



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:48 pm GMT

PDB ID : 1IT6
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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

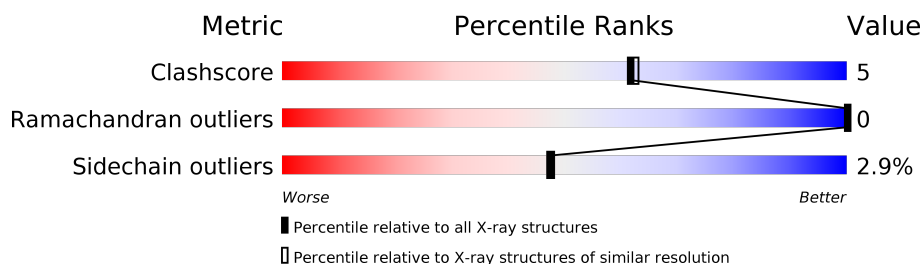
1 Overall quality at a glance

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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	 81% 9% • 9%
1	B	323	 77% 13% • 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.

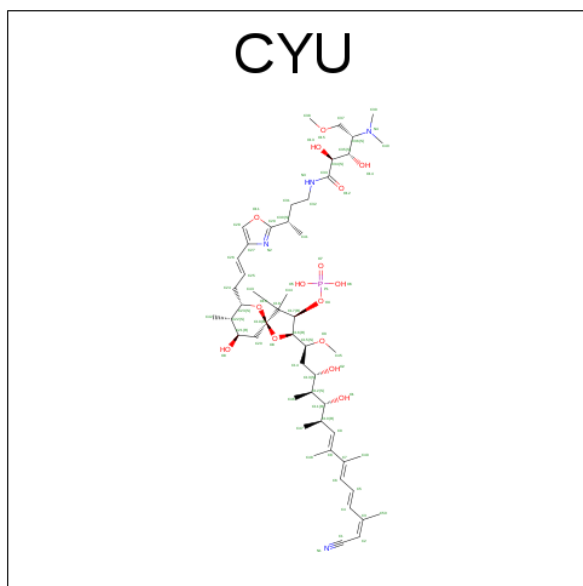
- Molecule 1 is a protein called SERINE/THREONINE PROTEIN PHOSPHATASE 1 GAMMA (PP1-GAMMA) CATALYTIC SUBUNIT.

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 (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is CALYCULIN A (three-letter code: CYU) (formula: $C_{50}H_{81}N_4O_{15}P$).



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		

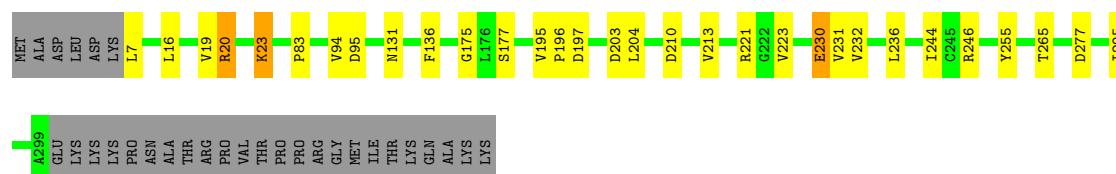
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.


Note EDS was not executed.

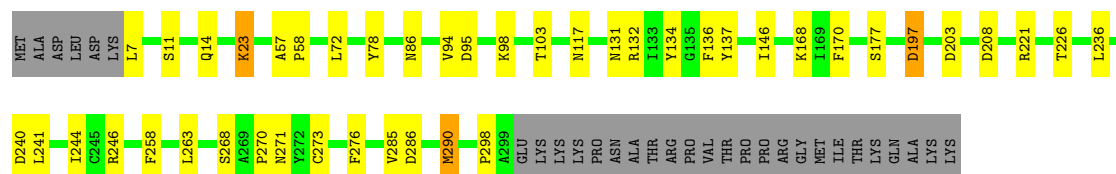
- Molecule 1: SERINE/THREONINE PROTEIN PHOSPHATASE 1 GAMMA (PP1-GAMMA) CATALYTIC SUBUNIT

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 [i](#)

5.1 Standard geometry [i](#)

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	0.40	0/2416	0.65	0/3263
1	B	0.41	0/2416	0.68	1/3263 (0.0%)
All	All	0.41	0/4832	0.66	1/6526 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	TYR	N-CA-C	5.08	124.71	111.00

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	2362	0	2332	21	0
1	B	2362	0	2332	24	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4936	0	4782	49	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 (49) 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: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:HH11	1:A:20:ARG:HB2	1.59	0.68
1:A:23:LYS:HD2	1:A:23:LYS:H	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
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:H23	3:A:501:CYU:H452	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:132:ARG:HA	1:B:137:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LYS:N	1:B:98:LYS:HD2	2.31	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: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%)	252 (97%)	7 (3%)	50	51
1	B	259/285 (91%)	251 (97%)	8 (3%)	45	44
All	All	518/570 (91%)	503 (97%)	15 (3%)	48	47

All (15) 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	83	PRO
1	A	230	GLU
1	A	246	ARG
1	A	277	ASP
1	B	7	LEU
1	B	23	LYS
1	B	78	TYR
1	B	197	ASP
1	B	240	ASP
1	B	246	ARG
1	B	273	CYS
1	B	290	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	86	ASN
1	A	271	ASN
1	B	86	ASN
1	B	117	ASN
1	B	181	GLN
1	B	262	GLN

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Mol	Chain	Res	Type
1	B	271	ASN
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 carbohydrates 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	-	51,58,72	3.03	24 (47%)	64,85,104	2.84	23 (35%)
3	CYU	B	1501	-	51,58,72	2.95	24 (47%)	64,85,104	2.89	23 (35%)

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	-	-	0/50/98/121	0/2/3/3
3	CYU	B	1501	-	-	0/50/98/121	0/2/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1501	CYU	C29-C30	-6.07	1.39	1.50
3	A	501	CYU	C29-C30	-5.52	1.40	1.50
3	A	501	CYU	O9-C21	-3.90	1.34	1.43
3	B	1501	CYU	O9-C21	-3.29	1.36	1.43
3	A	501	CYU	C2-C1	-2.13	1.39	1.42
3	A	501	CYU	C12-C11	2.04	1.60	1.54
3	B	1501	CYU	C32-C31	2.06	1.63	1.50
3	B	1501	CYU	C31-C30	2.10	1.63	1.50
3	A	501	CYU	C32-C31	2.11	1.64	1.50
3	A	501	CYU	C27-N2	2.13	1.44	1.37
3	B	1501	CYU	C12-C11	2.15	1.60	1.54
3	A	501	CYU	O8-C16	2.21	1.46	1.43
3	B	1501	CYU	C14-C13	2.25	1.58	1.53
3	B	1501	CYU	O3-C45	2.26	1.50	1.42
3	A	501	CYU	C24-C25	2.27	1.57	1.50
3	B	1501	CYU	C24-C25	2.31	1.57	1.50
3	B	1501	CYU	C27-N2	2.34	1.44	1.37
3	A	501	CYU	C1-N1	2.36	1.20	1.14
3	A	501	CYU	C14-C13	2.44	1.58	1.53
3	B	1501	CYU	C49-C7	2.52	1.57	1.50
3	A	501	CYU	C49-C7	2.56	1.57	1.50
3	B	1501	CYU	C1-N1	2.63	1.20	1.14
3	A	501	CYU	C24-C23	2.99	1.59	1.52
3	A	501	CYU	C20-C19	3.21	1.58	1.52
3	B	1501	CYU	C46-C12	3.24	1.60	1.53
3	A	501	CYU	C46-C12	3.27	1.60	1.53
3	B	1501	CYU	C20-C19	3.43	1.59	1.52
3	B	1501	CYU	C24-C23	3.43	1.60	1.52
3	B	1501	CYU	C22-C21	3.59	1.64	1.53
3	B	1501	CYU	C6-C7	3.65	1.46	1.34
3	A	501	CYU	C6-C7	3.74	1.47	1.34
3	A	501	CYU	C22-C21	3.79	1.64	1.53
3	A	501	CYU	C10-C11	3.88	1.69	1.54
3	B	1501	CYU	C10-C11	3.99	1.70	1.54
3	B	1501	CYU	C5-C4	4.29	1.45	1.34
3	A	501	CYU	C10-C9	4.30	1.60	1.51
3	A	501	CYU	C20-C21	4.38	1.59	1.53
3	B	1501	CYU	C10-C9	4.49	1.61	1.51
3	B	1501	CYU	C20-C21	5.02	1.60	1.53
3	A	501	CYU	O10-C19	5.68	1.53	1.43
3	B	1501	CYU	O10-C19	5.68	1.53	1.43
3	A	501	CYU	C5-C6	5.79	1.61	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1501	CYU	C5-C6	5.93	1.61	1.43
3	A	501	CYU	C5-C4	5.99	1.49	1.34
3	B	1501	CYU	C12-C13	7.21	1.67	1.54
3	B	1501	CYU	C4-C3	7.24	1.61	1.45
3	A	501	CYU	C12-C13	7.58	1.67	1.54
3	A	501	CYU	C4-C3	8.07	1.63	1.45

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1501	CYU	C5-C4-C3	-9.14	100.73	126.42
3	A	501	CYU	C5-C4-C3	-8.92	101.37	126.42
3	A	501	CYU	C6-C5-C4	-6.22	104.15	123.23
3	B	1501	CYU	C6-C5-C4	-5.99	104.86	123.23
3	B	1501	CYU	C2-C1-N1	-5.76	163.80	177.35
3	A	501	CYU	C2-C1-N1	-5.27	164.96	177.35
3	A	501	CYU	C10-C9-C8	-4.34	114.60	126.33
3	B	1501	CYU	C10-C9-C8	-4.24	114.86	126.33
3	B	1501	CYU	C5-C6-C7	-4.22	113.50	126.74
3	A	501	CYU	C5-C6-C7	-4.20	113.58	126.74
3	A	501	CYU	C50-C3-C2	-4.18	109.08	122.81
3	B	1501	CYU	C50-C3-C2	-4.11	109.33	122.81
3	A	501	CYU	C11-C10-C9	-3.30	103.20	110.67
3	A	501	CYU	C14-C15-C16	-3.28	106.99	113.48
3	B	1501	CYU	C47-C10-C11	-3.24	103.87	111.13
3	A	501	CYU	C24-C23-C22	-3.24	106.15	113.67
3	B	1501	CYU	C24-C23-C22	-3.22	106.20	113.67
3	A	501	CYU	C47-C10-C11	-3.12	104.15	111.13
3	B	1501	CYU	C14-C15-C16	-2.92	107.71	113.48
3	B	1501	CYU	C46-C12-C13	-2.89	107.28	111.36
3	B	1501	CYU	C11-C10-C9	-2.84	104.23	110.67
3	B	1501	CYU	C20-C21-C22	-2.79	105.79	110.94
3	B	1501	CYU	O3-C15-C14	-2.70	102.88	109.16
3	A	501	CYU	C13-C14-C15	-2.69	105.96	112.74
3	B	1501	CYU	C13-C14-C15	-2.69	105.98	112.74
3	A	501	CYU	C20-C21-C22	-2.68	106.00	110.94
3	A	501	CYU	O3-C15-C14	-2.59	103.13	109.16
3	A	501	CYU	C46-C12-C13	-2.41	107.96	111.36
3	A	501	CYU	O10-C23-C24	-2.15	99.94	105.13
3	B	1501	CYU	O10-C23-C24	-2.06	100.15	105.13
3	B	1501	CYU	O8-C19-C20	2.25	113.69	109.89
3	A	501	CYU	O8-C19-C20	2.27	113.71	109.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1501	CYU	C48-C8-C7	2.50	127.53	118.00
3	A	501	CYU	C44-C18-C19	2.70	118.50	110.20
3	A	501	CYU	C48-C8-C7	2.70	128.28	118.00
3	B	1501	CYU	C44-C18-C19	2.82	118.88	110.20
3	B	1501	CYU	O8-C16-C17	3.04	107.37	103.80
3	A	501	CYU	O8-C16-C17	3.10	107.45	103.80
3	A	501	CYU	C49-C7-C8	3.15	129.97	118.00
3	B	1501	CYU	C49-C7-C8	3.37	130.81	118.00
3	A	501	CYU	C42-C22-C23	3.54	118.85	112.00
3	B	1501	CYU	C42-C22-C23	3.72	119.21	112.00
3	A	501	CYU	C50-C3-C4	8.39	131.47	118.10
3	B	1501	CYU	C50-C3-C4	8.74	132.02	118.10
3	A	501	CYU	C30-C29-N2	8.97	142.19	124.96
3	B	1501	CYU	C30-C29-N2	9.07	142.38	124.96

There are no chirality outliers.

There are no torsion outliers.

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

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.