



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 AM UTC

PDB ID : 6TC7 / pdb_00006tc7
Title : PAS-GAF bidomain of Glycine max phytochromeA
Authors : Nagano, S.; Guan, K.; Shenkutie, S.M.; Hughes, J.E.
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 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

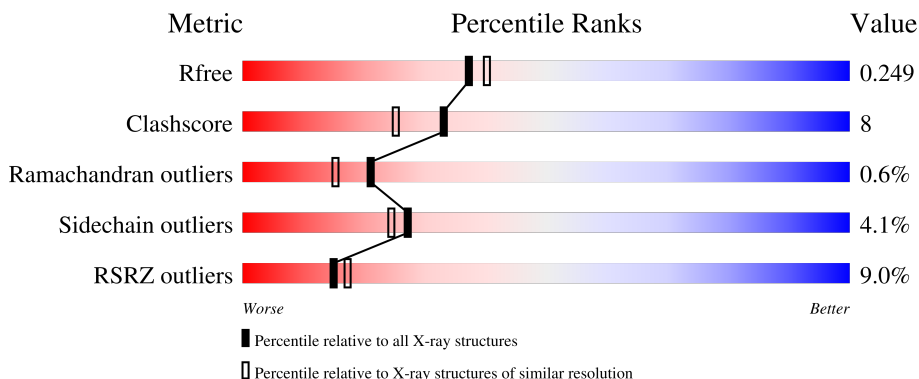
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 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}	180053	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (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 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	AAA	359	
1	BBB	359	

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 [i](#)

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.

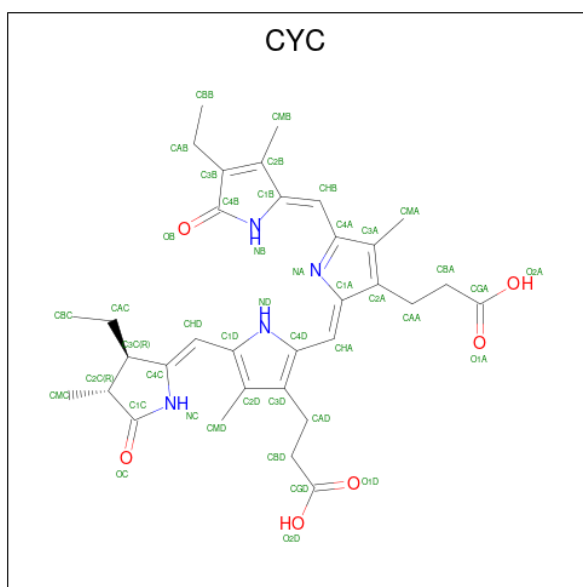
- Molecule 1 is a protein called Phytochrome.

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

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 (CCD ID: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

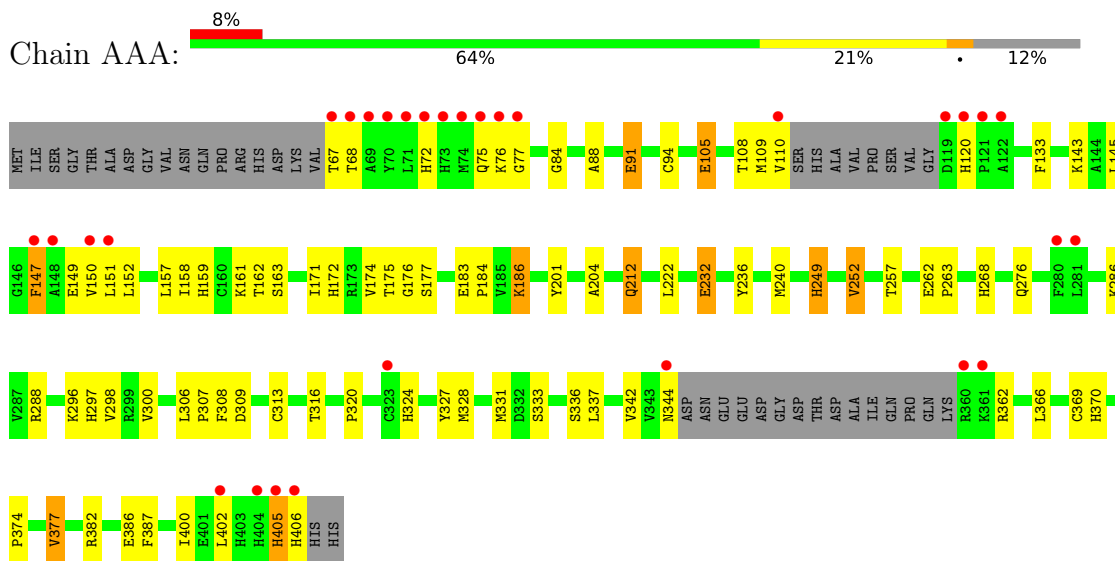
- Molecule 4 is water.

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

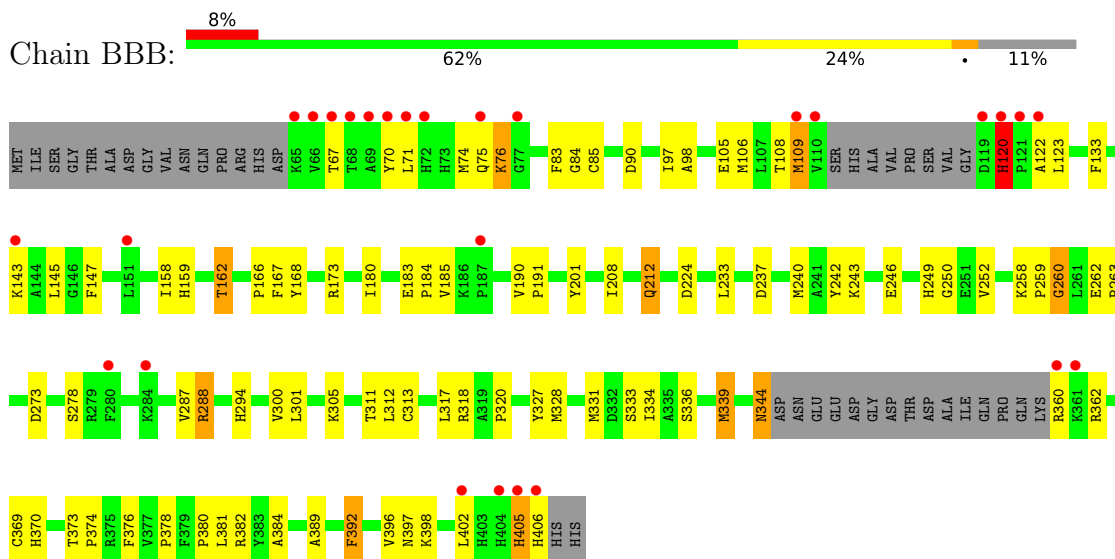
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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



- 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)	Xtrriage
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 (3.96%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtrriage
Anisotropy	0.170	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	1.58	27/2554 (1.1%)	1.68	23/3461 (0.7%)
1	BBB	1.57	20/2558 (0.8%)	1.68	26/3468 (0.7%)
All	All	1.57	47/5112 (0.9%)	1.68	49/6929 (0.7%)

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 (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	159	HIS	CE1-NE2	8.91	1.41	1.32
1	BBB	184	PRO	C-O	-7.98	1.14	1.23
1	BBB	90	ASP	C-O	-7.87	1.14	1.23
1	BBB	263	PRO	C-O	-7.54	1.15	1.23
1	AAA	75	GLN	C-O	7.51	1.31	1.23
1	AAA	297	HIS	CE1-NE2	7.39	1.40	1.32
1	AAA	105	GLU	C-O	-6.95	1.15	1.24
1	BBB	98	ALA	C-O	6.93	1.32	1.23
1	AAA	184	PRO	C-O	-6.90	1.15	1.23
1	AAA	316	THR	C-O	-6.87	1.15	1.24
1	BBB	145	LEU	C-O	-6.85	1.15	1.24
1	AAA	175	THR	C-O	6.79	1.31	1.24
1	BBB	305	LYS	C-O	-6.72	1.15	1.24
1	AAA	172	HIS	CE1-NE2	6.71	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	171	ILE	C-O	6.41	1.31	1.24
1	AAA	174	VAL	C-O	6.41	1.31	1.24
1	BBB	147	PHE	C-O	6.38	1.32	1.24
1	AAA	362	ARG	C-O	6.21	1.31	1.23
1	AAA	204	ALA	C-O	-6.18	1.16	1.24
1	AAA	313	CYS	C-O	-6.16	1.16	1.24
1	AAA	298	VAL	C-O	6.12	1.30	1.24
1	AAA	252	VAL	C-O	6.09	1.30	1.23
1	AAA	300	VAL	C-O	-6.08	1.16	1.24
1	BBB	294	HIS	CE1-NE2	5.94	1.38	1.32
1	AAA	337	LEU	C-O	5.87	1.30	1.23
1	BBB	250	GLY	C-O	5.79	1.31	1.23
1	AAA	374	PRO	C-O	-5.74	1.16	1.23
1	AAA	307	PRO	C-O	-5.67	1.16	1.24
1	BBB	212	GLN	C-O	-5.67	1.17	1.24
1	BBB	224	ASP	C-O	-5.64	1.17	1.24
1	AAA	88	ALA	C-O	5.59	1.30	1.24
1	AAA	163	SER	CA-CB	-5.59	1.44	1.53
1	BBB	180	ILE	C-O	-5.58	1.18	1.24
1	BBB	301	LEU	C-O	5.52	1.30	1.23
1	BBB	339	MET	C-O	5.44	1.30	1.24
1	BBB	259	PRO	C-O	5.44	1.31	1.24
1	BBB	260	GLY	CA-C	5.42	1.59	1.51
1	AAA	84	GLY	N-CA	5.38	1.50	1.45
1	BBB	105	GLU	CD-OE1	5.37	1.35	1.25
1	AAA	147	PHE	C-O	5.28	1.30	1.24
1	AAA	222	LEU	C-O	5.22	1.30	1.24
1	BBB	97	ILE	N-CA	5.19	1.51	1.46
1	BBB	123	LEU	C-O	-5.05	1.17	1.23
1	AAA	268	HIS	CE1-NE2	5.05	1.37	1.32
1	AAA	249	HIS	C-O	5.05	1.30	1.23
1	AAA	366	LEU	C-O	5.03	1.30	1.23
1	BBB	162	THR	C-O	5.03	1.29	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	161	LYS	CA-C-N	-9.64	104.02	122.53
1	AAA	161	LYS	C-N-CA	-9.64	104.02	122.53
1	AAA	382	ARG	NE-CZ-NH2	9.00	127.30	119.20
1	AAA	382	ARG	NE-CZ-NH1	-8.78	112.72	121.50
1	BBB	382	ARG	NE-CZ-NH2	8.69	127.02	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	382	ARG	NE-CZ-NH1	-8.67	112.83	121.50
1	AAA	175	THR	CA-CB-OG1	-8.29	97.16	109.60
1	BBB	288	ARG	CG-CD-NE	7.70	128.94	112.00
1	AAA	377	VAL	N-CA-CB	-7.59	100.58	111.21
1	AAA	120	HIS	CA-CB-CG	7.37	121.17	113.80
1	BBB	120	HIS	CA-CB-CG	6.98	120.78	113.80
1	AAA	162	THR	CB-CA-C	6.96	121.04	109.56
1	AAA	186	LYS	CB-CA-C	6.50	119.83	109.62
1	BBB	147	PHE	CA-CB-CG	6.44	120.24	113.80
1	AAA	186	LYS	O-C-N	-6.33	115.67	121.30
1	AAA	296	LYS	CB-CA-C	6.33	119.75	110.26
1	AAA	288	ARG	CG-CD-NE	6.25	125.75	112.00
1	BBB	362	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	BBB	145	LEU	CA-C-O	-6.18	112.31	119.61
1	BBB	273	ASP	CA-CB-CG	6.05	118.66	112.60
1	BBB	288	ARG	CB-CG-CD	5.91	124.89	111.30
1	AAA	320	PRO	CA-C-O	-5.90	114.23	121.31
1	AAA	306	LEU	N-CA-C	-5.88	100.86	109.50
1	AAA	257	THR	CA-CB-OG1	-5.87	100.79	109.60
1	AAA	161	LYS	CA-C-O	-5.87	114.66	120.70
1	BBB	311	THR	CA-C-O	-5.84	114.00	120.60
1	AAA	232	GLU	CB-CG-CD	5.78	122.42	112.60
1	BBB	382	ARG	CB-CG-CD	-5.75	98.07	111.30
1	AAA	387	PHE	N-CA-C	-5.74	105.10	111.36
1	BBB	344	ASN	CB-CA-C	-5.73	99.21	110.10
1	BBB	109	MET	CA-C-N	5.71	131.98	121.70
1	BBB	109	MET	C-N-CA	5.71	131.98	121.70
1	AAA	386	GLU	N-CA-C	-5.63	105.14	111.28
1	BBB	90	ASP	CA-C-O	-5.57	114.40	120.81
1	BBB	362	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	BBB	173	ARG	NE-CZ-NH1	-5.52	115.98	121.50
1	AAA	175	THR	CB-CA-C	5.49	119.65	110.92
1	BBB	320	PRO	CB-CA-C	-5.41	104.31	111.23
1	AAA	400	ILE	CA-C-O	-5.37	115.09	121.05
1	BBB	334	ILE	N-CA-C	-5.27	104.37	111.44
1	BBB	108	THR	CA-C-N	-5.26	114.97	123.23
1	BBB	108	THR	C-N-CA	-5.26	114.97	123.23
1	AAA	236	TYR	CA-C-O	-5.26	115.61	121.81
1	BBB	392	PHE	N-CA-C	-5.21	105.50	111.07
1	AAA	377	VAL	CA-CB-CG1	5.18	119.21	110.40
1	BBB	384	ALA	CA-C-O	-5.16	115.06	120.63
1	BBB	122	ALA	CA-C-N	-5.12	114.02	121.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	122	ALA	C-N-CA	-5.12	114.02	121.76
1	BBB	287	VAL	CA-C-O	-5.08	115.14	120.27

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 [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	AAA	2490	0	2522	32	0
1	BBB	2497	0	2524	49	0
2	AAA	43	0	36	3	0
2	BBB	43	0	36	5	0
3	AAA	7	0	10	0	0
3	BBB	7	0	10	7	0
4	AAA	79	0	0	4	0
4	BBB	97	0	0	2	0
All	All	5263	0	5138	80	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 8.

All (80) 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:BBB:106:MET:HE3	1:BBB:167:PHE:HE2	1.53	0.72
1:BBB:327:TYR:CE2	1:BBB:331:MET:HE1	2.24	0.72
1:BBB:85:CYS:SG	1:BBB:106:MET:HE2	2.34	0.68
1:AAA:76:LYS:HD2	1:AAA:309:ASP:OD2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:378:PRO:HB3	3:BBB:501:PEG:H31	1.80	0.64
1:AAA:157:LEU:C	1:AAA:157:LEU:HD13	2.22	0.64
1:AAA:331:MET:HE3	4:AAA:632:HOH:O	1.98	0.63
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:339:MET:HE2	1:BBB:389:ALA:HB2	1.82	0.60
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:327:TYR:CD2	1:BBB:331:MET:HE1	2.40	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:AAA:344:ASN:OD1	1:AAA:344:ASN:C	2.51	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:O	1:BBB:402:LEU:HD23	2.08	0.53
1:AAA:370:HIS:CE1	2:AAA:500:CYC:OB	2.63	0.52
1:BBB:70:TYR:OH	2:BBB:500:CYC:HBC3	2.10	0.52
2:AAA:500:CYC:HMA2	4:AAA:647:HOH:O	2.10	0.51
1:AAA:327:TYR:CE2	1:AAA:331:MET:HE1	2.45	0.51
1:BBB:67:THR:O	1:BBB:71:LEU:HB2	2.11	0.51
1:BBB:84:GLY:HA2	1:BBB:106:MET:HE1	1.92	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:BBB:106:MET:HE3	1:BBB:167:PHE:CE2	2.39	0.50
1:BBB:133:PHE:CD1	1:BBB:158:ILE:HD13	2.47	0.50
1:AAA:147:PHE:CD1	1:AAA:151:LEU:HD23	2.48	0.49
1:AAA:157:LEU:C	1:AAA:157:LEU:CD1	2.86	0.49
1:BBB:76:LYS:N	1:BBB:76:LYS:HD3	2.27	0.49
1:AAA:402:LEU:O	1:AAA:402:LEU:HD23	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:405:HIS:O	1:BBB:406:HIS:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:328:MET:HB3	1:BBB:333:SER:O	2.16	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:BBB:242:TYR:CE2	2:BBB:500:CYC:HBB3	2.53	0.44
1:AAA:402:LEU:HD23	1:AAA:402:LEU:C	2.43	0.44
1:AAA:405:HIS:O	1:AAA:406:HIS:C	2.60	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
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:83:PHE:CZ	1:BBB:317:LEU:HD23	2.54	0.43
1:BBB:376:PHE:CE2	3:BBB:501:PEG:H21	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: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
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: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:AAA:286:LYS:HE2	1:AAA:342:VAL:HG21	2.02	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:168:TYR:CD2	3:BBB:501:PEG:H12	2.54	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: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 [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	AAA	312/359 (87%)	298 (96%)	12 (4%)	2 (1%)	21	15
1	BBB	313/359 (87%)	303 (97%)	8 (3%)	2 (1%)	21	15
All	All	625/718 (87%)	601 (96%)	20 (3%)	4 (1%)	21	15

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 [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	AAA	272/307 (89%)	260 (96%)	12 (4%)	25	22
1	BBB	272/307 (89%)	262 (96%)	10 (4%)	30	29
All	All	544/614 (89%)	522 (96%)	22 (4%)	27	25

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

Mol	Chain	Res	Type
1	AAA	67	THR
1	AAA	68	THR

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Mol	Chain	Res	Type
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

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

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](#)

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	AAA	500	1	46,46,46	2.49	15 (32%)	63,67,67	2.25	24 (38%)
3	PEG	BBB	501	-	6,6,6	1.14	1 (16%)	5,5,5	1.07	0
2	CYC	BBB	500	1	46,46,46	2.36	12 (26%)	63,67,67	2.11	18 (28%)
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	AAA	500	1	-	10/26/74/74	0/4/4/4
3	PEG	BBB	501	-	-	3/4/4/4	-
2	CYC	BBB	500	1	-	9/26/74/74	0/4/4/4
3	PEG	AAA	501	-	-	2/4/4/4	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	500	CYC	C4B-C3B	-8.51	1.32	1.48
2	BBB	500	CYC	C4B-C3B	-8.51	1.32	1.48
2	AAA	500	CYC	C1A-C2A	-6.31	1.35	1.45
2	BBB	500	CYC	C1A-C2A	-5.20	1.37	1.45
2	BBB	500	CYC	C1B-C2B	-4.58	1.36	1.45
2	AAA	500	CYC	C1B-C2B	-4.52	1.37	1.45
2	AAA	500	CYC	CMA-C3A	4.51	1.60	1.50
2	BBB	500	CYC	CBA-CGA	4.35	1.60	1.50
2	AAA	500	CYC	C2C-C1C	3.91	1.55	1.52
2	BBB	500	CYC	C4A-C3A	-3.63	1.38	1.45
2	AAA	500	CYC	C4A-C3A	-3.62	1.38	1.45
2	BBB	500	CYC	C1D-C2D	-3.34	1.33	1.41
2	AAA	500	CYC	C3C-C4C	3.22	1.57	1.50
2	BBB	500	CYC	CMA-C3A	3.18	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	500	CYC	CMB-C2B	3.17	1.57	1.50
2	AAA	500	CYC	C4D-C3D	-3.10	1.35	1.42
2	BBB	500	CYC	C4D-C3D	-3.07	1.36	1.42
2	AAA	500	CYC	CMD-C2D	3.01	1.56	1.50
2	AAA	500	CYC	C1D-C2D	-2.79	1.34	1.41
2	BBB	500	CYC	C1B-NB	-2.72	1.33	1.37
2	AAA	500	CYC	CAC-C3C	2.55	1.58	1.54
2	BBB	500	CYC	C3C-C4C	2.42	1.55	1.50
2	AAA	500	CYC	O1A-CGA	2.30	1.29	1.22
2	AAA	500	CYC	C1C-NC	-2.18	1.34	1.37
3	BBB	501	PEG	O1-C1	2.12	1.52	1.42
2	BBB	500	CYC	O2D-CGD	-2.11	1.23	1.30
2	AAA	500	CYC	C1A-NA	-2.03	1.34	1.38
2	BBB	500	CYC	CMD-C2D	2.01	1.54	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	500	CYC	C3B-C4B-NB	6.36	111.84	106.77
2	BBB	500	CYC	OC-C1C-C2C	-6.29	121.17	126.17
2	AAA	500	CYC	C2C-C1C-NC	6.09	113.35	108.29
2	BBB	500	CYC	C2C-C1C-NC	5.51	112.87	108.29
2	BBB	500	CYC	OB-C4B-C3B	-5.31	122.46	128.03
2	AAA	500	CYC	OB-C4B-C3B	-5.20	122.57	128.03
2	AAA	500	CYC	C3B-C4B-NB	4.94	110.71	106.77
2	AAA	500	CYC	CBC-CAC-C3C	4.50	122.97	113.41
2	AAA	500	CYC	C1B-NB-C4B	-3.87	105.91	110.66
2	BBB	500	CYC	C1B-NB-C4B	-3.82	105.97	110.66
2	AAA	500	CYC	CMA-C3A-C4A	3.46	130.47	125.10
2	AAA	500	CYC	C1A-C2A-C3A	3.38	110.38	106.73
2	AAA	500	CYC	OC-C1C-C2C	-3.34	123.52	126.17
2	AAA	500	CYC	CBA-CAA-C2A	-3.20	103.68	112.53
2	AAA	500	CYC	CHB-C4A-C3A	3.04	132.68	124.87
2	BBB	500	CYC	CBA-CAA-C2A	-3.02	104.17	112.53
2	AAA	500	CYC	CMB-C2B-C1B	3.01	127.82	124.16
2	BBB	500	CYC	CMB-C2B-C1B	2.98	127.79	124.16
2	AAA	500	CYC	CHA-C4D-ND	2.98	132.03	125.29
2	BBB	500	CYC	CHB-C4A-C3A	2.93	132.39	124.87
2	BBB	500	CYC	CBD-CAD-C3D	-2.89	104.56	112.53
2	AAA	500	CYC	CHB-C4A-NA	-2.87	118.75	124.95
2	AAA	500	CYC	CAA-C2A-C3A	-2.68	122.84	127.87
2	AAA	500	CYC	CBD-CAD-C3D	-2.66	105.18	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	500	CYC	CHA-C4D-ND	2.64	131.27	125.29
2	AAA	500	CYC	CBB-CAB-C3B	-2.58	105.42	112.42
2	BBB	500	CYC	CHB-C4A-NA	-2.58	119.38	124.95
2	AAA	500	CYC	CAB-C3B-C2B	2.54	132.22	127.56
2	AAA	500	CYC	CHD-C1D-ND	2.44	130.79	125.29
2	AAA	500	CYC	O2A-CGA-O1A	2.43	129.57	123.33
2	AAA	500	CYC	C2A-C1A-NA	-2.40	106.64	110.04
2	AAA	500	CYC	CHD-C4C-NC	2.39	128.61	125.63
2	AAA	500	CYC	CHD-C1D-C2D	-2.38	121.69	127.53
2	BBB	500	CYC	CBC-CAC-C3C	-2.35	108.42	113.41
2	BBB	500	CYC	C2C-C3C-C4C	2.29	104.76	101.34
2	AAA	500	CYC	CHA-C4D-C3D	-2.22	122.44	127.22
2	BBB	500	CYC	CHD-C1D-ND	2.11	130.06	125.29
2	BBB	500	CYC	C2A-C1A-NA	-2.11	107.06	110.04
2	AAA	500	CYC	O1A-CGA-CBA	-2.07	116.53	123.09
2	BBB	500	CYC	CAB-C3B-C2B	2.04	131.31	127.56
2	BBB	500	CYC	CHA-C4D-C3D	-2.02	122.88	127.22
2	BBB	500	CYC	CHD-C4C-NC	2.00	128.13	125.63

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	C4C-C3C-CAC-CBC
2	AAA	500	CYC	C3A-C4A-CHB-C1B
2	BBB	500	CYC	C3A-C4A-CHB-C1B
3	BBB	501	PEG	O1-C1-C2-O2
3	BBB	501	PEG	O2-C3-C4-O4
2	BBB	500	CYC	NA-C4A-CHB-C1B
3	AAA	501	PEG	O2-C3-C4-O4
2	BBB	500	CYC	C2C-C3C-CAC-CBC
2	AAA	500	CYC	NB-C1B-CHB-C4A
3	AAA	501	PEG	C1-C2-O2-C3
2	BBB	500	CYC	CAD-CBD-CGD-O2D
2	BBB	500	CYC	CAA-CBA-CGA-O1A
2	BBB	500	CYC	CAD-CBD-CGD-O1D
2	BBB	500	CYC	NB-C1B-CHB-C4A
2	BBB	500	CYC	CAA-CBA-CGA-O2A
2	AAA	500	CYC	CAA-CBA-CGA-O1A

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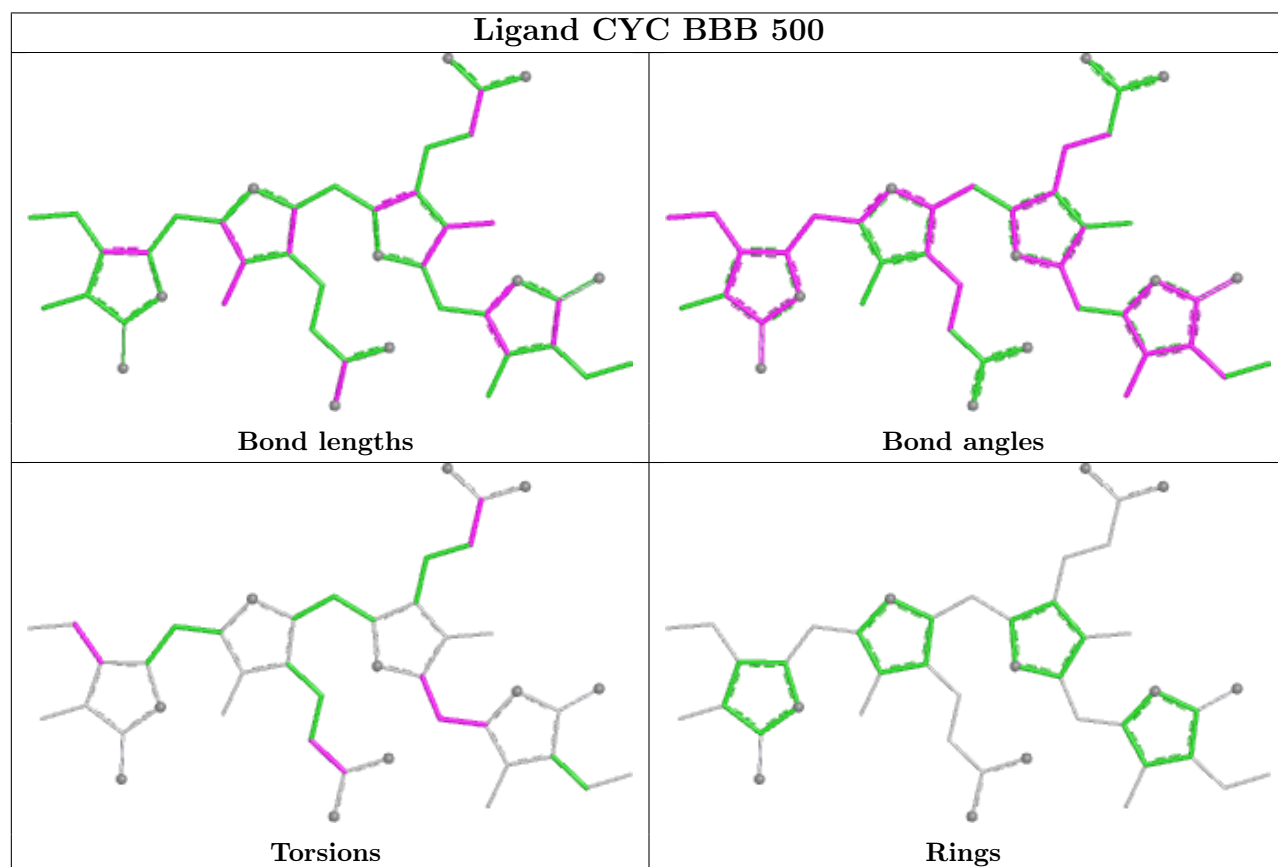
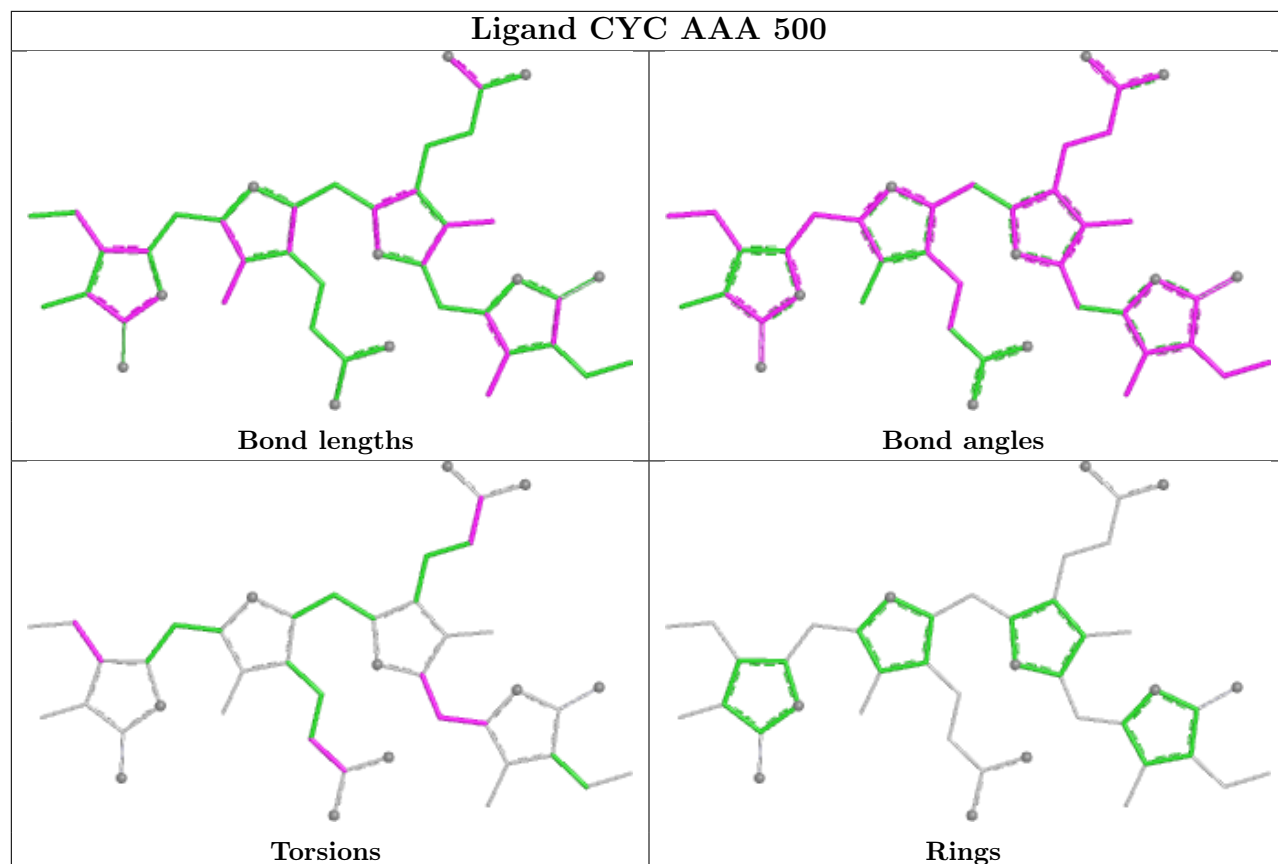
Mol	Chain	Res	Type	Atoms
2	AAA	500	CYC	CAD-CBD-CGD-O2D
2	AAA	500	CYC	CAA-CBA-CGA-O2A
2	AAA	500	CYC	CAD-CBD-CGD-O1D
2	AAA	500	CYC	C2B-C1B-CHB-C4A
3	BBB	501	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	AAA	500	CYC	3	0
3	BBB	501	PEG	7	0
2	BBB	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

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%)	0.30	30 (9%) 14 16	20, 44, 108, 161	1 (0%)
1	BBB	319/359 (88%)	0.24	27 (8%) 16 19	26, 42, 100, 145	0
All	All	636/718 (88%)	0.27	57 (8%) 15 17	20, 43, 105, 161	1 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	110	VAL	8.3
1	AAA	148	ALA	5.8
1	AAA	71	LEU	5.4
1	BBB	69	ALA	5.0
1	BBB	121	PRO	5.0
1	AAA	120	HIS	4.9
1	AAA	70	TYR	4.8
1	AAA	67	THR	4.6
1	AAA	147	PHE	4.6
1	AAA	150	VAL	4.6
1	BBB	122	ALA	4.5
1	BBB	71	LEU	4.4
1	AAA	119	ASP	4.2
1	AAA	110	VAL	4.2
1	BBB	67	THR	4.1
1	BBB	72	HIS	4.1
1	AAA	151	LEU	3.9
1	BBB	361	LYS	3.9
1	BBB	66	VAL	3.9
1	BBB	280	PHE	3.7
1	BBB	68	THR	3.5
1	AAA	121	PRO	3.5
1	AAA	69	ALA	3.3
1	BBB	119	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	AAA	280	PHE	3.2
1	AAA	402	LEU	3.2
1	AAA	73	HIS	3.2
1	BBB	120	HIS	3.1
1	AAA	74	MET	3.1
1	AAA	361	LYS	3.1
1	BBB	404	HIS	2.8
1	AAA	77	GLY	2.7
1	BBB	65	LYS	2.7
1	BBB	70	TYR	2.7
1	AAA	76	LYS	2.6
1	AAA	72	HIS	2.6
1	BBB	75	GLN	2.6
1	AAA	68	THR	2.6
1	BBB	151	LEU	2.6
1	AAA	75	GLN	2.4
1	BBB	402	LEU	2.4
1	BBB	360	ARG	2.4
1	AAA	404	HIS	2.4
1	AAA	405	HIS	2.4
1	BBB	406	HIS	2.4
1	AAA	122	ALA	2.3
1	BBB	187	PRO	2.3
1	AAA	281	LEU	2.3
1	BBB	405	HIS	2.3
1	BBB	284	LYS	2.3
1	BBB	109	MET	2.3
1	AAA	406	HIS	2.2
1	AAA	344	ASN	2.2
1	AAA	360	ARG	2.1
1	AAA	323	CYS	2.1
1	BBB	143	LYS	2.1
1	BBB	77	GLY	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 oligosaccharides in this entry.

6.4 Ligands

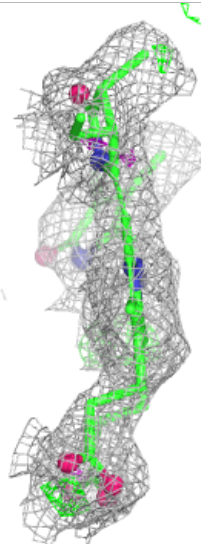
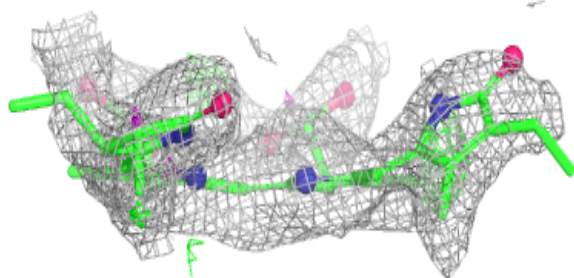
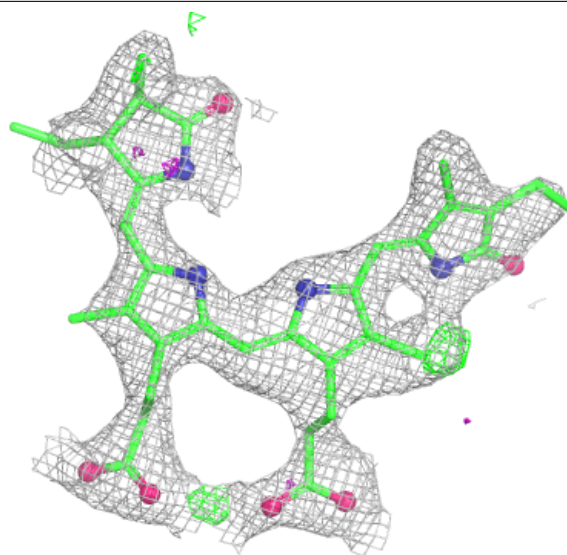
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PEG	AAA	501	7/7	0.81	0.23	36,60,89,90	0
2	CYC	AAA	500	43/43	0.82	0.16	47,86,95,105	0
3	PEG	BBB	501	7/7	0.83	0.22	13,23,29,30	7
2	CYC	BBB	500	43/43	0.86	0.14	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.

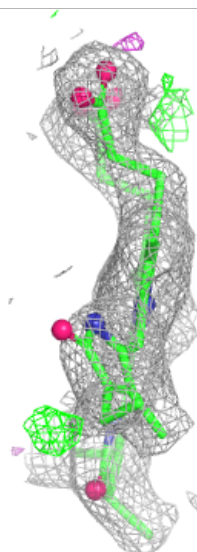
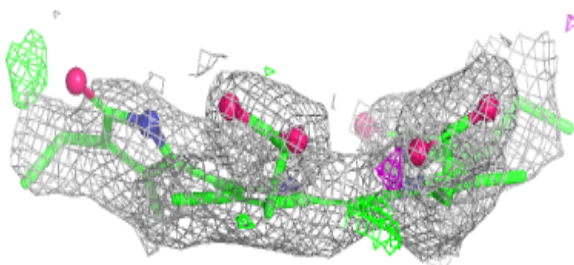
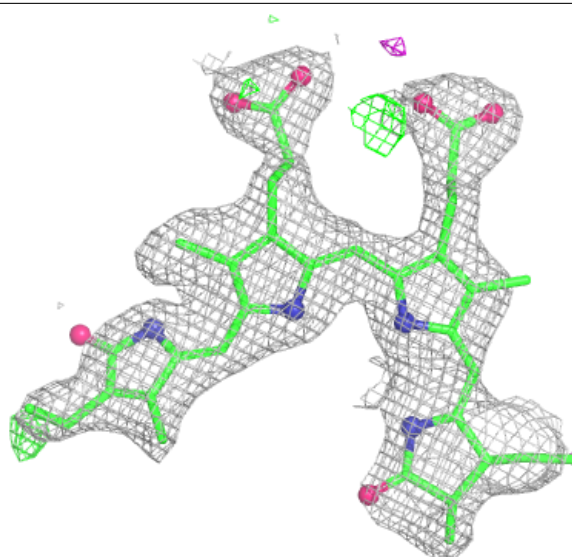
Electron density around CYC AAA 500:

$2mF_o-DF_c$ (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 [\(i\)](#)

There are no such residues in this entry.