WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:24 am GMT

PDB ID : 2QA1

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
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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

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.
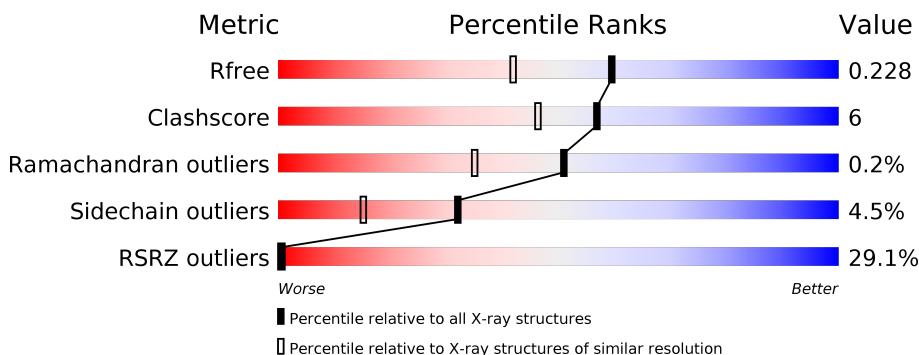
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (1.80-1.80)

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 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 <=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
3	FAD	A	500	-	-	-	X
4	EDO	A	603	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	604	-	-	-	X
5	GOL	A	605	-	-	-	X
5	GOL	A	607	-	-	-	X
5	GOL	A	608	-	-	-	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
1	A	488	Total 3718	C 2328	N 673	O 699	S 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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
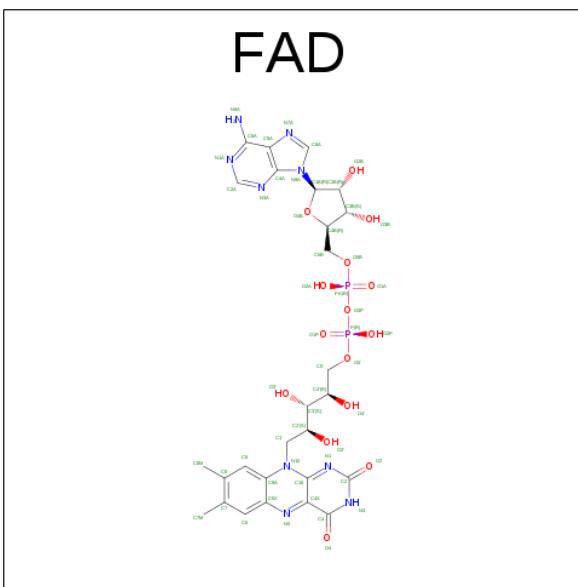
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
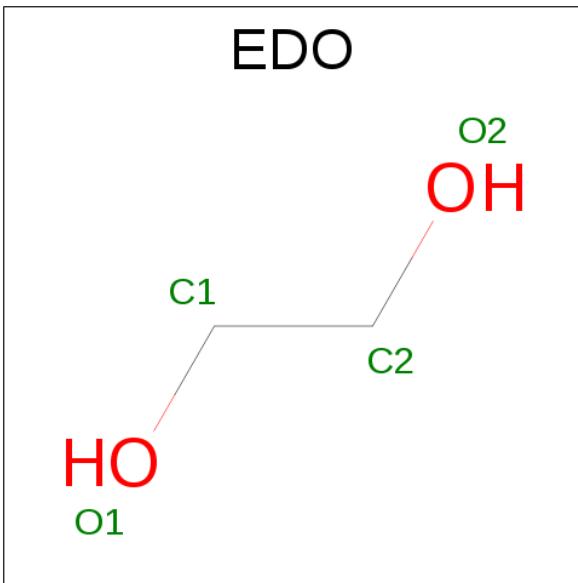
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
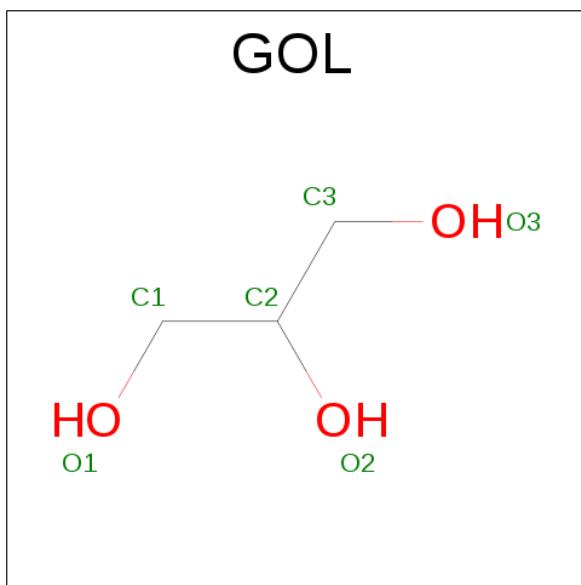
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 6	C 3	O 3	0	0
5	A	1	Total 6	C 3	O 3	0	0
5	A	1	Total 6	C 3	O 3	0	0
5	A	1	Total 6	C 3	O 3	0	0

- Molecule 6 is water.

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

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 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
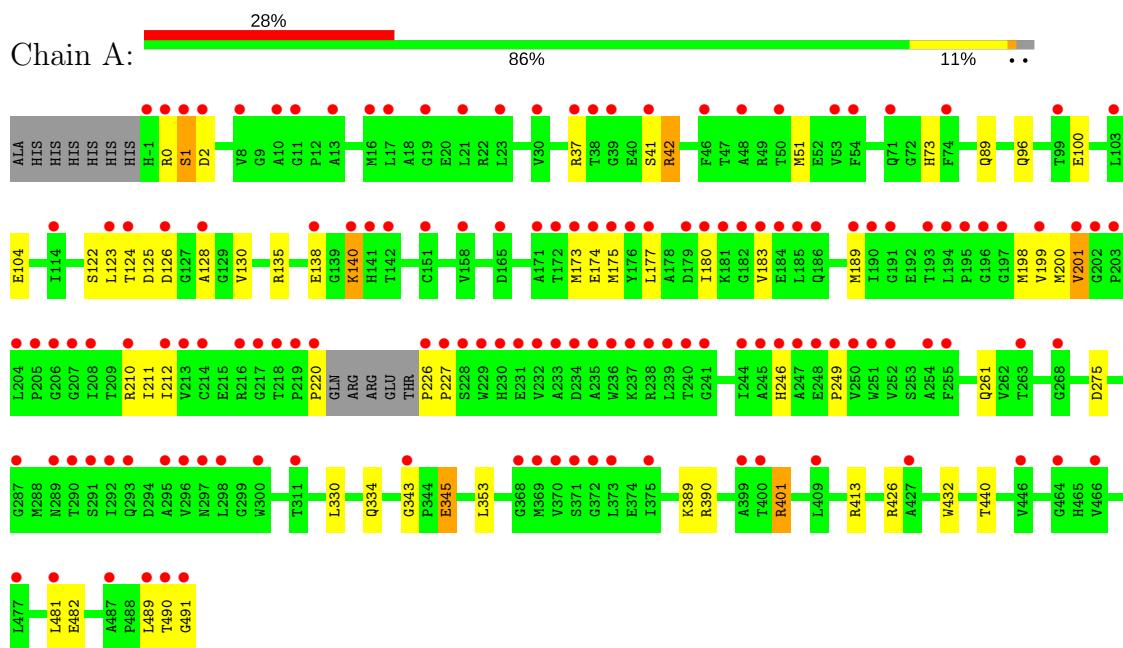
4 Data and refinement statistics (i)

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 36.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (36.96-1.80) 99.3 (36.92-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 1.81Å)	Xtriage
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 (5.31%)	DCC
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4166	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage'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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, ZN, EDO, FAD

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	0.50	0/3814	0.61	0/5180

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.

There are no bond angle outliers.

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	41	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	43	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 (43) 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: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: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:123:LEU:HD12	1:A:123:LEU:C	2.26	0.55
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:401:ARG:NH1	4:A:603:EDO:C2	2.74	0.51
1:A:426:ARG:HD3	1:A:440:THR:OG1	2.12	0.49
1:A:173[B]:MET:HE3	1:A:175:MET:HG3	1.97	0.47
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:CD2	1:A:246:HIS:H	2.33	0.47
1:A:345[A]:GLU:H	1:A:345[A]:GLU:CD	2.19	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
1:A:126:ASP:C	1:A:128:ALA:H	2.18	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ARG:HG2	5:A:607:GOL:H2	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:389:LYS:HE2	6:A:653:HOH:O	2.19	0.41
1:A:125:ASP:OD1	1:A:125:ASP:C	2.58	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:HA	1:A:489:LEU:HD23	1.94	0.41
1:A:180:ILE:HG22	1:A:249:PRO:HA	2.04	0.41
1:A:73:HIS:NE2	4:A:602:EDO:H22	2.35	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 ⓘ

5.3.1 Protein backbone ⓘ

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%)	51	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	SER

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	385/386 (100%)	366 (95%)	19 (5%)	29	12

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	ASP
1	A	42	ARG
1	A	122	SER
1	A	138	GLU
1	A	140[A]	LYS
1	A	140[B]	LYS
1	A	177	LEU
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	401	ARG
1	A	482	GLU

Some 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 ⓘ

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	#$|Z| > 2$
3	FAD	A	500	-	51,58,58	1.55	7 (13%)	54,89,89	2.19	8 (14%)
4	EDO	A	602	-	3,3,3	0.43	0	2,2,2	0.29	0
4	EDO	A	603	-	3,3,3	0.37	0	2,2,2	0.66	0
4	EDO	A	604	-	3,3,3	0.47	0	2,2,2	0.24	0
5	GOL	A	605	-	5,5,5	0.26	0	5,5,5	0.46	0
5	GOL	A	606	-	5,5,5	0.29	0	5,5,5	0.38	0
5	GOL	A	607	-	5,5,5	0.35	0	5,5,5	0.35	0
5	GOL	A	608	-	5,5,5	0.26	0	5,5,5	0.47	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
3	FAD	A	500	-	-	0/28/50/50	0/6/6/6
4	EDO	A	602	-	-	0/1/1/1	0/0/0/0
4	EDO	A	603	-	-	0/1/1/1	0/0/0/0
4	EDO	A	604	-	-	0/1/1/1	0/0/0/0
5	GOL	A	605	-	-	0/4/4/4	0/0/0/0
5	GOL	A	606	-	-	0/4/4/4	0/0/0/0
5	GOL	A	607	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	608	-	-	0/4/4/4	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	FAD	C5X-N5	2.30	1.38	1.35
3	A	500	FAD	C4A-N3A	2.97	1.39	1.35
3	A	500	FAD	C4-N3	3.48	1.39	1.33
3	A	500	FAD	C2A-N1A	3.51	1.40	1.33
3	A	500	FAD	C4X-N5	3.69	1.38	1.33
3	A	500	FAD	C10-N1	3.91	1.38	1.33
3	A	500	FAD	C2A-N3A	5.21	1.40	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	FAD	N3A-C2A-N1A	-11.74	118.63	128.86
3	A	500	FAD	C1B-N9A-C4A	-3.57	120.46	126.64
3	A	500	FAD	C4X-C4-N3	-2.61	119.77	123.48
3	A	500	FAD	N6A-C6A-N1A	2.42	123.57	118.77
3	A	500	FAD	C5X-C9A-N10	2.94	119.84	117.66
3	A	500	FAD	C1'-N10-C9A	3.17	121.25	118.35
3	A	500	FAD	C4X-N5-C5X	3.43	120.38	116.76
3	A	500	FAD	C4-N3-C2	5.58	120.04	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

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

5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	488/500 (97%)	1.67	142 (29%)	1	0	35, 42, 53, 75	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	PRO	9.8
1	A	205	PRO	9.4
1	A	229	TRP	8.9
1	A	1	SER	8.9
1	A	227	PRO	8.3
1	A	212	ILE	8.2
1	A	194	LEU	7.1
1	A	239	LEU	7.1
1	A	207	GLY	7.0
1	A	241	GLY	7.0
1	A	232	VAL	6.7
1	A	214	CYS	6.6
1	A	182	GLY	6.6
1	A	208	ILE	6.5
1	A	-1	HIS	6.3
1	A	186	GLN	6.1
1	A	219	PRO	6.0
1	A	226	PRO	5.9
1	A	0	ARG	5.9
1	A	179	ASP	5.6
1	A	38	THR	5.6
1	A	193	THR	5.6
1	A	185	LEU	5.4
1	A	204	LEU	5.3
1	A	39	GLY	5.1
1	A	250	VAL	5.1
1	A	180	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	126	ASP	5.0
1	A	195	PRO	5.0
1	A	248	GLU	4.6
1	A	191	GLY	4.6
1	A	176	TYR	4.6
1	A	236	TRP	4.5
1	A	183	VAL	4.5
1	A	230	HIS	4.5
1	A	206	GLY	4.5
1	A	247	ALA	4.5
1	A	203	PRO	4.5
1	A	235	ALA	4.4
1	A	141	HIS	4.3
1	A	190	ILE	4.3
1	A	245	ALA	4.3
1	A	228	SER	4.2
1	A	199	VAL	4.2
1	A	249	PRO	4.2
1	A	292	ILE	4.1
1	A	217	GLY	4.1
1	A	2	ASP	3.9
1	A	171	ALA	3.9
1	A	246	HIS	3.9
1	A	173[A]	MET	3.8
1	A	128	ALA	3.8
1	A	370	VAL	3.8
1	A	251	TRP	3.7
1	A	201	VAL	3.7
1	A	296	VAL	3.7
1	A	375	ILE	3.6
1	A	233	ALA	3.5
1	A	244	ILE	3.5
1	A	103	LEU	3.5
1	A	184	GLU	3.4
1	A	252	VAL	3.4
1	A	255	PHE	3.4
1	A	50	THR	3.4
1	A	177	LEU	3.4
1	A	37[B]	ARG	3.3
1	A	216	ARG	3.3
1	A	196	GLY	3.3
1	A	491	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	181	LYS	3.3
1	A	373	LEU	3.3
1	A	240	THR	3.2
1	A	400	THR	3.2
1	A	490	THR	3.2
1	A	17	LEU	3.2
1	A	489	LEU	3.1
1	A	53	VAL	3.1
1	A	124	THR	3.0
1	A	16	MET	3.0
1	A	290	THR	2.9
1	A	237	LYS	2.9
1	A	466	VAL	2.9
1	A	213	VAL	2.9
1	A	446	VAL	2.9
1	A	210	ARG	2.9
1	A	54	PHE	2.9
1	A	295	ALA	2.9
1	A	298	LEU	2.8
1	A	399	ALA	2.8
1	A	464	GLY	2.8
1	A	142	THR	2.7
1	A	254	ALA	2.7
1	A	189	MET	2.7
1	A	165[A]	ASP	2.6
1	A	343	GLY	2.6
1	A	30	VAL	2.6
1	A	172	THR	2.6
1	A	23	LEU	2.6
1	A	114	ILE	2.6
1	A	481	LEU	2.5
1	A	368	GLY	2.5
1	A	197	GLY	2.5
1	A	138	GLU	2.5
1	A	202	GLY	2.5
1	A	174	GLU	2.5
1	A	123	LEU	2.5
1	A	151	CYS	2.5
1	A	369[A]	MET	2.4
1	A	46	PHE	2.4
1	A	10	ALA	2.4
1	A	477	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	263	THR	2.4
1	A	372	GLY	2.4
1	A	158	VAL	2.4
1	A	409	LEU	2.3
1	A	371	SER	2.3
1	A	175	MET	2.3
1	A	289	ASN	2.3
1	A	218	THR	2.3
1	A	13	ALA	2.3
1	A	487	ALA	2.2
1	A	74	PHE	2.2
1	A	291	SER	2.2
1	A	234	ASP	2.2
1	A	238	ARG	2.2
1	A	297	ASN	2.2
1	A	293	GLN	2.2
1	A	300	TRP	2.2
1	A	231	GLU	2.2
1	A	71	GLN	2.1
1	A	99	THR	2.1
1	A	140[A]	LYS	2.1
1	A	21	LEU	2.1
1	A	48	ALA	2.1
1	A	287	GLY	2.1
1	A	427	ALA	2.0
1	A	19	GLY	2.0
1	A	41	SER	2.0
1	A	8	VAL	2.0
1	A	11	GLY	2.0
1	A	268	GLY	2.0
1	A	311	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
5	GOL	A	608	6/6	0.74	0.33	11.37	50,53,53,55	0
5	GOL	A	605	6/6	0.61	0.34	4.17	69,70,71,71	0
5	GOL	A	607	6/6	0.88	0.27	3.58	54,55,55,55	0
4	EDO	A	604	4/4	0.88	0.27	3.16	39,42,45,45	0
3	FAD	A	500	53/53	0.82	0.28	2.43	34,41,71,73	0
4	EDO	A	603	4/4	0.75	0.27	1.45	59,60,60,60	0
2	ZN	A	601	1/1	0.97	0.27	0.09	62,62,62,62	0
4	EDO	A	602	4/4	0.93	0.09	-2.32	46,47,49,49	0
5	GOL	A	606	6/6	0.77	0.30	-	82,83,83,83	0

6.5 Other polymers ⓘ

There are no such residues in this entry.