



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 11:45 PM UTC

PDB ID : 2QA1 / pdb_00002qa1
Title : Crystal structure of PgaE, an aromatic hydroxylase involved in angucycline biosynthesis
Authors : Koskiniemi, H.; Dobritzsch, D.; Metsa-Ketela, M.; Kallio, P.; Niemi, J.; Schneider, G.
Deposited on : 2007-06-14
Resolution : 1.80 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)
Xtrriage (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

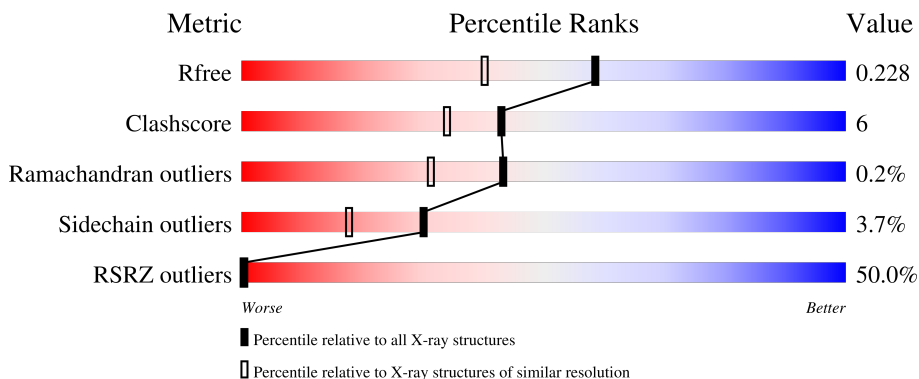
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	500	

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	EDO	A	603	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4166 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 Polyketide oxygenase PgaE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	488	3718	2328	673	699	18	0	10	0

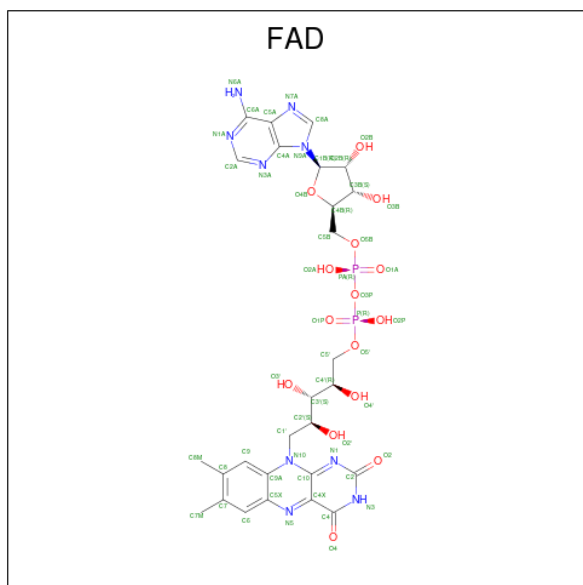
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ALA	-	expression tag	UNP Q93LY7
A	-7	HIS	-	expression tag	UNP Q93LY7
A	-6	HIS	-	expression tag	UNP Q93LY7
A	-5	HIS	-	expression tag	UNP Q93LY7
A	-4	HIS	-	expression tag	UNP Q93LY7
A	-3	HIS	-	expression tag	UNP Q93LY7
A	-2	HIS	-	expression tag	UNP Q93LY7
A	-1	HIS	-	expression tag	UNP Q93LY7
A	0	ARG	-	expression tag	UNP Q93LY7
A	1	SER	-	expression tag	UNP Q93LY7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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



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

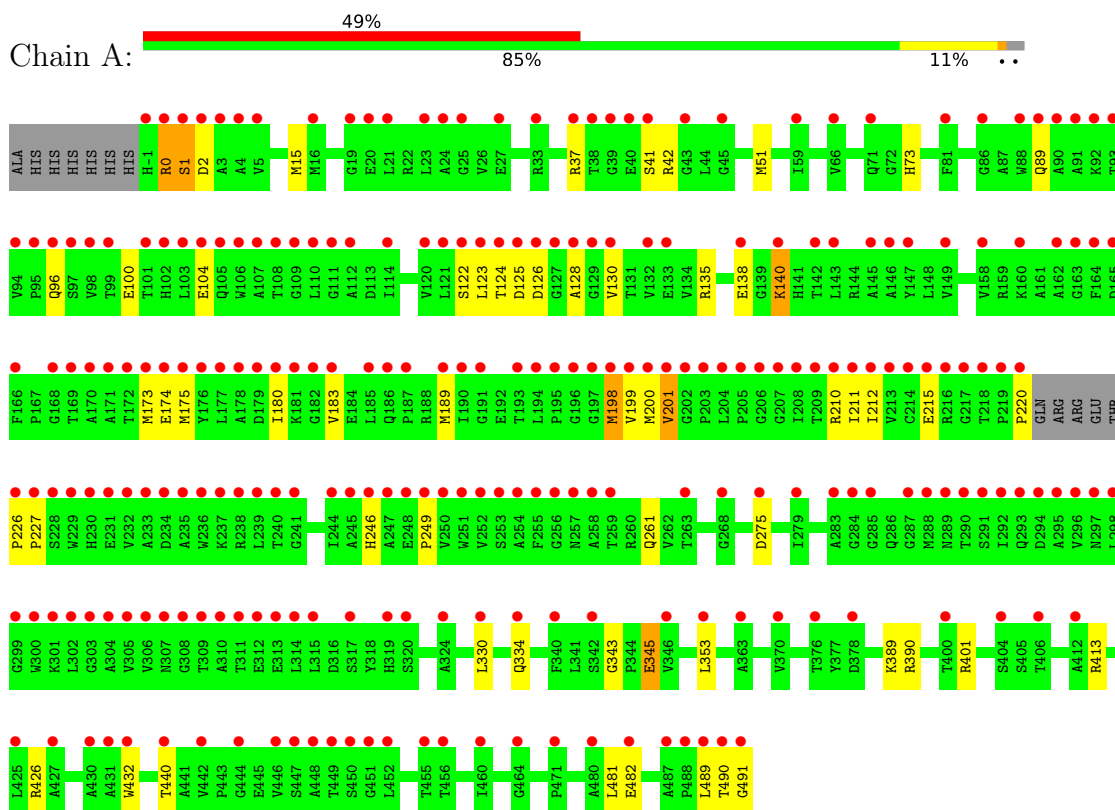
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	358	Total O 358 358	0	0

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: Polyketide oxygenase PgaE



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	66.23Å 171.53Å 212.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.96 – 1.80 36.96 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.96-1.80) 99.3 (36.96-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.195 , 0.224 0.198 , 0.228	Depositor DCC
R_{free} test set	2801 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtrriage
Anisotropy	0.454	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4166	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

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	0.62	0/3814	0.80	1/5180 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	0	ARG	N-CA-C	7.45	121.03	110.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	ARG	Peptide

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	3718	0	3714	45	0
2	A	1	0	0	0	0
3	A	53	0	31	2	0
4	A	12	0	18	6	0
5	A	24	0	32	4	0
6	A	358	0	0	6	0
All	All	4166	0	3795	47	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 6.

All (47) 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:275:ASP:OD2	5:A:608:GOL:H32	1.64	0.98
1:A:51[B]:MET:SD	1:A:89:GLN:O	2.34	0.86
1:A:490:THR:HA	6:A:960:HOH:O	1.81	0.80
1:A:200:MET:HB2	1:A:212:ILE:HB	1.72	0.70
1:A:15:MET:HA	1:A:15:MET:HE2	1.78	0.65
1:A:126:ASP:O	1:A:128:ALA:N	2.30	0.65
1:A:401:ARG:NH1	4:A:603:EDO:H22	2.12	0.63
1:A:491:GLY:HA3	6:A:955:HOH:O	2.00	0.62
1:A:174:GLU:HB2	1:A:220:PRO:HA	1.81	0.61
1:A:343:GLY:HA3	1:A:345[A]:GLU:OE1	2.01	0.60
1:A:123:LEU:C	1:A:123:LEU:HD12	2.26	0.60
1:A:37[C]:ARG:NH2	1:A:104:GLU:OE1	2.34	0.59
1:A:140[A]:LYS:H	1:A:140[A]:LYS:HD2	1.66	0.59
1:A:401:ARG:HH11	4:A:603:EDO:H22	1.71	0.56
1:A:41:SER:HA	1:A:96:GLN:HB3	1.87	0.55
1:A:401:ARG:HH11	4:A:603:EDO:C2	2.21	0.54
1:A:140[A]:LYS:H	1:A:140[A]:LYS:CD	2.21	0.54
1:A:37[B]:ARG:NH2	1:A:104:GLU:OE1	2.40	0.53
1:A:345[A]:GLU:H	1:A:345[A]:GLU:CD	2.19	0.51
1:A:401:ARG:NH1	4:A:603:EDO:C2	2.74	0.51
1:A:126:ASP:C	1:A:128:ALA:H	2.18	0.49
1:A:426:ARG:HD3	1:A:440:THR:OG1	2.12	0.49
1:A:334:GLN:NE2	6:A:904:HOH:O	2.48	0.47
1:A:210:ARG:NH1	6:A:910:HOH:O	2.47	0.47
1:A:246:HIS:H	1:A:246:HIS:CD2	2.33	0.47
1:A:173[A]:MET:HG3	1:A:175:MET:HE2	1.97	0.46
1:A:432:TRP:CE3	1:A:481:LEU:HD13	2.50	0.46
5:A:607:GOL:H31	6:A:911:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:C	1:A:125:ASP:OD1	2.58	0.45
1:A:173[B]:MET:HE1	1:A:215:GLU:O	2.16	0.44
1:A:37[B]:ARG:NH1	1:A:100:GLU:OE1	2.48	0.44
1:A:42:ARG:H	1:A:42:ARG:HG2	1.60	0.44
1:A:413:ARG:HG2	5:A:607:GOL:H2	1.99	0.43
1:A:198:MET:HE1	1:A:200:MET:HG3	1.99	0.43
1:A:261:GLN:HB2	1:A:330:LEU:HD11	2.01	0.43
1:A:73:HIS:HE2	4:A:602:EDO:H22	1.84	0.43
1:A:42:ARG:HB2	3:A:500:FAD:C7	2.49	0.42
1:A:226:PRO:HA	1:A:227:PRO:HD3	1.82	0.42
1:A:126:ASP:C	1:A:128:ALA:N	2.76	0.41
1:A:389:LYS:HE2	6:A:653:HOH:O	2.19	0.41
3:A:500:FAD:H1'1	5:A:608:GOL:H2	2.01	0.41
1:A:135:ARG:HD3	1:A:140[B]:LYS:HE3	2.02	0.41
1:A:124:THR:O	1:A:130:VAL:HG13	2.21	0.41
1:A:489:LEU:HD23	1:A:489:LEU:HA	1.94	0.41
1:A:73:HIS:NE2	4:A:602:EDO:H22	2.35	0.41
1:A:180:ILE:HG22	1:A:249:PRO:HA	2.04	0.41
1:A:201:VAL:HG12	1:A:211:ILE:HG22	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	494/500 (99%)	484 (98%)	9 (2%)	1 (0%)	43 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	SER

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	385/386 (100%)	369 (96%)	16 (4%)	26 14

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	ASP
1	A	122	SER
1	A	138	GLU
1	A	140[A]	LYS
1	A	140[B]	LYS
1	A	183	VAL
1	A	189	MET
1	A	198	MET
1	A	199	VAL
1	A	201	VAL
1	A	345[A]	GLU
1	A	345[B]	GLU
1	A	353	LEU
1	A	390	ARG
1	A	482	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	246	HIS

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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
5	GOL	A	608	-	5,5,5	0.31	0	5,5,5	0.53	0
3	FAD	A	500	-	58,58,58	1.35	7 (12%)	85,89,89	1.68	21 (24%)
5	GOL	A	607	-	5,5,5	0.37	0	5,5,5	0.37	0
4	EDO	A	603	-	3,3,3	0.35	0	2,2,2	0.66	0
4	EDO	A	604	-	3,3,3	0.46	0	2,2,2	0.25	0
4	EDO	A	602	-	3,3,3	0.41	0	2,2,2	0.31	0
5	GOL	A	606	-	5,5,5	0.34	0	5,5,5	0.42	0
5	GOL	A	605	-	5,5,5	0.31	0	5,5,5	0.49	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
5	GOL	A	608	-	-	0/4/4/4	-
3	FAD	A	500	-	-	3/34/50/50	0/6/6/6
5	GOL	A	607	-	-	2/4/4/4	-
4	EDO	A	603	-	-	0/1/1/1	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	A	602	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	606	-	-	4/4/4/4	-
5	GOL	A	605	-	-	4/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	FAD	C2A-N3A	3.89	1.40	1.33
3	A	500	FAD	C2A-N1A	3.69	1.40	1.33
3	A	500	FAD	C4X-N5	3.65	1.38	1.30
3	A	500	FAD	C8A-N7A	3.45	1.38	1.31
3	A	500	FAD	C4A-N3A	2.95	1.39	1.34
3	A	500	FAD	C10-N1	2.73	1.38	1.33
3	A	500	FAD	C6A-N1A	2.33	1.42	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	FAD	N3A-C2A-N1A	-6.57	118.63	128.58
3	A	500	FAD	N9A-C8A-N7A	-4.41	107.68	113.94
3	A	500	FAD	C5A-N7A-C8A	3.26	108.58	103.45
3	A	500	FAD	C2A-N3A-C4A	3.24	119.75	111.83
3	A	500	FAD	C4A-N9A-C8A	3.18	109.08	105.74
3	A	500	FAD	C4-N3-C2	-3.16	120.04	125.64
3	A	500	FAD	C5A-C4A-N3A	-3.05	122.52	126.72
3	A	500	FAD	O2P-P-O3P	3.03	115.47	107.27
3	A	500	FAD	C4X-C10-N10	3.01	120.79	116.48
3	A	500	FAD	C4A-N9A-C1B	-2.64	120.46	126.63
3	A	500	FAD	C4X-C4-N3	2.56	119.77	113.25
3	A	500	FAD	C10-C4X-N5	-2.49	119.73	124.81
3	A	500	FAD	C4A-C5A-N7A	-2.43	107.80	110.58
3	A	500	FAD	C5A-C6A-N6A	-2.33	117.51	123.29
3	A	500	FAD	N6A-C6A-N1A	2.33	123.57	118.38
3	A	500	FAD	O4-C4-C4X	-2.21	120.71	126.53
3	A	500	FAD	C4X-C10-N1	-2.13	119.37	124.59
3	A	500	FAD	C5X-C9A-N10	2.07	119.84	117.97
3	A	500	FAD	N3A-C4A-N9A	2.04	130.63	127.17
3	A	500	FAD	C9A-C5X-N5	-2.03	120.30	122.45
3	A	500	FAD	C2A-N1A-C6A	2.02	122.05	118.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

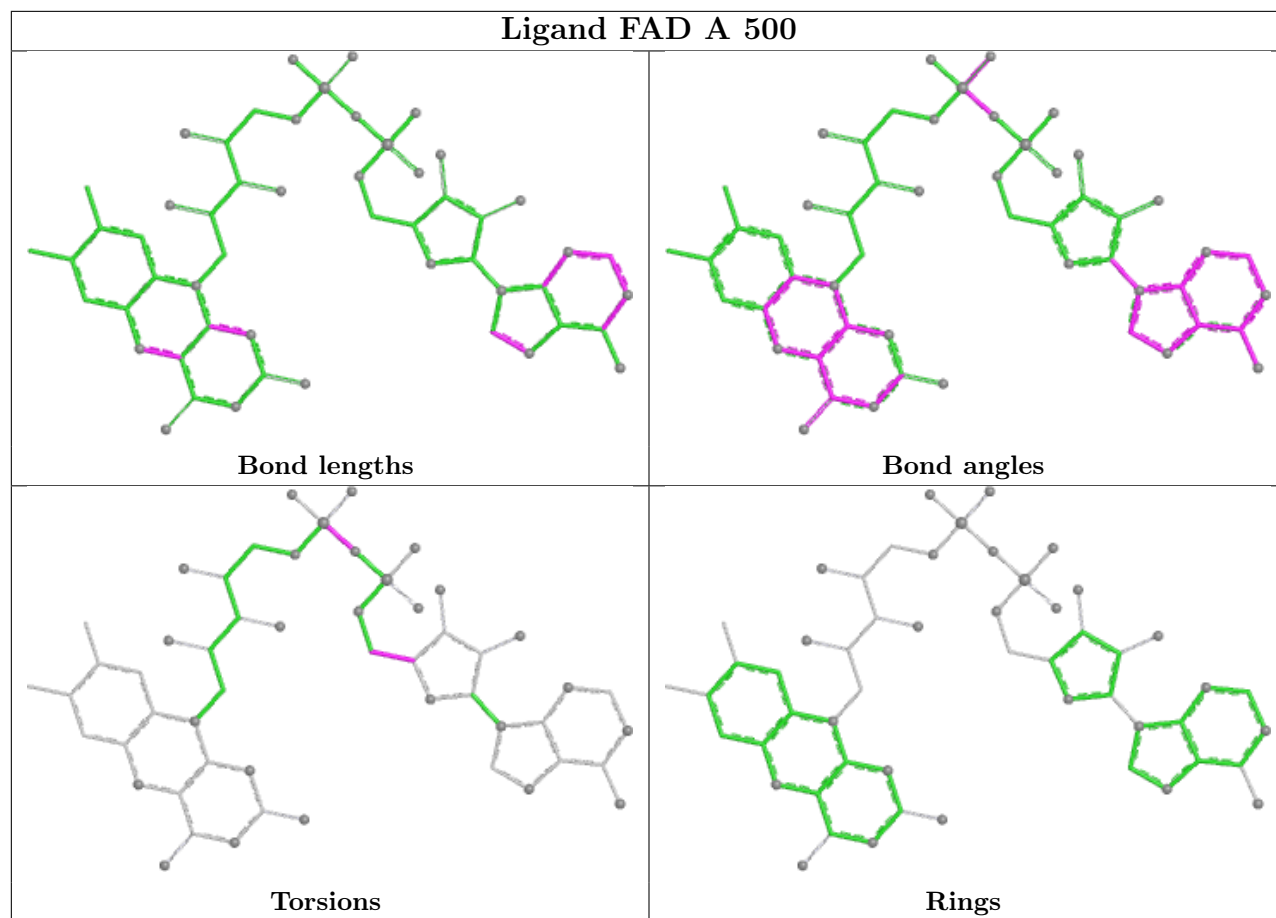
Mol	Chain	Res	Type	Atoms
5	A	606	GOL	O1-C1-C2-C3
5	A	606	GOL	C1-C2-C3-O3
5	A	606	GOL	O1-C1-C2-O2
5	A	605	GOL	O1-C1-C2-C3
5	A	605	GOL	C1-C2-C3-O3
5	A	607	GOL	C1-C2-C3-O3
5	A	606	GOL	O2-C2-C3-O3
5	A	605	GOL	O2-C2-C3-O3
5	A	605	GOL	O1-C1-C2-O2
3	A	500	FAD	PA-O3P-P-O5'
3	A	500	FAD	O4B-C4B-C5B-O5B
5	A	607	GOL	O2-C2-C3-O3
3	A	500	FAD	C3B-C4B-C5B-O5B

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	608	GOL	2	0
3	A	500	FAD	2	0
5	A	607	GOL	2	0
4	A	603	EDO	4	0
4	A	602	EDO	2	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

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	488/500 (97%)	2.30	244 (50%) 0 0	20, 42, 52, 75	10 (2%)

All (244) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	ALA	7.8
1	A	232	VAL	7.3
1	A	226	PRO	7.1
1	A	217	GLY	7.0
1	A	229	TRP	6.5
1	A	239	LEU	6.3
1	A	-1	HIS	6.1
1	A	90	ALA	5.9
1	A	190	ILE	5.8
1	A	230	HIS	5.6
1	A	88	TRP	5.5
1	A	218	THR	5.5
1	A	1	SER	5.4
1	A	196	GLY	5.4
1	A	98	VAL	5.4
1	A	255	PHE	5.4
1	A	183	VAL	5.3
1	A	212	ILE	5.3
1	A	171	ALA	5.2
1	A	199	VAL	5.2
1	A	283	ALA	5.2
1	A	107	ALA	5.1
1	A	41	SER	5.1
1	A	177	LEU	4.9
1	A	304	ALA	4.8
1	A	23	LEU	4.8
1	A	110	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	106	TRP	4.7
1	A	236	TRP	4.7
1	A	208	ILE	4.7
1	A	220	PRO	4.7
1	A	111	GLY	4.6
1	A	38	THR	4.6
1	A	296	VAL	4.6
1	A	109	GLY	4.6
1	A	233	ALA	4.5
1	A	124	THR	4.5
1	A	94	VAL	4.5
1	A	214	CYS	4.4
1	A	256	GLY	4.4
1	A	219	PRO	4.4
1	A	309	THR	4.4
1	A	128	ALA	4.4
1	A	193	THR	4.3
1	A	39	GLY	4.3
1	A	103	LEU	4.2
1	A	295	ALA	4.2
1	A	203	PRO	4.2
1	A	123	LEU	4.2
1	A	194	LEU	4.2
1	A	490	THR	4.1
1	A	127	GLY	4.1
1	A	213	VAL	4.1
1	A	306	VAL	4.1
1	A	91	ALA	4.1
1	A	205	PRO	4.1
1	A	176	TYR	4.1
1	A	179	ASP	4.1
1	A	200	MET	4.1
1	A	216	ARG	4.0
1	A	249	PRO	4.0
1	A	311	THR	3.9
1	A	241	GLY	3.9
1	A	299	GLY	3.9
1	A	251	TRP	3.9
1	A	300	TRP	3.9
1	A	108	THR	3.8
1	A	168	GLY	3.8
1	A	246	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	227	PRO	3.8
1	A	37[B]	ARG	3.8
1	A	101	THR	3.7
1	A	237	LYS	3.7
1	A	245	ALA	3.7
1	A	89	GLN	3.7
1	A	95	PRO	3.7
1	A	112	ALA	3.7
1	A	254	ALA	3.6
1	A	182	GLY	3.6
1	A	102	HIS	3.5
1	A	252	VAL	3.5
1	A	165[A]	ASP	3.5
1	A	97	SER	3.5
1	A	93	THR	3.5
1	A	279	ILE	3.4
1	A	268	GLY	3.4
1	A	310	ALA	3.4
1	A	292	ILE	3.4
1	A	206	GLY	3.3
1	A	247	ALA	3.3
1	A	173[A]	MET	3.3
1	A	489	LEU	3.3
1	A	147	TYR	3.3
1	A	201	VAL	3.3
1	A	185	LEU	3.3
1	A	289	ASN	3.3
1	A	211	ILE	3.2
1	A	126	ASP	3.2
1	A	207	GLY	3.2
1	A	240	THR	3.2
1	A	303	GLY	3.2
1	A	444	GLY	3.2
1	A	178	ALA	3.2
1	A	92	LYS	3.2
1	A	140[A]	LYS	3.1
1	A	146	ALA	3.1
1	A	180	ILE	3.1
1	A	162	ALA	3.1
1	A	198	MET	3.1
1	A	447	SER	3.1
1	A	287	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	96	GLN	3.1
1	A	297	ASN	3.1
1	A	169	THR	3.1
1	A	312	GLU	3.1
1	A	314	LEU	3.0
1	A	313	GLU	3.0
1	A	175	MET	3.0
1	A	305	VAL	3.0
1	A	25	GLY	3.0
1	A	3	ALA	3.0
1	A	122	SER	2.9
1	A	293	GLN	2.9
1	A	172	THR	2.9
1	A	197	GLY	2.9
1	A	378	ASP	2.9
1	A	370	VAL	2.9
1	A	19	GLY	2.9
1	A	45	GLY	2.9
1	A	170	ALA	2.9
1	A	430	ALA	2.9
1	A	448	ALA	2.9
1	A	129	GLY	2.9
1	A	191	GLY	2.9
1	A	346[A]	VAL	2.9
1	A	455	THR	2.9
1	A	317	SER	2.9
1	A	99	THR	2.8
1	A	71	GLN	2.8
1	A	81	PHE	2.8
1	A	288	MET	2.8
1	A	204	LEU	2.8
1	A	244	ILE	2.8
1	A	0	ARG	2.8
1	A	189	MET	2.8
1	A	301	LYS	2.8
1	A	440	THR	2.8
1	A	290	THR	2.8
1	A	66	VAL	2.8
1	A	259	THR	2.7
1	A	33	ARG	2.7
1	A	4	ALA	2.7
1	A	215	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	324	ALA	2.7
1	A	285	GLY	2.7
1	A	400	THR	2.7
1	A	406	THR	2.7
1	A	284	GLY	2.7
1	A	121	LEU	2.7
1	A	487	ALA	2.6
1	A	234	ASP	2.6
1	A	164	PHE	2.6
1	A	307	ASN	2.6
1	A	59	ILE	2.6
1	A	452	LEU	2.6
1	A	210	ARG	2.6
1	A	174	GLU	2.6
1	A	187	PRO	2.6
1	A	195	PRO	2.6
1	A	43	GLY	2.6
1	A	130	VAL	2.6
1	A	491	GLY	2.5
1	A	160	LYS	2.5
1	A	308	GLY	2.5
1	A	253	SER	2.5
1	A	450	SER	2.5
1	A	449	THR	2.5
1	A	275	ASP	2.5
1	A	163	GLY	2.5
1	A	238	ARG	2.5
1	A	16	MET	2.5
1	A	2	ASP	2.5
1	A	298	LEU	2.4
1	A	460	ILE	2.4
1	A	258	ALA	2.4
1	A	376	THR	2.4
1	A	5	VAL	2.4
1	A	319	HIS	2.4
1	A	404	SER	2.4
1	A	181	LYS	2.4
1	A	263	THR	2.4
1	A	24	ALA	2.4
1	A	250	VAL	2.4
1	A	432	TRP	2.4
1	A	105	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	186	GLN	2.4
1	A	202	GLY	2.4
1	A	291	SER	2.4
1	A	320	SER	2.4
1	A	302	LEU	2.4
1	A	340	PHE	2.4
1	A	363	ALA	2.4
1	A	412	ALA	2.4
1	A	133	GLU	2.4
1	A	353	LEU	2.3
1	A	114	ILE	2.3
1	A	120	VAL	2.3
1	A	166	PHE	2.3
1	A	257	ASN	2.3
1	A	442	VAL	2.3
1	A	27	GLU	2.3
1	A	427	ALA	2.3
1	A	471	PRO	2.3
1	A	464	GLY	2.3
1	A	334	GLN	2.3
1	A	21	LEU	2.3
1	A	138	GLU	2.2
1	A	342	SER	2.2
1	A	132	VAL	2.2
1	A	482	GLU	2.2
1	A	451	GLY	2.2
1	A	145	ALA	2.2
1	A	456	THR	2.2
1	A	294	ASP	2.2
1	A	431	ALA	2.2
1	A	40	GLU	2.2
1	A	248	GLU	2.2
1	A	446	VAL	2.2
1	A	480	ALA	2.2
1	A	209	THR	2.1
1	A	86	GLY	2.1
1	A	228	SER	2.1
1	A	20	GLU	2.1
1	A	104	GLU	2.1
1	A	143	LEU	2.1
1	A	315	LEU	2.1
1	A	125	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	142	THR	2.1
1	A	330	LEU	2.1
1	A	425	LEU	2.1
1	A	488	PRO	2.0
1	A	231	GLU	2.0
1	A	149	VAL	2.0
1	A	158	VAL	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](#)

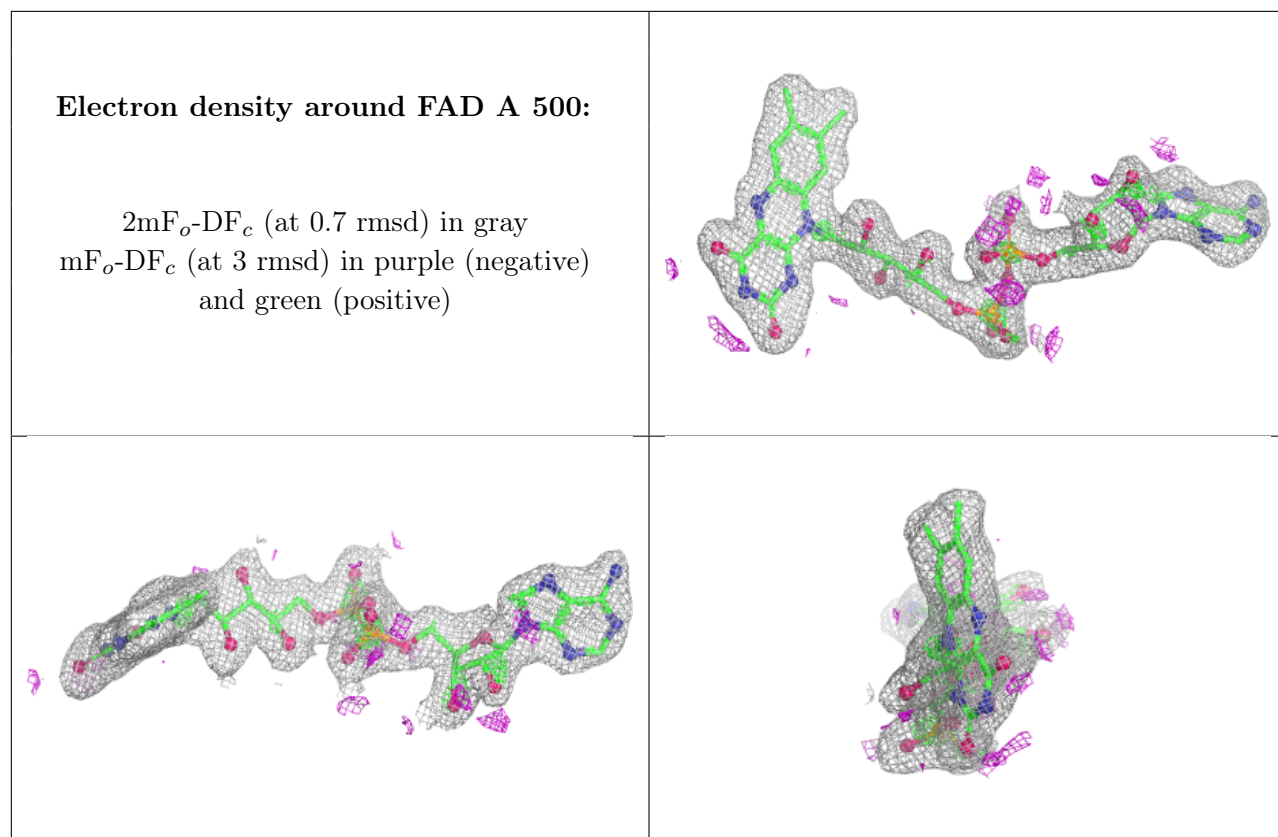
There are no oligosaccharides in this entry.

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(Å ²)	Q<0.9
5	GOL	A	606	6/6	0.65	0.22	82,83,83,83	0
5	GOL	A	605	6/6	0.78	0.19	69,70,71,71	0
4	EDO	A	603	4/4	0.79	0.19	59,60,60,60	0
5	GOL	A	607	6/6	0.83	0.16	54,55,55,55	0
4	EDO	A	604	4/4	0.84	0.21	39,42,45,45	0
5	GOL	A	608	6/6	0.85	0.17	50,53,53,55	0
2	ZN	A	601	1/1	0.89	0.21	62,62,62,62	0
4	EDO	A	602	4/4	0.89	0.15	46,47,49,49	0
3	FAD	A	500	53/53	0.93	0.15	34,41,71,73	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.