



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:10 PM UTC

PDB ID : 2VOU / pdb_00002vou
Title : Structure of 2,6-dihydroxypyridine-3-hydroxylase from *Arthrobacter nicotinovorans*
Authors : Treiber, N.; Schulz, G.E.
Deposited on : 2008-02-21
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 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

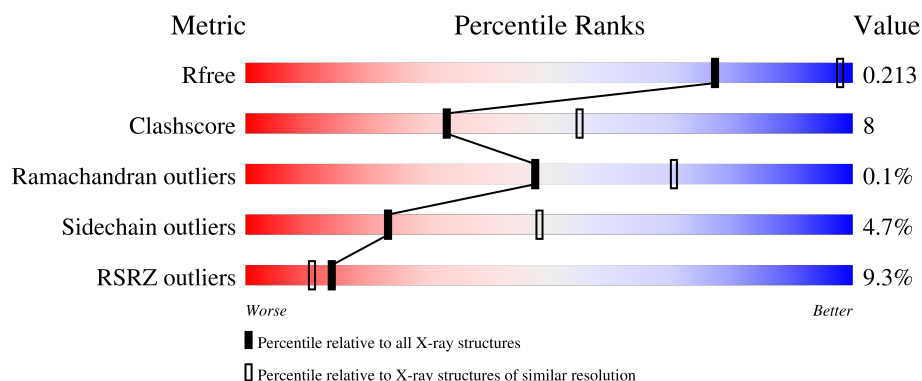
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	397	5% 82% 16% ..
1	B	397	18% 78% 18% ..
1	C	397	5% 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
4	ACT	A	1397	-	-	X	-
4	ACT	B	1391	-	-	X	-
4	ACT	C	1391	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9590 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.

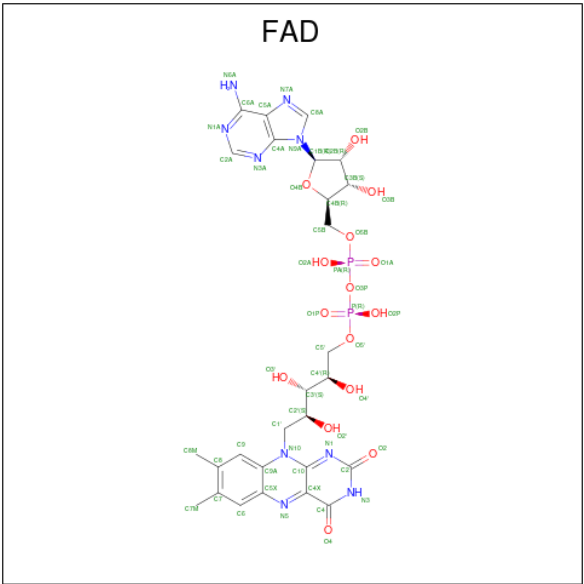
- Molecule 1 is a protein called 2,6-DIHYDROXYPYRIDINE HYDROXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			3034	1916	530	581	7			
1	B	387	Total	C	N	O	S	0	0	0
			2990	1889	524	570	7			
1	C	387	Total	C	N	O	S	0	0	0
			2990	1889	524	570	7			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	SER	CYS	engineered mutation	UNP Q93NG3
B	323	SER	CYS	engineered mutation	UNP Q93NG3
C	323	SER	CYS	engineered mutation	UNP Q93NG3

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



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

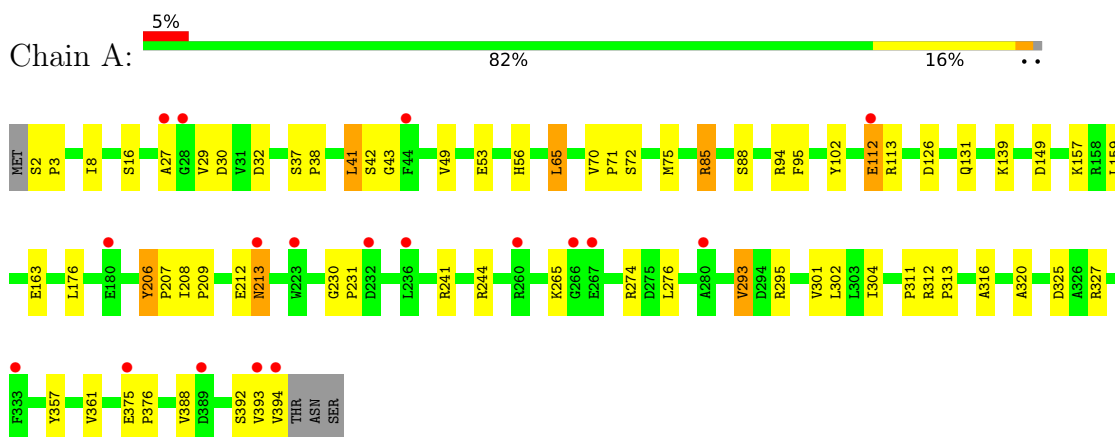
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	192	Total	O	0	0
			192	192		
5	B	127	Total	O	0	0
			127	127		
5	C	68	Total	O	0	0
			68	68		

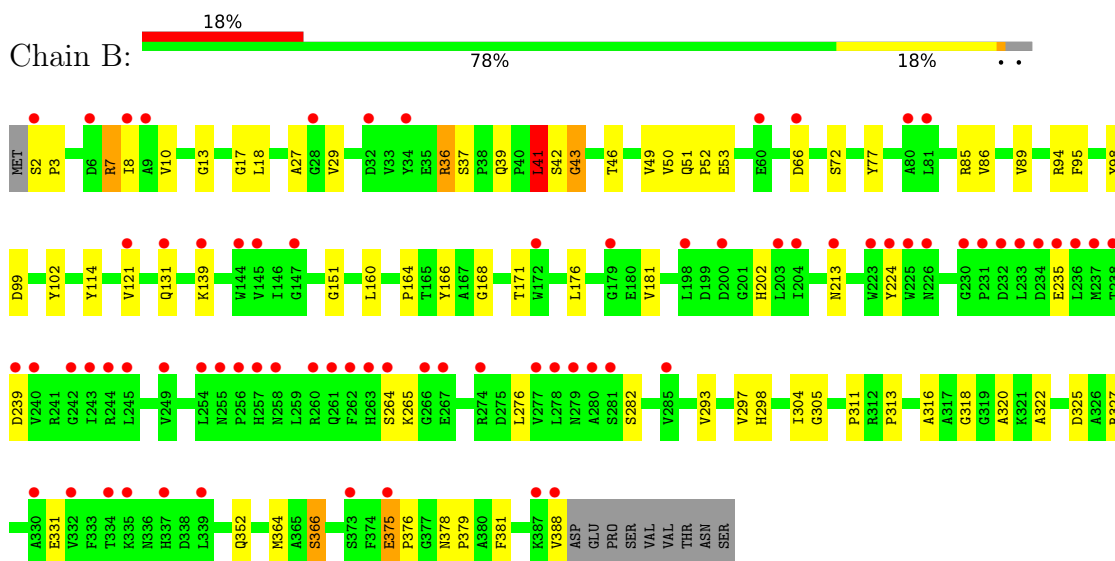
3 Residue-property plots [i](#)

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.

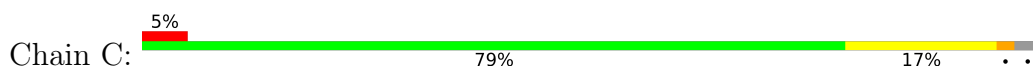
• Molecule 1: 2,6-DIHYDROXYPYRIDINE HYDROXYLASE

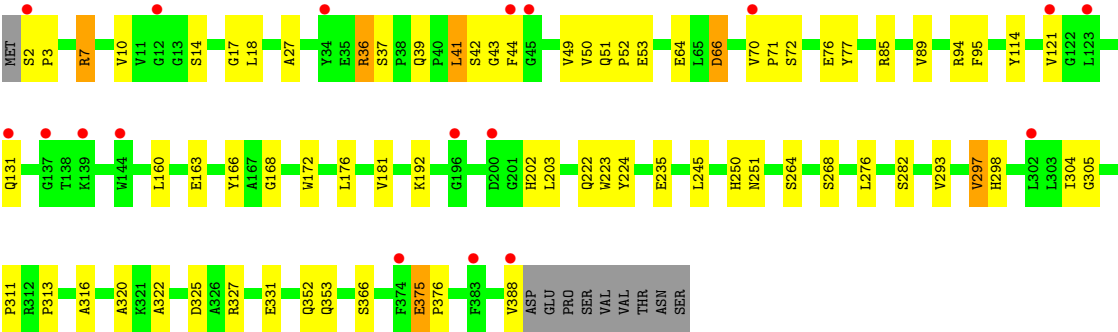


• Molecule 1: 2,6-DIHYDROXYPYRIDINE HYDROXYLASE



• Molecule 1: 2,6-DIHYDROXYPYRIDINE HYDROXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.96Å 185.96Å 104.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.92 – 2.60 27.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (27.92-2.60) 99.7 (27.92-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.185 , 0.222 0.178 , 0.213	Depositor DCC
R_{free} test set	3205 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9590	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% 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: ACT, FAD, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.92	0/3110	1.07	6/4235 (0.1%)
1	B	0.76	0/3065	0.94	6/4172 (0.1%)
1	C	0.65	0/3065	0.89	2/4172 (0.0%)
All	All	0.79	0/9240	0.97	14/12579 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	GLY	N-CA-C	-8.54	95.97	111.25
1	B	43	GLY	N-CA-C	-7.61	102.32	112.82
1	A	312	ARG	N-CA-C	-7.18	100.13	110.40
1	B	41	LEU	N-CA-C	6.88	119.41	110.53
1	C	43	GLY	N-CA-C	-6.82	103.41	112.82
1	A	41	LEU	N-CA-C	5.66	118.17	110.35
1	A	388	VAL	N-CA-C	-5.43	107.56	112.12
1	C	41	LEU	N-CA-C	5.26	117.66	110.55
1	B	282	SER	N-CA-C	5.25	118.87	110.73
1	A	206	TYR	N-CA-C	5.17	112.87	108.22
1	B	85	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	A	71	PRO	N-CA-C	5.08	118.34	111.22
1	B	43	GLY	CA-C-N	-5.03	115.09	122.83
1	B	43	GLY	C-N-CA	-5.03	115.09	122.83

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	3034	0	2938	39	0
1	B	2990	0	2898	49	0
1	C	2990	0	2898	48	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
2	C	53	0	31	1	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
4	A	4	0	3	8	0
4	B	4	0	3	7	0
4	C	4	0	3	3	0
5	A	192	0	0	8	0
5	B	127	0	0	7	0
5	C	68	0	0	7	0
All	All	9590	0	8860	141	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 (141) 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)
4:A:1397:ACT:H2	5:A:2159:HOH:O	1.55	1.03
1:A:42:SER:HB3	5:A:2013:HOH:O	1.69	0.91
1:C:7:ARG:HH11	1:C:7:ARG:HG3	1.36	0.90
1:B:7:ARG:HG3	1:B:7:ARG:HH11	1.34	0.89
4:A:1397:ACT:CH3	5:A:2159:HOH:O	2.20	0.85
1:B:375:GLU:HA	1:B:375:GLU:OE1	1.82	0.76
1:C:7:ARG:HH11	1:C:7:ARG:CG	1.99	0.76
1:B:7:ARG:HH11	1:B:7:ARG:CG	1.98	0.76
1:C:375:GLU:OE1	1:C:375:GLU:HA	1.87	0.75
1:B:36:ARG:HG3	1:B:37:SER:N	2.05	0.70
1:A:313:PRO:HA	4:A:1397:ACT:C	2.24	0.67
1:C:313:PRO:HA	4:C:1391:ACT:C	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:SER:N	5:C:2001:HOH:O	2.27	0.66
1:A:157:LYS:HE3	1:A:163:GLU:CD	2.21	0.66
4:B:1391:ACT:CH3	5:B:2109:HOH:O	2.46	0.64
2:A:1395:FAD:C1'	4:A:1397:ACT:H1	2.32	0.59
1:B:352:GLN:HE21	1:B:388:VAL:HG11	1.68	0.59
1:B:121:VAL:HG22	1:C:235:GLU:HG3	1.85	0.59
1:C:36:ARG:HG3	1:C:37:SER:N	2.16	0.58
1:C:18:LEU:HD21	1:C:114:TYR:HE1	1.68	0.58
1:C:50:VAL:HG11	1:C:94:ARG:HB2	1.85	0.58
1:C:352:GLN:HE21	1:C:388:VAL:HG11	1.68	0.58
2:A:1395:FAD:H1'1	4:A:1397:ACT:H1	1.86	0.57
1:C:192:LYS:NZ	5:C:2032:HOH:O	2.36	0.57
1:A:72:SER:HB3	1:A:95:PHE:HE2	1.69	0.57
1:A:72:SER:HB3	1:A:95:PHE:CE2	2.39	0.57
1:B:50:VAL:HG11	1:B:94:ARG:HB2	1.88	0.56
1:A:41:LEU:HB2	1:A:102:TYR:CZ	2.40	0.55
1:A:293:VAL:HG13	1:A:295:ARG:O	2.06	0.55
2:B:1389:FAD:C1'	4:B:1391:ACT:H1	2.37	0.55
1:B:50:VAL:HG12	1:B:94:ARG:O	2.09	0.53
1:C:327:ARG:CZ	1:C:327:ARG:HB2	2.38	0.53
1:B:18:LEU:HD21	1:B:114:TYR:HE1	1.74	0.53
1:A:393:VAL:HG21	1:C:298:HIS:C	2.34	0.52
1:A:3:PRO:HG3	1:A:27:ALA:O	2.09	0.52
1:C:353:GLN:HG3	5:C:2064:HOH:O	2.09	0.52
1:A:30:ASP:HA	5:A:2009:HOH:O	2.09	0.52
1:A:176:LEU:HD13	1:A:276:LEU:HD22	1.92	0.52
2:B:1389:FAD:H1'2	4:B:1391:ACT:H1	1.92	0.52
1:C:160:LEU:HD21	1:C:298:HIS:CE1	2.44	0.52
1:A:274:ARG:HD3	5:A:2138:HOH:O	2.11	0.51
1:C:176:LEU:HD13	1:C:276:LEU:HD22	1.92	0.51
1:C:49:VAL:HB	1:C:316:ALA:HB1	1.92	0.50
1:C:297:VAL:HG12	5:C:2059:HOH:O	2.10	0.50
1:A:112:GLU:HG2	1:A:113:ARG:HG3	1.92	0.50
1:B:72:SER:HB3	1:B:95:PHE:HE2	1.76	0.50
1:B:213:ASN:HA	5:B:2050:HOH:O	2.10	0.50
1:C:72:SER:HB3	1:C:95:PHE:HE2	1.77	0.50
1:C:10:VAL:HG11	1:C:17:GLY:HA2	1.93	0.49
1:B:327:ARG:CZ	1:B:327:ARG:HB2	2.40	0.49
1:A:357:TYR:OH	4:A:1397:ACT:O	2.30	0.49
1:B:49:VAL:HB	1:B:316:ALA:HB1	1.93	0.49
1:A:85:ARG:HE	1:A:85:ARG:HB3	1.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:VAL:CG1	1:C:94:ARG:HB2	2.43	0.48
1:A:376:PRO:HD2	1:B:366:SER:HB3	1.94	0.48
1:A:49:VAL:HB	1:A:316:ALA:HB1	1.96	0.48
1:B:265:LYS:HE2	5:B:2087:HOH:O	2.14	0.48
1:B:235:GLU:HG3	1:C:121:VAL:HG22	1.95	0.48
1:B:239:ASP:OD1	1:B:239:ASP:C	2.56	0.48
1:B:10:VAL:HG11	1:B:17:GLY:HA2	1.95	0.47
1:C:7:ARG:CG	1:C:7:ARG:NH1	2.68	0.47
1:B:160:LEU:HD21	1:B:298:HIS:CE1	2.49	0.47
1:C:7:ARG:HG3	1:C:7:ARG:NH1	2.17	0.47
1:A:149:ASP:OD1	1:A:149:ASP:N	2.47	0.47
1:A:126:ASP:C	1:A:126:ASP:OD1	2.58	0.46
1:C:51:GLN:HG2	5:C:2067:HOH:O	2.16	0.46
1:C:76:GLU:HG3	1:C:192:LYS:HD3	1.98	0.46
1:A:2:SER:HA	1:A:3:PRO:HD2	1.82	0.46
1:A:357:TYR:O	1:A:361:VAL:HG22	2.15	0.46
1:B:43:GLY:N	1:B:99:ASP:OD1	2.35	0.46
1:B:50:VAL:CG1	1:B:94:ARG:HB2	2.46	0.46
1:B:327:ARG:O	1:B:331:GLU:HG3	2.16	0.46
1:A:75:MET:HE1	5:A:2063:HOH:O	2.16	0.46
1:B:77:TYR:CZ	1:B:376:PRO:HA	2.50	0.45
1:C:311:PRO:HG2	4:C:1391:ACT:H3	1.97	0.45
1:B:313:PRO:HA	4:B:1391:ACT:C	2.46	0.45
1:B:2:SER:HA	5:B:2002:HOH:O	2.16	0.45
1:B:166:TYR:CE2	1:B:168:GLY:HA2	2.51	0.45
1:B:41:LEU:HB2	1:B:102:TYR:CZ	2.52	0.45
1:A:32:ASP:CG	1:A:113:ARG:HH21	2.25	0.45
1:B:318:GLY:H	4:B:1391:ACT:C	2.30	0.45
1:C:172:TRP:O	1:C:222:GLN:HA	2.17	0.44
1:B:3:PRO:HG3	1:B:27:ALA:O	2.17	0.44
1:C:245:LEU:HD11	5:C:2042:HOH:O	2.18	0.44
1:A:53:GLU:HB2	1:A:320:ALA:HB1	2.00	0.44
1:C:327:ARG:O	1:C:331:GLU:HG3	2.18	0.44
1:B:51:GLN:O	1:B:52:PRO:C	2.60	0.44
1:A:311:PRO:CG	4:A:1397:ACT:H3	2.48	0.44
1:B:176:LEU:HD13	1:B:276:LEU:HD22	1.99	0.44
1:B:8:ILE:HD12	1:B:29:VAL:HG11	2.01	0.43
1:B:18:LEU:HD21	1:B:114:TYR:CE1	2.52	0.43
1:C:18:LEU:HD21	1:C:114:TYR:CE1	2.52	0.43
1:C:70:VAL:HG22	1:C:71:PRO:HD2	2.00	0.43
1:B:98:TYR:C	1:B:98:TYR:CD2	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ASP:OD1	1:C:66:ASP:N	2.49	0.43
1:A:304:ILE:HB	1:A:325:ASP:HB3	2.00	0.43
1:B:151:GLY:O	1:B:164:PRO:HG3	2.19	0.43
1:C:3:PRO:HG3	1:C:27:ALA:O	2.19	0.43
1:C:202:HIS:CE1	1:C:224:TYR:CD2	3.07	0.43
1:B:13:GLY:C	1:B:18:LEU:HD23	2.44	0.43
1:A:8:ILE:HD12	1:A:29:VAL:HG11	2.01	0.43
1:A:241:ARG:NH1	5:A:2118:HOH:O	2.40	0.43
1:A:208:ILE:HB	1:A:209:PRO:CD	2.49	0.42
1:B:311:PRO:HG2	4:B:1391:ACT:H3	2.00	0.42
1:C:14:SER:HB3	2:C:1389:FAD:O5B	2.19	0.42
1:C:166:TYR:CE2	1:C:168:GLY:HA2	2.55	0.42
1:A:56:HIS:HB3	1:A:327:ARG:NH2	2.35	0.42
4:B:1391:ACT:H2	5:B:2109:HOH:O	2.18	0.42
1:A:37:SER:HA	1:A:38:PRO:HD3	1.93	0.42
1:C:251:ASN:ND2	1:C:282:SER:HA	2.34	0.42
1:C:311:PRO:HG2	4:C:1391:ACT:CH3	2.50	0.42
1:C:53:GLU:HB2	1:C:320:ALA:HB1	2.02	0.42
1:B:378:ASN:HA	1:B:379:PRO:HD2	1.92	0.41
1:A:230:GLY:O	1:A:231:PRO:C	2.62	0.41
1:A:265:LYS:NZ	5:A:2135:HOH:O	2.45	0.41
1:B:364:MET:HG2	1:B:381:PHE:CD1	2.55	0.41
1:A:159:LEU:HD11	1:A:301:VAL:HG11	2.02	0.41
1:B:7:ARG:CG	1:B:7:ARG:NH1	2.68	0.41
1:A:131:GLN:HB3	1:A:139:LYS:NZ	2.35	0.41
1:B:53:GLU:HB2	1:B:320:ALA:HB1	2.01	0.41
1:B:304:ILE:HB	1:B:325:ASP:HB3	2.02	0.41
1:B:305:GLY:HA2	1:B:322:ALA:HA	2.03	0.41
1:C:305:GLY:HA2	1:C:322:ALA:HA	2.02	0.41
1:A:65:LEU:HD13	1:A:94:ARG:HD2	2.01	0.41
1:B:375:GLU:OE1	1:B:375:GLU:CA	2.62	0.41
1:C:304:ILE:HB	1:C:325:ASP:HB3	2.03	0.41
5:B:2077:HOH:O	1:C:121:VAL:HG21	2.19	0.41
1:A:206:TYR:HB2	1:A:207:PRO:HD2	2.02	0.41
2:A:1395:FAD:C10	4:A:1397:ACT:OXT	2.69	0.41
1:B:7:ARG:HG3	1:B:7:ARG:NH1	2.16	0.41
1:B:171:THR:HB	1:B:224:TYR:CD1	2.56	0.41
1:C:51:GLN:O	1:C:52:PRO:C	2.64	0.41
1:A:56:HIS:HB3	1:A:327:ARG:CZ	2.51	0.40
1:A:212:GLU:O	1:A:213:ASN:C	2.64	0.40
1:B:202:HIS:CE1	1:B:224:TYR:CD2	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:PHE:CD2	1:C:250:HIS:CD2	3.09	0.40
1:B:10:VAL:HG11	1:B:17:GLY:CA	2.51	0.40
1:B:46:THR:HB	5:B:2040:HOH:O	2.21	0.40
1:C:77:TYR:CZ	1:C:376:PRO:HA	2.57	0.40
1:C:163:GLU:HG3	5:C:2026:HOH:O	2.21	0.40
1:C:203:LEU:HG	1:C:223:TRP:CD1	2.56	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	391/397 (98%)	371 (95%)	19 (5%)	1 (0%)	36	58
1	B	385/397 (97%)	368 (96%)	17 (4%)	0	100	100
1	C	385/397 (97%)	365 (95%)	20 (5%)	0	100	100
All	All	1161/1191 (98%)	1104 (95%)	56 (5%)	1 (0%)	48	70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	213	ASN

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	324/328 (99%)	312 (96%)	12 (4%)	30	57
1	B	318/328 (97%)	302 (95%)	16 (5%)	22	46
1	C	318/328 (97%)	301 (95%)	17 (5%)	20	43
All	All	960/984 (98%)	915 (95%)	45 (5%)	23	48

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	SER
1	A	65	LEU
1	A	70	VAL
1	A	85	ARG
1	A	88	SER
1	A	112	GLU
1	A	244	ARG
1	A	293	VAL
1	A	302	LEU
1	A	375	GLU
1	A	392	SER
1	A	394	VAL
1	B	7	ARG
1	B	36	ARG
1	B	39	GLN
1	B	41	LEU
1	B	42	SER
1	B	66	ASP
1	B	86	VAL
1	B	89	VAL
1	B	131	GLN
1	B	139	LYS
1	B	181	VAL
1	B	264	SER
1	B	293	VAL
1	B	297	VAL
1	B	366	SER
1	B	375	GLU
1	C	7	ARG
1	C	36	ARG
1	C	39	GLN
1	C	41	LEU
1	C	42	SER
1	C	64	GLU

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Mol	Chain	Res	Type
1	C	66	ASP
1	C	85	ARG
1	C	89	VAL
1	C	131	GLN
1	C	181	VAL
1	C	264	SER
1	C	268	SER
1	C	293	VAL
1	C	297	VAL
1	C	366	SER
1	C	375	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	258	ASN
1	A	261	GLN
1	A	370	HIS
1	B	131	GLN
1	B	213	ASN
1	B	257	HIS
1	B	261	GLN
1	B	352	GLN
1	B	370	HIS
1	C	250	HIS
1	C	251	ASN
1	C	261	GLN
1	C	352	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	1395	-	58,58,58	1.11	5 (8%)	85,89,89	1.83	19 (22%)
2	FAD	B	1389	-	58,58,58	1.09	5 (8%)	85,89,89	1.54	15 (17%)
2	FAD	C	1389	-	58,58,58	1.12	5 (8%)	85,89,89	1.57	19 (22%)
4	ACT	A	1397	-	3,3,3	1.18	0	3,3,3	0.85	0
3	GOL	B	1390	-	5,5,5	0.44	0	5,5,5	0.28	0
4	ACT	B	1391	-	3,3,3	0.92	0	3,3,3	1.26	0
3	GOL	C	1390	-	5,5,5	0.34	0	5,5,5	0.37	0
3	GOL	A	1396	-	5,5,5	0.43	0	5,5,5	0.45	0
4	ACT	C	1391	-	3,3,3	0.92	0	3,3,3	1.31	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	1395	-	-	0/34/50/50	0/6/6/6
2	FAD	B	1389	-	-	0/34/50/50	0/6/6/6
2	FAD	C	1389	-	-	2/34/50/50	0/6/6/6
3	GOL	B	1390	-	-	0/4/4/4	-
3	GOL	C	1390	-	-	0/4/4/4	-
3	GOL	A	1396	-	-	2/4/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1389	FAD	C4X-N5	3.75	1.38	1.30
2	A	1395	FAD	C4X-N5	3.57	1.38	1.30
2	C	1389	FAD	C4X-N5	3.53	1.38	1.30
2	C	1389	FAD	C2A-N1A	3.26	1.39	1.33
2	C	1389	FAD	C2A-N3A	2.85	1.39	1.33
2	B	1389	FAD	C2A-N3A	2.83	1.39	1.33
2	B	1389	FAD	C2A-N1A	2.70	1.38	1.33
2	C	1389	FAD	C10-N1	2.70	1.38	1.33
2	A	1395	FAD	C2A-N1A	2.58	1.38	1.33
2	C	1389	FAD	C8A-N7A	2.46	1.36	1.31
2	B	1389	FAD	C8A-N7A	2.38	1.36	1.31
2	A	1395	FAD	C8A-N7A	2.34	1.36	1.31
2	A	1395	FAD	O4B-C4B	-2.21	1.40	1.45
2	B	1389	FAD	C10-N1	2.18	1.37	1.33
2	A	1395	FAD	O2'-C2'	-2.16	1.38	1.43

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1395	FAD	N3A-C2A-N1A	-6.07	119.39	128.58
2	B	1389	FAD	N3A-C2A-N1A	-5.83	119.76	128.58
2	C	1389	FAD	N3A-C2A-N1A	-5.56	120.16	128.58
2	A	1395	FAD	C5A-C4A-N3A	-5.07	119.74	126.72
2	A	1395	FAD	N9A-C8A-N7A	-4.52	107.53	113.94
2	B	1389	FAD	C5A-C4A-N3A	-4.36	120.72	126.72
2	C	1389	FAD	N9A-C8A-N7A	-4.09	108.13	113.94
2	C	1389	FAD	C5A-C4A-N3A	-3.98	121.23	126.72
2	A	1395	FAD	C2A-N3A-C4A	3.89	121.34	111.83
2	A	1395	FAD	C5A-N7A-C8A	3.67	109.22	103.45
2	B	1389	FAD	C2A-N3A-C4A	3.52	120.42	111.83
2	B	1389	FAD	N9A-C8A-N7A	-3.51	108.95	113.94
2	C	1389	FAD	C5A-N7A-C8A	3.49	108.93	103.45
2	A	1395	FAD	N3A-C4A-N9A	3.46	133.05	127.17
2	A	1395	FAD	C4-C4X-N5	3.46	122.99	118.21
2	A	1395	FAD	C9A-C5X-N5	-3.38	118.87	122.45
2	A	1395	FAD	C4-N3-C2	-3.35	119.69	125.64
2	C	1389	FAD	C4-N3-C2	-3.17	120.00	125.64
2	B	1389	FAD	C5X-C9A-N10	2.98	120.66	117.97
2	C	1389	FAD	C2A-N3A-C4A	2.97	119.08	111.83
2	A	1395	FAD	C4X-C4-N3	2.93	120.72	113.25
2	B	1389	FAD	C5A-N7A-C8A	2.89	107.98	103.45
2	B	1389	FAD	C4-N3-C2	-2.80	120.67	125.64
2	A	1395	FAD	C4X-C10-N10	2.78	120.47	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1389	FAD	N3A-C4A-N9A	2.75	131.85	127.17
2	B	1389	FAD	C4X-C10-N10	2.73	120.39	116.48
2	A	1395	FAD	C10-C4X-N5	-2.66	119.38	124.81
2	B	1389	FAD	C4X-C4-N3	2.62	119.93	113.25
2	C	1389	FAD	C4A-C5A-N7A	-2.61	107.60	110.58
2	C	1389	FAD	C10-C4X-N5	-2.53	119.64	124.81
2	A	1395	FAD	O3P-PA-O1A	-2.53	103.09	110.70
2	C	1389	FAD	N3A-C4A-N9A	2.52	131.45	127.17
2	A	1395	FAD	C4A-C5A-N7A	-2.50	107.72	110.58
2	C	1389	FAD	O3B-C3B-C4B	-2.49	103.93	111.08
2	A	1395	FAD	O3B-C3B-C4B	-2.49	103.94	111.08
2	C	1389	FAD	C4X-C4-N3	2.48	119.58	113.25
2	A	1395	FAD	C4A-N9A-C8A	2.44	108.30	105.74
2	C	1389	FAD	C4X-C10-N10	2.44	119.97	116.48
2	C	1389	FAD	C9A-C5X-N5	-2.41	119.89	122.45
2	C	1389	FAD	O4-C4-C4X	-2.31	120.43	126.53
2	C	1389	FAD	C4X-C10-N1	-2.30	118.95	124.59
2	B	1389	FAD	C4A-C5A-N7A	-2.28	107.98	110.58
2	A	1395	FAD	O2A-PA-O3P	2.23	113.29	107.27
2	C	1389	FAD	C6A-C5A-C4A	2.21	120.19	117.18
2	C	1389	FAD	C4A-N9A-C8A	2.18	108.02	105.74
2	C	1389	FAD	C4-C4X-C10	2.14	120.60	116.93
2	B	1389	FAD	O4-C4-C4X	-2.12	120.94	126.53
2	A	1395	FAD	C4'-C3'-C2'	-2.07	110.13	113.57
2	B	1389	FAD	C9-C9A-N10	-2.05	119.10	121.85
2	C	1389	FAD	C4'-C3'-C2'	-2.04	110.17	113.57
2	B	1389	FAD	C10-C4X-N5	-2.03	120.66	124.81
2	A	1395	FAD	C10-N1-C2	2.03	121.25	116.85
2	B	1389	FAD	C4X-C10-N1	-2.02	119.64	124.59

There are no chirality outliers.

All (4) torsion outliers are listed below:

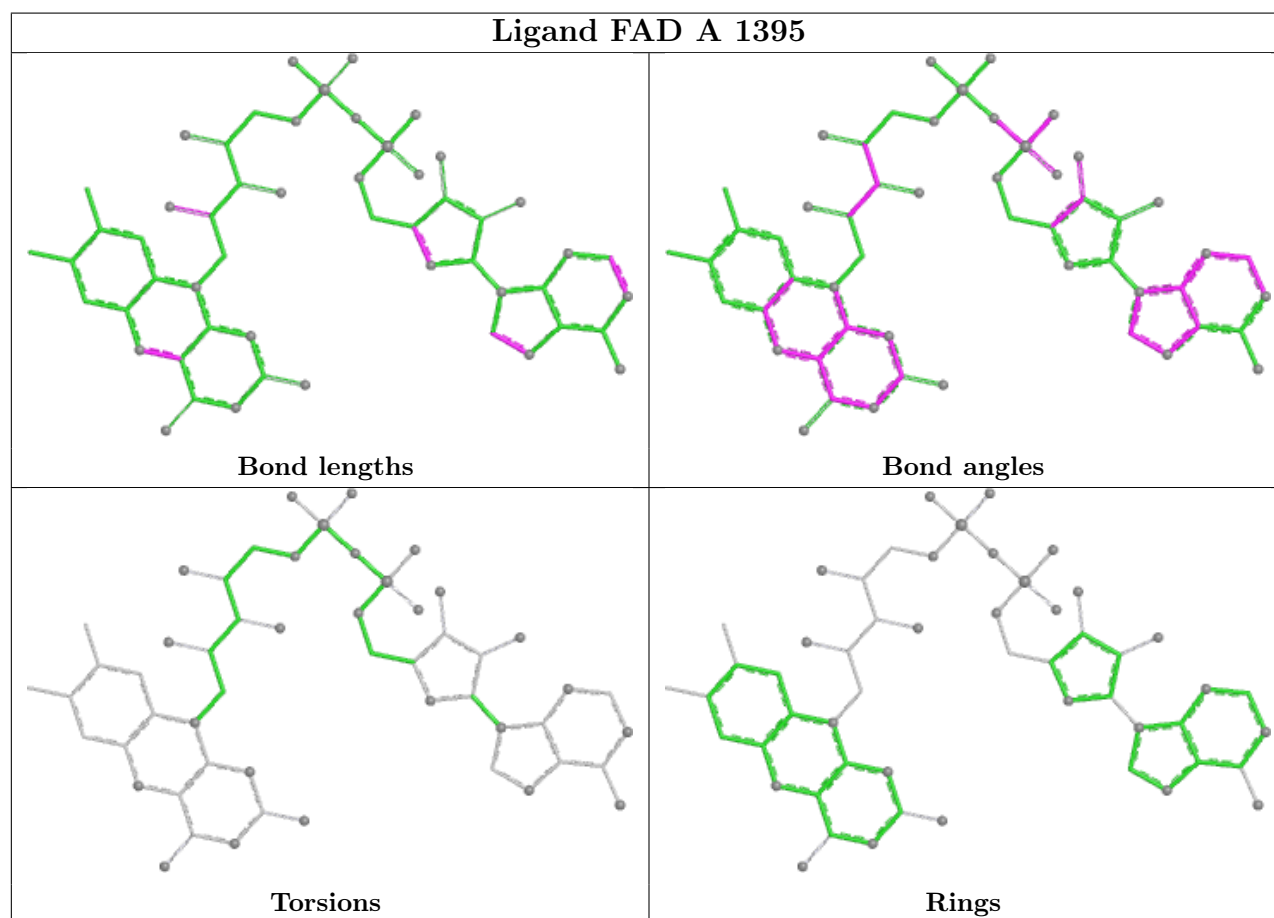
Mol	Chain	Res	Type	Atoms
3	A	1396	GOL	C1-C2-C3-O3
2	C	1389	FAD	C3B-C4B-C5B-O5B
2	C	1389	FAD	O4B-C4B-C5B-O5B
3	A	1396	GOL	O2-C2-C3-O3

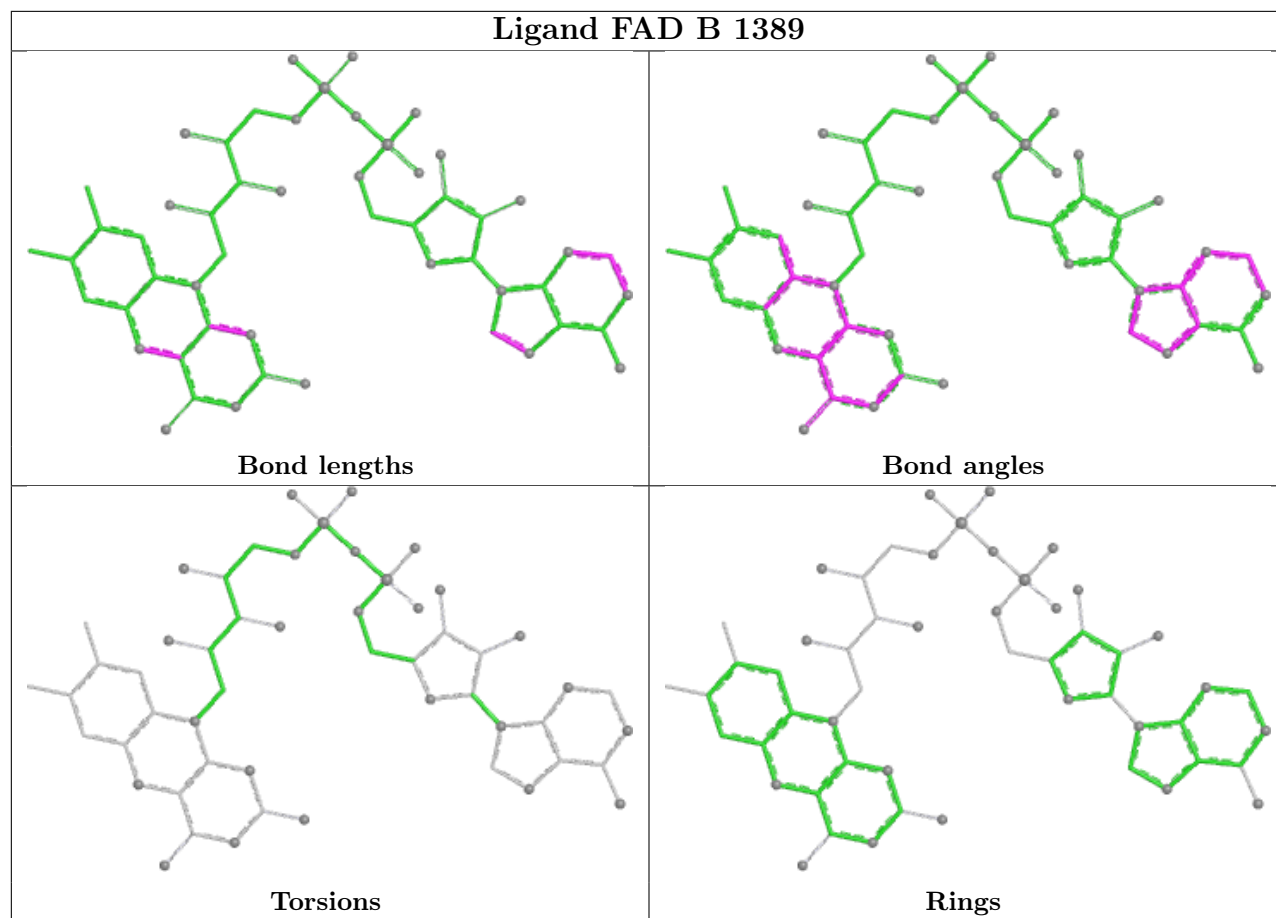
There are no ring outliers.

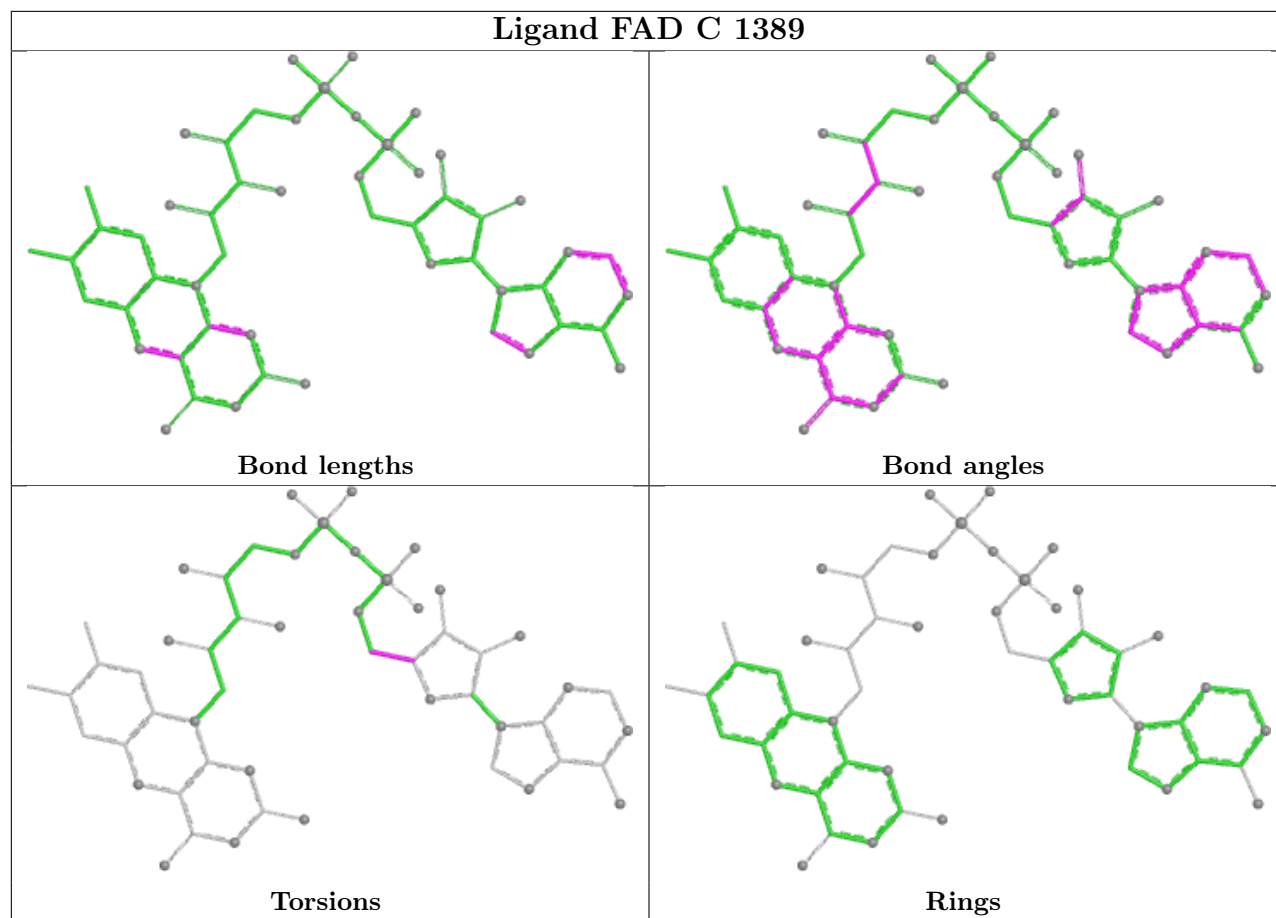
6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1395	FAD	3	0
2	B	1389	FAD	2	0
2	C	1389	FAD	1	0
4	A	1397	ACT	8	0
4	B	1391	ACT	7	0
4	C	1391	ACT	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	393/397 (98%)	0.74	18 (4%) 37 32	58, 66, 80, 99	0
1	B	387/397 (97%)	1.23	73 (18%) 3 2	64, 66, 70, 76	0
1	C	387/397 (97%)	0.69	18 (4%) 36 30	64, 66, 70, 76	0
All	All	1167/1191 (97%)	0.89	109 (9%) 14 11	58, 66, 73, 99	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	VAL	4.3
1	B	388	VAL	4.3
1	B	231	PRO	4.2
1	B	235	GLU	3.7
1	B	213	ASN	3.7
1	B	223	TRP	3.5
1	B	278	LEU	3.4
1	C	374	PHE	3.4
1	B	121	VAL	3.3
1	B	257	HIS	3.3
1	B	240	VAL	3.3
1	B	172	TRP	3.3
1	B	334	THR	3.3
1	B	238	THR	3.3
1	B	198	LEU	3.1
1	B	32	ASP	3.1
1	B	9	ALA	3.1
1	B	255	ASN	3.0
1	B	144	TRP	3.0
1	B	243	ILE	3.0
1	B	387	LYS	2.9
1	B	233	LEU	2.9
1	C	139	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	232	ASP	2.8
1	B	330	ALA	2.8
1	B	262	PHE	2.8
1	B	200	ASP	2.8
1	B	224	TYR	2.8
1	B	264	SER	2.7
1	B	179	GLY	2.7
1	B	242	GLY	2.7
1	B	263	HIS	2.7
1	B	80	ALA	2.7
1	C	388	VAL	2.7
1	B	260	ARG	2.7
1	B	254	LEU	2.7
1	C	44	PHE	2.7
1	B	258	ASN	2.6
1	B	335	LYS	2.6
1	B	337	HIS	2.6
1	C	12	GLY	2.6
1	B	225	TRP	2.6
1	B	236	LEU	2.6
1	C	123	LEU	2.6
1	C	302	LEU	2.6
1	B	279	ASN	2.5
1	A	393	VAL	2.5
1	B	145	VAL	2.5
1	B	277	VAL	2.5
1	B	8	ILE	2.5
1	C	45	GLY	2.5
1	B	131	GLN	2.5
1	B	281	SER	2.4
1	C	144	TRP	2.4
1	C	200	ASP	2.4
1	B	244	ARG	2.4
1	A	389	ASP	2.3
1	B	2	SER	2.3
1	C	137	GLY	2.3
1	B	204	ILE	2.3
1	C	34	TYR	2.3
1	C	121	VAL	2.3
1	B	203	LEU	2.3
1	B	339	LEU	2.3
1	C	383	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	213	ASN	2.3
1	B	66	ASP	2.3
1	B	256	PRO	2.3
1	B	261	GLN	2.3
1	A	44	PHE	2.3
1	B	230	GLY	2.3
1	B	81	LEU	2.3
1	A	27	ALA	2.2
1	A	260	ARG	2.2
1	B	239	ASP	2.2
1	C	2	SER	2.2
1	B	332	VAL	2.2
1	C	70	VAL	2.2
1	A	280	ALA	2.2
1	B	375	GLU	2.2
1	B	245	LEU	2.2
1	A	236	LEU	2.2
1	B	373	SER	2.2
1	C	131	GLN	2.2
1	A	232	ASP	2.2
1	A	375	GLU	2.1
1	B	274	ARG	2.1
1	B	28	GLY	2.1
1	C	196	GLY	2.1
1	B	285	VAL	2.1
1	B	280	ALA	2.1
1	A	112	GLU	2.1
1	B	60	GLU	2.1
1	B	237	MET	2.1
1	A	28	GLY	2.1
1	A	180	GLU	2.1
1	B	249	VAL	2.1
1	B	6	ASP	2.1
1	B	267	GLU	2.1
1	B	226	ASN	2.1
1	B	266	GLY	2.1
1	A	333	PHE	2.1
1	A	267	GLU	2.0
1	A	223	TRP	2.0
1	A	266	GLY	2.0
1	B	147	GLY	2.0
1	B	34	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	234	ASP	2.0
1	B	139	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

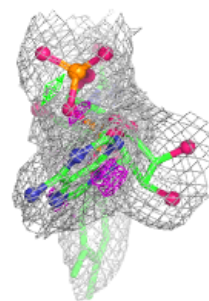
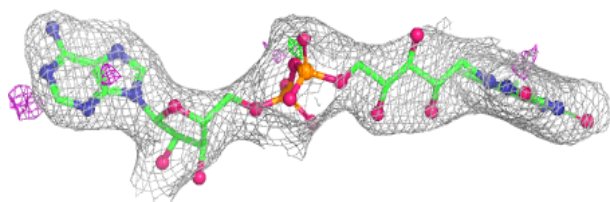
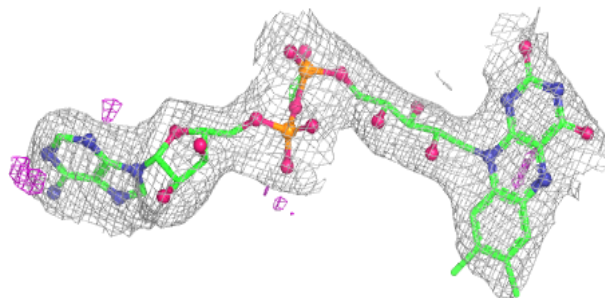
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACT	C	1391	4/4	0.81	0.22	128,129,129,129	0
4	ACT	B	1391	4/4	0.86	0.23	94,94,94,95	0
4	ACT	A	1397	4/4	0.86	0.38	59,60,61,62	0
2	FAD	C	1389	53/53	0.93	0.11	57,68,76,77	0
3	GOL	C	1390	6/6	0.94	0.16	93,95,95,96	0
3	GOL	A	1396	6/6	0.95	0.21	50,60,62,63	0
2	FAD	B	1389	53/53	0.96	0.09	61,70,73,75	0
2	FAD	A	1395	53/53	0.97	0.08	60,66,72,73	0
3	GOL	B	1390	6/6	0.97	0.15	74,77,78,80	0

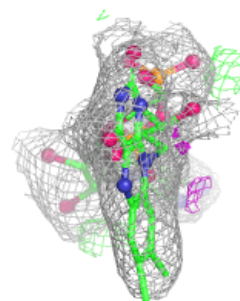
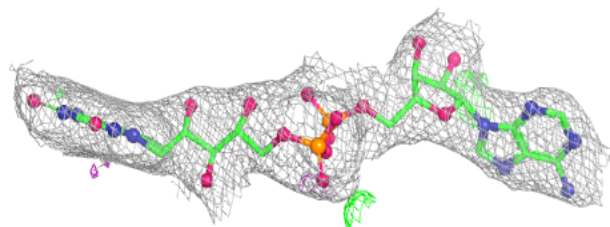
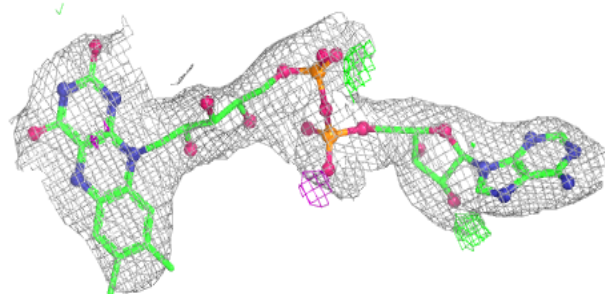
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

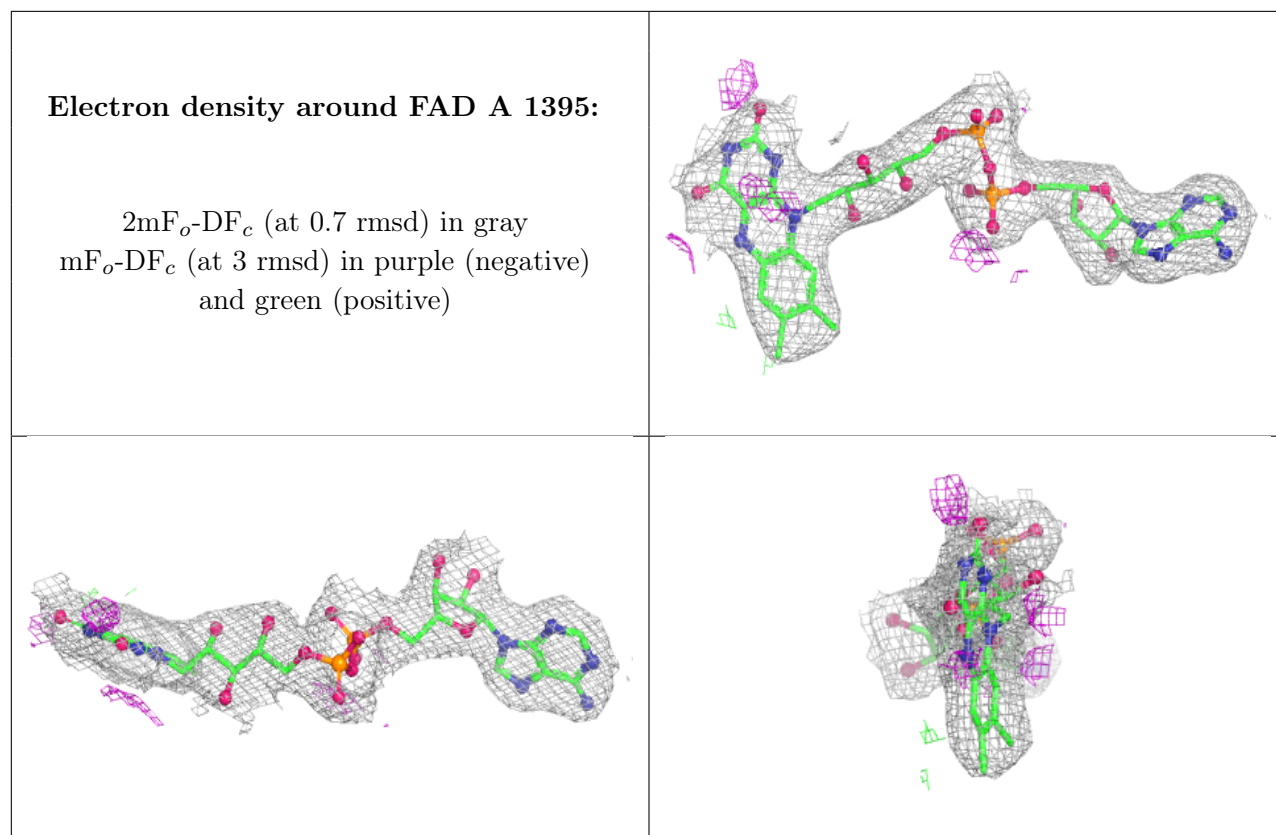
Electron density around FAD C 1389:

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

**Electron density around FAD B 1389:**

$2mF_o-DF_c$ (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.