



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 14, 2017 – 05:30 pm GMT

PDB ID : 2VLC
Title : CRYSTAL STRUCTURE OF NATURAL CINNAMOMIN (ISOFORM III)
Authors : Azzi, A.; Wang, T.; Zhu, D.-W.; Zou, Y.-S.; Liu, W.-Y.; Lin, S.-X.
Deposited on : 2008-01-11
Resolution : 2.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

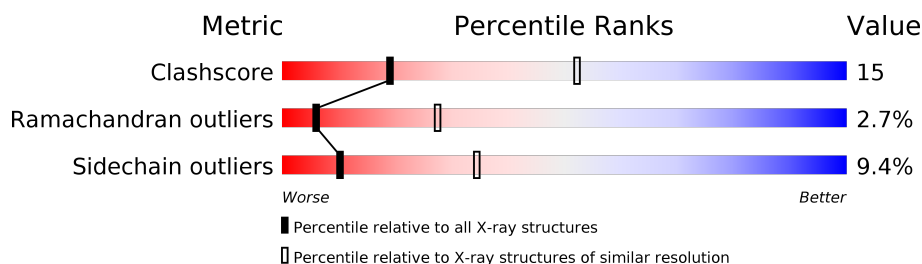
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)

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	570	
1	B	570	

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
2	AS5	A	1549	X	-	-	-
2	AS5	A	1550	X	-	-	-
2	AS5	A	1551	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AS5	B	1550	X	-	X	-
2	AS5	B	1551	X	-	-	-
2	AS5	B	1552	X	-	-	-
3	BMA	B	1549	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8406 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.

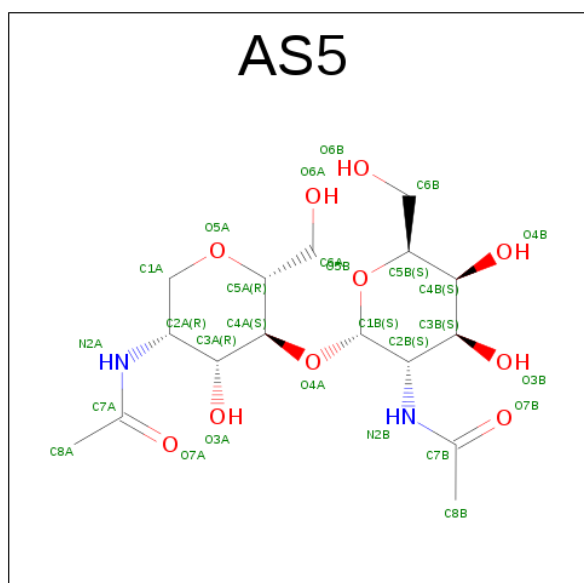
- Molecule 1 is a protein called TYPE 2 RIBOSOME-INACTIVATING PROTEIN CINNAMOMIN III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	518	Total	C	N	O	S	4	0	0
			4036	2529	713	773	21			
1	B	518	Total	C	N	O	S	5	0	0
			4038	2529	713	775	21			

There are 4 discrepancies between the modelled and reference sequences:

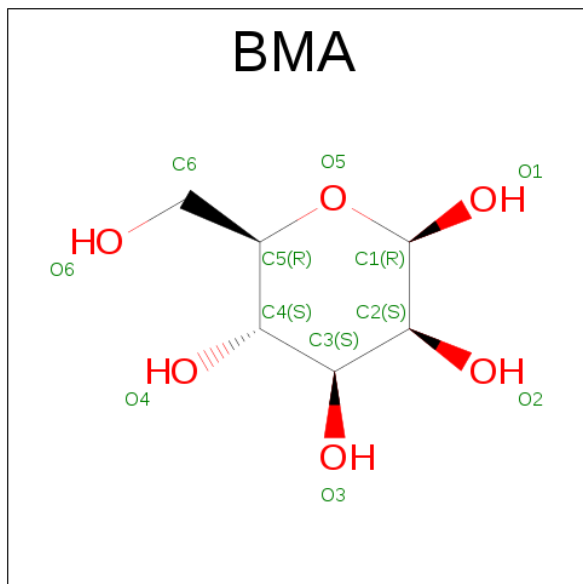
Chain	Residue	Modelled	Actual	Comment	Reference
A	183	SER	THR	CONFLICT	UNP Q94BW3
A	307	ARG	ASP	CONFLICT	UNP Q94BW3
B	183	SER	THR	CONFLICT	UNP Q94BW3
B	307	ARG	ASP	CONFLICT	UNP Q94BW3

- Molecule 2 is 2-(ACETYLAMINO)-4-O-[2-(ACETYLAMINO)-2-DEOXY-ALPHA-L-GULOPYRANOSYL]-1,5-ANHYDRO-2-DEOXY-D-MANNITOL (three-letter code: AS5) (formula: $C_{16}H_{28}N_2O_{10}$).



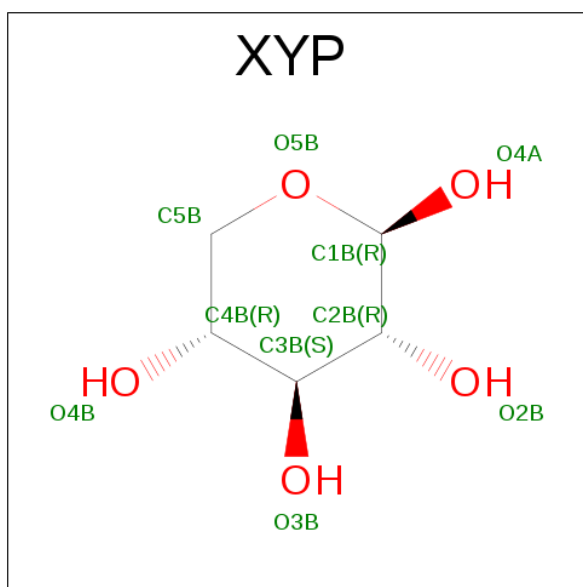
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	16	2	10		
2	A	1	Total	C	N	O	0	0
			28	16	2	10		
2	A	1	Total	C	N	O	0	0
			28	16	2	10		
2	B	1	Total	C	N	O	0	0
			28	16	2	10		
2	B	1	Total	C	N	O	0	0
			28	16	2	10		
2	B	1	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



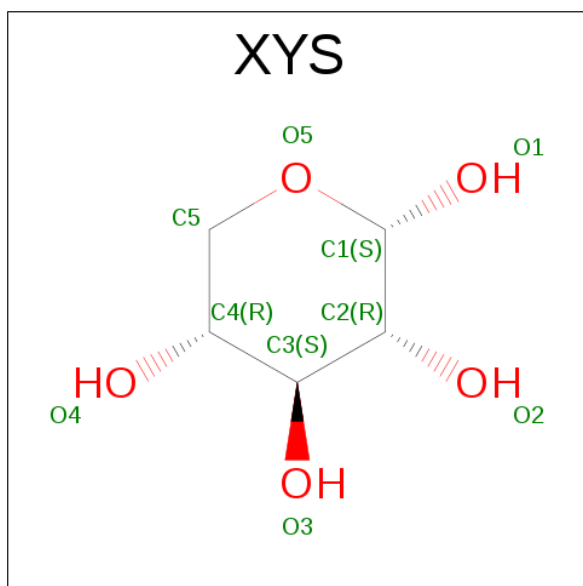
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is SUGAR (BETA-D-XYLOPYRANOSE) (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 5 is SUGAR (XYLOPYRANOSE) (three-letter code: XYS) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	5	5		

- Molecule 6 is water.

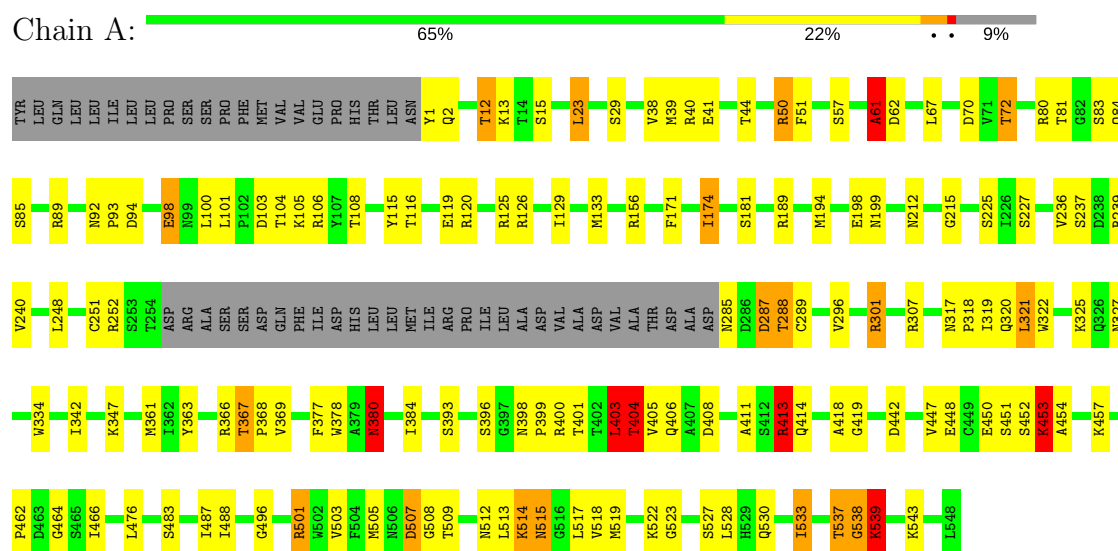
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	68	Total 68	O 68	0	0
6	B	52	Total 52	O 52	0	0

3 Residue-property plots

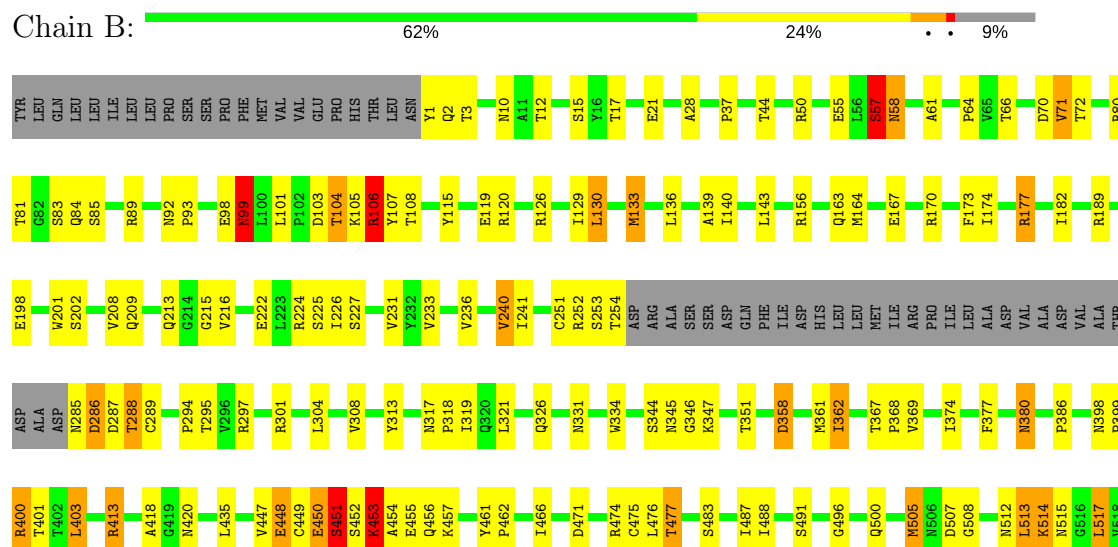
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: TYPE 2 RIBOSOME-INACTIVATING PROTEIN CINNAMOMIN III



• Molecule 1: TYPE 2 RIBOSOME-INACTIVATING PROTEIN CINNAMOMIN III





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 21	Depositor
Cell constants a, b, c, α , β , γ	52.39Å 126.33Å 161.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 2.95	Depositor
% Data completeness (in resolution range)	98.9 (17.00-2.95)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8406	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: XYP, XYS, BMA, AS5

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	1.05	4/4122 (0.1%)	0.91	13/5610 (0.2%)
1	B	0.89	4/4124 (0.1%)	1.71	15/5612 (0.3%)
All	All	0.98	8/8246 (0.1%)	1.37	28/11222 (0.2%)

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	A	0	9
1	B	0	6
All	All	0	15

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	368	PRO	N-CD	-41.24	0.90	1.47
1	B	358	ASP	CG-OD2	23.72	1.79	1.25
1	A	462	PRO	N-CD	-16.64	1.24	1.47
1	B	462	PRO	CB-CG	-15.91	0.70	1.50
1	A	462	PRO	CB-CG	-14.95	0.75	1.50

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ASP	CB-CG-OD2	-104.02	24.69	118.30
1	B	462	PRO	CA-N-CD	-15.55	89.73	111.50
1	B	368	PRO	CA-N-CD	-13.82	92.16	111.50
1	B	358	ASP	OD1-CG-OD2	-12.96	98.68	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	368	PRO	N-CD-CG	11.04	119.77	103.20

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	367	THR	Peptide
1	A	403	LEU	Peptide
1	A	57	SER	Peptide
1	A	61	ALA	Peptide
1	A	98	GLU	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	A	4036	0	3954	95	0
1	B	4038	0	3954	112	0
2	A	84	0	75	16	0
2	B	84	0	79	28	0
3	A	12	0	9	5	0
3	B	12	0	11	14	0
4	A	10	0	9	2	0
5	B	10	0	10	2	0
6	A	68	0	0	3	0
6	B	52	0	0	4	0
All	All	8406	0	8101	239	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 15.

The worst 5 of 239 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)
2:A:1549:AS5:HA	3:A:1552:BMA:O3	1.27	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1549:BMA:C6	2:B:1550:AS5:H1B	1.63	1.25
2:B:1552:AS5:O7B	6:B:2051:HOH:O	1.56	1.21
1:A:380:ASN:ND2	1:A:513:LEU:HD11	1.55	1.18
3:B:1549:BMA:O6	2:B:1550:AS5:C4B	1.96	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	514/570 (90%)	467 (91%)	33 (6%)	14 (3%)	6	27
1	B	514/570 (90%)	469 (91%)	31 (6%)	14 (3%)	6	27
All	All	1028/1140 (90%)	936 (91%)	64 (6%)	28 (3%)	6	27

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ASP
1	A	288	THR
1	A	404	THR
1	A	514	LYS
1	A	538	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/496 (90%)	406 (91%)	40 (9%)	11	37
1	B	446/496 (90%)	402 (90%)	44 (10%)	9	32
All	All	892/992 (90%)	808 (91%)	84 (9%)	10	34

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	528	LEU
1	B	83	SER
1	B	505	MET
1	A	539	LYS
1	B	3	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	B	213	GLN
1	B	285	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

10 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	AS5	A	1549	-	29,29,29	1.77	6 (20%)	36,41,41	5.16	16 (44%)
2	AS5	A	1550	-	29,29,29	1.07	1 (3%)	36,41,41	2.42	8 (22%)
2	AS5	A	1551	-	29,29,29	1.87	2 (6%)	36,41,41	2.68	15 (41%)
3	BMA	A	1552	-	12,12,12	0.72	0	17,17,17	2.39	7 (41%)
4	XYP	A	1553	-	10,10,10	1.37	1 (10%)	14,14,14	1.53	4 (28%)
3	BMA	B	1549	-	12,12,12	0.79	0	17,17,17	1.92	5 (29%)
2	AS5	B	1550	-	29,29,29	1.93	1 (3%)	36,41,41	2.65	12 (33%)
2	AS5	B	1551	-	29,29,29	0.76	1 (3%)	36,41,41	7.07	8 (22%)
2	AS5	B	1552	-	29,29,29	1.05	2 (6%)	36,41,41	2.48	12 (33%)
5	XYS	B	1553	-	10,10,10	1.38	1 (10%)	14,14,14	1.52	3 (21%)

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	AS5	A	1549	-	1/1/11/13	0/16/53/53	0/2/2/2
2	AS5	A	1550	-	3/3/11/13	0/16/53/53	0/2/2/2
2	AS5	A	1551	-	2/2/11/13	0/16/53/53	1/2/2/2
3	BMA	A	1552	-	-	0/2/22/22	0/1/1/1
4	XYP	A	1553	-	-	0/0/17/17	0/1/1/1
3	BMA	B	1549	-	-	0/2/22/22	0/1/1/1
2	AS5	B	1550	-	1/1/11/13	0/16/53/53	0/2/2/2
2	AS5	B	1551	-	2/2/11/13	0/16/53/53	0/2/2/2
2	AS5	B	1552	-	6/6/11/13	0/16/53/53	0/2/2/2
5	XYS	B	1553	-	-	0/0/17/17	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1550	AS5	O3B-C3B	-9.85	1.20	1.43
2	A	1551	AS5	O3B-C3B	-8.92	1.22	1.43
2	A	1549	AS5	O3B-C3B	-4.36	1.32	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1553	XYP	O5B-C1B	-3.94	1.37	1.43
5	B	1553	XYS	O5-C1	-3.66	1.37	1.43

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1551	AS5	O7B-C7B-C8B	-22.85	80.46	122.06
2	B	1551	AS5	O7B-C7B-N2B	-22.16	79.26	121.92
2	A	1549	AS5	O3B-C3B-C4B	-10.34	87.86	110.36
2	A	1551	AS5	O5A-C1A-C2A	-5.26	104.15	111.47
3	A	1552	BMA	O6-C6-C5	-4.61	95.82	111.34

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1550	AS5	C4B
2	A	1551	AS5	C2B
2	A	1551	AS5	C3B
2	A	1549	AS5	C3B
2	A	1550	AS5	C2B

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1551	AS5	C1A-C2A-C3A-C4A-C5A-O5A

10 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1549	AS5	7	0
2	A	1550	AS5	1	0
2	A	1551	AS5	8	0
3	A	1552	BMA	5	0
4	A	1553	XYP	2	0
3	B	1549	BMA	14	0
2	B	1550	AS5	22	0
2	B	1551	AS5	2	0
2	B	1552	AS5	4	0
5	B	1553	XYS	2	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.