1	A	374	HIS	3.2
1	B	317	ASN	3.1
1	B	575	ASN	3.1
1	B	576	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	276	LEU	3.1
1	A	283	TYR	3.1
1	B	445	LEU	3.0
1	A	502	LEU	3.0
1	B	282	VAL	3.0
1	A	506	GLU	2.9
1	A	577	ILE	2.9
1	A	367	PHE	2.9
1	B	465	LEU	2.9
1	B	461	ALA	2.9
1	B	319	GLY	2.9
1	A	51	SER	2.8
1	B	277	VAL	2.8
1	B	281	MET	2.8
1	B	578	THR	2.8
1	B	451	PRO	2.8
1	B	462	ALA	2.8
1	B	467	CYS	2.8
1	B	444	GLN	2.7
1	A	467	CYS	2.7
1	A	406	TRP	2.7
1	A	364	ALA	2.7
1	B	261	VAL	2.6
1	A	575	ASN	2.6
1	A	363	ALA	2.6
1	A	505	PHE	2.5
1	A	272	VAL	2.5
1	A	542	ASP	2.5
1	A	275	GLN	2.5
1	B	280	THR	2.5
1	A	659	LEU	2.5
1	B	316	HIS	2.4
1	B	468	ARG	2.4
1	B	459	GLY	2.4
1	B	577	ILE	2.4
1	B	318	GLY	2.4
1	B	448	GLY	2.4
1	B	77	ILE	2.4
1	B	320	ILE	2.3
1	A	261	VAL	2.3
1	A	355	TYR	2.3
1	A	274	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	272	VAL	2.3
1	A	361	ARG	2.3
1	A	424	GLU	2.2
1	A	658	GLN	2.2
1	A	53	ARG	2.2
1	A	574	THR	2.2
1	A	52	ASN	2.2
1	B	283	TYR	2.1
1	B	657	GLN	2.1
1	B	449	LYS	2.1
1	A	366	ASP	2.1
1	A	459	GLY	2.1
1	B	279	GLY	2.1
1	B	453	GLY	2.1
1	A	466	GLN	2.1
1	A	269	PRO	2.1
1	B	358	VAL	2.1
1	A	2[A]	GLU	2.0
1	B	259	SER	2.1
1	B	363	ALA	2.1
1	A	354	LEU	2.0
1	A	271	ASP	2.0
1	B	2	GLU	2.0
1	B	367	PHE	2.0
1	A	314	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

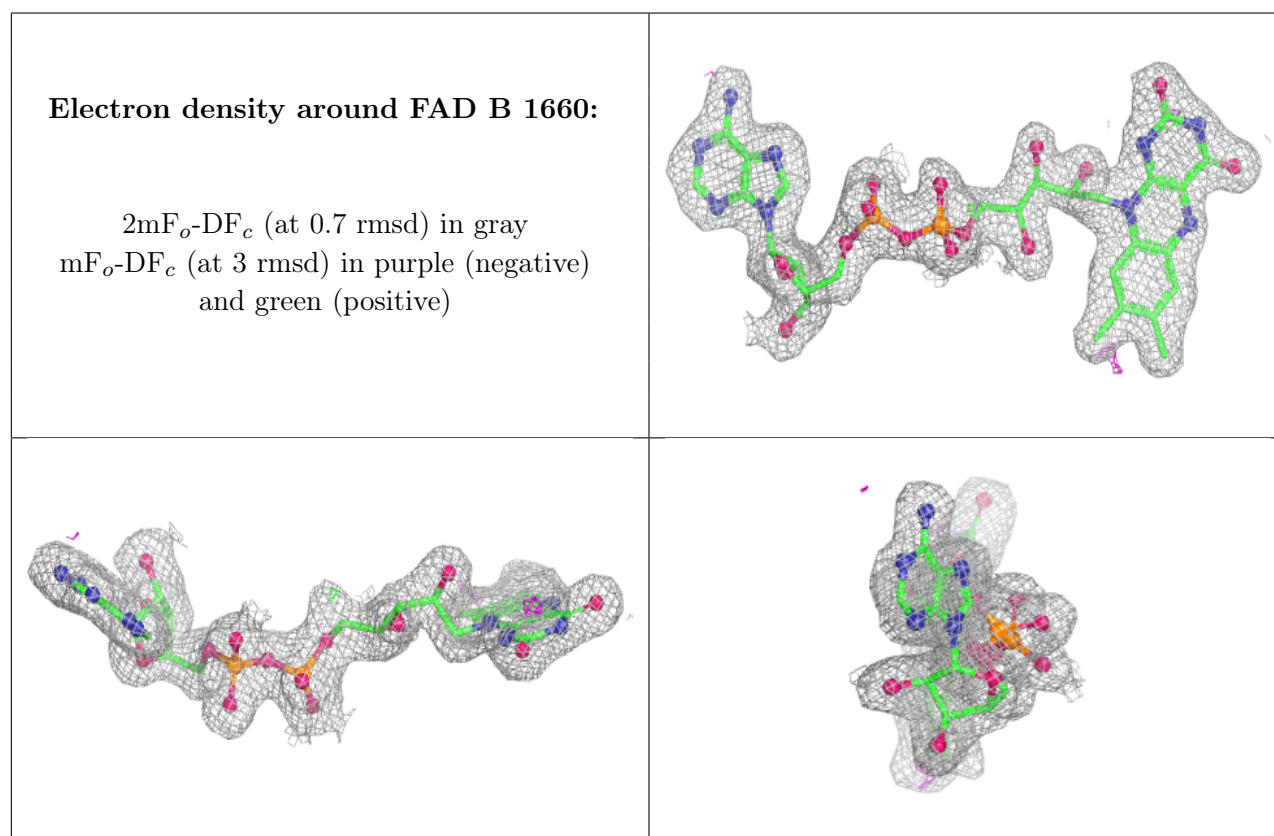
There are no oligosaccharides in this entry.

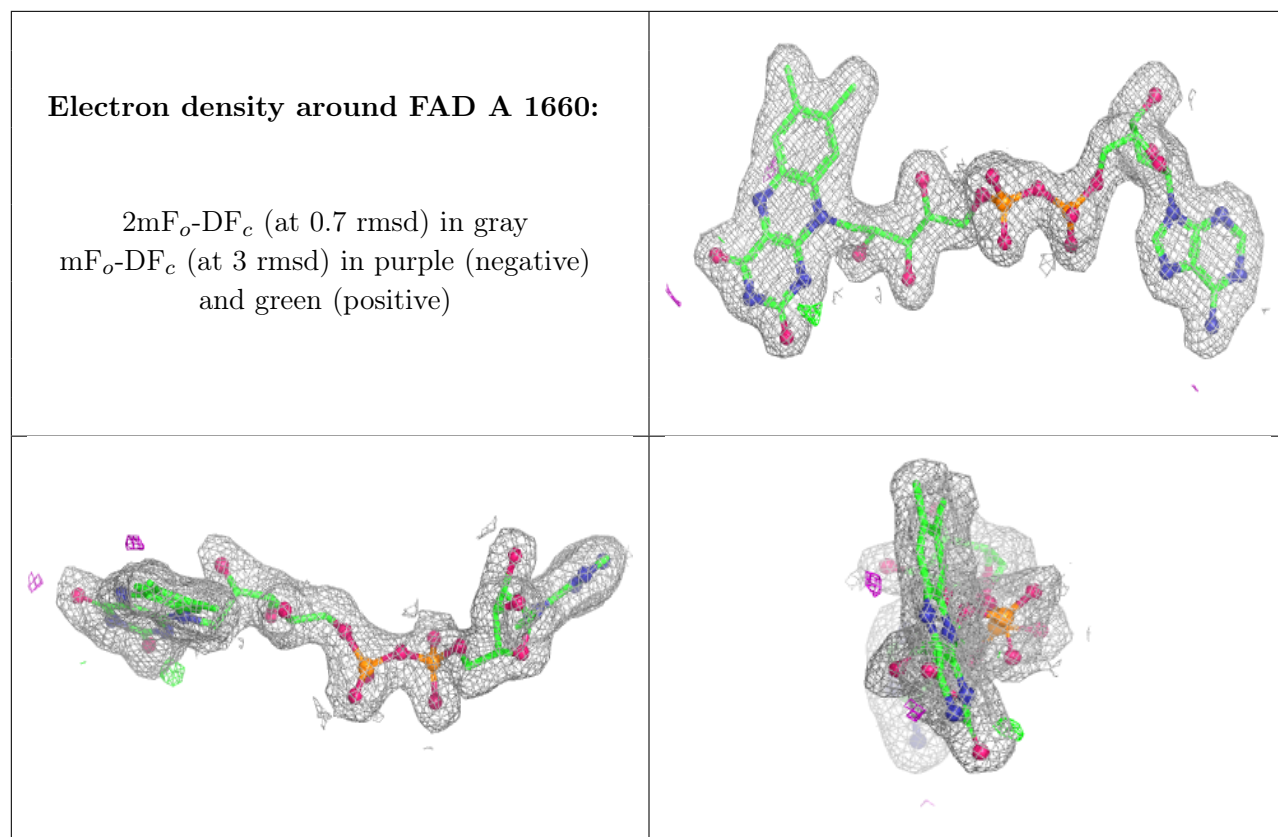
6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PT	A	1665	1/1	0.88	0.15	128,128,128,128	0
5	PT	B	1663	1/1	0.88	0.25	144,144,144,144	0
4	CL	A	1662	1/1	0.94	0.07	38,38,38,38	0
2	FAD	B	1660	53/53	0.96	0.06	12,17,23,25	0
5	PT	B	1662	1/1	0.96	0.07	63,63,63,63	0
2	FAD	A	1660	53/53	0.96	0.06	7,19,24,26	0
5	PT	B	1664	1/1	0.96	0.10	88,88,88,88	0
5	PT	A	1663	1/1	0.99	0.05	58,58,58,58	0
5	PT	A	1664	1/1	0.99	0.04	41,41,41,41	0
3	CA	A	1661	1/1	1.00	0.03	20,20,20,20	0
4	CL	B	1661	1/1	1.00	0.02	18,18,18,18	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.