



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:58 PM GMT

PDB ID : 1W07
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

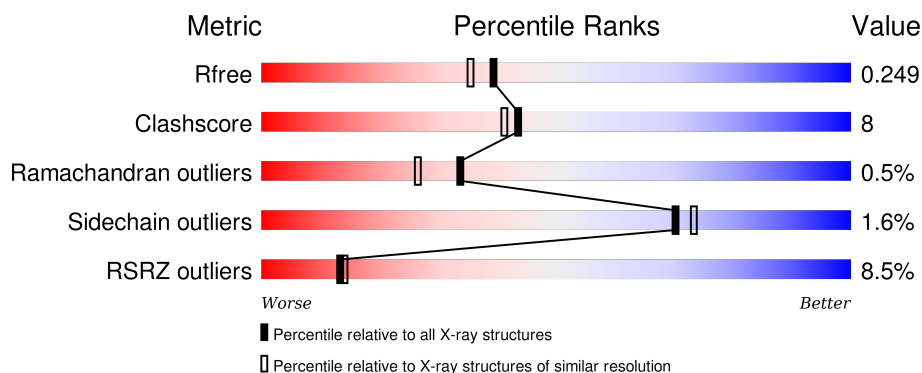
1 Overall quality at a glance

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>9%</div> <div>81%</div> <div>18%</div> <div>..</div> </div>
1	B	659	<div> <div>8%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>

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.

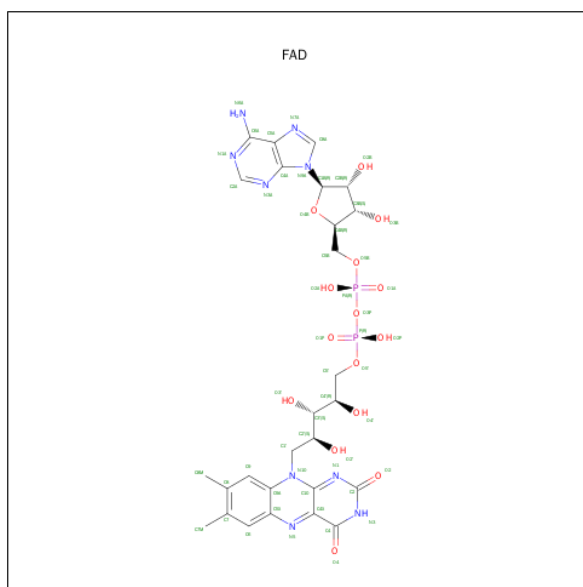
- Molecule 1 is a protein called ACYL-COA OXIDASE.

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

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 (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		

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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 (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is PLATINUM (II) ION (three-letter code: PT) (formula: Pt).

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

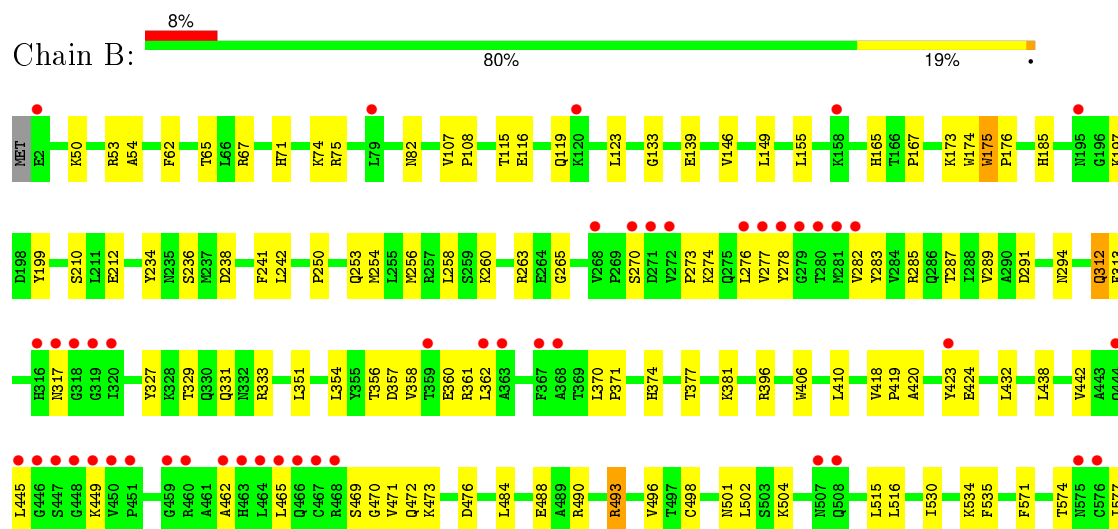
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.59-2.00) 95.4 (29.59-1.98)	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	4342 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 87331 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, PT, FAD, 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	0.38	0/5243	0.55	0/7109
1	B	0.38	0/5276	0.55	0/7155
All	All	0.38	0/10519	0.55	0/14264

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5136	0	5049	90	0
1	B	5166	0	5098	86	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	7	0
6	B	385	0	0	7	0
All	All	11165	0	10209	168	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 8.

All (168) 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:648:GLN:H	1:B:648:GLN:NE2	1.91	0.69
1:B:258:LEU:HD11	1:B:277:VAL:HG23	1.75	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
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:465:LEU:HD11	1:B:496:VAL:HG21	1.86	0.56
1:B:282:VAL:HG13	1:B:377:THR:HG21	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:358:VAL:O	1:B:362:LEU:HB2	2.08	0.53
1:A:205:ILE:O	1:A:253:GLN:HG2	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:N	1:A:52:ASN:HD22	1.97	0.52
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:B:260:LYS:HE2	1:B:270:SER:HB3	1.92	0.51
1:A:101:LEU:HD13	1:A:177:GLY:CA	2.40	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:B:273:PRO:HD2	1:B:276:LEU:HD12	1.92	0.51
1:A:626:TYR:HB2	1:A:627:PRO:HD3	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:71:HIS:O	1:B:75:ARG:HG2	2.11	0.50
1:B:54:ALA:HB2	1:B:406:TRP:CE2	2.47	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:B:578:THR:HG22	1:B:581:GLN:CG	2.40	0.50
1:B:432:LEU:HD22	1:B:516:LEU:HD22	1.93	0.50
1:A:178:GLY:HA2	1:A:238:ASP:OD1	2.12	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:VAL:HG22	1:B:659:LEU:HD21	1.96	0.48
1:A:530:ILE:O	1:A:534:LYS:HG2	2.14	0.48
1:B:396:ARG:HA	1:B:410:LEU:HD13	1.96	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:363:ALA:C	1:A:365:SER:H	2.16	0.47
1:B:258:LEU:HA	1:B:270:SER:OG	2.14	0.47
1:A:29:ARG:O	1:A:33[B]:GLU:HG3	2.15	0.47
1:A:486:ALA:HB1	1:A:577:ILE:HD11	1.97	0.47
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:B:312:GLN:O	1:B:313:PHE:HB2	2.16	0.46
1:B:119:GLN:O	1:B:123:LEU:HB2	2.15	0.46
1:A:173:LYS:O	1:A:241:PHE:HA	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:A:219:ASN:HB3	1:A:245:ASP:HB3	1.97	0.46
1:A:174:TRP:C	1:A:176:PRO:HD3	2.36	0.45
1:A:53:ARG:HB3	6:A:2227:HOH:O	2.16	0.45
1:B:210:SER:OG	1:B:212:GLU:HG2	2.15	0.45
1:A:283:TYR:O	1:A:287:THR:HG23	2.16	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: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:490:ARG:HD2	1:A:571:PHE:CZ	2.51	0.45
1:A:479:ASN:HD22	1:A:480:PRO:CD	2.29	0.45
1:B:501:ASN:O	1:B:504:LYS:HG2	2.16	0.44
1:A:354:LEU:O	1:A:358:VAL:HG23	2.17	0.44
1:B:175:TRP:N	1:B:176:PRO:CD	2.80	0.44
1:A:119:GLN:HB3	1:A:123:LEU:HD12	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:GLY:O	1:B:472:GLN:HG3	2.18	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
1:A:256:MET:HA	1:A:259:SER:O	2.18	0.43
1:A:133:GLY:HA2	1:A:185:HIS: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:A:479:ASN:C	1:A:479:ASN:HD22	2.22	0.43
1:B:432:LEU:CD2	1:B:516:LEU:HD22	2.48	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:507:ASN:HB3	1:A:510:GLN:CB	2.49	0.42
1:A:420:ALA:HA	1:A:423:TYR:CZ	2.55	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:B:381:LYS:HD3	1:B:381:LYS:C	2.40	0.41
1:A:344:PHE:HA	1:A:347:VAL:HG12	2.02	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:355:TYR:O	1:A:359:THR:HG23	2.20	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:B:174:TRP:C	1:B:176:PRO:HD3	2.40	0.41
1:A:185:HIS:NE2	1:A:207:GLN:HG3	2.35	0.41
1:A:381:LYS:C	1:A:381:LYS:HD3	2.41	0.41
1:A:636:ASP:CG	1:A:637:PRO:HD2	2.41	0.41
1:A:167:PRO:HG3	6:A:2132:HOH:O	2.20	0.41
1:A:479:ASN:HD22	1:A:480:PRO:N	2.18	0.41
1:A:12:ASN:ND2	6:A:2023:HOH:O	2.53	0.41
1:B:620:ARG:CD	1:B:628:LYS:HG3	2.51	0.41
1:A:281:MET:O	1:A:285:ARG:HD2	2.21	0.41
1:A:165:HIS:O	1:A:167:PRO:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:285:ARG:NH2	6:B:2194:HOH:O	2.51	0.40
1:B:155:LEU:HD23	1:B:265:GLY:HA2	2.02	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
1:A:113:GLN:HB2	1:A:255:LEU:HD13	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	653/659 (99%)	631 (97%)	20 (3%)	2 (0%)	46	41
1	B	659/659 (100%)	623 (94%)	32 (5%)	4 (1%)	30	22
All	All	1312/1318 (100%)	1254 (96%)	52 (4%)	6 (0%)	34	26

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 ⓘ

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%)	532 (99%)	6 (1%)	80	83
1	B	543/550 (99%)	532 (98%)	11 (2%)	63	65
All	All	1081/1100 (98%)	1064 (98%)	17 (2%)	70	73

All (17) 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	479	ASN
1	A	535	PHE
1	A	630	PHE
1	B	50	LYS
1	B	234	TYR
1	B	263	ARG
1	B	291	ASP
1	B	312	GLN
1	B	317	ASN
1	B	374	HIS
1	B	490	ARG
1	B	493	ARG
1	B	535	PHE
1	B	648	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	52	ASN
1	A	246	HIS
1	A	294	ASN
1	A	479	ASN

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Mol	Chain	Res	Type
1	A	508	GLN
1	A	553	ASN
1	A	554	ASN
1	A	588	GLN
1	A	615	ASN
1	B	253	GLN
1	B	444	GLN
1	B	510	GLN
1	B	588	GLN
1	B	648	GLN
1	B	656	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 carbohydrates 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	A	1660	-	48,58,58	1.46	6 (12%)	54,89,89	2.16	8 (14%)
2	FAD	B	1660	-	48,58,58	1.44	6 (12%)	54,89,89	2.16	8 (14%)

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	1660	-	-	0/30/50/50	0/6/6/6
2	FAD	B	1660	-	-	0/30/50/50	0/6/6/6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1660	FAD	O4B-C1B	2.36	1.44	1.41
2	A	1660	FAD	O4B-C1B	2.38	1.44	1.41
2	A	1660	FAD	C10-N1	2.92	1.40	1.35
2	B	1660	FAD	C10-N1	3.02	1.40	1.35
2	B	1660	FAD	C5X-N5	3.05	1.40	1.35
2	A	1660	FAD	C5X-N5	3.26	1.40	1.35
2	B	1660	FAD	C2A-N1A	3.38	1.40	1.33
2	A	1660	FAD	C2A-N1A	3.49	1.40	1.33
2	B	1660	FAD	C4-N3	3.97	1.40	1.33
2	A	1660	FAD	C4-N3	4.05	1.40	1.33
2	A	1660	FAD	C4X-N5	4.68	1.40	1.33
2	B	1660	FAD	C4X-N5	4.73	1.40	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1660	FAD	N3A-C2A-N1A	-11.81	119.85	128.89
2	A	1660	FAD	N3A-C2A-N1A	-11.60	120.01	128.89
2	A	1660	FAD	P-O3P-PA	-3.95	121.65	132.73
2	B	1660	FAD	P-O3P-PA	-3.48	122.95	132.73
2	B	1660	FAD	C4X-C4-N3	-2.58	120.05	123.59
2	A	1660	FAD	C4X-C4-N3	-2.52	120.14	123.59
2	B	1660	FAD	C4A-C5A-N7A	-2.28	107.38	109.48
2	A	1660	FAD	C9A-C5X-N5	-2.15	119.17	122.36
2	B	1660	FAD	C2B-C1B-N9A	-2.07	111.12	114.29
2	A	1660	FAD	C2B-C1B-N9A	-2.01	111.22	114.29
2	B	1660	FAD	C5X-C9A-N10	2.21	119.30	117.62
2	A	1660	FAD	C5X-C9A-N10	2.93	119.84	117.62
2	A	1660	FAD	C4X-N5-C5X	3.68	121.00	116.76
2	B	1660	FAD	C4X-N5-C5X	3.95	121.31	116.76
2	B	1660	FAD	C4-N3-C2	5.81	120.27	115.25
2	A	1660	FAD	C4-N3-C2	5.88	120.33	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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%)	0.38	61 (9%) 11 11	10, 24, 47, 60	0
1	B	658/659 (99%)	0.28	50 (7%) 17 18	10, 24, 46, 55	0
All	All	1313/1318 (99%)	0.33	111 (8%) 13 14	10, 24, 46, 60	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	TYR	8.8
1	B	450	VAL	8.5
1	A	363	ALA	8.4
1	A	356	THR	8.0
1	A	273	PRO	7.8
1	A	280	THR	7.8
1	A	272	VAL	7.5
1	A	279	GLY	7.4
1	B	446	GLY	7.3
1	B	448	GLY	7.2
1	A	367	PHE	7.0
1	A	277	VAL	6.8
1	A	276	LEU	6.7
1	A	365	SER	6.4
1	A	283	TYR	6.1
1	A	576	CYS	5.7
1	A	362	LEU	5.7
1	B	276	LEU	5.5
1	A	358	VAL	5.5
1	B	467	CYS	5.2
1	B	319	GLY	5.2
1	A	364	ALA	5.0
1	B	468	ARG	5.0
1	A	368	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	275	GLN	4.8
1	B	316	HIS	4.8
1	A	270	SER	4.7
1	A	366	ASP	4.7
1	A	361	ARG	4.6
1	B	447	SER	4.6
1	A	274	LYS	4.5
1	A	355	TYR	4.5
1	B	318	GLY	4.2
1	A	370	LEU	4.2
1	A	659	LEU	4.2
1	B	362	LEU	4.2
1	A	282	VAL	4.2
1	A	575	ASN	4.2
1	B	445	LEU	4.0
1	B	363	ALA	4.0
1	B	277	VAL	3.9
1	B	278	TYR	3.9
1	A	450	VAL	3.9
1	A	466	GLN	3.6
1	B	575	ASN	3.6
1	B	465	LEU	3.6
1	A	360	GLU	3.5
1	B	120	LYS	3.5
1	B	464	LEU	3.5
1	B	463	HIS	3.5
1	A	54	ALA	3.5
1	B	449	LYS	3.4
1	A	507	ASN	3.4
1	A	263	ARG	3.4
1	B	451	PRO	3.3
1	A	271	ASP	3.3
1	B	317	ASN	3.3
1	A	467	CYS	3.2
1	B	2	GLU	3.2
1	B	195	ASN	3.1
1	B	272	VAL	3.1
1	B	271	ASP	3.0
1	B	282	VAL	3.0
1	B	462	ALA	2.9
1	A	371	PRO	2.9
1	B	657	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	354	LEU	2.9
1	B	423	TYR	2.9
1	A	315	ALA	2.8
1	B	507	ASN	2.8
1	A	314	GLY	2.8
1	A	2[A]	GLU	2.7
1	A	359	THR	2.7
1	B	281	MET	2.6
1	B	576	CYS	2.6
1	A	505	PHE	2.6
1	A	406	TRP	2.5
1	B	459	GLY	2.5
1	A	353	TRP	2.5
1	A	374	HIS	2.4
1	A	468	ARG	2.4
1	B	280	THR	2.4
1	B	368	ALA	2.4
1	A	658	GLN	2.3
1	B	268	VAL	2.3
1	A	116	GLU	2.3
1	A	452	VAL	2.3
1	B	279	GLY	2.3
1	B	466	GLN	2.3
1	B	460	ARG	2.3
1	A	281	MET	2.3
1	B	444	GLN	2.3
1	A	459	GLY	2.2
1	B	270	SER	2.2
1	A	542	ASP	2.2
1	B	359	THR	2.2
1	B	367	PHE	2.2
1	B	508	GLN	2.2
1	A	264	GLU	2.2
1	A	574	THR	2.2
1	A	423	TYR	2.2
1	B	658	GLN	2.1
1	A	51	SER	2.1
1	A	503	SER	2.1
1	A	508	GLN	2.1
1	A	186	ALA	2.1
1	A	258	LEU	2.0
1	B	79	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	120	LYS	2.0
1	B	158	LYS	2.0
1	B	320	ILE	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	CL	A	1662	1/1	0.93	0.14	0.51	38,38,38,38	0
2	FAD	B	1660	53/53	0.96	0.11	-0.25	12,17,23,25	0
2	FAD	A	1660	53/53	0.96	0.10	-0.55	7,19,24,26	0
4	CL	B	1661	1/1	1.00	0.07	-1.52	18,18,18,18	0
5	PT	B	1664	1/1	0.94	0.05	-	88,88,88,88	0
5	PT	B	1662	1/1	0.94	0.04	-	63,63,63,63	0
3	CA	A	1661	1/1	0.99	0.05	-	20,20,20,20	0
5	PT	A	1665	1/1	0.70	0.06	-	128,128,128,128	0
5	PT	A	1664	1/1	0.99	0.05	-	41,41,41,41	0
5	PT	B	1663	1/1	0.90	0.09	-	144,144,144,144	0
5	PT	A	1663	1/1	0.99	0.03	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.