



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:54 AM UTC

PDB ID : 9F4I / pdb_00009f4i
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

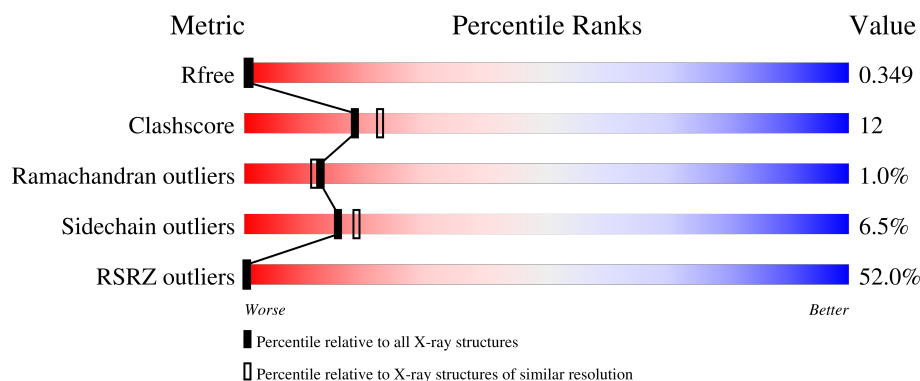
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	359	51% 64% 18% • 17%
1	B	359	36% 54% 27% • 17%

2 Entry composition

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.

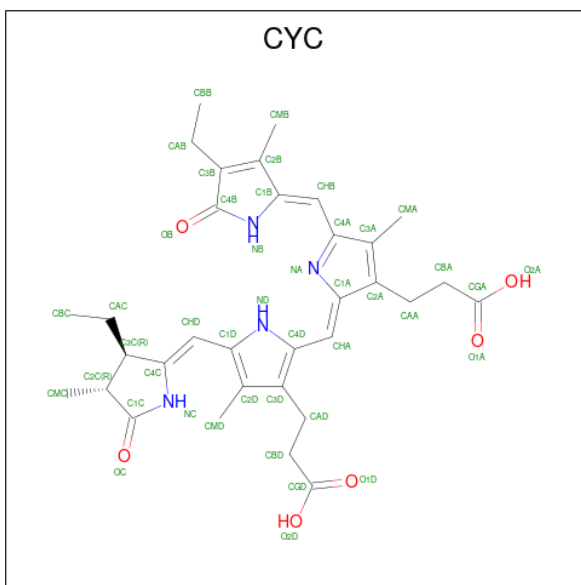
- Molecule 1 is a protein called Phytochrome A-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2315	1494	389	410	22			
1	B	299	Total	C	N	O	S	0	0	0
			2333	1505	392	414	22			

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 (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$).



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

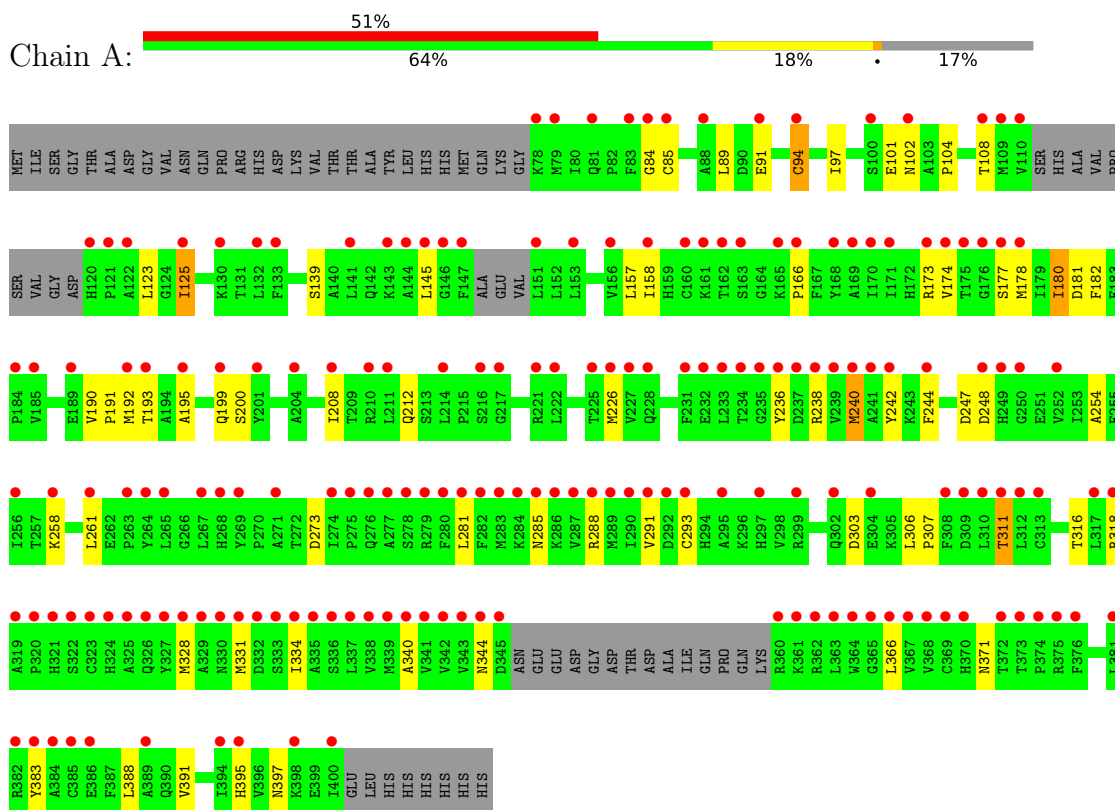
- Molecule 3 is water.

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

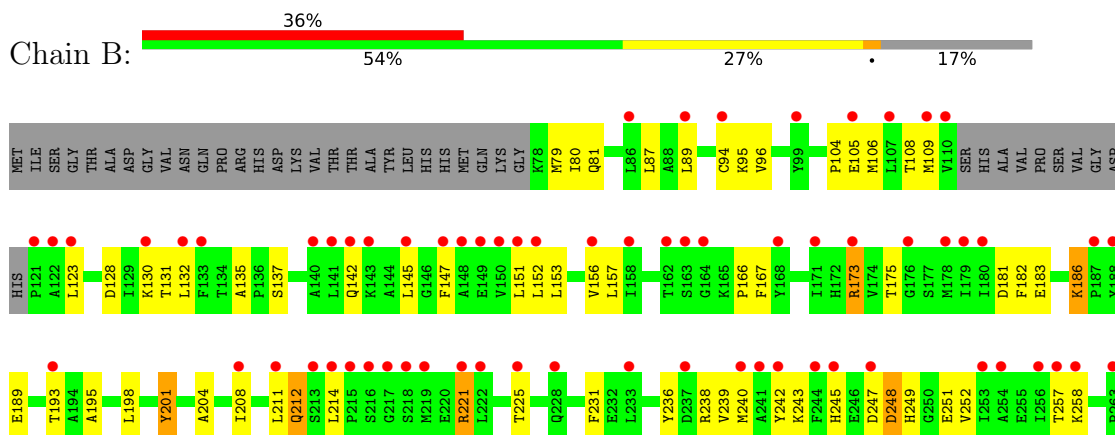
3 Residue-property plots

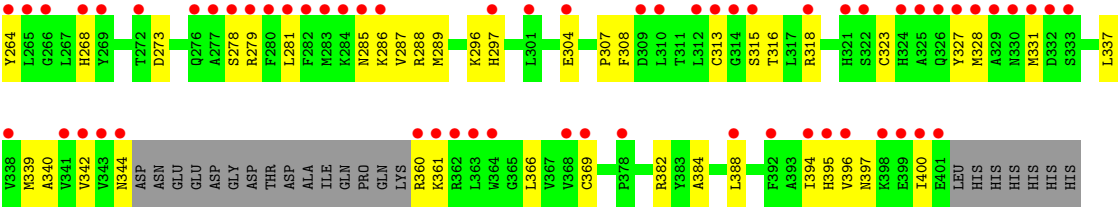
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Phytochrome A-2





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)	99.9 (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 2.19Å)	Xtriage
Refinement program	PHENIX 1.21rc_5156	Depositor
R, R_{free}	0.191 , 0.231 0.326 , 0.349	Depositor DCC
R_{free} test set	2311 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	45.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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: 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	0.32	0/2368	0.55	0/3209
1	B	0.53	0/2386	0.79	0/3233
All	All	0.44	0/4754	0.68	0/6442

There are no bond length outliers.

There are no bond angle outliers.

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	49	0
1	B	2333	0	2380	68	0
2	A	43	0	36	5	0
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	115	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 12.

All (115) 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:226:MET:HE1	1:A:388:LEU:HG	1.67	0.77
1:A:344:ASN:OD1	1:A:397:ASN:ND2	2.13	0.76
1:B:297:HIS:NE2	3:B:605:HOH:O	2.17	0.76
1:B:251:GLU:OE1	1:B:268:HIS:NE2	2.23	0.72
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:A:192:MET:HE1	1:B:156:VAL:HG22	1.76	0.67
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:B:183:GLU:CD	1:B:382:ARG:HH22	2.05	0.64
1:A:288:ARG:HG2	3:A:625:HOH:O	1.97	0.64
1:B:201:TYR:OH	3:B:603:HOH:O	2.13	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:B:240:MET:HE2	1:B:242:TYR:HE1	1.65	0.62
1:A:285:ASN:HD21	1:A:318:ARG:HH12	1.49	0.60
1:B:106:MET:HE2	1:B:167:PHE:CE2	2.37	0.60
1:B:327:TYR:O	1:B:331:MET:HG2	2.02	0.60
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:A:85:CYS:SG	1:A:182:PHE:HB2	2.46	0.55
1:B:106:MET:HE2	1:B:167:PHE:HE2	1.72	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
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:273:ASP:HB3	2:A:500:CYC:HHB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HBB	1.94	0.49
1:A:191:PRO:HG3	3:B:645:HOH:O	2.12	0.49
1:A:145:LEU:HA	1:A:178:MET:HE1	1.93	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: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:258:LYS:NZ	3:A:612:HOH:O	2.42	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:331:MET:HE3	1:B:331:MET:HB2	1.67	0.47
2:A:500:CYC:HMB3	2:A:500:CYC:HMA2	1.98	0.46
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:288:ARG:C	1:B:288:ARG:HD3	2.42	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:A:173:ARG:HD3	1:A:178:MET:HE2	1.99	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:285:ASN:C	3:B:637:HOH:O	2.61	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:A:240:MET:HE3	1:A:240:MET:HB3	1.59	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:181:ASP:OD2	1:B:316:THR:OG1	2.29	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:A:340:ALA:HA	1:A:366:LEU:HD23	2.03	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
1:A:331:MET:HE1	2:A:500:CYC:HMB2	2.04	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%)	36	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%)	12	11

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%)	246 (97%)	8 (3%)	35	48
1	B	256/307 (83%)	231 (90%)	25 (10%)	7	8
All	All	510/614 (83%)	477 (94%)	33 (6%)	15	18

All (33) 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	180	ILE
1	A	200	SER
1	A	240	MET
1	A	311	THR
1	B	79	MET
1	B	81	GLN
1	B	105	GLU
1	B	109	MET
1	B	131	THR
1	B	137	SER
1	B	142	GLN
1	B	157	LEU
1	B	173	ARG
1	B	186	LYS
1	B	201	TYR
1	B	211	LEU
1	B	212	GLN
1	B	214	LEU
1	B	221	ARG
1	B	278	SER
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
1	B	394	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	390	GLN
1	B	285	ASN
1	B	297	HIS
1	B	324	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 oligosaccharides 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	46,46,46	0.77	0	63,67,67	0.97	3 (4%)
2	CYC	B	500	1	46,46,46	0.83	1 (2%)	63,67,67	0.89	2 (3%)

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	-	10/26/74/74	0/4/4/4
2	CYC	B	500	1	-	9/26/74/74	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	CYC	CHD-C4C	2.12	1.40	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	CYC	CMB-C2B-C1B	4.01	129.04	124.16
2	B	500	CYC	CMB-C2B-C1B	3.62	128.56	124.16
2	A	500	CYC	C1B-CHB-C4A	3.05	135.53	128.06
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 (19) 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	CAD-CBD-CGD-O1D
2	A	500	CYC	CAD-CBD-CGD-O2D
2	A	500	CYC	CAA-CBA-CGA-O1A
2	A	500	CYC	CAA-CBA-CGA-O2A
2	B	500	CYC	CAD-CBD-CGD-O2D
2	B	500	CYC	CAD-CBD-CGD-O1D
2	B	500	CYC	CAA-CBA-CGA-O2A

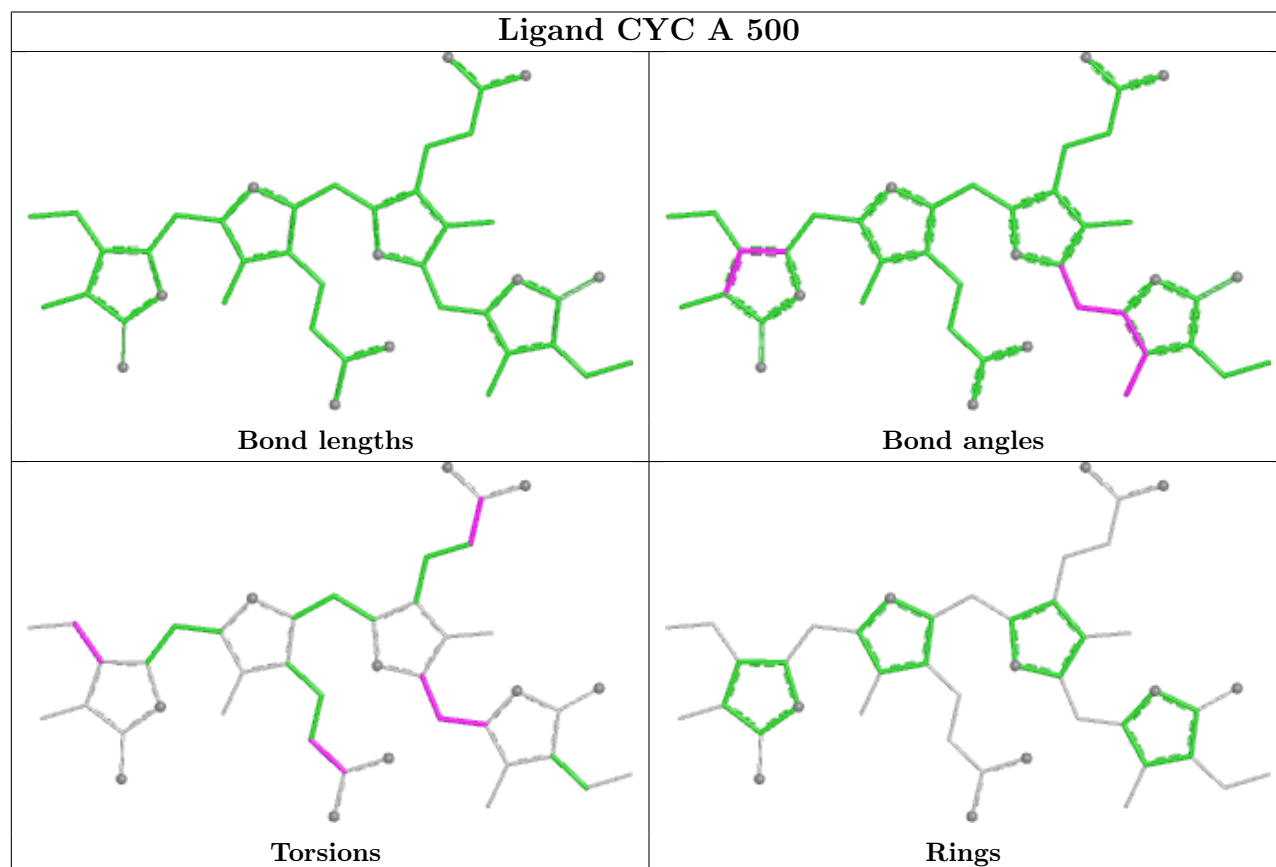
There are no ring outliers.

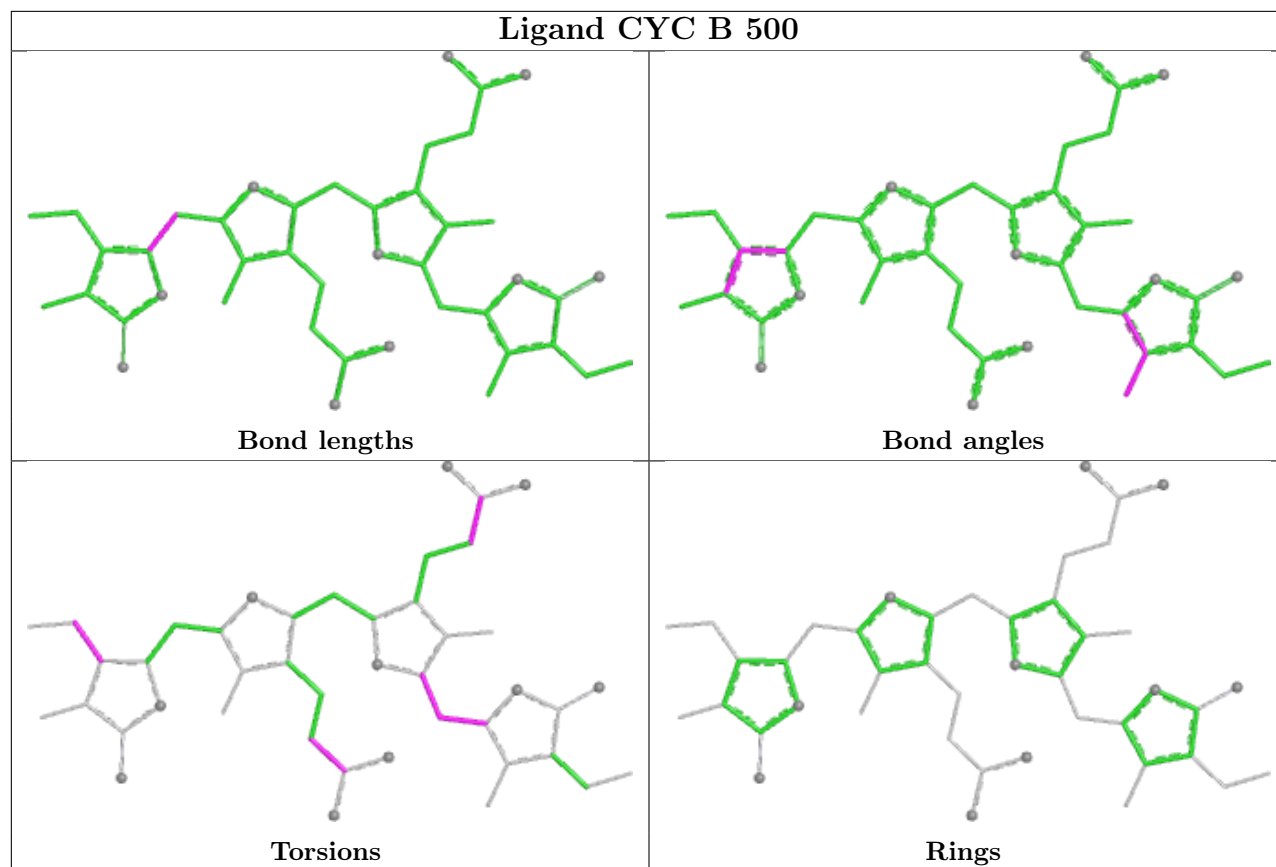
2 monomers are involved in 8 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	297/359 (82%)	2.38	182 (61%) 0 0	34, 50, 86, 132	0
1	B	299/359 (83%)	2.03	128 (42%) 0 0	34, 48, 89, 143	0
All	All	596/718 (83%)	2.21	310 (52%) 0 0	34, 49, 87, 143	0

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	242	TYR	9.7
1	B	242	TYR	8.5
1	A	145	LEU	8.0
1	A	282	PHE	7.0
1	B	121	PRO	6.7
1	A	327	TYR	6.5
1	B	110	VAL	6.1
1	B	247	ASP	6.1
1	A	280	PHE	5.9
1	B	330	ASN	5.9
1	A	269	TYR	5.8
1	A	325	ALA	5.6
1	A	369	CYS	5.5
1	B	277	ALA	5.4
1	A	285	ASN	5.4
1	B	282	PHE	5.2
1	B	269	TYR	5.2
1	B	280	PHE	5.1
1	B	109	MET	5.0
1	A	110	VAL	5.0
1	B	278	SER	5.0
1	A	324	HIS	4.9
1	B	327	TYR	4.8
1	B	150	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	147	PHE	4.6
1	A	175	THR	4.6
1	B	147	PHE	4.5
1	B	148	ALA	4.5
1	B	152	LEU	4.4
1	A	281	LEU	4.3
1	A	334	ILE	4.3
1	A	328	MET	4.3
1	A	120	HIS	4.3
1	B	213	SER	4.3
1	A	176	GLY	4.3
1	A	288	ARG	4.2
1	A	279	ARG	4.2
1	B	122	ALA	4.2
1	A	151	LEU	4.2
1	A	385	CYS	4.1
1	B	368	VAL	4.1
1	B	328	MET	4.1
1	B	145	LEU	4.1
1	A	121	PRO	4.1
1	B	322	SER	4.1
1	B	240	MET	4.0
1	A	340	ALA	4.0
1	B	151	LEU	4.0
1	B	149	GLU	4.0
1	B	399	GLU	4.0
1	A	211	LEU	4.0
1	B	343	VAL	3.9
1	A	337	LEU	3.9
1	A	235	GLY	3.9
1	A	291	VAL	3.8
1	A	372	THR	3.8
1	A	304	GLU	3.8
1	A	256	ILE	3.8
1	A	326	GLN	3.8
1	A	290	ILE	3.8
1	B	341	VAL	3.8
1	B	331	MET	3.7
1	B	364	TRP	3.7
1	A	109	MET	3.7
1	A	264	TYR	3.7
1	A	177	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	283	MET	3.6
1	A	193	THR	3.6
1	B	285	ASN	3.6
1	A	252	VAL	3.6
1	A	231	PHE	3.5
1	A	189	GLU	3.5
1	B	142	GLN	3.5
1	A	250	GLY	3.5
1	A	329	ALA	3.5
1	A	331	MET	3.5
1	A	320	PRO	3.4
1	B	286	LYS	3.4
1	A	286	LYS	3.4
1	A	244	PHE	3.4
1	A	310	LEU	3.4
1	B	143	LYS	3.4
1	A	311	THR	3.4
1	A	368	VAL	3.4
1	A	384	ALA	3.4
1	B	329	ALA	3.4
1	B	362	ARG	3.4
1	B	281	LEU	3.3
1	A	178	MET	3.3
1	A	275	PRO	3.3
1	B	401	GLU	3.3
1	A	366	LEU	3.2
1	A	323	CYS	3.2
1	A	336	SER	3.2
1	A	91	GLU	3.2
1	B	276	GLN	3.2
1	B	219	MET	3.2
1	A	338	VAL	3.2
1	B	211	LEU	3.2
1	A	241	ALA	3.2
1	A	192	MET	3.2
1	A	78	LYS	3.1
1	A	330	ASN	3.1
1	A	367	VAL	3.1
1	B	344	ASN	3.1
1	B	99	TYR	3.1
1	B	301	LEU	3.1
1	B	361	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	386	GLU	3.1
1	A	292	ASP	3.1
1	A	141	LEU	3.1
1	A	374	PRO	3.1
1	A	163	SER	3.1
1	B	244	PHE	3.1
1	B	310	LEU	3.1
1	B	264	TYR	3.1
1	B	324	HIS	3.1
1	A	332	ASP	3.1
1	A	321	HIS	3.0
1	A	345	ASP	3.0
1	B	221	ARG	3.0
1	B	217	GLY	3.0
1	A	271	ALA	3.0
1	A	199	GLN	3.0
1	B	360	ARG	3.0
1	A	237	ASP	3.0
1	B	313	CYS	3.0
1	A	158	ILE	3.0
1	A	236	TYR	3.0
1	A	216	SER	3.0
1	A	226	MET	3.0
1	A	319	ALA	2.9
1	B	237	ASP	2.9
1	B	89	LEU	2.9
1	A	302	GLN	2.9
1	A	322	SER	2.9
1	B	178	MET	2.9
1	A	284	LYS	2.9
1	A	173	ARG	2.9
1	B	215	PRO	2.9
1	A	261	LEU	2.9
1	A	239	VAL	2.9
1	A	364	TRP	2.9
1	B	283	MET	2.9
1	A	339	MET	2.8
1	B	179	ILE	2.8
1	A	217	GLY	2.8
1	A	363	LEU	2.8
1	A	287	VAL	2.8
1	B	253	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	256	ILE	2.8
1	B	309	ASP	2.8
1	B	266	GLY	2.8
1	B	326	GLN	2.8
1	A	394	ILE	2.7
1	B	171	ILE	2.7
1	B	225	THR	2.7
1	A	293	CYS	2.7
1	A	313	CYS	2.7
1	B	188	TYR	2.7
1	B	257	THR	2.7
1	A	361	LYS	2.7
1	A	221	ARG	2.7
1	B	107	LEU	2.7
1	A	295	ALA	2.7
1	A	370	HIS	2.7
1	B	321	HIS	2.7
1	A	342	VAL	2.7
1	B	272	THR	2.7
1	B	216	SER	2.7
1	B	94	CYS	2.7
1	B	156	VAL	2.7
1	B	342	VAL	2.7
1	A	162	THR	2.7
1	B	394	ILE	2.7
1	A	240	MET	2.7
1	A	144	ALA	2.6
1	B	392	PHE	2.6
1	B	332	ASP	2.6
1	B	105	GLU	2.6
1	A	248	ASP	2.6
1	A	208	ILE	2.6
1	B	400	ILE	2.6
1	A	153	LEU	2.6
1	B	132	LEU	2.6
1	B	222	LEU	2.6
1	A	335	ALA	2.6
1	B	254	ALA	2.6
1	B	318	ARG	2.6
1	B	314	GLY	2.6
1	A	233	LEU	2.6
1	B	140	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	166	PRO	2.6
1	A	100	SER	2.6
1	A	228	GLN	2.5
1	A	79	MET	2.5
1	A	184	PRO	2.5
1	A	376	PHE	2.5
1	A	395	HIS	2.5
1	B	268	HIS	2.5
1	B	297	HIS	2.5
1	A	360	ARG	2.5
1	B	241	ALA	2.5
1	B	398	LYS	2.5
1	A	333	SER	2.5
1	A	132	LEU	2.5
1	A	234	THR	2.5
1	B	228	GLN	2.5
1	A	278	SER	2.5
1	B	218	SER	2.5
1	A	274	ILE	2.5
1	A	400	ILE	2.5
1	A	201	TYR	2.5
1	A	383	TYR	2.5
1	A	88	ALA	2.5
1	B	187	PRO	2.5
1	A	160	CYS	2.4
1	A	375	ARG	2.4
1	A	222	LEU	2.4
1	A	210	ARG	2.4
1	A	225	THR	2.4
1	B	315	SER	2.4
1	A	317	LEU	2.4
1	A	249	HIS	2.4
1	A	238	ARG	2.4
1	A	318	ARG	2.4
1	A	344	ASN	2.4
1	A	382	ARG	2.4
1	A	174	VAL	2.4
1	B	141	LEU	2.4
1	B	168	TYR	2.4
1	A	289	MET	2.4
1	A	308	PHE	2.4
1	B	158	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	208	ILE	2.4
1	A	185	VAL	2.3
1	B	338	VAL	2.3
1	A	102	ASN	2.3
1	A	130	LYS	2.3
1	B	258	LYS	2.3
1	A	277	ALA	2.3
1	B	333	SER	2.3
1	A	171	ILE	2.3
1	B	233	LEU	2.3
1	A	84	GLY	2.3
1	A	232	GLU	2.3
1	A	341	VAL	2.3
1	A	343	VAL	2.3
1	A	146	GLY	2.3
1	B	176	GLY	2.3
1	A	297	HIS	2.3
1	B	395	HIS	2.3
1	A	81	GLN	2.3
1	B	123	LEU	2.2
1	B	363	LEU	2.2
1	A	263	PRO	2.2
1	A	276	GLN	2.2
1	B	284	LYS	2.2
1	A	125	ILE	2.2
1	A	214	LEU	2.2
1	B	214	LEU	2.2
1	A	133	PHE	2.2
1	B	133	PHE	2.2
1	A	309	ASP	2.2
1	A	94	CYS	2.2
1	A	299	ARG	2.2
1	B	263	PRO	2.2
1	A	165	LYS	2.2
1	A	156	VAL	2.2
1	A	108	THR	2.2
1	B	162	THR	2.2
1	B	163	SER	2.2
1	B	193	THR	2.2
1	A	227	VAL	2.2
1	A	83	PHE	2.2
1	A	258	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	365	GLY	2.2
1	A	169	ALA	2.2
1	A	373	THR	2.2
1	B	279	ARG	2.1
1	B	265	LEU	2.1
1	B	164	GLY	2.1
1	A	362	ARG	2.1
1	A	265	LEU	2.1
1	B	86	LEU	2.1
1	B	130	LYS	2.1
1	B	388	LEU	2.1
1	B	245	HIS	2.1
1	A	143	LYS	2.1
1	A	161	LYS	2.1
1	A	267	LEU	2.1
1	B	304	GLU	2.1
1	A	168	TYR	2.1
1	A	268	HIS	2.1
1	B	396	VAL	2.1
1	A	85	CYS	2.1
1	B	325	ALA	2.1
1	A	312	LEU	2.1
1	B	312	LEU	2.1
1	A	170	ILE	2.1
1	B	173	ARG	2.1
1	A	195	ALA	2.0
1	A	204	ALA	2.0
1	A	389	ALA	2.0
1	B	369	CYS	2.0
1	A	381	LEU	2.0
1	B	378	PRO	2.0
1	A	398	LYS	2.0
1	A	122	ALA	2.0
1	B	180	ILE	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

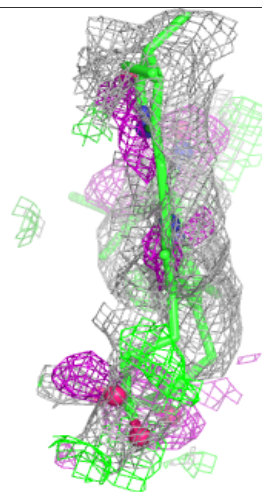
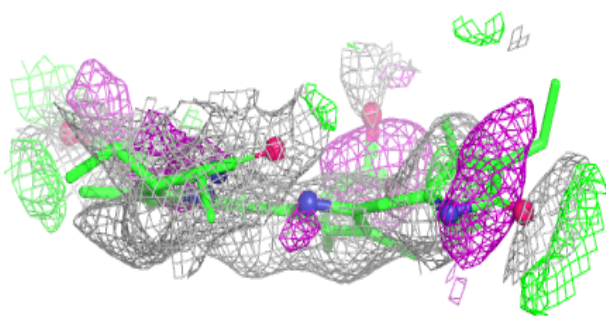
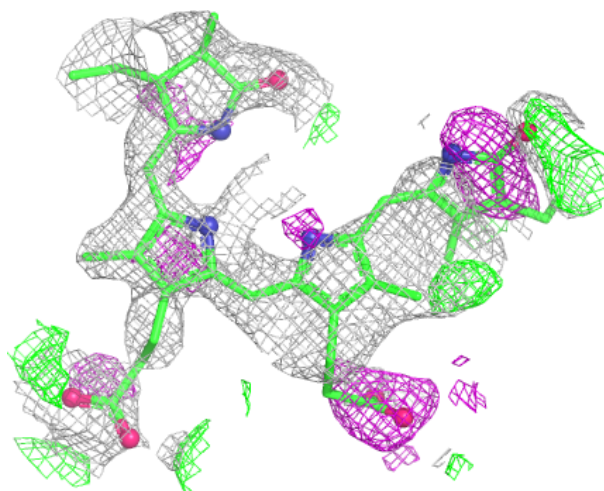
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

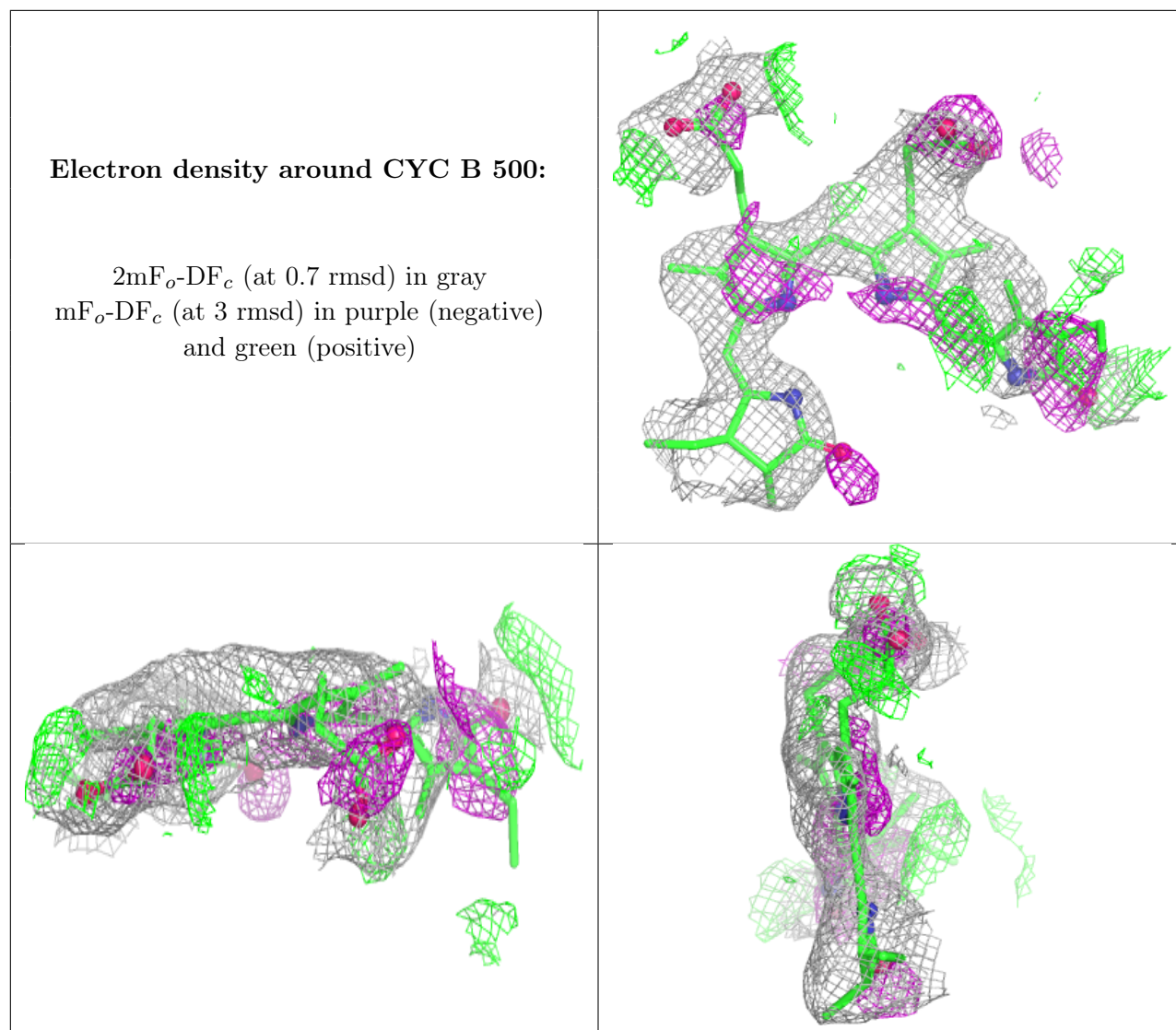
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CYC	A	500	43/43	0.31	0.30	58,75,89,91	0
2	CYC	B	500	43/43	0.44	0.28	40,63,80,95	0

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.

Electron density around CYC A 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.