WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Mar 26, 2024 – 01:05 pm GMT

PDB ID	:	9ER4
Title	:	Room temperature structure of Glycine max phyA in Pr
Deposited on	:	2024-03-22
Resolution	:	2.20 Å(reported)

This wwPDB validation report is for manuscript review

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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 (i) symbol.

The types of validation reports are described at
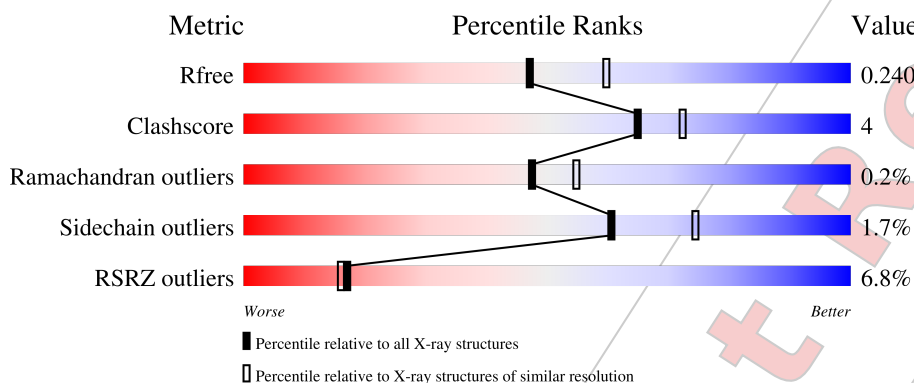http://www.wwpdb.org/validation/2017/FAQs#types.

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 2.20 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	Percentile Ranks	Value
Rfree		0.240
Clashscore		4
Ramachandran outliers		0.2%
Sidechain outliers		1.7%
RSRZ outliers		6.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 <=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	359	6% 76% 9% 15%
1	B	359	5% 80% 6% 14%

Validation Pipeline (wwPDB-VP) : 2.36

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5027 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 Phytochrome A-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total 2387	C 1538	N 404	O 422	S 23	0	0	0
1	B	309	Total 2416	C 1557	N 408	O 428	S 23	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	initiating methionine	UNP B4YB07
A	403	HIS	-	expression tag	UNP B4YB07
A	404	HIS	-	expression tag	UNP B4YB07
A	405	HIS	-	expression tag	UNP B4YB07
A	406	HIS	-	expression tag	UNP B4YB07
A	407	HIS	-	expression tag	UNP B4YB07
A	408	HIS	-	expression tag	UNP B4YB07
B	50	MET	-	initiating methionine	UNP B4YB07
B	403	HIS	-	expression tag	UNP B4YB07
B	404	HIS	-	expression tag	UNP B4YB07
B	405	HIS	-	expression tag	UNP B4YB07
B	406	HIS	-	expression tag	UNP B4YB07
B	407	HIS	-	expression tag	UNP B4YB07
B	408	HIS	-	expression tag	UNP B4YB07

- Molecule 2 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).

CYC

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 43	C 33	N 4	O 6	0	0
2	B	1	Total 43	C 33	N 4	O 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total 65	O 65	0	0
3	B	73	Total 73	O 73	0	0

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: Phytochrome A-2

Chain A:

• Molecule 1: Phytochrome A-2

Chain B:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.45Å 115.05Å 69.80Å 90.00° 92.68° 90.00°	Depositor
Resolution (Å)	20.48 – 2.20 20.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.48-2.20) 99.9 (20.48-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.39 (at 2.19Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5156	Depositor
R, R_{free}	0.204 , 0.241 0.204 , 0.240	Depositor DCC
R_{free} test set	2308 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 46.4	EDS
L-test for twinning[2]	$<\|L\|> = 0.49$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5027	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CYC

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	0.51	0/2442	0.79	1/3307 (0.0%)
1	B	0.50	0/2472	0.79	1/3348 (0.0%)
All	All	0.50	0/4914	0.79	2/6655 (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	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	161	LYS	CD-CE-NZ	5.07	123.37	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	ARG	Sidechain
1	A	382	ARG	Sidechain

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	2387	0	2418	20	0
1	B	2416	0	2456	18	0
2	A	43	0	36	3	0
2	B	43	0	37	1	0
3	A	65	0	0	3	0
3	B	73	0	0	1	0
All	All	5027	0	4947	40	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 4.

All (40) 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:101:GLU:OE1	3:A:601:HOH:O	2.04	0.76
1:A:74:MET:HE1	2:A:500:CYC:HAD1	1.70	0.74
1:B:130:LYS:HE3	1:B:142:GLN:HE22	1.56	0.70
1:B:173:ARG:HG2	1:B:173:ARG:HH11	1.56	0.70
1:B:326:GLN:OE1	1:B:330:ASN:ND2	2.27	0.68
1:A:279:ARG:NH2	3:A:602:HOH:O	2.22	0.67
1:B:173:ARG:HH12	1:B:178:MET:HB2	1.59	0.66
1:A:327:TYR:CE2	1:A:331:MET:HE1	2.32	0.65
1:A:74:MET:CE	2:A:500:CYC:HAD1	2.27	0.63
1:B:106:MET:HE3	1:B:167:PHE:HE2	1.64	0.62
1:B:304:GLU:HG3	3:B:668:HOH:O	2.05	0.56
1:B:360:ARG:HG3	1:B:360:ARG:HH11	1.71	0.54
1:A:121:PRO:O	1:A:123:LEU:N	2.41	0.53
1:B:173:ARG:HG2	1:B:173:ARG:NH1	2.21	0.53
1:A:176:GLY:HA3	1:A:308:PHE:CZ	2.43	0.53
1:B:190:VAL:O	1:B:193:THR:HG23	2.09	0.53
1:A:210:ARG:NE	1:A:229:GLU:OE2	2.33	0.52
1:B:91:GLU:HB2	1:B:173:ARG:HH22	1.75	0.51
1:B:106:MET:HE3	1:B:167:PHE:CE2	2.46	0.51
1:B:360:ARG:HG3	1:B:360:ARG:NH1	2.26	0.51
1:A:108:THR:O	1:A:109:MET:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LYS:HE3	1:B:142:GLN:NE2	2.25	0.48
1:A:147:PHE:HD1	1:A:151:LEU:HD13	1.79	0.47
2:A:500:CYC:NB	2:A:500:CYC:HMA1	2.29	0.47
1:A:147:PHE:HB3	1:A:151:LEU:HB3	1.97	0.47
1:A:72:HIS:CD2	1:A:76:LYS:HD2	2.49	0.46
1:B:246:GLU:OE1	1:B:246:GLU:O	2.33	0.46
1:B:331:MET:HE3	1:B:331:MET:HB3	1.80	0.46
1:A:248:ASP:HB3	1:A:279:ARG:NH2	2.33	0.44
1:A:71:LEU:HG	1:A:277:ALA:HB2	1.99	0.44
1:A:306:LEU:HA	1:A:307:PRO:HD3	1.90	0.44
1:A:145:LEU:HD12	1:A:173:ARG:HH12	1.81	0.43
1:A:261:LEU:HD23	1:A:261:LEU:HA	1.82	0.43
1:B:242:TYR:CZ	1:B:250:GLY:HA3	2.53	0.42
1:B:238:ARG:HG3	1:B:257:THR:HG22	2.01	0.42
2:B:500:CYC:NB	2:B:500:CYC:HMA1	2.35	0.41
1:A:183:GLU:OE1	3:A:603:HOH:O	2.22	0.41
1:B:305:LYS:HB2	1:B:305:LYS:HE2	1.90	0.41
1:A:145:LEU:HA	1:A:173:ARG:HH22	1.86	0.41
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.95	0.41

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	298/359 (83%)	292 (98%)	5 (2%)	1 (0%)	41	46
1	B	303/359 (84%)	300 (99%)	3 (1%)	0	100	100
All	All	601/718 (84%)	592 (98%)	8 (1%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/307 (85%)	255 (98%)	6 (2%)	50	63
1	B	264/307 (86%)	261 (99%)	3 (1%)	73	85
All	All	525/614 (86%)	516 (98%)	9 (2%)	60	74

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	CYS
1	A	139	SER
1	A	201	TYR
1	A	276	GLN
1	A	288	ARG
1	A	331	MET
1	B	92	LYS
1	B	201	TYR
1	B	360	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	A	370	HIS
1	B	142	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	CYC	A	500	1	42,46,46	1.06	2 (4%)	50,67,67	1.29	8 (16%)
2	CYC	B	500	1	42,46,46	1.16	3 (7%)	50,67,67	1.44	5 (10%)

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	CYC	A	500	1	-	12/25/74/74	0/4/4/4
2	CYC	B	500	1	-	8/25/74/74	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	CYC	CHA-C1A	4.85	1.39	1.35
2	A	500	CYC	CHA-C1A	2.95	1.37	1.35
2	B	500	CYC	CHB-C4A	2.26	1.45	1.40
2	B	500	CYC	CBA-CGA	2.10	1.55	1.50
2	A	500	CYC	CHB-C4A	2.03	1.45	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	CYC	C4D-CHA-C1A	6.72	136.84	128.81
2	A	500	CYC	C4D-CHA-C1A	3.99	133.58	128.81
2	A	500	CYC	CHA-C1A-NA	-2.65	125.14	128.83
2	A	500	CYC	OC-C1C-C2C	2.44	128.11	126.17
2	B	500	CYC	CHD-C4C-NC	2.43	128.09	125.20
2	B	500	CYC	C2C-C3C-C4C	2.39	104.91	101.34
2	A	500	CYC	CAB-C3B-C4B	2.36	125.11	121.38
2	A	500	CYC	C2C-C3C-C4C	2.29	104.77	101.34
2	B	500	CYC	CBD-CAD-C3D	-2.23	108.81	112.62
2	A	500	CYC	CHD-C4C-NC	2.21	127.83	125.20
2	A	500	CYC	CMD-C2D-C3D	2.18	129.05	124.94
2	A	500	CYC	CHB-C4A-NA	-2.16	120.41	124.93
2	B	500	CYC	CMA-C3A-C4A	2.10	128.30	125.06

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	CYC	NA-C4A-CHB-C1B
2	A	500	CYC	ND-C1D-CHD-C4C
2	A	500	CYC	C2D-C1D-CHD-C4C
2	B	500	CYC	NA-C4A-CHB-C1B
2	B	500	CYC	C3A-C4A-CHB-C1B
2	A	500	CYC	C2B-C3B-CAB-CBB
2	A	500	CYC	C4B-C3B-CAB-CBB
2	B	500	CYC	C2B-C3B-CAB-CBB
2	A	500	CYC	C3A-C4A-CHB-C1B
2	A	500	CYC	NB-C1B-CHB-C4A
2	B	500	CYC	CAD-CBD-CGD-O1D
2	A	500	CYC	C2B-C1B-CHB-C4A
2	A	500	CYC	CAD-CBD-CGD-O1D
2	B	500	CYC	CAD-CBD-CGD-O2D
2	B	500	CYC	CAA-CBA-CGA-O2A
2	A	500	CYC	CAA-CBA-CGA-O1A
2	A	500	CYC	CAA-CBA-CGA-O2A
2	B	500	CYC	CAA-CBA-CGA-O1A
2	A	500	CYC	CAD-CBD-CGD-O2D
2	B	500	CYC	NB-C1B-CHB-C4A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	CYC	3	0
2	B	500	CYC	1	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 then 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.

Ligand CYC A 500

Bond lengths

Bond angles

Torsions

Rings

Ligand CYC B 500

Bond lengths

Bond angles

Torsions

Rings
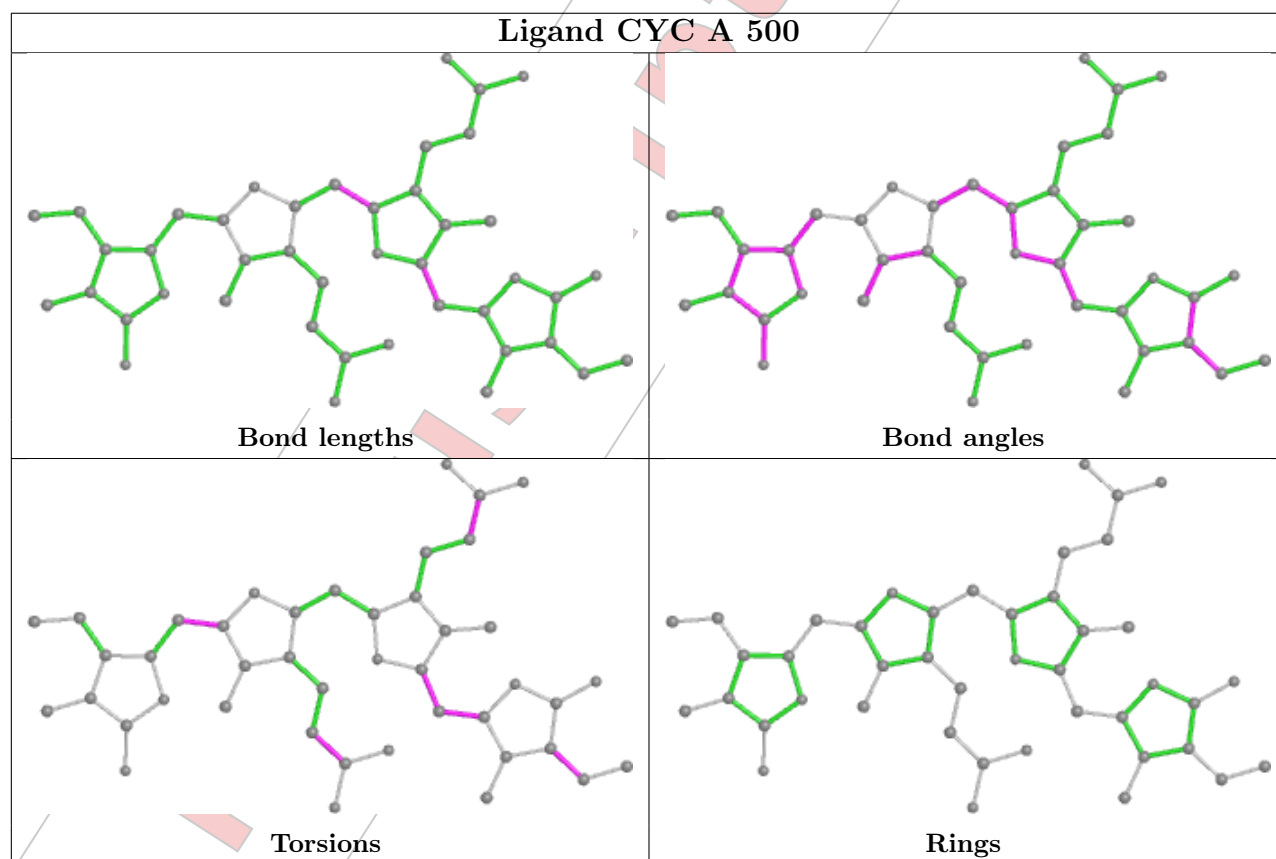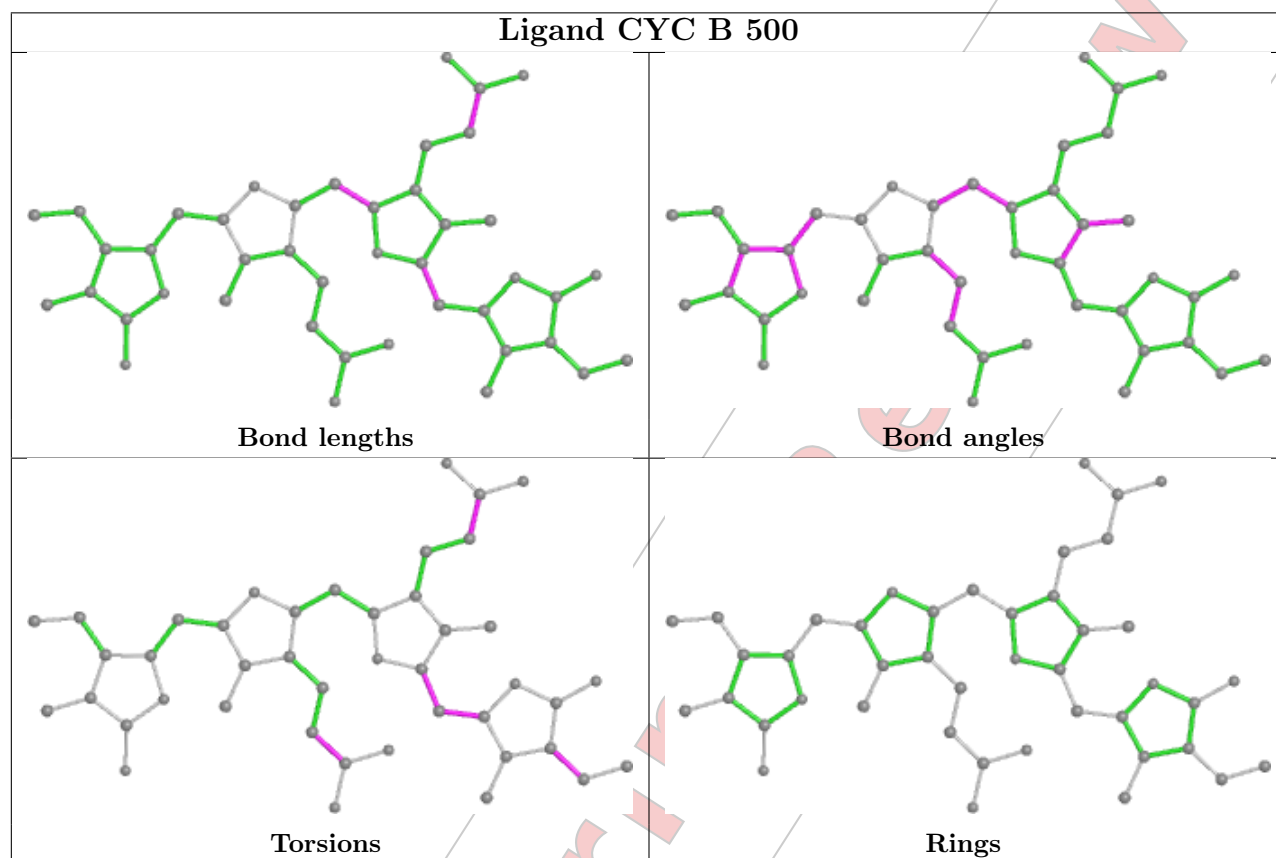
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	306/359 (85%)	0.14	23 (7%)	14	13	26, 43, 78, 131	0
1	B	309/359 (86%)	-0.03	19 (6%)	21	20	28, 42, 72, 96	0
All	All	615/718 (85%)	0.06	42 (6%)	17	16	26, 43, 77, 131	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	73	HIS	8.8
1	B	110	VAL	8.3
1	B	121	PRO	8.0
1	A	120	HIS	7.9
1	A	71	LEU	7.6
1	A	119	ASP	6.8
1	A	72	HIS	6.4
1	B	69	ALA	5.0
1	B	71	LEU	4.7
1	B	147	PHE	4.6
1	A	121	PRO	4.6
1	A	217	GLY	4.3
1	B	150	VAL	4.3
1	A	76	LYS	4.0
1	A	75	GLN	4.0
1	A	326	GLN	4.0
1	B	109	MET	3.9
1	A	74	MET	3.8
1	B	149	GLU	3.6
1	B	360	ARG	3.1
1	A	360	ARG	3.1
1	A	280	PHE	3.0
1	A	361	LYS	2.9
1	B	72	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	162	THR	2.8
1	A	77	GLY	2.7
1	B	75	GLN	2.7
1	B	151	LEU	2.6
1	A	147	PHE	2.5
1	A	401	GLU	2.4
1	B	280	PHE	2.4
1	A	330	ASN	2.4
1	B	70	TYR	2.3
1	B	217	GLY	2.2
1	A	109	MET	2.2
1	A	345	ASP	2.2
1	A	329	ALA	2.1
1	B	146	GLY	2.1
1	B	330	ASN	2.0
1	A	162	THR	2.0
1	B	122	ALA	2.0
1	A	220	GLU	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 monosaccharides 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. 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
2	CYC	A	500	43/43	0.85	0.20	51,60,68,68	0
2	CYC	B	500	43/43	0.91	0.14	43,50,58,62	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.
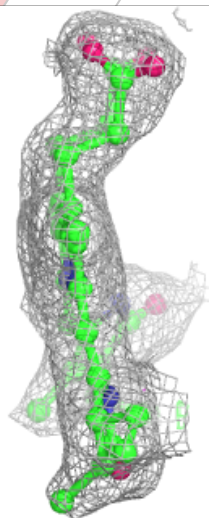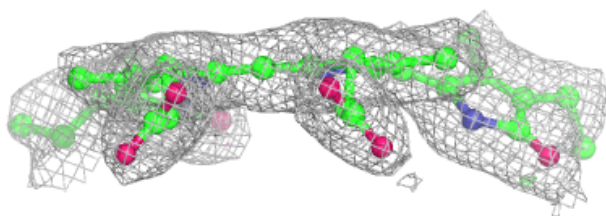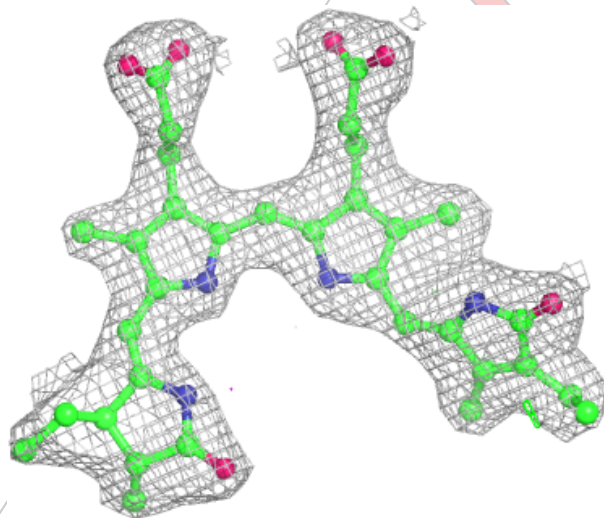
Electron density around CYC A 500:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
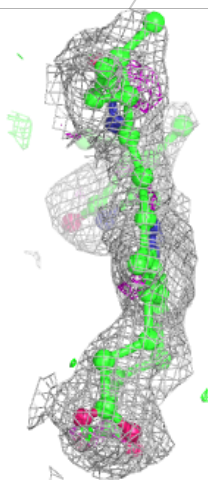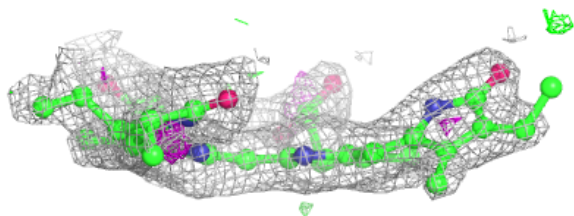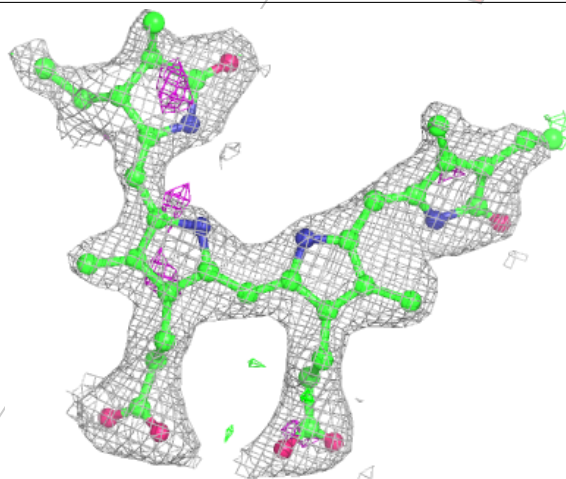
Electron density around CYC B 500:

$2mF_o$-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 ⓘ

There are no such residues in this entry.