



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:32 PM UTC

PDB ID : 1IT6 / pdb_00001it6
Title : CRYSTAL STRUCTURE OF THE COMPLEX BETWEEN CALYCULIN A
AND THE CATALYTIC SUBUNIT OF PROTEIN PHOSPHATASE 1
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Deposited on : 2002-01-09
Resolution : 2.00 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

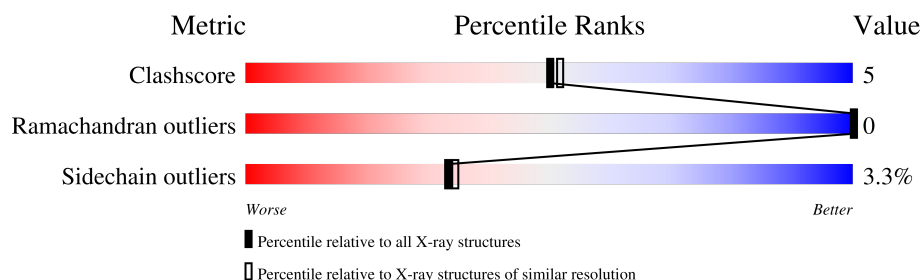
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	 78% 12% • 9%
1	B	323	 75% 15% • 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4936 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.

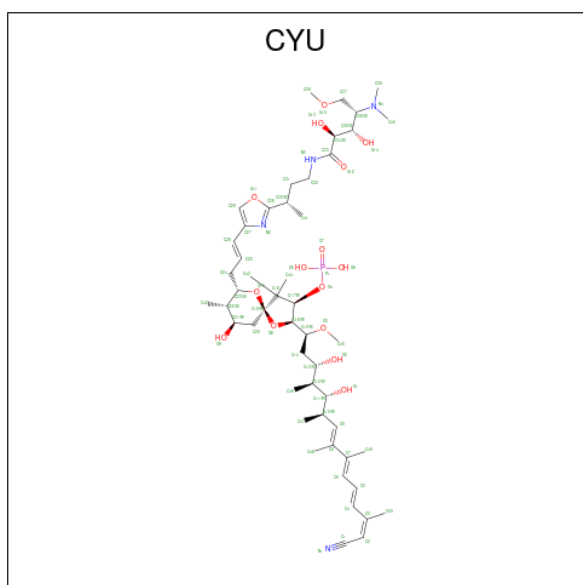
- Molecule 1 is a protein called SERINE/THREONINE PROTEIN PHOSPHATASE 1 GAMMA (PP1-GAMMA) CATALYTIC SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2362	1516	396	432	18			
1	B	293	Total	C	N	O	S	0	0	0
			2362	1516	396	432	18			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is CALYCULIN A (CCD ID: CYU) (formula: C₅₀H₈₁N₄O₁₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			56	42	2	11	1		
3	B	1	Total	C	N	O	P	0	0
			56	42	2	11	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	43	Total	O	0	0
			43	43		

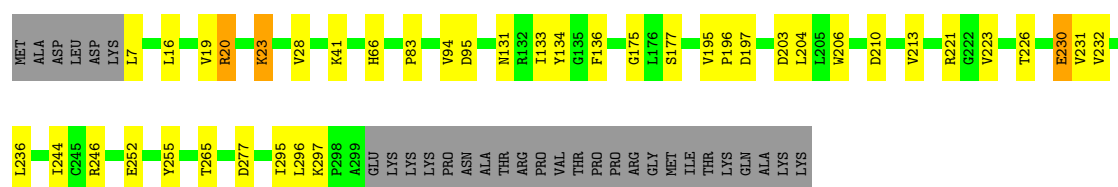
3 Residue-property plots [i](#)

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.

Note EDS was not executed.

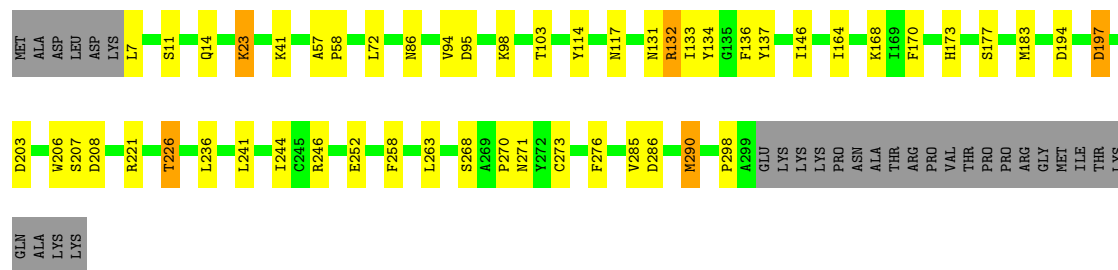
- Molecule 1: SERINE/THREONINE PROTEIN PHOSPHATASE 1 GAMMA (PP1-GAMMA) CATALYTIC SUBUNIT

Chain A: 



- Molecule 1: SERINE/THREONINE PROTEIN PHOSPHATASE 1 GAMMA (PP1-GAMMA) CATALYTIC SUBUNIT

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.09Å 136.36Å 61.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.182 , 0.218	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4936	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.46	0/2416	0.93	7/3263 (0.2%)
1	B	0.45	0/2416	0.98	11/3263 (0.3%)
All	All	0.45	0/4832	0.96	18/6526 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	TYR	N-CA-C	10.52	124.71	112.93
1	A	134	TYR	N-CA-C	8.75	123.56	113.15
1	A	252	GLU	N-CA-C	6.50	120.07	111.75
1	A	206	TRP	N-CA-C	6.07	122.14	114.31
1	B	226	THR	N-CA-C	-5.96	100.19	109.72
1	B	194	ASP	N-CA-C	-5.66	102.08	110.46
1	B	173	HIS	N-CA-C	5.66	117.31	111.03
1	A	28	VAL	N-CA-C	-5.62	99.46	107.77
1	A	226	THR	N-CA-C	-5.53	101.12	109.85
1	A	133	ILE	N-CA-C	5.45	116.51	111.45
1	B	206	TRP	N-CA-C	5.18	121.00	114.31
1	B	207	SER	N-CA-C	5.15	117.33	110.53
1	B	114	TYR	CA-C-N	5.14	124.81	119.56
1	B	114	TYR	C-N-CA	5.14	124.81	119.56
1	B	252	GLU	N-CA-C	5.14	117.55	111.33
1	B	133	ILE	N-CA-C	5.05	116.15	111.45
1	A	66	HIS	N-CA-C	5.02	118.17	111.24
1	B	132	ARG	N-CA-C	-5.01	105.53	111.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2362	0	2332	21	0
1	B	2362	0	2332	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	56	0	59	5	0
3	B	56	0	59	4	0
4	A	53	0	0	0	0
4	B	43	0	0	0	0
All	All	4936	0	4782	51	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 5.

All (51) 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:164:ILE:HD11	1:B:183:MET:HE3	1.72	0.71
1:A:197:ASP:HA	3:A:501:CYU:H503	1.71	0.71
1:B:197:ASP:HA	3:B:1501:CYU:H503	1.74	0.69
1:A:20:ARG:HB2	1:A:20:ARG:HH11	1.59	0.68
1:A:23:LYS:H	1:A:23:LYS:HD2	1.60	0.65
1:A:221:ARG:HG2	3:A:501:CYU:H453	1.79	0.64
1:B:268:SER:O	1:B:270:PRO:HD3	1.99	0.63
1:A:255:TYR:HE1	1:A:295:ILE:HD11	1.64	0.61
1:A:223:VAL:HG21	3:A:501:CYU:H501	1.83	0.59
1:A:236:LEU:HD21	1:A:244:ILE:HG13	1.86	0.57
1:B:271:ASN:HA	1:B:276:PHE:O	2.05	0.56
1:A:255:TYR:CE1	1:A:295:ILE:HD11	2.41	0.56
1:A:255:TYR:HE1	1:A:295:ILE:CD1	2.19	0.56
1:B:221:ARG:HG2	3:B:1501:CYU:H453	1.89	0.53
1:A:23:LYS:H	1:A:23:LYS:CD	2.22	0.53
1:A:255:TYR:HA	1:A:265:THR:O	2.09	0.53
3:B:1501:CYU:H452	3:B:1501:CYU:H23	1.90	0.52
1:B:57:ALA:HB1	1:B:58:PRO:HA	1.91	0.51
1:B:208:ASP:O	1:B:226:THR:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ASP:OD1	1:B:290:MET:HB3	2.12	0.50
1:B:11:SER:HA	1:B:14:GLN:HG2	1.93	0.50
1:B:23:LYS:HD2	1:B:23:LYS:H	1.76	0.50
1:B:137:TYR:CE1	1:B:146:ILE:HD12	2.48	0.49
1:B:177:SER:HB2	1:B:203:ASP:HB2	1.93	0.49
1:A:94:VAL:O	1:A:95:ASP:HB2	2.13	0.49
1:A:230:GLU:OE1	1:A:231:VAL:HG23	2.14	0.48
1:B:131:ASN:HB2	1:B:136:PHE:HB3	1.96	0.48
1:B:94:VAL:O	1:B:95:ASP:HB2	2.12	0.48
3:A:501:CYU:H452	3:A:501:CYU:H23	1.97	0.47
1:B:170:PHE:HB2	1:B:241:LEU:HD13	1.98	0.46
1:B:23:LYS:HD2	1:B:23:LYS:N	2.30	0.46
1:A:177:SER:HB2	1:A:203:ASP:HB2	1.98	0.46
1:B:86:ASN:ND2	1:B:117:ASN:HB3	2.30	0.46
1:B:98:LYS:HD2	1:B:98:LYS:N	2.31	0.46
1:B:132:ARG:HA	1:B:137:TYR:HB2	1.97	0.46
1:A:16:LEU:O	1:A:19:VAL:HG22	2.16	0.45
1:A:175:GLY:O	1:A:204:LEU:HD23	2.17	0.45
1:B:58:PRO:HA	1:B:285:VAL:O	2.18	0.44
1:A:210:ASP:HB3	1:A:213:VAL:HG12	1.99	0.44
1:B:170:PHE:CD1	1:B:183:MET:HE1	2.52	0.44
1:B:271:ASN:HB2	1:B:298:PRO:HB3	2.00	0.43
1:B:236:LEU:HD21	1:B:244:ILE:HG13	2.01	0.42
1:A:20:ARG:HH11	1:A:20:ARG:CB	2.28	0.42
1:A:131:ASN:HB2	1:A:136:PHE:HB3	2.00	0.42
3:B:1501:CYU:H491	3:B:1501:CYU:H9	1.82	0.42
1:B:258:PHE:HB3	1:B:263:LEU:HD22	2.01	0.42
1:B:168:LYS:HA	1:B:168:LYS:HD3	1.91	0.41
1:A:232:VAL:HG13	1:A:244:ILE:HD12	2.02	0.41
1:B:72:LEU:HD22	1:B:103:THR:HG23	2.02	0.41
3:A:501:CYU:H491	3:A:501:CYU:H9	1.79	0.41
1:A:195:VAL:HA	1:A:196:PRO:HD3	1.94	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	A	291/323 (90%)	278 (96%)	13 (4%)	0	100	100
1	B	291/323 (90%)	274 (94%)	17 (6%)	0	100	100
All	All	582/646 (90%)	552 (95%)	30 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/285 (91%)	249 (96%)	10 (4%)	28	28
1	B	259/285 (91%)	252 (97%)	7 (3%)	39	42
All	All	518/570 (91%)	501 (97%)	17 (3%)	33	34

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	20	ARG
1	A	23	LYS
1	A	41	LYS
1	A	83	PRO
1	A	230	GLU
1	A	246	ARG
1	A	277	ASP
1	A	296	LEU
1	A	297	LYS
1	B	7	LEU
1	B	23	LYS
1	B	41	LYS
1	B	197	ASP

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Mol	Chain	Res	Type
1	B	246	ARG
1	B	273	CYS
1	B	290	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	31	GLN
1	A	86	ASN
1	A	117	ASN
1	A	262	GLN
1	B	14	GLN
1	B	68	GLN
1	B	86	ASN
1	B	181	GLN
1	B	262	GLN
1	B	294	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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
3	CYU	A	501	-	56,58,72	3.02	30 (53%)	69,85,104	2.90	29 (42%)
3	CYU	B	1501	-	56,58,72	2.94	29 (51%)	69,85,104	2.95	30 (43%)

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
3	CYU	A	501	-	-	7/55/98/121	0/3/3/3
3	CYU	B	1501	-	-	5/55/98/121	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	CYU	C4-C3	8.17	1.63	1.46
3	B	1501	CYU	C4-C3	7.33	1.61	1.46
3	A	501	CYU	C12-C13	7.26	1.67	1.54
3	B	1501	CYU	C12-C13	6.90	1.67	1.54
3	B	1501	CYU	O10-C19	6.00	1.53	1.43
3	A	501	CYU	O10-C19	6.00	1.53	1.43
3	B	1501	CYU	C5-C6	6.00	1.61	1.43
3	A	501	CYU	C5-C6	5.85	1.61	1.43
3	A	501	CYU	C5-C4	5.84	1.49	1.34
3	B	1501	CYU	C20-C21	5.15	1.60	1.53
3	B	1501	CYU	C10-C9	4.87	1.61	1.51
3	A	501	CYU	C10-C9	4.66	1.60	1.51
3	A	501	CYU	C6-C7	4.56	1.47	1.34
3	A	501	CYU	C20-C21	4.50	1.59	1.53
3	B	1501	CYU	C6-C7	4.45	1.46	1.34
3	B	1501	CYU	C10-C11	4.45	1.70	1.54
3	A	501	CYU	C10-C11	4.33	1.69	1.54
3	B	1501	CYU	C5-C4	4.17	1.45	1.34
3	A	501	CYU	C22-C21	4.10	1.64	1.53
3	A	501	CYU	O9-C21	-4.08	1.34	1.43
3	B	1501	CYU	C22-C21	3.88	1.64	1.53
3	B	1501	CYU	C20-C19	3.73	1.59	1.52
3	B	1501	CYU	C30-C29	-3.59	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	CYU	C46-C12	3.58	1.60	1.53
3	B	1501	CYU	C28-C27	3.56	1.41	1.35
3	B	1501	CYU	C46-C12	3.54	1.60	1.53
3	B	1501	CYU	C24-C23	3.52	1.60	1.52
3	A	501	CYU	C20-C19	3.49	1.58	1.52
3	B	1501	CYU	O9-C21	-3.44	1.36	1.43
3	A	501	CYU	O11-C29	3.39	1.42	1.36
3	A	501	CYU	C28-C27	3.28	1.41	1.35
3	A	501	CYU	C30-C29	-3.25	1.40	1.50
3	B	1501	CYU	O11-C29	3.15	1.41	1.36
3	B	1501	CYU	C27-N2	3.08	1.44	1.38
3	A	501	CYU	C24-C23	3.07	1.59	1.52
3	A	501	CYU	C49-C7	2.84	1.57	1.50
3	B	1501	CYU	C49-C7	2.79	1.57	1.50
3	A	501	CYU	C27-N2	2.77	1.44	1.38
3	B	1501	CYU	C29-N2	2.69	1.33	1.29
3	A	501	CYU	C14-C13	2.59	1.58	1.53
3	B	1501	CYU	C24-C25	2.55	1.57	1.50
3	A	501	CYU	C24-C25	2.50	1.57	1.50
3	B	1501	CYU	C12-C11	2.48	1.60	1.54
3	A	501	CYU	C29-N2	2.47	1.33	1.29
3	B	1501	CYU	C1-N1	2.44	1.20	1.14
3	B	1501	CYU	C14-C13	2.39	1.58	1.53
3	B	1501	CYU	O3-C45	2.39	1.50	1.42
3	A	501	CYU	C12-C11	2.36	1.60	1.54
3	A	501	CYU	C2-C1	-2.28	1.39	1.42
3	A	501	CYU	C32-C31	2.25	1.64	1.51
3	A	501	CYU	C18-C17	2.24	1.56	1.52
3	A	501	CYU	O8-C16	2.20	1.46	1.43
3	B	1501	CYU	C32-C31	2.20	1.63	1.51
3	A	501	CYU	C1-N1	2.19	1.20	1.14
3	B	1501	CYU	C18-C17	2.07	1.56	1.52
3	B	1501	CYU	C31-C30	2.06	1.63	1.51
3	A	501	CYU	O3-C45	2.03	1.49	1.42
3	A	501	CYU	C44-C18	2.01	1.59	1.53
3	B	1501	CYU	C44-C18	2.00	1.59	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1501	CYU	C5-C4-C3	-9.35	100.73	126.36
3	B	1501	CYU	C50-C3-C4	9.12	132.02	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	CYU	C5-C4-C3	-9.12	101.37	126.36
3	A	501	CYU	C50-C3-C4	8.76	131.47	118.09
3	A	501	CYU	C6-C5-C4	-6.57	104.15	123.20
3	B	1501	CYU	C2-C1-N1	-6.49	163.80	177.43
3	B	1501	CYU	C6-C5-C4	-6.33	104.86	123.20
3	B	1501	CYU	C30-C29-N2	6.17	142.38	129.16
3	A	501	CYU	C30-C29-N2	6.08	142.19	129.16
3	A	501	CYU	C2-C1-N1	-5.94	164.96	177.43
3	B	1501	CYU	C28-C27-N2	-5.90	98.86	107.69
3	A	501	CYU	C28-C27-N2	-5.68	99.19	107.69
3	B	1501	CYU	C5-C6-C7	-4.65	113.50	126.64
3	A	501	CYU	C5-C6-C7	-4.62	113.58	126.64
3	A	501	CYU	C10-C9-C8	-4.50	114.60	126.41
3	B	1501	CYU	C10-C9-C8	-4.41	114.86	126.41
3	A	501	CYU	C50-C3-C2	-4.09	109.08	122.59
3	B	1501	CYU	C50-C3-C2	-4.02	109.33	122.59
3	B	1501	CYU	C42-C22-C23	3.98	119.21	111.89
3	A	501	CYU	C42-C22-C23	3.79	118.85	111.89
3	B	1501	CYU	O11-C28-C27	3.71	113.60	108.85
3	A	501	CYU	C27-N2-C29	3.68	115.43	105.11
3	B	1501	CYU	C27-N2-C29	3.63	115.28	105.11
3	A	501	CYU	O11-C28-C27	3.55	113.39	108.85
3	B	1501	CYU	C47-C10-C11	-3.54	103.87	111.45
3	B	1501	CYU	C49-C7-C8	3.48	130.81	117.80
3	A	501	CYU	C47-C10-C11	-3.41	104.15	111.45
3	A	501	CYU	C24-C23-C22	-3.40	106.15	113.68
3	B	1501	CYU	C24-C23-C22	-3.37	106.20	113.68
3	A	501	CYU	C14-C15-C16	-3.31	106.99	113.34
3	A	501	CYU	C49-C7-C8	3.26	129.97	117.80
3	A	501	CYU	O8-C16-C17	3.14	107.45	103.83
3	B	1501	CYU	O8-C16-C17	3.07	107.37	103.83
3	B	1501	CYU	C14-C15-C16	-2.94	107.71	113.34
3	B	1501	CYU	C26-C27-N2	2.89	126.37	122.37
3	B	1501	CYU	C20-C21-C22	-2.81	105.79	111.16
3	A	501	CYU	C48-C8-C7	2.81	128.28	117.80
3	A	501	CYU	C11-C10-C9	-2.80	103.20	109.55
3	A	501	CYU	C13-C12-C11	-2.79	103.38	111.19
3	A	501	CYU	C13-C14-C15	-2.76	105.96	113.09
3	B	1501	CYU	C13-C14-C15	-2.76	105.98	113.09
3	B	1501	CYU	C44-C18-C19	2.71	118.88	110.42
3	A	501	CYU	C20-C21-C22	-2.70	106.00	111.16
3	A	501	CYU	O11-C29-N2	-2.69	105.77	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1501	CYU	C13-C12-C11	-2.66	103.76	111.19
3	B	1501	CYU	C48-C8-C7	2.60	127.53	117.80
3	B	1501	CYU	O11-C29-N2	-2.59	106.03	113.34
3	A	501	CYU	C44-C18-C19	2.59	118.50	110.42
3	A	501	CYU	C26-C27-N2	2.48	125.80	122.37
3	B	1501	CYU	O3-C15-C14	-2.47	102.88	110.27
3	B	1501	CYU	C46-C12-C13	-2.39	107.28	111.09
3	A	501	CYU	O3-C15-C14	-2.38	103.13	110.27
3	B	1501	CYU	C11-C10-C9	-2.35	104.23	109.55
3	A	501	CYU	O8-C19-C20	2.27	113.71	109.89
3	B	1501	CYU	O8-C19-C20	2.25	113.69	109.89
3	A	501	CYU	O10-C23-C24	-2.21	99.94	105.18
3	B	1501	CYU	O10-C23-C24	-2.12	100.15	105.18
3	B	1501	CYU	O10-C19-C20	-2.01	107.84	111.82
3	A	501	CYU	O8-C19-O10	-2.00	108.76	110.62

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1501	CYU	O11-C29-C30-C41
3	A	501	CYU	O11-C29-C30-C31
3	B	1501	CYU	O11-C29-C30-C31
3	A	501	CYU	C14-C15-C16-O8
3	B	1501	CYU	C14-C15-C16-O8
3	A	501	CYU	C11-C12-C13-O2
3	B	1501	CYU	C11-C12-C13-O2
3	A	501	CYU	C22-C23-C24-C25
3	A	501	CYU	C17-O4-P1-O7
3	B	1501	CYU	C17-O4-P1-O7
3	A	501	CYU	O11-C29-C30-C41
3	A	501	CYU	N2-C29-C30-C41

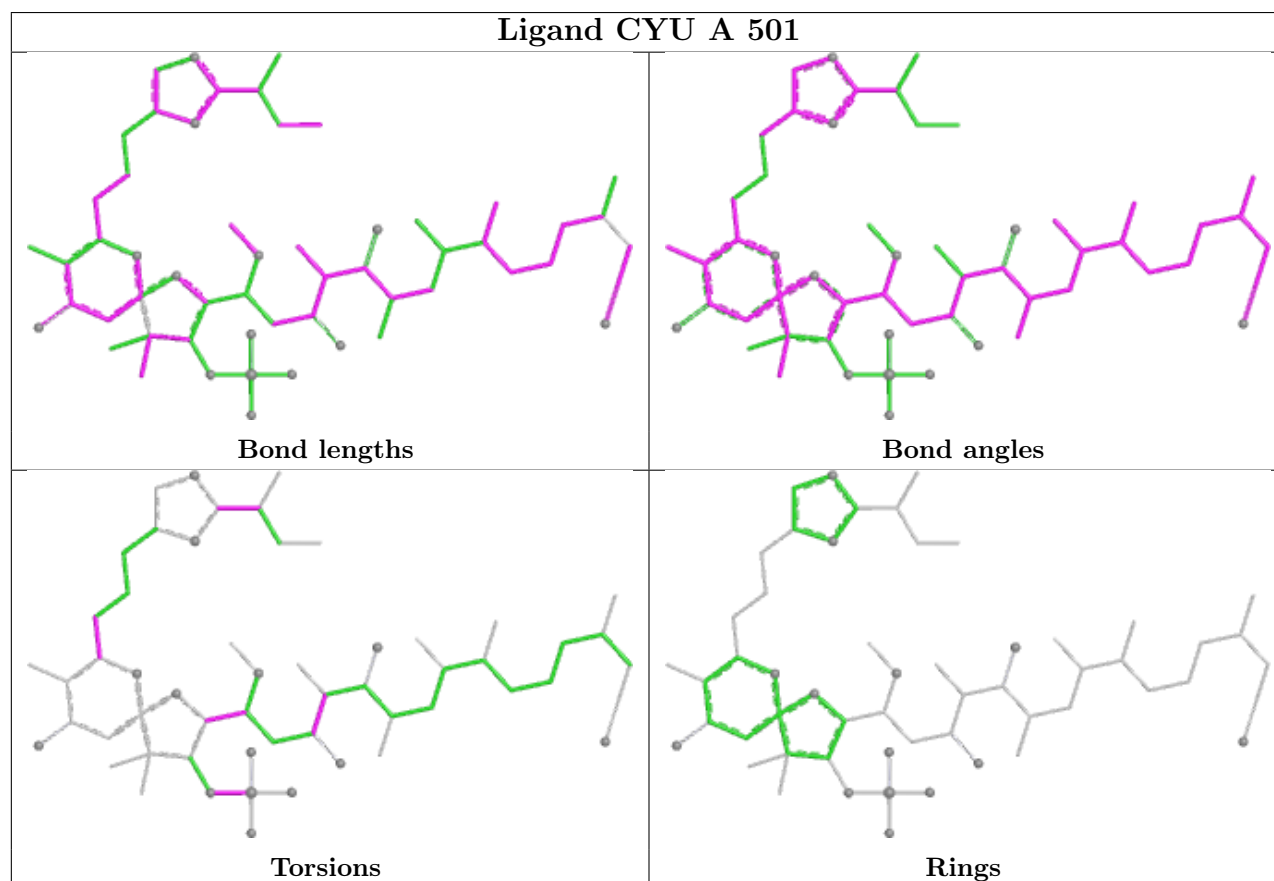
There are no ring outliers.

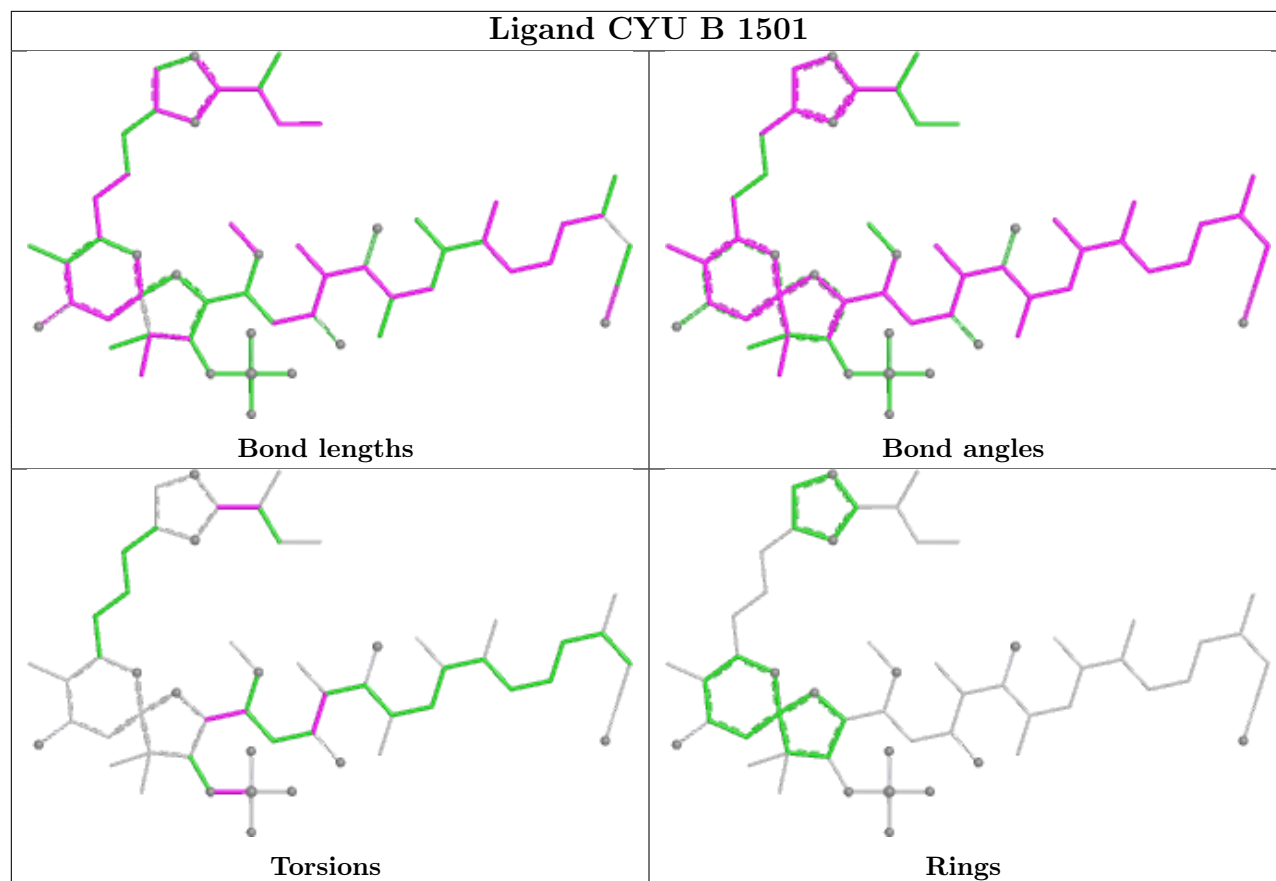
2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	CYU	5	0
3	B	1501	CYU	4	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.