



# Full wwPDB X-ray Structure Validation Report i

Jan 2, 2025 – 12:11 pm GMT

PDB ID : 9F4I  
Title : Room temperature structure of Glycine max phyA in Pfr  
Authors : Nagano, S.; Hughes, J.  
Deposited on : 2024-04-28  
Resolution : 2.20 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

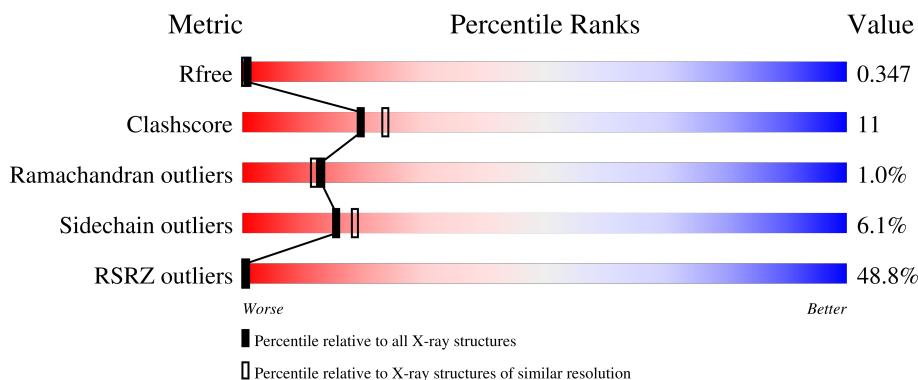
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

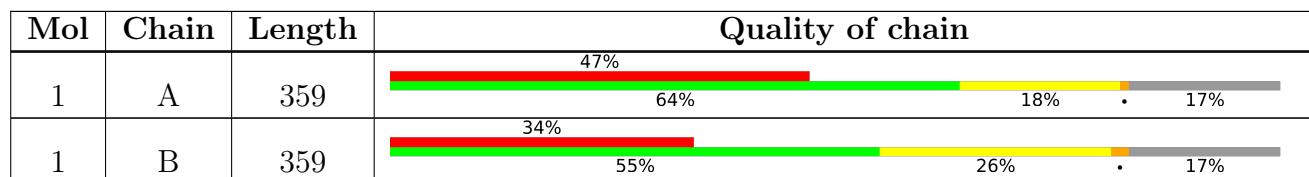
The reported resolution of this entry is 2.20 Å.

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (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  $\geq 3$ , 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  $\leq 5\%$



## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4866 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.

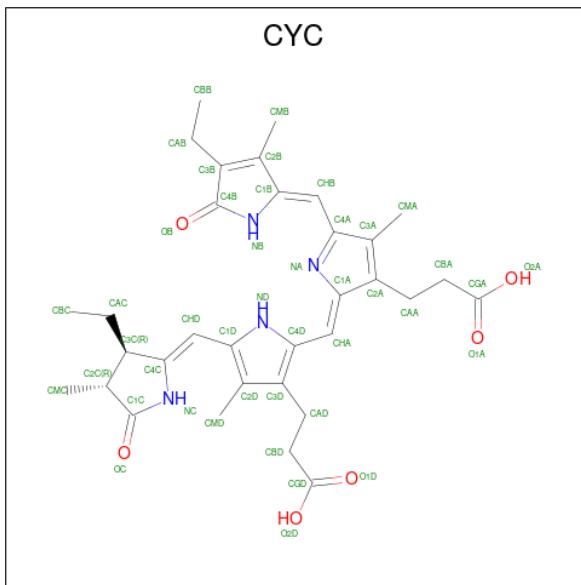
- Molecule 1 is a protein called Phytochrome A-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C 2315	N 1494	O 389	S 410	22	0	0
1	B	299	Total	C 2333	N 1505	O 392	S 414	22	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<sub>33</sub>H<sub>40</sub>N<sub>4</sub>O<sub>6</sub>).



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

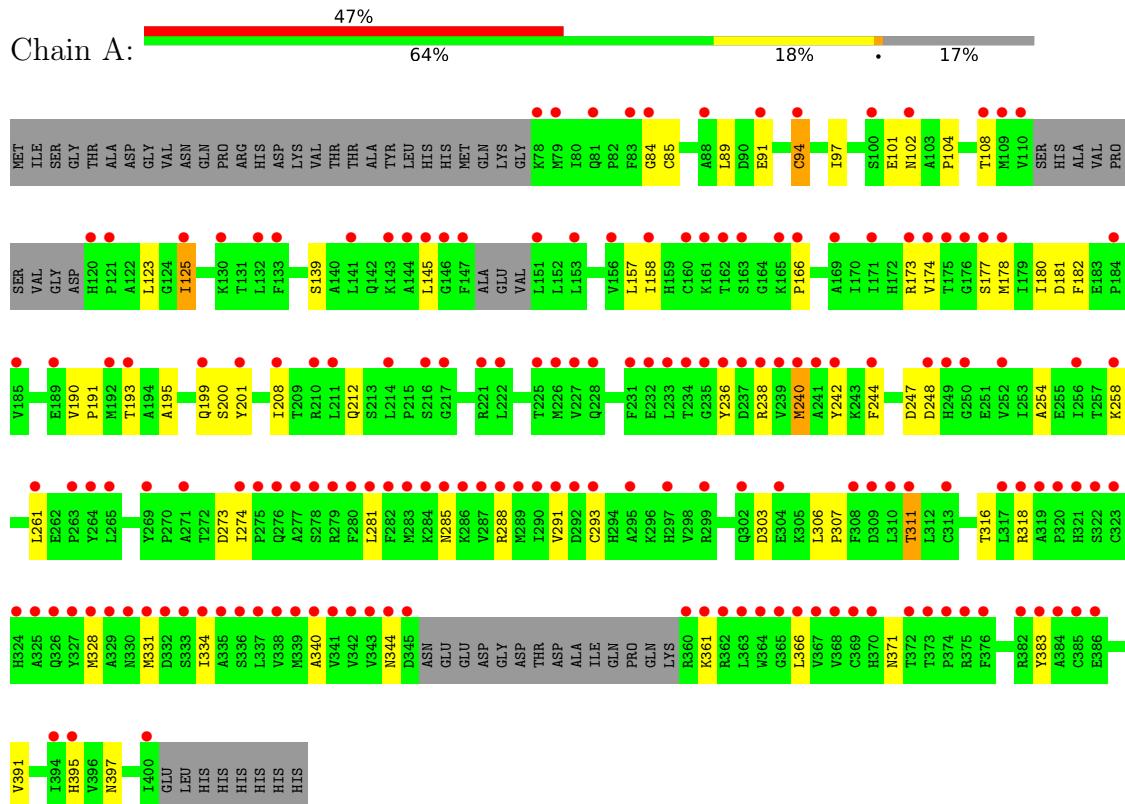
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	60	Total O 60 60	0	0
3	B	72	Total O 72 72	0	0

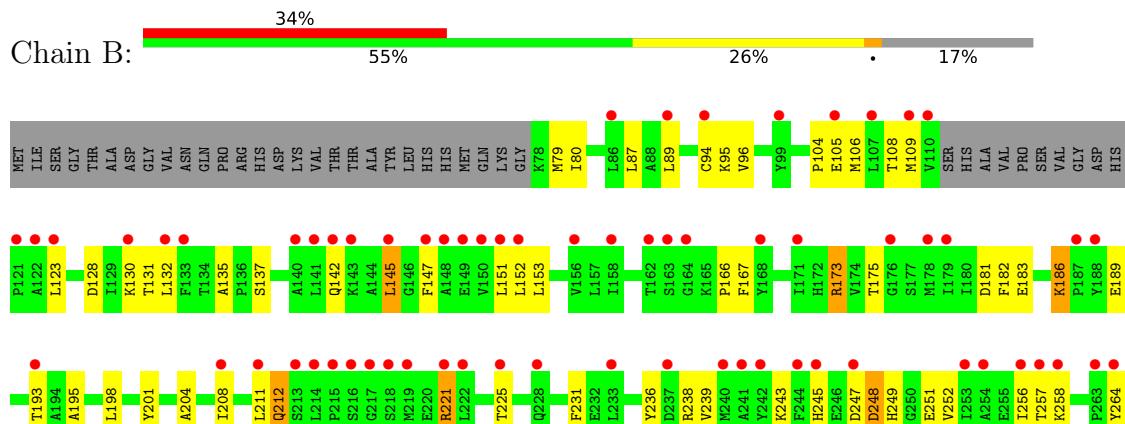
### 3 Residue-property plots [\(i\)](#)

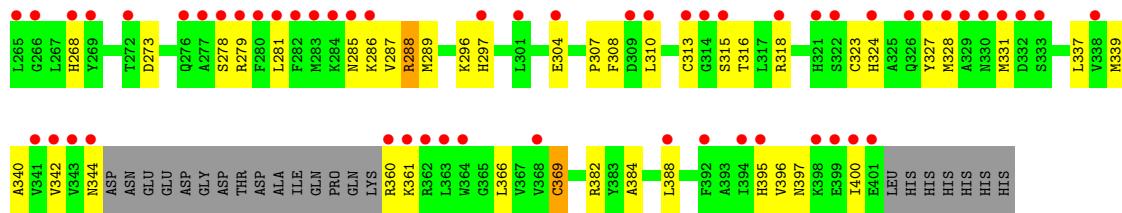
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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



- Molecule 1: Phytochrome A-2





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.45 Å    115.05 Å    69.80 Å 90.00°    92.68°    90.00°	Depositor
Resolution (Å)	20.48 – 2.20 20.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.48-2.20) 99.8 (20.48-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	1.18 (at 2.19 Å)	Xtriage
Refinement program	PHENIX 1.21rc_5156	Depositor
$R$ , $R_{free}$	0.191 , 0.231 0.325 , 0.347	Depositor DCC
$R_{free}$ test set	2310 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.37	0/2368	0.61	0/3209
1	B	0.59	1/2386 (0.0%)	0.79	2/3233 (0.1%)
All	All	0.49	1/4754 (0.0%)	0.70	2/6442 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	CYS	CB-SG	-6.52	1.71	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	145	LEU	CB-CG-CD1	-8.40	96.73	111.00
1	B	310	LEU	CA-CB-CG	5.20	127.25	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts i

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2315	0	2352	46	0
1	B	2333	0	2380	65	0
2	A	43	0	36	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	36	3	0
3	A	60	0	0	10	0
3	B	72	0	0	14	0
All	All	4866	0	4804	109	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 11.

All (109) 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:B:279:ARG:NH2	3:B:601:HOH:O	1.93	1.00
1:A:311:THR:O	3:A:601:HOH:O	1.90	0.90
1:B:285:ASN:HD21	1:B:318:ARG:HH21	1.25	0.84
1:A:101:GLU:O	3:A:602:HOH:O	2.00	0.78
1:A:344:ASN:OD1	1:A:397:ASN:ND2	2.13	0.76
1:B:251:GLU:OE1	1:B:268:HIS:NE2	2.23	0.72
1:B:186:LYS:NZ	3:B:602:HOH:O	2.06	0.71
1:A:212:GLN:OE1	1:B:212:GLN:NE2	2.25	0.69
1:A:208:ILE:HG23	1:A:391:VAL:HG11	1.73	0.68
1:B:285:ASN:ND2	1:B:318:ARG:HH21	1.93	0.66
1:B:186:LYS:HE3	1:B:186:LYS:H	1.61	0.66
1:A:173:ARG:NH2	1:A:174:VAL:O	2.29	0.66
1:A:288:ARG:HG2	3:A:625:HOH:O	1.97	0.64
3:A:619:HOH:O	1:B:195:ALA:HB1	1.98	0.63
1:A:244:PHE:O	3:A:603:HOH:O	2.15	0.63
1:A:285:ASN:HD21	1:A:318:ARG:HH12	1.49	0.60
1:B:183:GLU:CD	1:B:382:ARG:HH22	2.05	0.60
1:B:327:TYR:O	1:B:331:MET:HG2	2.02	0.60
1:B:324:HIS:ND1	3:B:611:HOH:O	2.32	0.59
1:B:135:ALA:N	3:B:604:HOH:O	2.17	0.58
1:A:212:GLN:HG2	1:A:395:HIS:NE2	2.19	0.58
1:B:247:ASP:O	1:B:248:ASP:HB2	2.03	0.57
1:A:101:GLU:OE1	3:A:604:HOH:O	2.18	0.57
1:B:243:LYS:HE2	1:B:245:HIS:HD2	1.69	0.56
1:B:95:LYS:HE3	1:B:128:ASP:HB2	1.89	0.55
1:B:297:HIS:NE2	3:B:605:HOH:O	2.17	0.55
1:A:85:CYS:SG	1:A:182:PHE:HB2	2.46	0.55
1:B:264:TYR:CE2	2:B:500:CYC:HBB1	2.43	0.54
2:B:500:CYC:NA	3:B:611:HOH:O	2.33	0.54
1:B:183:GLU:OE1	1:B:382:ARG:NH2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:MET:HG2	3:B:649:HOH:O	2.08	0.53
1:B:318:ARG:HA	3:B:623:HOH:O	2.09	0.53
1:B:342:VAL:HG12	3:B:644:HOH:O	2.08	0.53
1:A:84:GLY:O	1:A:102:ASN:ND2	2.39	0.53
1:B:208:ILE:O	1:B:212:GLN:HG2	2.09	0.53
1:B:231:PHE:HD1	1:B:239:VAL:HG23	1.73	0.52
1:A:258:LYS:NZ	3:A:612:HOH:O	2.42	0.52
1:A:274:ILE:HD11	2:A:500:CYC:HMA3	1.91	0.52
1:A:273:ASP:HB3	2:A:500:CYC:HHB	1.93	0.51
1:B:208:ILE:HG13	1:B:388:LEU:HD13	1.92	0.51
1:A:177:SER:OG	1:A:178:MET:N	2.44	0.50
1:B:130:LYS:HG3	3:B:663:HOH:O	2.11	0.50
1:A:208:ILE:HD13	1:A:391:VAL:HG21	1.94	0.50
1:B:273:ASP:HB3	2:B:500:CYC:HHB	1.94	0.49
1:A:191:PRO:HG3	3:B:645:HOH:O	2.12	0.49
1:B:238:ARG:HG3	1:B:257:THR:HG22	1.95	0.49
1:B:189:GLU:O	1:B:193:THR:HG23	2.13	0.48
1:B:258:LYS:HA	1:B:258:LYS:HE2	1.95	0.48
1:B:212:GLN:HA	1:B:395:HIS:HE1	1.79	0.48
1:B:397:ASN:HA	1:B:400:ILE:HD12	1.95	0.48
1:A:331:MET:HE1	2:A:500:CYC:HMB2	1.96	0.48
1:A:97:ILE:HD11	1:A:177:SER:HB2	1.96	0.47
1:A:125:ILE:HG21	1:A:303:ASP:HB2	1.95	0.47
1:A:181:ASP:OD2	1:A:316:THR:N	2.42	0.47
1:B:204:ALA:HB2	1:B:384:ALA:HB1	1.96	0.47
1:B:147:PHE:HD2	1:B:151:LEU:HB3	1.81	0.46
1:B:152:LEU:HD21	3:B:670:HOH:O	2.16	0.46
1:A:104:PRO:O	1:A:108:THR:OG1	2.26	0.45
1:A:285:ASN:ND2	1:A:318:ARG:HH12	2.14	0.45
1:B:285:ASN:O	1:B:287:VAL:N	2.48	0.45
1:B:212:GLN:HG2	1:B:212:GLN:H	1.53	0.45
1:B:245:HIS:ND1	1:B:249:HIS:CE1	2.85	0.45
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.73	0.45
1:B:94:CYS:SG	1:B:145:LEU:HD11	2.56	0.45
1:B:89:LEU:HD23	1:B:96:VAL:HA	1.98	0.44
1:B:285:ASN:HD21	1:B:318:ARG:NH2	2.04	0.44
1:A:254:ALA:HA	3:A:605:HOH:O	2.16	0.44
1:A:281:LEU:HA	1:A:281:LEU:HD23	1.84	0.44
1:B:396:VAL:O	1:B:400:ILE:HG13	2.18	0.44
1:A:236:TYR:CD2	1:A:371:ASN:HB2	2.52	0.44
1:B:87:LEU:HD12	1:B:182:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ALA:HA	1:B:366:LEU:HD23	2.00	0.44
1:A:306:LEU:HA	1:A:307:PRO:HD3	1.87	0.44
1:B:288:ARG:HD3	1:B:289:MET:N	2.33	0.43
1:A:247:ASP:O	1:A:248:ASP:HB2	2.18	0.43
1:B:80:ILE:HG22	3:B:623:HOH:O	2.18	0.43
1:B:344:ASN:O	1:B:361:LYS:HE2	2.17	0.43
1:A:240:MET:HE3	1:A:240:MET:HB3	1.85	0.43
1:B:181:ASP:OD2	1:B:316:THR:OG1	2.29	0.43
1:A:242:TYR:HE2	2:A:500:CYC:O2A	2.02	0.43
1:B:145:LEU:HA	1:B:173:ARG:NH2	2.34	0.43
1:A:195:ALA:HB1	1:B:153:LEU:HB3	2.00	0.43
1:B:236:TYR:CB	1:B:369:CYS:HB3	2.49	0.42
1:A:94:CYS:SG	1:A:145:LEU:HD13	2.59	0.42
1:B:108:THR:HG22	1:B:132:LEU:HD22	2.01	0.42
1:B:104:PRO:HD2	3:B:619:HOH:O	2.18	0.42
1:A:293:CYS:SG	1:A:334:ILE:HA	2.60	0.42
1:B:281:LEU:HB3	1:B:318:ARG:NH2	2.34	0.42
1:A:306:LEU:HD12	1:A:307:PRO:CD	2.50	0.42
1:A:328:MET:HG2	3:A:653:HOH:O	2.19	0.42
1:B:243:LYS:HE2	1:B:245:HIS:CD2	2.52	0.42
1:A:89:LEU:HD11	1:A:180:ILE:HD11	2.01	0.41
1:A:190:VAL:O	1:A:193:THR:HG23	2.20	0.41
1:A:199:GLN:HG2	1:B:153:LEU:HD21	2.02	0.41
1:B:221:ARG:O	1:B:225:THR:OG1	2.35	0.41
1:A:91:GLU:O	1:A:145:LEU:HD11	2.20	0.41
2:A:500:CYC:HC	2:A:500:CYC:HD	1.69	0.41
1:A:157:LEU:HD11	1:A:166:PRO:HB2	2.03	0.41
1:B:256:ILE:HG13	1:B:257:THR:N	2.36	0.41
1:A:340:ALA:HA	1:A:366:LEU:HD23	2.03	0.41
1:B:106:MET:CE	1:B:167:PHE:HE2	2.34	0.41
1:B:288:ARG:HD3	1:B:288:ARG:C	2.42	0.41
1:B:307:PRO:HG2	1:B:308:PHE:CD2	2.56	0.41
1:B:123:LEU:HD13	1:B:132:LEU:HD11	2.04	0.40
1:B:236:TYR:CG	1:B:369:CYS:HB3	2.56	0.40
1:B:245:HIS:ND1	1:B:249:HIS:HE1	2.18	0.40
1:A:291:VAL:HB	3:A:618:HOH:O	2.21	0.40
1:A:383:TYR:CD2	1:B:198:LEU:HD13	2.57	0.40
1:A:238:ARG:NH2	1:A:261:LEU:HD12	2.36	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	289/359 (80%)	280 (97%)	8 (3%)	1 (0%)	37 42
1	B	293/359 (82%)	277 (94%)	11 (4%)	5 (2%)	7 5
All	All	582/718 (81%)	557 (96%)	19 (3%)	6 (1%)	13 12

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	286	LYS
1	B	252	VAL
1	B	175	THR
1	B	248	ASP
1	B	166	PRO
1	A	125	ILE

### 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	254/307 (83%)	245 (96%)	9 (4%)	31 41
1	B	256/307 (83%)	234 (91%)	22 (9%)	8 9
All	All	510/614 (83%)	479 (94%)	31 (6%)	15 18

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	CYS
1	A	123	LEU
1	A	139	SER
1	A	158	ILE
1	A	200	SER
1	A	201	TYR
1	A	240	MET
1	A	311	THR
1	A	361	LYS
1	B	79	MET
1	B	105	GLU
1	B	109	MET
1	B	131	THR
1	B	137	SER
1	B	142	GLN
1	B	173	ARG
1	B	186	LYS
1	B	201	TYR
1	B	211	LEU
1	B	212	GLN
1	B	221	ARG
1	B	278	SER
1	B	288	ARG
1	B	296	LYS
1	B	304	GLU
1	B	313	CYS
1	B	315	SER
1	B	323	CYS
1	B	337	LEU
1	B	339	MET
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	390	GLN
1	B	285	ASN
1	B	297	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 [\(i\)](#)

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	B	500	1	42,46,46	1.10	1 (2%)	50,67,67	1.08	3 (6%)
2	CYC	A	500	1	42,46,46	1.14	1 (2%)	50,67,67	1.13	4 (8%)

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	B	500	1	-	10/25/74/74	0/4/4/4
2	CYC	A	500	1	-	10/25/74/74	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	CYC	CHA-C1A	5.85	1.40	1.35
2	B	500	CYC	CHA-C1A	5.14	1.39	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	CYC	CMB-C2B-C1B	3.90	129.04	124.17
2	B	500	CYC	CMB-C2B-C1B	3.52	128.56	124.17
2	A	500	CYC	C1B-CHB-C4A	3.05	135.53	128.08
2	B	500	CYC	CHA-C1A-NA	-2.75	125.02	128.83
2	A	500	CYC	CHA-C1A-NA	-2.46	125.41	128.83
2	B	500	CYC	C2C-C3C-C4C	2.23	104.68	101.34
2	A	500	CYC	C2C-C3C-C4C	2.16	104.57	101.34

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	CYC	C3A-C4A-CHB-C1B
2	A	500	CYC	NB-C1B-CHB-C4A
2	A	500	CYC	C2B-C1B-CHB-C4A
2	A	500	CYC	C2C-C3C-CAC-CBC
2	A	500	CYC	C4C-C3C-CAC-CBC
2	B	500	CYC	C3A-C4A-CHB-C1B
2	B	500	CYC	NB-C1B-CHB-C4A
2	B	500	CYC	C2B-C1B-CHB-C4A
2	B	500	CYC	C2C-C3C-CAC-CBC
2	B	500	CYC	C4C-C3C-CAC-CBC
2	A	500	CYC	NA-C4A-CHB-C1B
2	B	500	CYC	NA-C4A-CHB-C1B
2	A	500	CYC	CAA-CBA-CGA-O1A
2	A	500	CYC	CAD-CBD-CGD-O1D
2	A	500	CYC	CAA-CBA-CGA-O2A
2	A	500	CYC	CAD-CBD-CGD-O2D
2	B	500	CYC	CAD-CBD-CGD-O2D
2	B	500	CYC	CAD-CBD-CGD-O1D
2	B	500	CYC	CAA-CBA-CGA-O2A
2	B	500	CYC	CAA-CBA-CGA-O1A

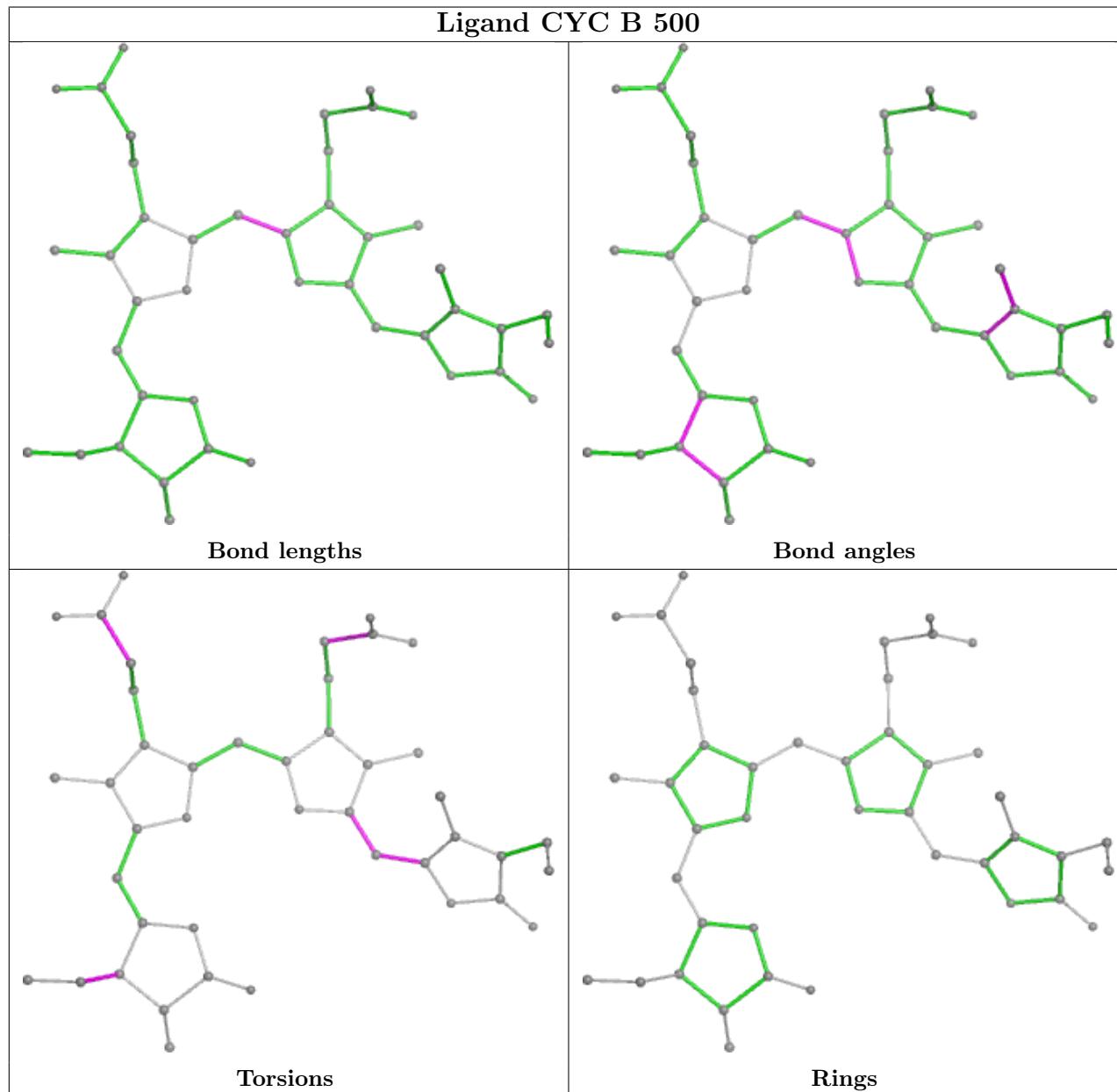
There are no ring outliers.

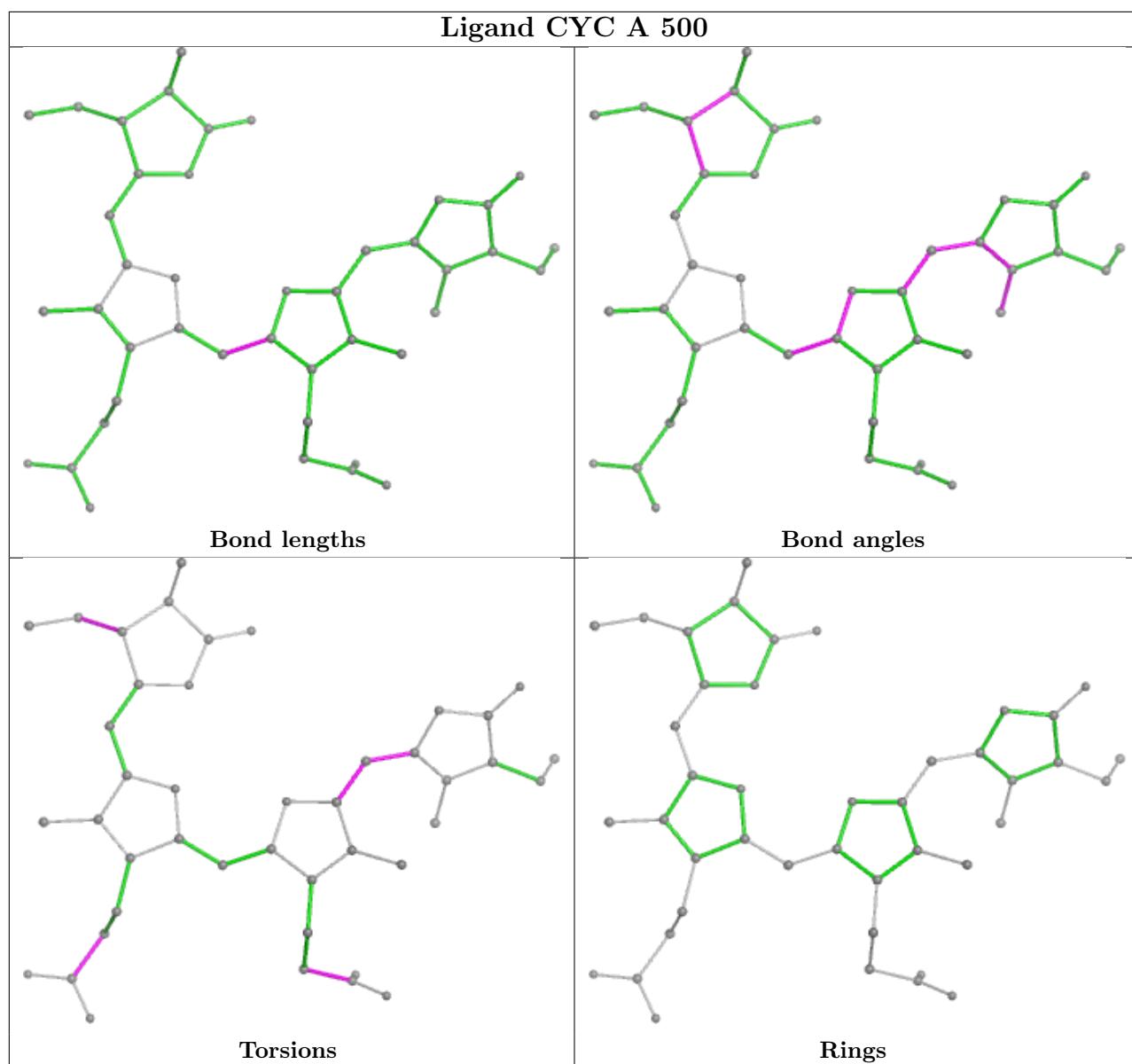
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	CYC	3	0
2	A	500	CYC	5	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

**Warning:** The R factor obtained from EDS is 0.3312, which does not match the depositor's R factor of 0.1907. Please interpret the results in this section carefully.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	297/359 (82%)	2.28	170 (57%) 0   0	34, 50, 86, 132	0
1	B	299/359 (83%)	1.93	121 (40%) 1   0	34, 48, 89, 143	0
All	All	596/718 (83%)	2.11	291 (48%) 0   0	34, 49, 87, 143	0

All (291) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	TYR	9.5
1	B	242	TYR	8.3
1	A	145	LEU	7.8
1	A	282	PHE	6.8
1	B	121	PRO	6.5
1	A	327	TYR	6.3
1	B	247	ASP	6.1
1	B	110	VAL	5.9
1	B	330	ASN	5.9
1	A	280	PHE	5.8
1	A	269	TYR	5.6
1	A	325	ALA	5.4
1	A	285	ASN	5.4
1	A	369	CYS	5.4
1	B	277	ALA	5.3
1	B	282	PHE	5.1
1	B	269	TYR	5.0
1	B	280	PHE	5.0
1	B	109	MET	5.0
1	B	278	SER	4.9
1	A	110	VAL	4.9
1	A	324	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	327	TYR	4.7
1	B	150	VAL	4.6
1	A	175	THR	4.5
1	A	147	PHE	4.5
1	B	147	PHE	4.4
1	B	148	ALA	4.4
1	B	152	LEU	4.3
1	A	288	ARG	4.2
1	A	334	ILE	4.2
1	A	281	LEU	4.2
1	A	328	MET	4.2
1	B	213	SER	4.2
1	A	120	HIS	4.2
1	A	279	ARG	4.2
1	A	176	GLY	4.1
1	B	328	MET	4.0
1	B	122	ALA	4.0
1	A	385	CYS	4.0
1	A	151	LEU	4.0
1	B	145	LEU	4.0
1	B	149	GLU	4.0
1	B	399	GLU	4.0
1	B	368	VAL	4.0
1	B	322	SER	4.0
1	A	121	PRO	4.0
1	B	240	MET	3.9
1	A	340	ALA	3.9
1	B	151	LEU	3.9
1	A	211	LEU	3.8
1	A	304	GLU	3.8
1	B	343	VAL	3.8
1	A	337	LEU	3.8
1	A	235	GLY	3.7
1	A	326	GLN	3.7
1	A	372	THR	3.7
1	A	256	ILE	3.7
1	A	291	VAL	3.7
1	B	331	MET	3.7
1	A	290	ILE	3.7
1	B	341	VAL	3.6
1	A	177	SER	3.6
1	A	109	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	364	TRP	3.6
1	A	283	MET	3.6
1	B	285	ASN	3.5
1	A	193	THR	3.5
1	A	189	GLU	3.5
1	A	264	TYR	3.5
1	B	286	LYS	3.5
1	A	252	VAL	3.5
1	B	142	GLN	3.4
1	A	286	LYS	3.4
1	A	231	PHE	3.4
1	A	331	MET	3.4
1	B	143	LYS	3.4
1	A	250	GLY	3.4
1	A	320	PRO	3.3
1	B	362	ARG	3.3
1	A	329	ALA	3.3
1	A	311	THR	3.3
1	A	244	PHE	3.3
1	B	401	GLU	3.3
1	A	310	LEU	3.3
1	A	368	VAL	3.2
1	B	281	LEU	3.2
1	A	384	ALA	3.2
1	B	329	ALA	3.2
1	A	91	GLU	3.2
1	A	178	MET	3.2
1	A	275	PRO	3.2
1	A	336	SER	3.2
1	B	276	GLN	3.1
1	A	78	LYS	3.1
1	A	323	CYS	3.1
1	A	366	LEU	3.1
1	B	361	LYS	3.1
1	A	386	GLU	3.1
1	B	219	MET	3.1
1	B	211	LEU	3.1
1	A	330	ASN	3.1
1	B	344	ASN	3.1
1	A	338	VAL	3.1
1	A	192	MET	3.1
1	A	292	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	241	ALA	3.0
1	B	301	LEU	3.0
1	A	163	SER	3.0
1	A	367	VAL	3.0
1	A	332	ASP	3.0
1	A	374	PRO	3.0
1	B	99	TYR	3.0
1	A	141	LEU	3.0
1	A	345	ASP	3.0
1	B	221	ARG	3.0
1	B	324	HIS	3.0
1	B	310	LEU	3.0
1	B	244	PHE	3.0
1	B	360	ARG	3.0
1	A	321	HIS	2.9
1	B	264	TYR	2.9
1	A	237	ASP	2.9
1	A	199	GLN	2.9
1	A	284	LYS	2.9
1	B	217	GLY	2.9
1	A	216	SER	2.9
1	B	313	CYS	2.9
1	B	237	ASP	2.9
1	A	271	ALA	2.9
1	A	226	MET	2.9
1	A	173	ARG	2.9
1	A	158	ILE	2.9
1	A	302	GLN	2.9
1	A	322	SER	2.8
1	A	236	TYR	2.8
1	A	319	ALA	2.8
1	B	178	MET	2.8
1	B	89	LEU	2.8
1	B	215	PRO	2.8
1	B	283	MET	2.8
1	A	261	LEU	2.8
1	A	239	VAL	2.7
1	A	339	MET	2.7
1	B	309	ASP	2.7
1	A	364	TRP	2.7
1	B	326	GLN	2.7
1	A	361	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	221	ARG	2.7
1	B	179	ILE	2.7
1	A	217	GLY	2.7
1	A	363	LEU	2.7
1	B	253	ILE	2.7
1	B	256	ILE	2.7
1	A	287	VAL	2.7
1	B	266	GLY	2.6
1	B	225	THR	2.6
1	A	293	CYS	2.6
1	A	313	CYS	2.6
1	A	394	ILE	2.6
1	B	171	ILE	2.6
1	B	257	THR	2.6
1	B	216	SER	2.6
1	A	370	HIS	2.6
1	B	321	HIS	2.6
1	B	105	GLU	2.6
1	B	188	TYR	2.6
1	B	107	LEU	2.6
1	B	272	THR	2.6
1	B	94	CYS	2.6
1	B	332	ASP	2.6
1	A	240	MET	2.6
1	A	295	ALA	2.6
1	A	342	VAL	2.6
1	A	162	THR	2.6
1	B	394	ILE	2.6
1	A	248	ASP	2.6
1	B	318	ARG	2.6
1	B	156	VAL	2.5
1	B	342	VAL	2.5
1	A	144	ALA	2.5
1	B	392	PHE	2.5
1	A	208	ILE	2.5
1	B	400	ILE	2.5
1	A	153	LEU	2.5
1	B	132	LEU	2.5
1	B	222	LEU	2.5
1	B	398	LYS	2.5
1	A	228	GLN	2.5
1	A	360	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	100	SER	2.5
1	B	314	GLY	2.5
1	A	335	ALA	2.5
1	B	254	ALA	2.5
1	A	233	LEU	2.5
1	A	166	PRO	2.5
1	A	79	MET	2.4
1	A	395	HIS	2.4
1	B	140	ALA	2.4
1	B	268	HIS	2.4
1	B	297	HIS	2.4
1	A	184	PRO	2.4
1	A	333	SER	2.4
1	A	375	ARG	2.4
1	B	228	GLN	2.4
1	A	376	PHE	2.4
1	A	278	SER	2.4
1	B	218	SER	2.4
1	A	210	ARG	2.4
1	A	132	LEU	2.4
1	B	241	ALA	2.4
1	A	234	THR	2.4
1	A	274	ILE	2.4
1	A	400	ILE	2.4
1	A	238	ARG	2.4
1	A	318	ARG	2.4
1	A	382	ARG	2.4
1	A	160	CYS	2.4
1	B	187	PRO	2.3
1	B	315	SER	2.3
1	A	201	TYR	2.3
1	A	383	TYR	2.3
1	A	222	LEU	2.3
1	A	88	ALA	2.3
1	A	344	ASN	2.3
1	A	225	THR	2.3
1	A	249	HIS	2.3
1	A	317	LEU	2.3
1	A	130	LYS	2.3
1	B	258	LYS	2.3
1	A	289	MET	2.3
1	B	141	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	174	VAL	2.3
1	B	158	ILE	2.3
1	B	208	ILE	2.3
1	A	232	GLU	2.2
1	B	168	TYR	2.2
1	A	102	ASN	2.2
1	A	308	PHE	2.2
1	B	333	SER	2.2
1	A	185	VAL	2.2
1	B	338	VAL	2.2
1	A	171	ILE	2.2
1	B	284	LYS	2.2
1	B	233	LEU	2.2
1	A	277	ALA	2.2
1	A	81	GLN	2.2
1	A	165	LYS	2.2
1	A	84	GLY	2.2
1	A	299	ARG	2.2
1	A	297	HIS	2.2
1	B	395	HIS	2.2
1	A	276	GLN	2.2
1	A	341	VAL	2.2
1	A	343	VAL	2.2
1	A	309	ASP	2.2
1	A	146	GLY	2.1
1	B	176	GLY	2.1
1	B	123	LEU	2.1
1	B	363	LEU	2.1
1	A	263	PRO	2.1
1	A	258	LYS	2.1
1	A	125	ILE	2.1
1	A	94	CYS	2.1
1	A	214	LEU	2.1
1	B	214	LEU	2.1
1	B	263	PRO	2.1
1	A	133	PHE	2.1
1	B	133	PHE	2.1
1	B	163	SER	2.1
1	B	279	ARG	2.1
1	B	130	LYS	2.1
1	A	108	THR	2.1
1	B	162	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	193	THR	2.1
1	A	156	VAL	2.1
1	A	362	ARG	2.1
1	A	143	LYS	2.1
1	A	161	LYS	2.1
1	A	373	THR	2.1
1	B	304	GLU	2.0
1	A	227	VAL	2.0
1	A	83	PHE	2.0
1	A	365	GLY	2.0
1	B	265	LEU	2.0
1	A	169	ALA	2.0
1	B	164	GLY	2.0
1	B	245	HIS	2.0
1	A	265	LEU	2.0
1	B	86	LEU	2.0
1	B	388	LEU	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 [\(i\)](#)

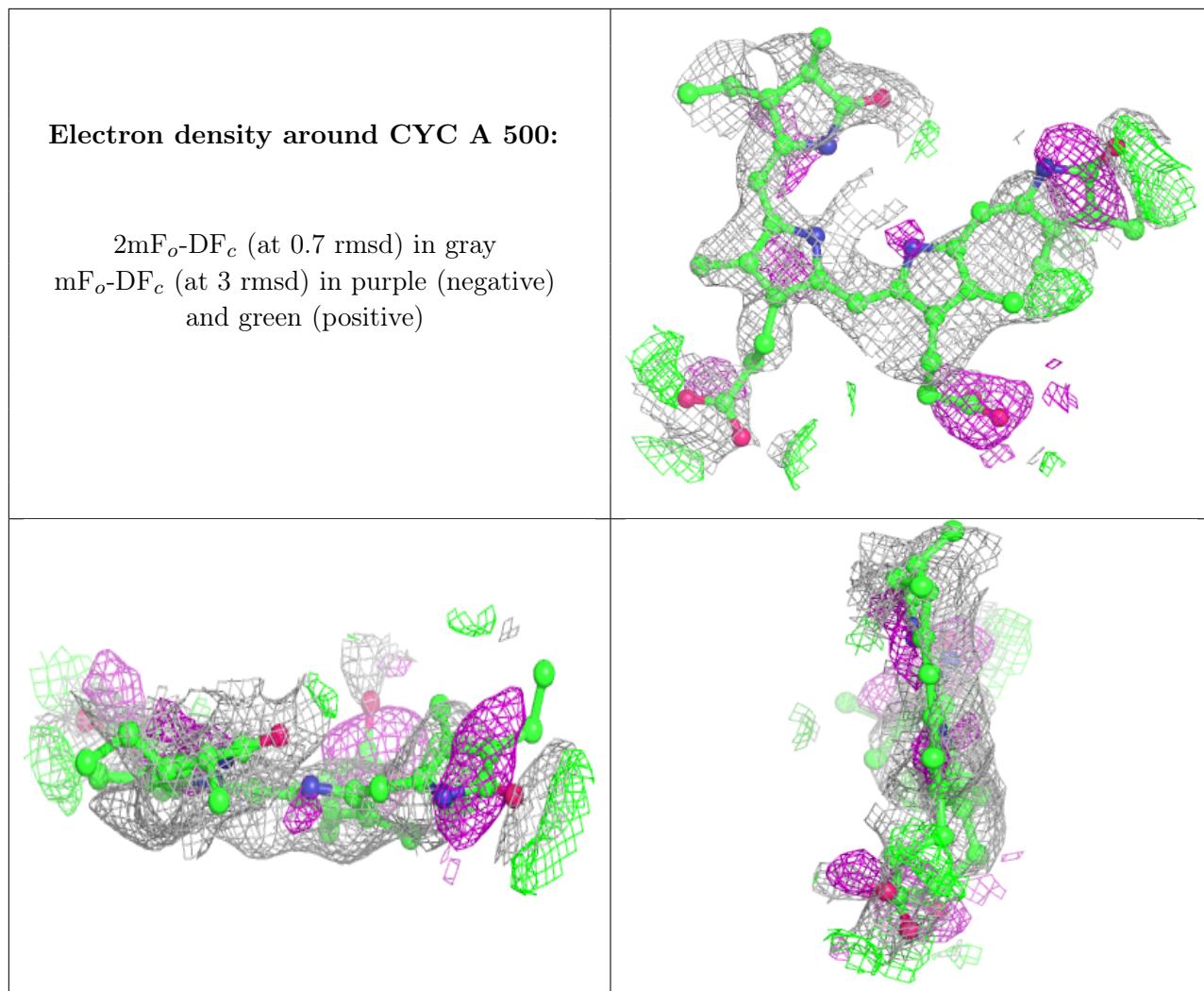
There are no monosaccharides in this entry.

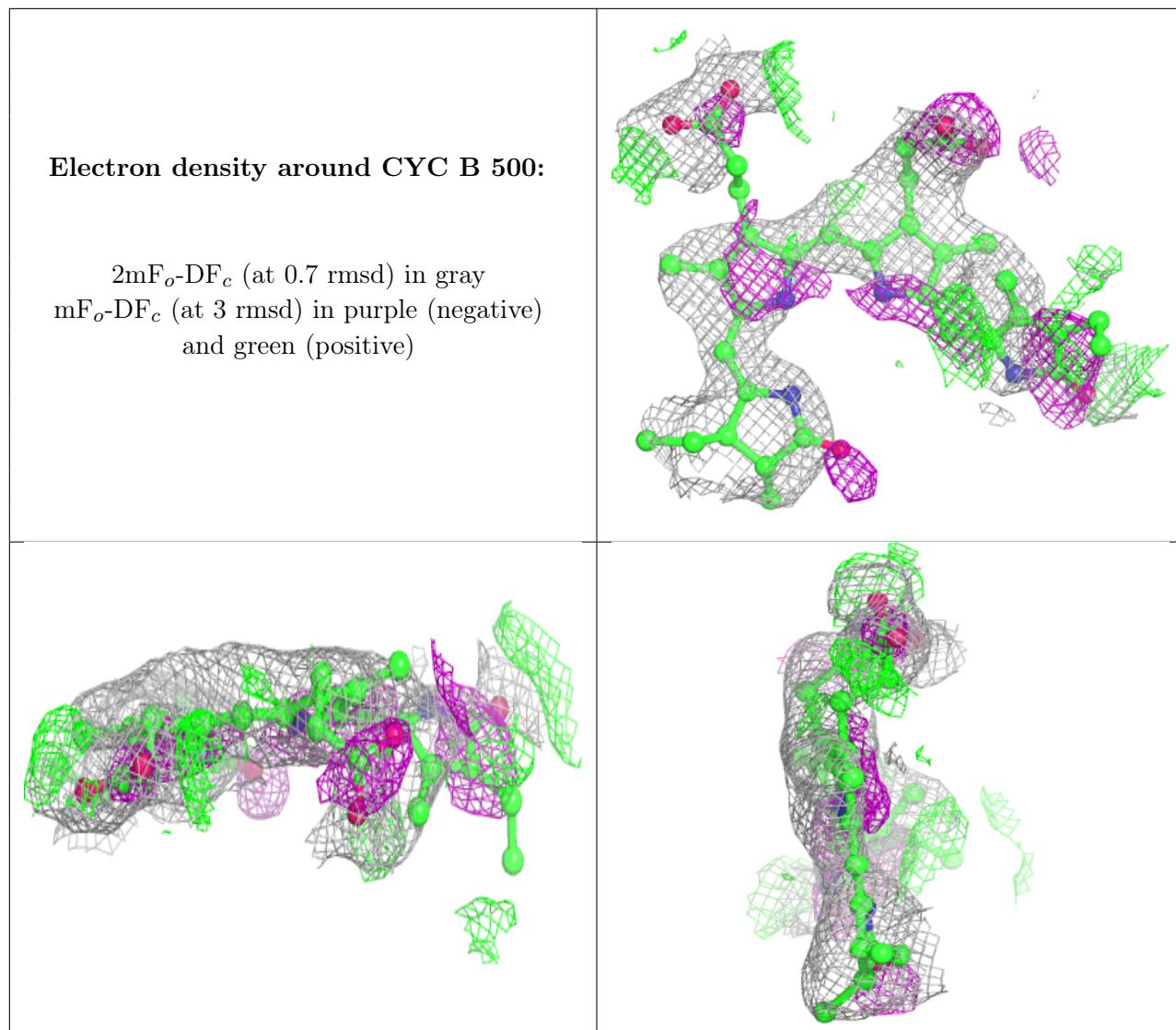
## 6.4 Ligands [\(i\)](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	CYC	A	500	43/43	0.31	0.30	58,75,89,91	0
2	CYC	B	500	43/43	0.44	0.28	40,63,80,95	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.