



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:25 AM UTC

PDB ID : 1C0P / pdb_00001c0p
Title : D-AMINO ACID OXIDASE IN COMPLEX WITH D-ALANINE AND A PARTIALLY OCCUPIED BIATOMIC SPECIES
Authors : Umhau, S.; Pollegioni, L.; Molla, G.; Diederichs, K.; Welte, W.; Pilone, S.M.; Ghisla, S.
Deposited on : 1999-07-19
Resolution : 1.20 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

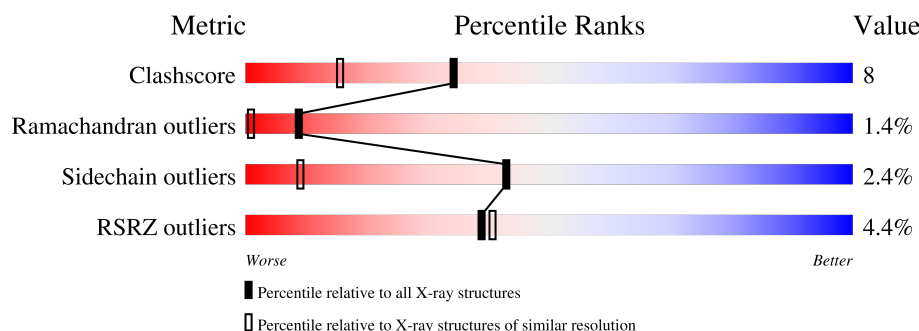
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.20 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))
Clashscore	190562	1265 (1.20-1.20)
Ramachandran outliers	187476	1226 (1.20-1.20)
Sidechain outliers	187428	1226 (1.20-1.20)
RSRZ outliers	180081	1214 (1.20-1.20)

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	363	4% 79% 17% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DAL	A	1364	-	-	X	-
4	PER	A	1365	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	1366	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3478 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.

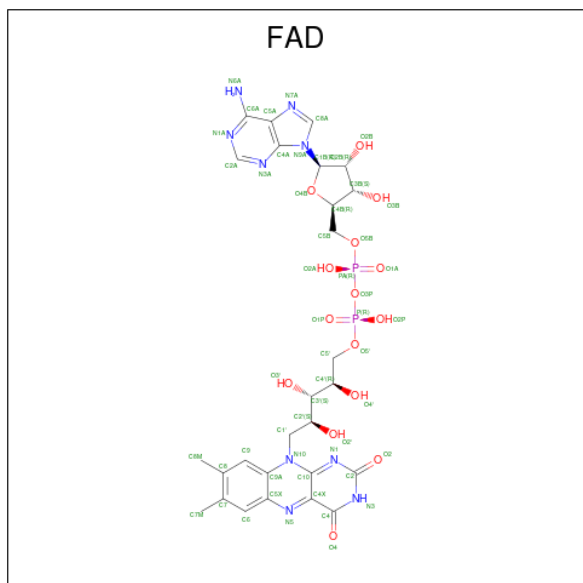
- Molecule 1 is a protein called D-AMINO ACID OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2799	1763	500	525	11	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

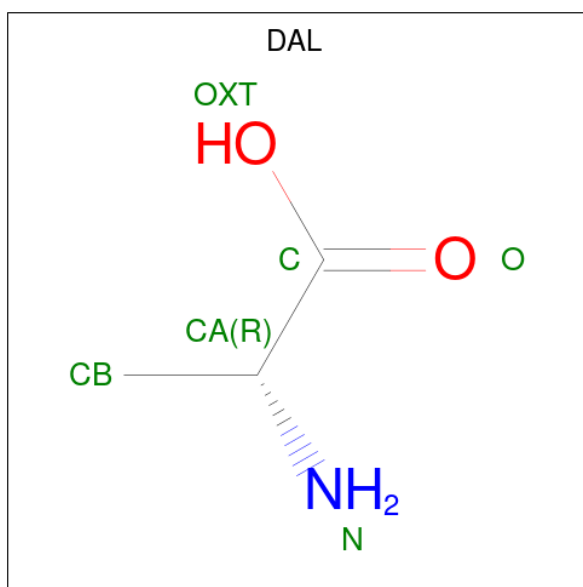
Chain	Residue	Modelled	Actual	Comment	Reference
A	999	LEU	-	cloning artifact	UNP P80324
A	1000	MET	-	cloning artifact	UNP P80324

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



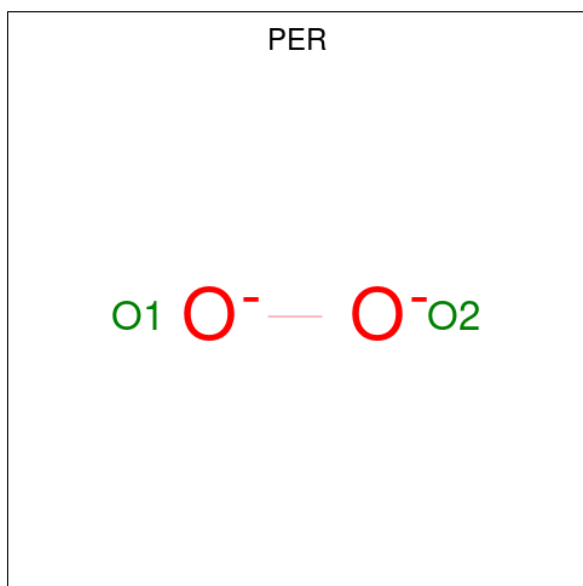
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	53	27	9	15	2	0	0

- Molecule 3 is D-ALANINE (CCD ID: DAL) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	3	1	2		

- Molecule 4 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

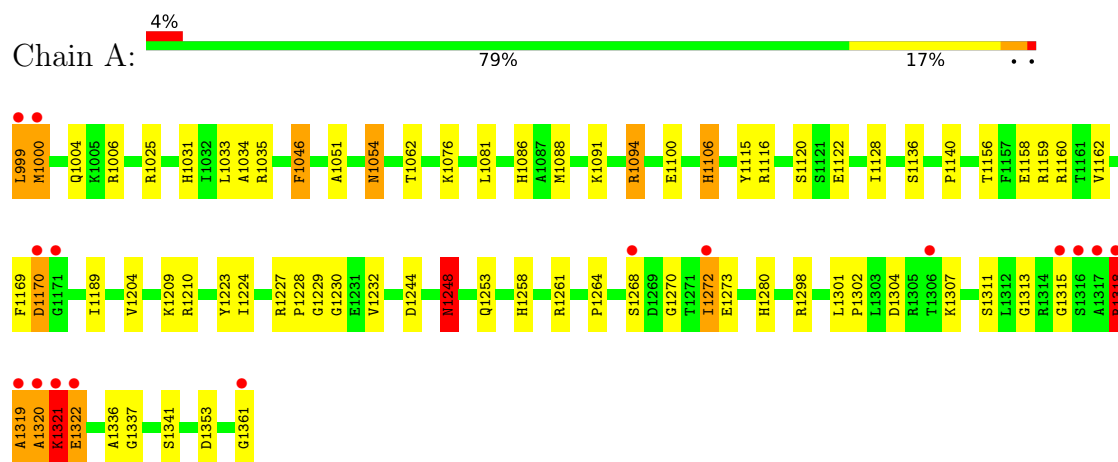
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	612	Total	O	0	0
			612	612		

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: D-AMINO ACID OXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.89Å 120.89Å 136.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 1.20 90.46 – 1.20	Depositor EDS
% Data completeness (in resolution range)	5.3 (100.00-1.20) 98.8 (90.46-1.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 1.20Å)	Xtriage
Refinement program	SHELXL-97, CNS	Depositor
R, R_{free}	0.125 , 0.150 0.138 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 83.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3478	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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: DAL, GOL, FAD, PER

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	2.17	2/2881 (0.1%)	1.69	70/3915 (1.8%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1361	GLY	C-OXT	104.61	3.32	1.23
1	A	1088	MET	SD-CE	-5.17	1.66	1.79

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1318	ARG	CA-C-N	19.54	158.87	121.54
1	A	1318	ARG	C-N-CA	19.54	158.87	121.54
1	A	1319	ALA	CA-C-N	17.07	154.13	121.54
1	A	1319	ALA	C-N-CA	17.07	154.13	121.54
1	A	1298	ARG	NE-CZ-NH2	13.84	131.66	119.20
1	A	1062	THR	O-C-N	-9.71	111.09	122.15
1	A	1062	THR	CA-C-N	9.55	133.86	120.29
1	A	1062	THR	C-N-CA	9.55	133.86	120.29
1	A	1321	LYS	CA-C-O	-9.46	106.99	120.51
1	A	1094	ARG	CD-NE-CZ	9.01	137.01	124.40
1	A	1315	GLY	CA-C-N	8.87	133.05	120.28
1	A	1315	GLY	C-N-CA	8.87	133.05	120.28
1	A	1094	ARG	CG-CD-NE	8.29	130.24	112.00
1	A	1272	ILE	CB-CA-C	-7.94	101.42	112.14
1	A	1046	PHE	CA-CB-CG	7.92	121.72	113.80
1	A	1170[A]	ASP	CA-C-O	7.56	129.00	120.84
1	A	1170[B]	ASP	CA-C-O	7.56	129.00	120.84
1	A	1116	ARG	NE-CZ-NH1	7.38	128.88	121.50
1	A	1228	PRO	CA-C-O	7.18	129.14	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1270	GLY	CA-C-N	-7.13	111.39	122.59
1	A	1270	GLY	C-N-CA	-7.13	111.39	122.59
1	A	1298	ARG	NE-CZ-NH1	-7.10	114.40	121.50
1	A	1227	ARG	O-C-N	6.89	126.93	121.55
1	A	1353	ASP	CA-CB-CG	6.83	119.43	112.60
1	A	1162	VAL	CA-C-N	6.82	132.94	122.24
1	A	1162	VAL	C-N-CA	6.82	132.94	122.24
1	A	1094	ARG	NE-CZ-NH2	6.64	125.18	119.20
1	A	1261	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	A	1189	ILE	N-CA-C	-6.46	105.41	111.48
1	A	1169	PHE	CA-C-N	6.42	131.78	122.85
1	A	1169	PHE	C-N-CA	6.42	131.78	122.85
1	A	1106	HIS	CB-CG-ND1	6.39	132.29	122.70
1	A	1268	SER	CA-C-O	6.37	127.31	120.55
1	A	1318	ARG	CD-NE-CZ	6.14	133.00	124.40
1	A	1315	GLY	CA-C-O	-6.13	113.78	120.40
1	A	1170[A]	ASP	O-C-N	-6.08	115.39	122.87
1	A	1170[B]	ASP	O-C-N	-6.08	115.39	122.87
1	A	1311	SER	CA-C-O	6.05	127.97	121.55
1	A	1035	ARG	CA-C-N	6.02	131.31	123.00
1	A	1035	ARG	C-N-CA	6.02	131.31	123.00
1	A	1004	GLN	O-C-N	-5.99	114.89	122.26
1	A	1227	ARG	CA-C-O	-5.95	114.75	120.64
1	A	1122	GLU	CB-CG-CD	5.94	122.69	112.60
1	A	1025	ARG	CD-NE-CZ	-5.85	116.21	124.40
1	A	1248	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	A	1004	GLN	CA-C-O	5.69	126.67	119.95
1	A	1307	LYS	CB-CG-CD	5.69	124.39	111.30
1	A	1315	GLY	O-C-N	5.59	128.17	122.24
1	A	1000	MET	CB-CG-SD	-5.48	96.27	112.70
1	A	1321	LYS	O-C-N	5.43	129.81	122.59
1	A	1227	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	A	1336	ALA	CA-C-N	5.40	125.97	119.98
1	A	1336	ALA	C-N-CA	5.40	125.97	119.98
1	A	1116	ARG	CD-NE-CZ	5.38	131.93	124.40
1	A	1280	HIS	CA-CB-CG	-5.37	108.43	113.80
1	A	1162	VAL	O-C-N	-5.35	116.62	122.83
1	A	1229	GLY	N-CA-C	5.30	122.43	114.95
1	A	1261	ARG	CG-CD-NE	5.30	123.67	112.00
1	A	1258	HIS	ND1-CG-CD2	-5.29	100.81	106.10
1	A	1086	HIS	CA-CB-CG	-5.26	108.53	113.80
1	A	1244	ASP	CA-CB-CG	5.22	117.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1081	LEU	CA-C-N	-5.14	117.00	120.24
1	A	1081	LEU	C-N-CA	-5.14	117.00	120.24
1	A	1253	GLN	CB-CG-CD	5.11	121.28	112.60
1	A	1054	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	1210	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	A	1223	TYR	CA-CB-CG	5.07	123.03	113.90
1	A	1128	ILE	CA-CB-CG1	5.06	119.00	110.40
1	A	1230	GLY	CA-C-O	5.03	124.84	119.06
1	A	1313	GLY	O-C-N	-5.01	118.14	122.90

There are no chirality outliers.

There are no planarity outliers.

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	2799	0	2776	28	0
2	A	53	0	31	4	0
3	A	6	0	6	5	0
4	A	2	0	0	8	0
5	A	6	0	6	0	0
6	A	612	0	0	10	0
All	All	3478	0	2819	36	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 (36) 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)
3:A:1364:DAL:CA	4:A:1365:PER:O2	2.09	1.00
3:A:1364:DAL:HA	4:A:1365:PER:O2	1.70	0.89
3:A:1364:DAL:C	4:A:1365:PER:O1	2.24	0.85
1:A:1033:LEU:HD11	1:A:1170[B]:ASP:OD2	1.86	0.76
2:A:1363:FAD:C10	4:A:1365:PER:O2	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:LEU:O	1:A:1322:GLU:HA	1.92	0.70
1:A:1321:LYS:O	1:A:1322:GLU:HB2	1.93	0.68
2:A:1363:FAD:N10	4:A:1365:PER:O1	2.27	0.68
1:A:1209:LYS:HE2	6:A:3246:HOH:O	1.99	0.61
1:A:1106:HIS:HD2	1:A:1115:TYR:OH	1.84	0.60
1:A:1031:HIS:HD2	1:A:1156:THR:OG1	1.85	0.59
3:A:1364:DAL:O	4:A:1365:PER:O2	2.10	0.56
1:A:1224:ILE:HG23	1:A:1232[B]:VAL:HG21	1.89	0.55
1:A:1031:HIS:HE1	1:A:1158:GLU:OE1	1.91	0.54
1:A:1091:LYS:HE2	6:A:3449:HOH:O	2.09	0.53
1:A:1248:ASN:C	1:A:1248:ASN:HD22	2.17	0.53
3:A:1364:DAL:N	4:A:1365:PER:O2	2.44	0.51
1:A:1136:SER:HB2	6:A:3002:HOH:O	2.10	0.51
1:A:1100:GLU:OE1	1:A:1106:HIS:HE1	1.93	0.50
1:A:1204:VAL:HB	1:A:1232[B]:VAL:HG13	1.94	0.50
1:A:1006:ARG:HD2	6:A:3425:HOH:O	2.12	0.49
1:A:1272:ILE:HG12	6:A:3231:HOH:O	2.13	0.48
1:A:1000:MET:HE1	6:A:3563:HOH:O	2.14	0.46
1:A:1160:ARG:NH1	1:A:1170[B]:ASP:OD2	2.50	0.45
1:A:1273:GLU:OE2	1:A:1273:GLU:N	2.47	0.45
1:A:1302:PRO:HG2	1:A:1320:ALA:HB3	1.98	0.45
1:A:1051:ALA:HA	2:A:1363:FAD:C5X	2.46	0.44
1:A:999:LEU:N	6:A:3576:HOH:O	2.50	0.44
1:A:1140:PRO:HG3	6:A:3180:HOH:O	2.16	0.44
1:A:1264:PRO:HG3	6:A:3322:HOH:O	2.17	0.44
1:A:1304:ASP:OD1	1:A:1304:ASP:N	2.49	0.43
2:A:1363:FAD:C6	4:A:1365:PER:O1	2.58	0.43
1:A:1076:LYS:HG3	6:A:3069:HOH:O	2.17	0.43
1:A:1034:ALA:O	1:A:1159:ARG:HA	2.19	0.42
1:A:1106:HIS:CD2	1:A:1115:TYR:OH	2.69	0.41
1:A:1337:GLY:O	1:A:1341:SER:HB3	2.22	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	365/363 (101%)	346 (95%)	14 (4%)	5 (1%)	9 1

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1319	ALA
1	A	1320	ALA
1	A	1318	ARG
1	A	1322	GLU
1	A	1321	LYS

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	299/295 (101%)	292 (98%)	7 (2%)	44 9

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	999	LEU
1	A	1046	PHE
1	A	1054	ASN
1	A	1094	ARG
1	A	1120	SER
1	A	1248	ASN
1	A	1318	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1031	HIS
1	A	1054	ASN

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Mol	Chain	Res	Type
1	A	1098	GLN
1	A	1106	HIS
1	A	1138	HIS
1	A	1167	GLN
1	A	1248	ASN

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](#)

4 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	1363	4	58,58,58	1.72	13 (22%)	85,89,89	1.50	13 (15%)
5	GOL	A	1366	-	5,5,5	2.50	1 (20%)	5,5,5	4.36	5 (100%)
3	DAL	A	1364	4	5,5,5	1.96	2 (40%)	6,6,6	1.88	1 (16%)
4	PER	A	1365	2,3	1,1,1	0.12	0	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	1363	4	-	0/34/50/50	0/6/6/6
5	GOL	A	1366	-	-	2/4/4/4	-
3	DAL	A	1364	4	-	2/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1363	FAD	C4X-N5	5.70	1.43	1.30
5	A	1366	GOL	O2-C2	-5.01	1.28	1.43
2	A	1363	FAD	C5A-C4A	-4.81	1.30	1.39
2	A	1363	FAD	C4A-N3A	3.75	1.41	1.34
2	A	1363	FAD	C5'-C4'	-3.15	1.47	1.51
2	A	1363	FAD	C2A-N3A	3.12	1.39	1.33
2	A	1363	FAD	C9A-N10	3.01	1.46	1.41
3	A	1364	DAL	CA-N	-2.99	1.38	1.48
2	A	1363	FAD	C8A-N9A	2.62	1.42	1.37
3	A	1364	DAL	CA-C	-2.54	1.51	1.54
2	A	1363	FAD	C2B-C3B	-2.49	1.46	1.53
2	A	1363	FAD	C9A-C5X	2.40	1.45	1.41
2	A	1363	FAD	C1'-N10	-2.35	1.42	1.47
2	A	1363	FAD	O4-C4	2.28	1.27	1.23
2	A	1363	FAD	C1'-C2'	-2.13	1.49	1.52
2	A	1363	FAD	C4X-C4	-2.07	1.36	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1366	GOL	O3-C3-C2	-6.00	83.36	110.38
5	A	1366	GOL	O2-C2-C1	-5.64	85.84	109.18
2	A	1363	FAD	C5A-C4A-N9A	5.30	111.59	105.81
2	A	1363	FAD	C4A-N9A-C8A	-5.08	100.40	105.74
2	A	1363	FAD	N3A-C4A-N9A	-4.95	118.75	127.17
5	A	1366	GOL	O2-C2-C3	-3.21	95.88	109.18
5	A	1366	GOL	C3-C2-C1	-3.14	100.27	111.80
3	A	1364	DAL	CB-CA-C	3.07	117.18	110.29
2	A	1363	FAD	C5X-C9A-N10	-2.95	115.30	117.97
5	A	1366	GOL	O1-C1-C2	-2.65	98.43	110.38
2	A	1363	FAD	C4X-C10-N10	2.64	120.25	116.48
2	A	1363	FAD	C1'-C2'-C3'	2.35	116.04	109.66
2	A	1363	FAD	O3'-C3'-C4'	-2.23	103.85	108.93
2	A	1363	FAD	C4-C4X-C10	2.22	120.74	116.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1363	FAD	O2B-C2B-C3B	2.22	118.92	111.82
2	A	1363	FAD	C6-C5X-C9A	-2.11	116.14	119.05
2	A	1363	FAD	O3'-C3'-C2'	2.11	113.72	108.93
2	A	1363	FAD	C5A-C4A-N3A	2.11	129.62	126.72
2	A	1363	FAD	N3A-C2A-N1A	-2.00	125.55	128.58

There are no chirality outliers.

All (4) torsion outliers are listed below:

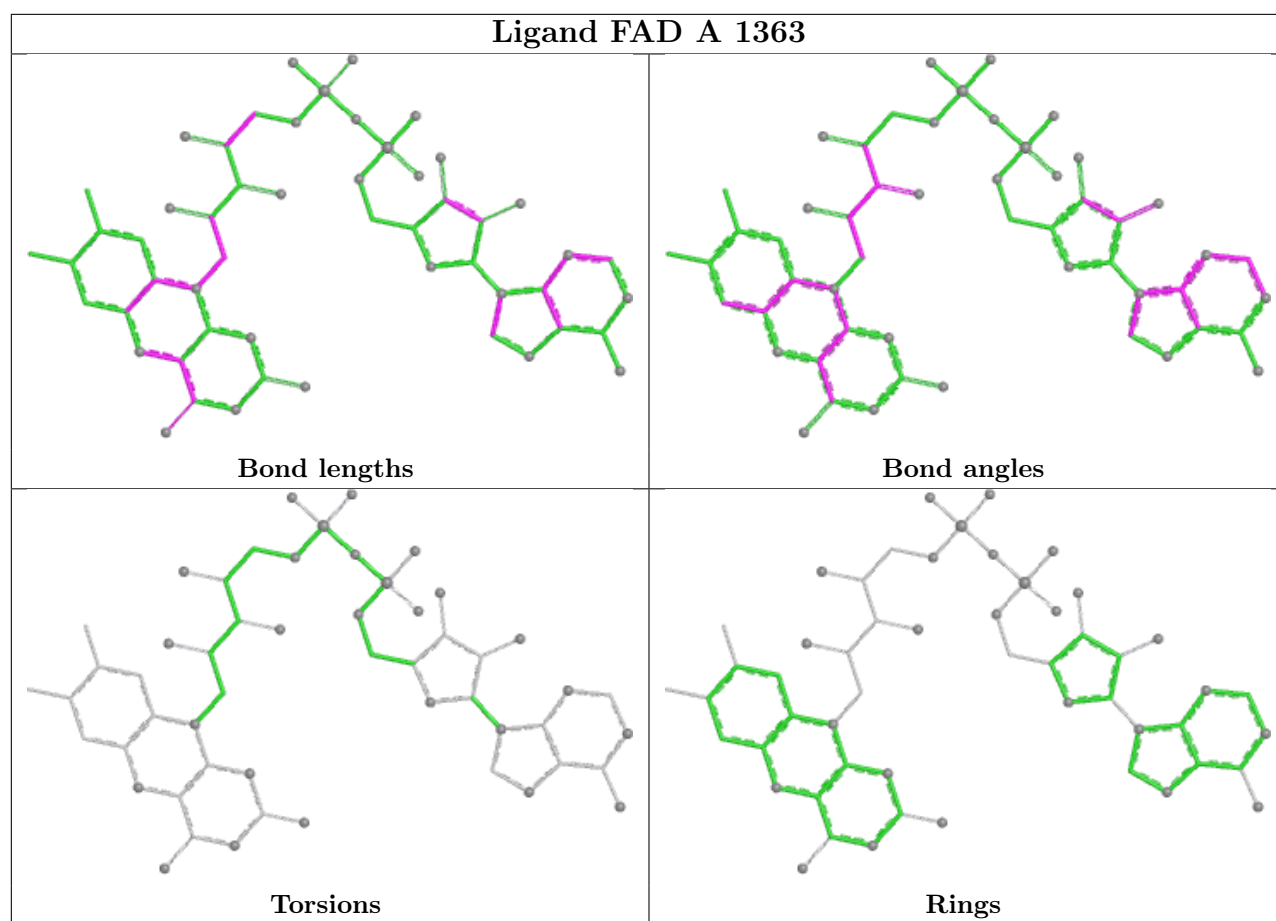
Mol	Chain	Res	Type	Atoms
3	A	1364	DAL	O-C-CA-CB
5	A	1366	GOL	O2-C2-C3-O3
3	A	1364	DAL	OXT-C-CA-CB
5	A	1366	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1363	FAD	4	0
3	A	1364	DAL	5	0
4	A	1365	PER	8	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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	363/363 (100%)	-0.08	16 (4%)	39 41	9, 14, 40, 128	4 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1317	ALA	6.3
1	A	1320	ALA	5.3
1	A	1361	GLY	5.0
1	A	1319	ALA	5.0
1	A	1318	ARG	4.5
1	A	1315	GLY	4.2
1	A	1321	LYS	3.9
1	A	1316	SER	3.6
1	A	999	LEU	3.4
1	A	1322	GLU	3.2
1	A	1268	SER	3.0
1	A	1170[A]	ASP	2.6
1	A	1171	GLY	2.5
1	A	1000	MET	2.3
1	A	1306	THR	2.2
1	A	1272	ILE	2.2

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](#)

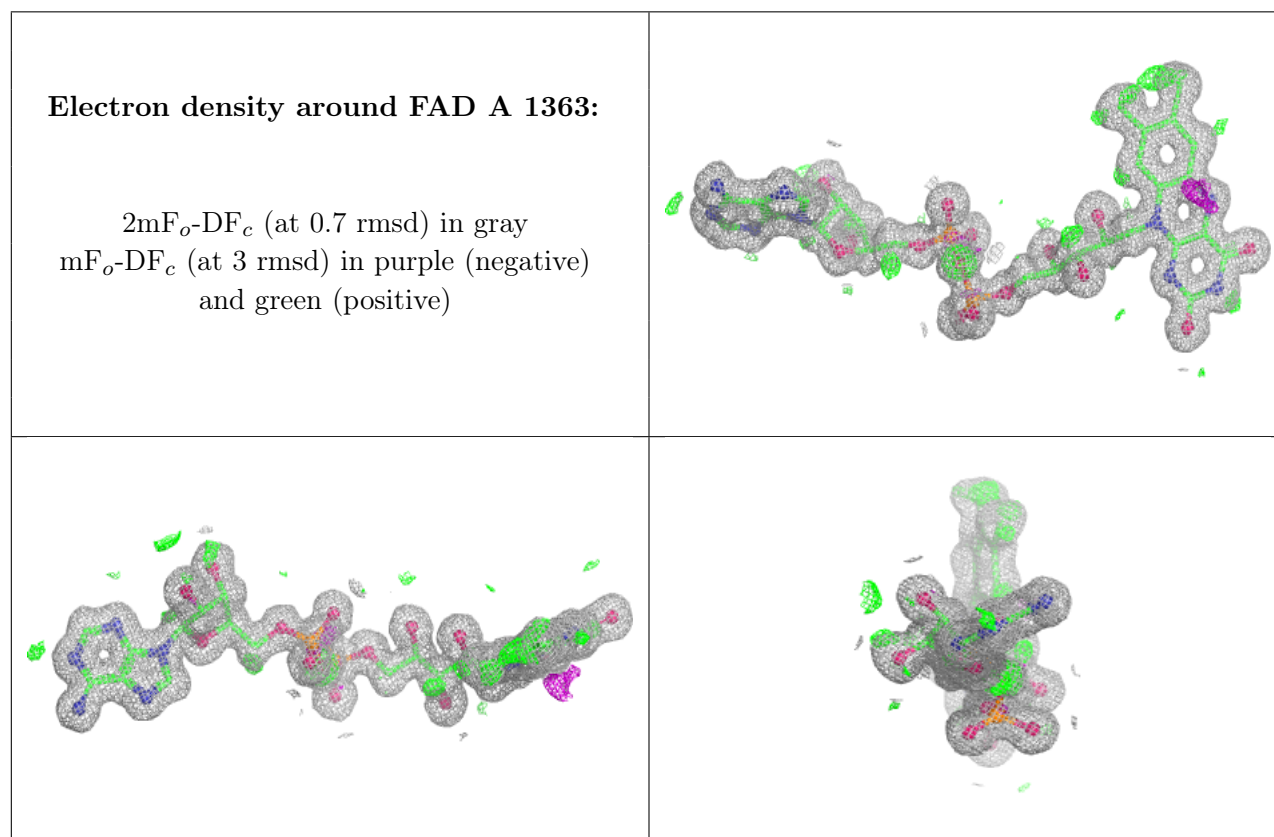
There are no oligosaccharides in this entry.

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
4	PER	A	1365	2/2	0.82	0.53	13,13,13,15	2
5	GOL	A	1366	6/6	0.92	0.14	18,33,37,42	0
3	DAL	A	1364	6/6	0.98	0.04	12,12,16,18	0
2	FAD	A	1363	53/53	0.99	0.04	8,10,12,15	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.