



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:18 pm BST

PDB ID : 6TC7
Title : PAS-GAF bidomain of Glycine max phytochromeA
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Deposited on : 2019-11-05
Resolution : 2.13 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

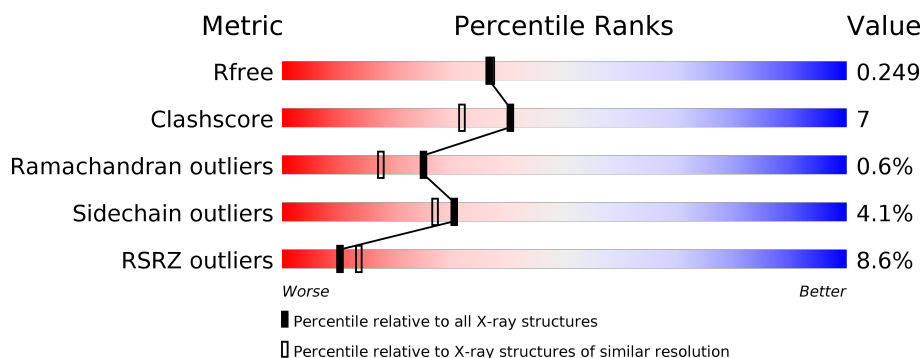
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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 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	AAA	359	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>14%</div> <div>•</div> <div>12%</div> </div> </div>
1	BBB	359	<div> <div>7%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>

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	PEG	BBB	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5263 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.

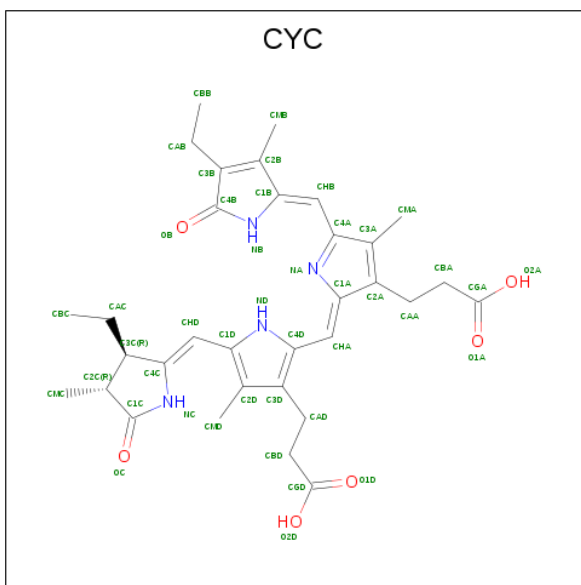
- Molecule 1 is a protein called Phytochrome.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	317	Total	C	N	O	S	0	1	0
			2490	1604	426	436	24			
1	BBB	319	Total	C	N	O	S	0	0	0
			2497	1608	428	438	23			

There are 14 discrepancies between the modelled and reference sequences:

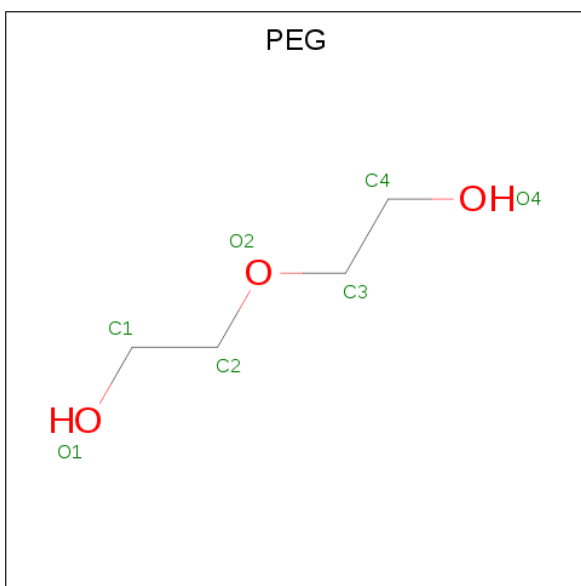
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	50	MET	-	initiating methionine	UNP B4YB07
AAA	403	HIS	-	expression tag	UNP B4YB07
AAA	404	HIS	-	expression tag	UNP B4YB07
AAA	405	HIS	-	expression tag	UNP B4YB07
AAA	406	HIS	-	expression tag	UNP B4YB07
AAA	407	HIS	-	expression tag	UNP B4YB07
AAA	408	HIS	-	expression tag	UNP B4YB07
BBB	50	MET	-	initiating methionine	UNP B4YB07
BBB	403	HIS	-	expression tag	UNP B4YB07
BBB	404	HIS	-	expression tag	UNP B4YB07
BBB	405	HIS	-	expression tag	UNP B4YB07
BBB	406	HIS	-	expression tag	UNP B4YB07
BBB	407	HIS	-	expression tag	UNP B4YB07
BBB	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 author).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $\text{C}_4\text{H}_{10}\text{O}_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 7 4 3	0	0
3	BBB	1	Total C O 7 4 3	0	0

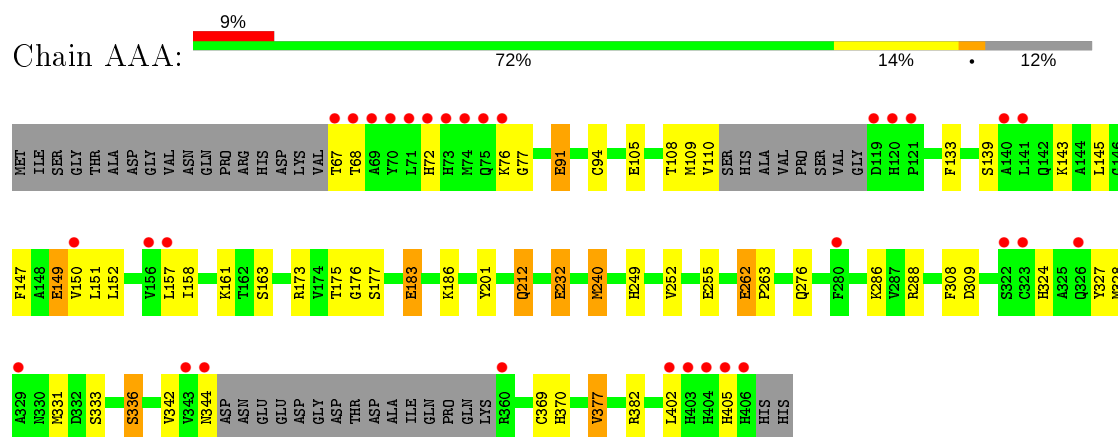
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	79	Total 79	O 79	0	0
4	BBB	97	Total 97	O 97	0	0

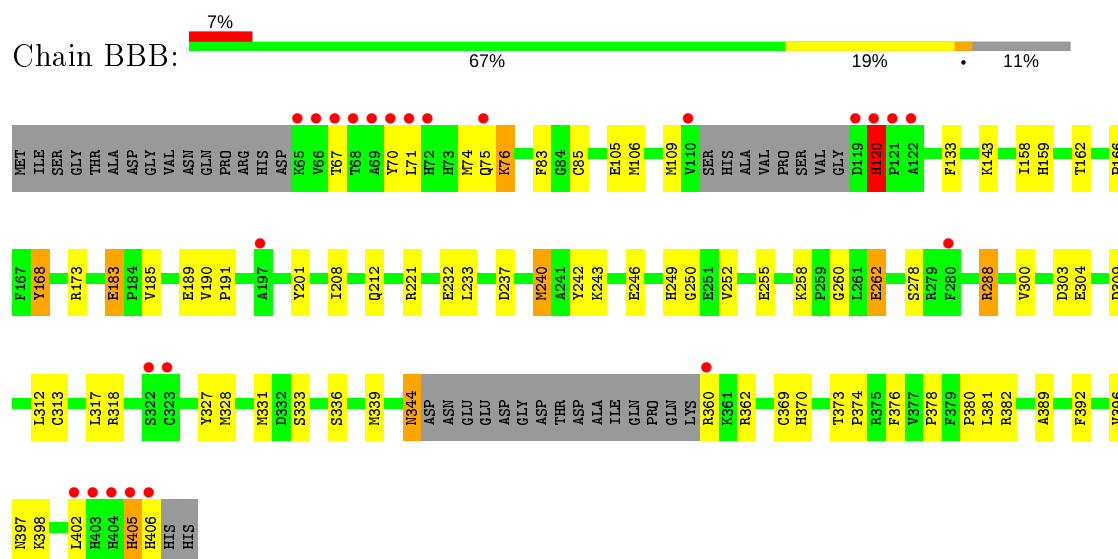
3 Residue-property plots [i](#)

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: Phytochrome



• Molecule 1: Phytochrome



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.42Å 113.23Å 68.46Å 90.00° 93.52° 90.00°	Depositor
Resolution (Å)	44.35 – 2.13 44.35 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.4 (44.35-2.13) 99.4 (44.35-2.13)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.189 , 0.241 0.195 , 0.249	Depositor DCC
R_{free} test set	1866 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5263	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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

5.1 Standard geometry

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

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	AAA	1.15	9/2554 (0.4%)	1.24	9/3461 (0.3%)
1	BBB	1.13	10/2558 (0.4%)	1.27	16/3468 (0.5%)
All	All	1.14	19/5112 (0.4%)	1.26	25/6929 (0.4%)

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	AAA	0	1
1	BBB	0	2
All	All	0	3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	105	GLU	CD-OE1	9.00	1.35	1.25
1	AAA	183	GLU	CD-OE1	7.94	1.34	1.25
1	AAA	183	GLU	CD-OE2	7.78	1.34	1.25
1	AAA	255	GLU	CD-OE2	7.77	1.34	1.25
1	BBB	183	GLU	CD-OE1	7.48	1.33	1.25
1	BBB	232	GLU	CD-OE1	6.73	1.33	1.25
1	BBB	304	GLU	CD-OE1	6.73	1.33	1.25
1	BBB	255	GLU	CD-OE1	6.72	1.33	1.25
1	AAA	232	GLU	CD-OE2	6.15	1.32	1.25
1	AAA	262	GLU	CD-OE1	6.04	1.32	1.25
1	AAA	149	GLU	CD-OE1	-5.96	1.19	1.25
1	AAA	163	SER	CA-CB	-5.87	1.44	1.52
1	AAA	139	SER	CB-OG	-5.74	1.34	1.42
1	BBB	189	GLU	CD-OE1	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	232	GLU	CD-OE2	5.41	1.31	1.25
1	BBB	344	ASN	C-O	5.37	1.33	1.23
1	BBB	262	GLU	CD-OE1	5.36	1.31	1.25
1	AAA	336	SER	CA-CB	-5.30	1.45	1.52
1	BBB	250	GLY	C-O	5.06	1.31	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	382	ARG	NE-CZ-NH1	-15.17	112.72	120.30
1	BBB	382	ARG	NE-CZ-NH1	-14.95	112.83	120.30
1	AAA	382	ARG	NE-CZ-NH2	14.00	127.30	120.30
1	BBB	382	ARG	NE-CZ-NH2	13.44	127.02	120.30
1	BBB	362	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	BBB	362	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	BBB	173	ARG	NE-CZ-NH1	-8.63	115.98	120.30
1	BBB	288	ARG	CG-CD-NE	8.16	128.94	111.80
1	AAA	161	LYS	C-N-CA	-7.07	104.02	121.70
1	AAA	288	ARG	CG-CD-NE	6.64	125.75	111.80
1	AAA	288	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	AAA	240	MET	CG-SD-CE	-6.41	89.94	100.20
1	BBB	240	MET	CG-SD-CE	-5.80	90.92	100.20
1	BBB	173	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	AAA	173	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	AAA	175	THR	CA-CB-OG1	-5.64	97.16	109.00
1	BBB	344	ASN	CB-CA-C	-5.60	99.21	110.40
1	AAA	377	VAL	CA-CB-CG1	5.54	119.21	110.90
1	BBB	309	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	BBB	262	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	BBB	382	ARG	CB-CG-CD	-5.20	98.07	111.60
1	BBB	303	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	BBB	221	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	BBB	288	ARG	CB-CG-CD	5.11	124.89	111.60
1	BBB	168	TYR	CB-CG-CD1	5.02	124.01	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	177	SER	Mainchain
1	BBB	120	HIS	Peptide
1	BBB	260	GLY	Peptide

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	AAA	2490	0	2522	29	0
1	BBB	2497	0	2524	45	0
2	AAA	43	0	36	3	0
2	BBB	43	0	36	6	0
3	AAA	7	0	10	0	0
3	BBB	7	0	10	7	0
4	AAA	79	0	0	3	0
4	BBB	97	0	0	2	0
All	All	5263	0	5138	74	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 7.

All (74) 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:AAA:76:LYS:HD2	1:AAA:309:ASP:OD2	1.94	0.67
1:BBB:378:PRO:HB3	3:BBB:501:PEG:H31	1.80	0.64
1:AAA:183:GLU:OE2	4:AAA:601:HOH:O	2.16	0.61
1:AAA:108:THR:O	1:AAA:109:MET:HB2	2.00	0.61
1:AAA:91:GLU:HA	1:AAA:145:LEU:HD11	1.83	0.60
1:BBB:85:CYS:N	1:BBB:106:MET:HE1	2.17	0.60
1:AAA:157:LEU:HD13	1:AAA:157:LEU:C	2.22	0.59
1:BBB:344:ASN:O	1:BBB:344:ASN:OD1	2.20	0.58
1:BBB:183:GLU:HB2	3:BBB:501:PEG:H11	1.85	0.58
1:AAA:149:GLU:HA	1:AAA:152:LEU:HD12	1.87	0.56
1:BBB:378:PRO:HB2	1:BBB:380:PRO:HD2	1.87	0.56
1:BBB:71:LEU:O	1:BBB:75:GLN:HG3	2.06	0.56
1:BBB:344:ASN:ND2	1:BBB:397:ASN:OD1	2.39	0.55
1:BBB:313:CYS:HA	1:BBB:318:ARG:HD3	1.89	0.54
1:BBB:278:SER:OG	2:BBB:500:CYC:HAD2	2.07	0.54
1:BBB:339:MET:CE	1:BBB:389:ALA:HB2	2.37	0.54
1:AAA:133:PHE:CD1	1:AAA:158:ILE:HD13	2.43	0.54
1:BBB:402:LEU:HD23	1:BBB:402:LEU:O	2.08	0.53
1:AAA:370:HIS:CE1	2:AAA:500:CYC:OB	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:70:TYR:OH	2:BBB:500:CYC:HBC3	2.10	0.52
1:BBB:67:THR:O	1:BBB:71:LEU:HB2	2.11	0.51
2:BBB:500:CYC:NB	2:BBB:500:CYC:HMA1	2.25	0.51
1:BBB:168:TYR:HD2	3:BBB:501:PEG:H12	1.74	0.51
1:AAA:370:HIS:HE1	2:AAA:500:CYC:OB	1.93	0.51
1:BBB:300:VAL:HG11	1:BBB:312:LEU:CD1	2.41	0.50
1:AAA:331:MET:HE3	4:AAA:632:HOH:O	2.11	0.50
1:BBB:133:PHE:CD1	1:BBB:158:ILE:HD13	2.47	0.50
1:AAA:344:ASN:C	1:AAA:344:ASN:OD1	2.51	0.49
1:AAA:147:PHE:CD1	1:AAA:151:LEU:HD23	2.48	0.49
1:BBB:339:MET:HE3	1:BBB:389:ALA:HB2	1.95	0.49
1:BBB:76:LYS:HD3	1:BBB:76:LYS:N	2.27	0.49
1:AAA:402:LEU:HD23	1:AAA:402:LEU:O	2.13	0.49
1:BBB:166:PRO:HG2	1:BBB:185:VAL:O	2.13	0.48
1:BBB:74:MET:O	1:BBB:313:CYS:HB3	2.14	0.47
1:BBB:233:LEU:HG	1:BBB:381:LEU:HD11	1.96	0.47
1:BBB:183:GLU:CB	3:BBB:501:PEG:H11	2.44	0.46
1:BBB:208:ILE:O	1:BBB:212:GLN:HG3	2.15	0.46
1:BBB:328:MET:HB3	1:BBB:333:SER:O	2.16	0.45
1:BBB:327:TYR:CE2	1:BBB:331:MET:HE1	2.52	0.45
1:AAA:328:MET:HB3	1:AAA:333:SER:O	2.17	0.45
1:AAA:212:GLN:O	1:AAA:212:GLN:NE2	2.50	0.45
1:BBB:159:HIS:HD2	4:BBB:631:HOH:O	1.99	0.45
1:AAA:157:LEU:C	1:AAA:157:LEU:CD1	2.86	0.44
1:BBB:242:TYR:CE2	2:BBB:500:CYC:HBB3	2.53	0.44
1:AAA:105:GLU:HA	1:AAA:110:VAL:HG23	2.00	0.44
1:AAA:176:GLY:HA3	1:AAA:308:PHE:CZ	2.53	0.44
2:AAA:500:CYC:NB	2:AAA:500:CYC:HMA1	2.33	0.44
1:BBB:237:ASP:HA	1:BBB:258:LYS:HD2	2.00	0.44
1:AAA:262:GLU:HG2	1:AAA:263:PRO:HD2	2.00	0.43
1:BBB:243:LYS:HE3	4:BBB:661:HOH:O	2.18	0.43
1:BBB:376:PHE:CE2	3:BBB:501:PEG:H21	2.54	0.43
1:BBB:83:PHE:CZ	1:BBB:317:LEU:HD23	2.54	0.43
1:AAA:91:GLU:HB3	1:AAA:176:GLY:O	2.18	0.42
1:AAA:212:GLN:OE1	1:BBB:212:GLN:HB3	2.19	0.42
1:BBB:109:MET:CE	1:BBB:162:THR:CG2	2.97	0.42
1:BBB:373:THR:HB	1:BBB:374:PRO:HD2	2.02	0.42
1:BBB:376:PHE:CZ	3:BBB:501:PEG:C2	3.02	0.42
1:BBB:405:HIS:O	1:BBB:406:HIS:C	2.58	0.42
1:AAA:157:LEU:HD13	1:AAA:158:ILE:N	2.35	0.42
1:BBB:300:VAL:HG11	1:BBB:312:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:240:MET:HB2	1:BBB:252:VAL:HG13	2.01	0.41
1:AAA:212:GLN:HG2	1:BBB:212:GLN:HB3	2.03	0.41
1:AAA:286:LYS:HE2	1:AAA:342:VAL:HG21	2.02	0.41
1:AAA:72:HIS:CE1	1:AAA:76:LYS:HG3	2.56	0.41
1:AAA:94:CYS:O	4:AAA:602:HOH:O	2.21	0.41
1:BBB:370:HIS:CE1	2:BBB:500:CYC:OB	2.74	0.41
1:BBB:190:VAL:HB	1:BBB:191:PRO:HD3	2.01	0.41
1:AAA:240:MET:HB2	1:AAA:252:VAL:HG13	2.01	0.41
1:AAA:324:HIS:O	1:AAA:327:TYR:HB3	2.20	0.41
1:BBB:336:SER:HA	1:BBB:369:CYS:O	2.21	0.41
1:BBB:392:PHE:O	1:BBB:396:VAL:HG23	2.20	0.41
1:BBB:168:TYR:CD2	3:BBB:501:PEG:H12	2.54	0.41
1:AAA:336:SER:HA	1:AAA:369:CYS:O	2.21	0.40
1:BBB:278:SER:OG	2:BBB:500:CYC:CAD	2.68	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	AAA	312/359 (87%)	298 (96%)	12 (4%)	2 (1%)	25	17
1	BBB	313/359 (87%)	303 (97%)	8 (3%)	2 (1%)	25	17
All	All	625/718 (87%)	601 (96%)	20 (3%)	4 (1%)	25	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	405	HIS
1	BBB	405	HIS
1	AAA	77	GLY
1	BBB	120	HIS

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	AAA	272/307 (89%)	260 (96%)	12 (4%)	28	24
1	BBB	272/307 (89%)	262 (96%)	10 (4%)	34	31
All	All	544/614 (89%)	522 (96%)	22 (4%)	30	28

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	67	THR
1	AAA	68	THR
1	AAA	91	GLU
1	AAA	143	LYS
1	AAA	150	VAL
1	AAA	186	LYS
1	AAA	201	TYR
1	AAA	212	GLN
1	AAA	232	GLU
1	AAA	249	HIS
1	AAA	276	GLN
1	AAA	377	VAL
1	BBB	76	LYS
1	BBB	120	HIS
1	BBB	143	LYS
1	BBB	201	TYR
1	BBB	246	GLU
1	BBB	249	HIS
1	BBB	262	GLU
1	BBB	288	ARG
1	BBB	360	ARG
1	BBB	398	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

4 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	BBB	500	1	36,46,46	2.41	10 (27%)	44,67,67	2.36	15 (34%)
2	CYC	AAA	500	1	36,46,46	2.65	12 (33%)	44,67,67	2.42	17 (38%)
3	PEG	BBB	501	-	6,6,6	1.13	1 (16%)	5,5,5	1.08	0
3	PEG	AAA	501	-	6,6,6	0.23	0	5,5,5	0.30	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
2	CYC	BBB	500	1	-	6/21/74/74	0/4/4/4
2	CYC	AAA	500	1	-	6/21/74/74	0/4/4/4
3	PEG	BBB	501	-	-	3/4/4/4	-
3	PEG	AAA	501	-	-	2/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	500	CYC	C4B-C3B	-8.27	1.32	1.48
2	BBB	500	CYC	C4B-C3B	-8.26	1.32	1.48
2	AAA	500	CYC	C1A-C2A	-6.19	1.35	1.45
2	BBB	500	CYC	C1A-C2A	-5.09	1.37	1.45
2	AAA	500	CYC	C3C-C4C	4.60	1.57	1.50
2	BBB	500	CYC	C1B-C2B	-4.56	1.36	1.45
2	AAA	500	CYC	C1B-C2B	-4.49	1.37	1.45
2	AAA	500	CYC	CMA-C3A	4.36	1.60	1.50
2	AAA	500	CYC	C2C-C1C	3.91	1.55	1.52
2	BBB	500	CYC	C4A-C3A	-3.65	1.38	1.45
2	AAA	500	CYC	C4A-C3A	-3.64	1.38	1.45
2	BBB	500	CYC	C3C-C4C	3.43	1.55	1.50
2	BBB	500	CYC	CHA-C1A	3.22	1.37	1.35
2	BBB	500	CYC	CMA-C3A	3.06	1.57	1.50
2	AAA	500	CYC	CMB-C2B	3.06	1.57	1.50
2	BBB	500	CYC	CAD-C3D	2.88	1.56	1.52
2	BBB	500	CYC	C1B-NB	-2.76	1.33	1.37
2	AAA	500	CYC	CMD-C2D	2.55	1.56	1.51
2	AAA	500	CYC	CAC-C3C	2.49	1.58	1.54
2	AAA	500	CYC	C1C-NC	-2.12	1.34	1.37
3	BBB	501	PEG	O1-C1	2.09	1.52	1.42
2	AAA	500	CYC	CHA-C1A	2.02	1.36	1.35
2	BBB	500	CYC	C4B-NB	-2.01	1.33	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	500	CYC	OC-C1C-C2C	-6.29	121.17	126.17
2	BBB	500	CYC	C3B-C4B-NB	6.27	111.84	106.78
2	AAA	500	CYC	C2C-C1C-NC	5.89	113.35	108.27
2	BBB	500	CYC	C2C-C1C-NC	5.34	112.87	108.27
2	BBB	500	CYC	OB-C4B-C3B	-5.15	122.46	128.04
2	AAA	500	CYC	OB-C4B-C3B	-5.04	122.57	128.04
2	AAA	500	CYC	C3B-C4B-NB	4.87	110.71	106.78
2	BBB	500	CYC	CBD-CAD-C3D	-4.30	104.56	112.49
2	AAA	500	CYC	CBC-CAC-C3C	4.27	122.97	113.47
2	AAA	500	CYC	CBD-CAD-C3D	-3.96	105.18	112.49
2	AAA	500	CYC	C1B-NB-C4B	-3.74	105.91	110.67
2	BBB	500	CYC	C1B-NB-C4B	-3.69	105.97	110.67
2	AAA	500	CYC	CMA-C3A-C4A	3.51	130.47	125.06
2	AAA	500	CYC	OC-C1C-C2C	-3.34	123.52	126.17
2	AAA	500	CYC	C1A-C2A-C3A	3.25	110.38	106.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	500	CYC	CHB-C4A-C3A	3.03	132.68	124.90
2	AAA	500	CYC	CHB-C4A-NA	-2.96	118.75	124.93
2	AAA	500	CYC	CMB-C2B-C1B	2.92	127.82	124.17
2	BBB	500	CYC	CHB-C4A-C3A	2.91	132.39	124.90
2	BBB	500	CYC	CMB-C2B-C1B	2.90	127.79	124.17
2	AAA	500	CYC	CHD-C4C-NC	2.86	128.61	125.20
2	AAA	500	CYC	CAB-C3B-C2B	2.74	132.22	127.53
2	AAA	500	CYC	CAA-C2A-C3A	-2.70	122.84	127.88
2	BBB	500	CYC	CHB-C4A-NA	-2.65	119.38	124.93
2	AAA	500	CYC	CBB-CAB-C3B	-2.54	105.42	112.43
2	BBB	500	CYC	CHD-C4C-NC	2.46	128.13	125.20
2	AAA	500	CYC	C2A-C1A-NA	-2.34	106.64	110.05
2	BBB	500	CYC	CAC-C3C-C2C	-2.34	108.41	114.26
2	BBB	500	CYC	C2C-C3C-C4C	2.29	104.76	101.34
2	BBB	500	CYC	CBC-CAC-C3C	-2.27	108.42	113.47
2	BBB	500	CYC	CAB-C3B-C2B	2.21	131.31	127.53
2	BBB	500	CYC	C2A-C1A-NA	-2.06	107.06	110.05

There are no chirality outliers.

All (17) torsion outliers are listed below:

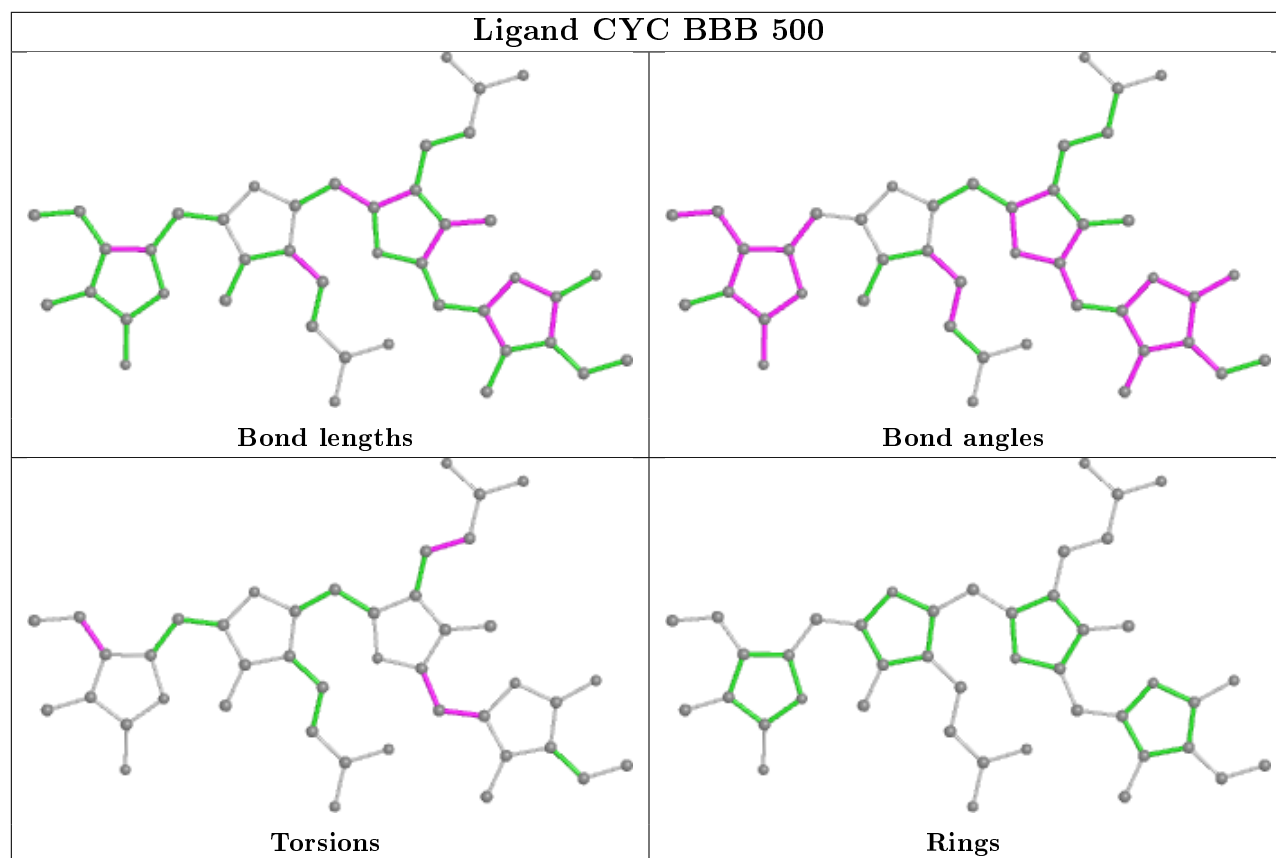
Mol	Chain	Res	Type	Atoms
2	BBB	500	CYC	C4C-C3C-CAC-CBC
2	AAA	500	CYC	NA-C4A-CHB-C1B
2	AAA	500	CYC	C2C-C3C-CAC-CBC
2	AAA	500	CYC	C4C-C3C-CAC-CBC
2	BBB	500	CYC	C3A-C4A-CHB-C1B
2	AAA	500	CYC	C3A-C4A-CHB-C1B
3	BBB	501	PEG	O2-C3-C4-O4
3	BBB	501	PEG	O1-C1-C2-O2
2	BBB	500	CYC	NA-C4A-CHB-C1B
2	BBB	500	CYC	C2C-C3C-CAC-CBC
3	AAA	501	PEG	O2-C3-C4-O4
2	AAA	500	CYC	NB-C1B-CHB-C4A
2	BBB	500	CYC	NB-C1B-CHB-C4A
3	AAA	501	PEG	C1-C2-O2-C3
2	AAA	500	CYC	C2B-C1B-CHB-C4A
3	BBB	501	PEG	C1-C2-O2-C3
2	BBB	500	CYC	C2A-CAA-CBA-CGA

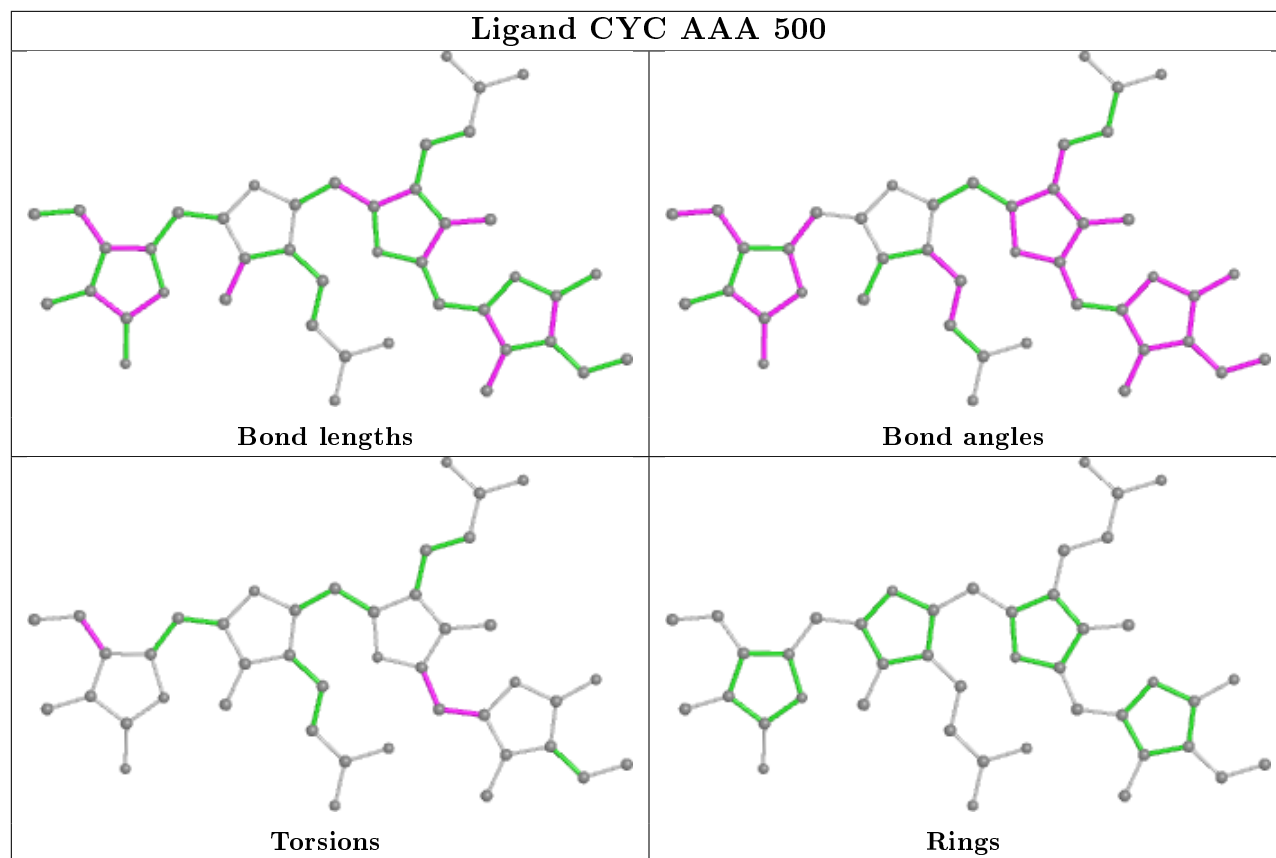
There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	500	CYC	6	0
2	AAA	500	CYC	3	0
3	BBB	501	PEG	7	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	AAA	317/359 (88%)	0.53	31 (9%) 7 10	26, 44, 108, 161	0
1	BBB	319/359 (88%)	0.30	24 (7%) 14 18	26, 42, 100, 145	0
All	All	636/718 (88%)	0.41	55 (8%) 10 13	26, 43, 105, 161	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	120	HIS	9.9
1	BBB	119	ASP	8.9
1	BBB	67	THR	8.9
1	AAA	67	THR	8.7
1	AAA	70	TYR	8.4
1	AAA	119	ASP	7.8
1	BBB	66	VAL	7.5
1	AAA	405	HIS	7.0
1	AAA	68	THR	6.8
1	BBB	72	HIS	6.6
1	AAA	71	LEU	6.3
1	AAA	406	HIS	6.1
1	AAA	69	ALA	5.7
1	AAA	72	HIS	5.5
1	BBB	121	PRO	5.5
1	AAA	404	HIS	5.5
1	AAA	75	GLN	5.3
1	AAA	76	LYS	5.1
1	BBB	405	HIS	4.8
1	BBB	69	ALA	4.7
1	BBB	402	LEU	4.7
1	BBB	120	HIS	4.4
1	BBB	404	HIS	4.3
1	AAA	73	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	AAA	360	ARG	4.1
1	AAA	344	ASN	4.1
1	BBB	70	TYR	4.0
1	AAA	74	MET	3.9
1	BBB	68	THR	3.8
1	BBB	122	ALA	3.8
1	AAA	402	LEU	3.8
1	AAA	280	PHE	3.7
1	AAA	326	GLN	3.6
1	BBB	75	GLN	3.4
1	AAA	150	VAL	3.2
1	AAA	329	ALA	3.1
1	BBB	406	HIS	3.1
1	BBB	360	ARG	3.1
1	AAA	121	PRO	3.1
1	AAA	323	CYS	3.0
1	AAA	322	SER	2.8
1	BBB	65	LYS	2.7
1	BBB	71	LEU	2.7
1	AAA	403	HIS	2.6
1	BBB	110	VAL	2.5
1	BBB	280	PHE	2.5
1	AAA	140	ALA	2.4
1	AAA	141	LEU	2.4
1	AAA	343	VAL	2.4
1	BBB	323	CYS	2.4
1	AAA	156	VAL	2.3
1	BBB	322	SER	2.3
1	BBB	197	ALA	2.2
1	AAA	157	LEU	2.1
1	BBB	403	HIS	2.1

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 [i](#)

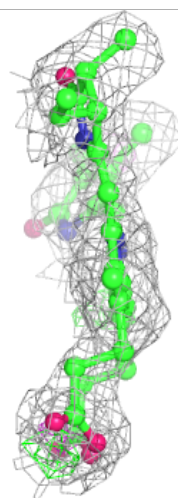
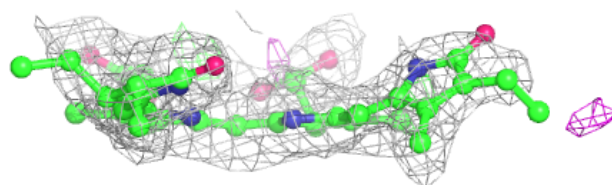
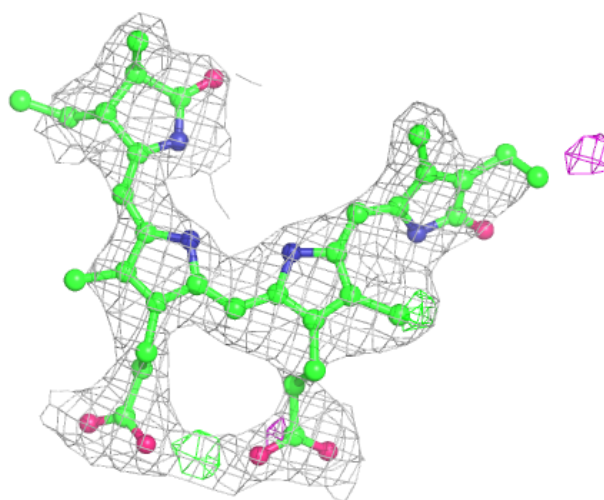
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CYC	AAA	500	43/43	0.82	0.28	47,86,95,105	0
3	PEG	AAA	501	7/7	0.84	0.23	36,60,89,90	0
3	PEG	BBB	501	7/7	0.86	0.46	13,23,29,30	7
2	CYC	BBB	500	43/43	0.90	0.24	48,73,91,100	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.

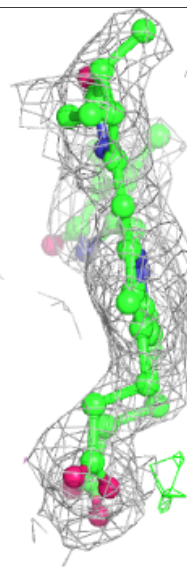
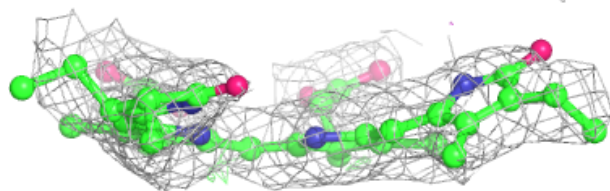
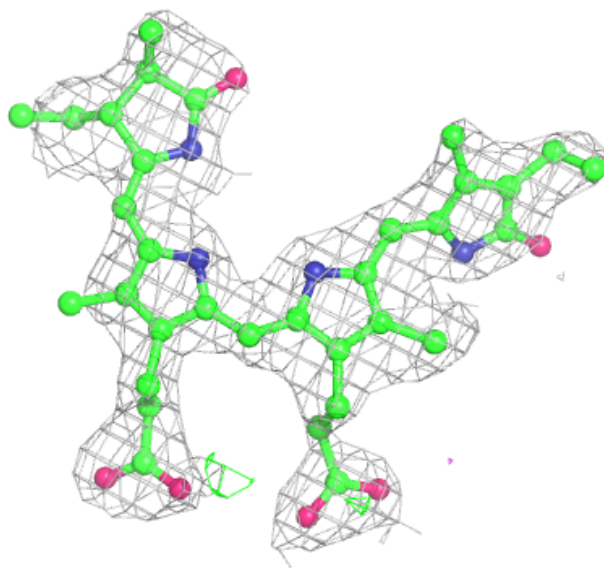
Electron density around CYC AAA 500:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CYC BBB 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.