



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:36 AM 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 full wwPDB 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/ValidationPDFNotes.html>

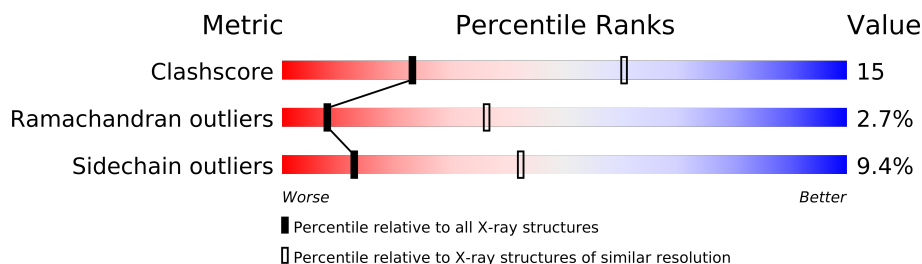
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	570	
1	B	570	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8406 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

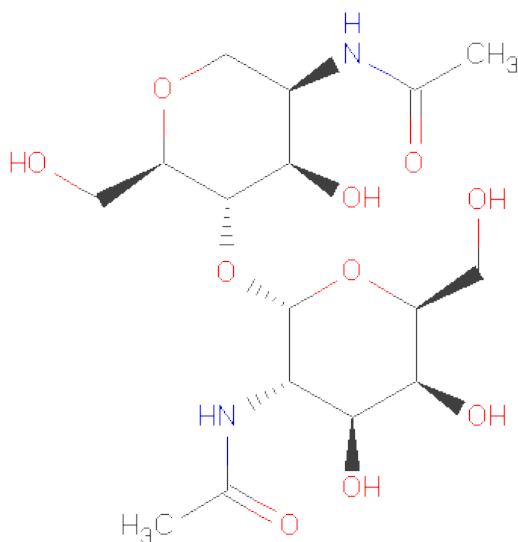
- Molecule 1 is a protein called TYPE 2 RIBOSOME-INACTIVATINGPROTEIN CINNAMOMIN III.

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:

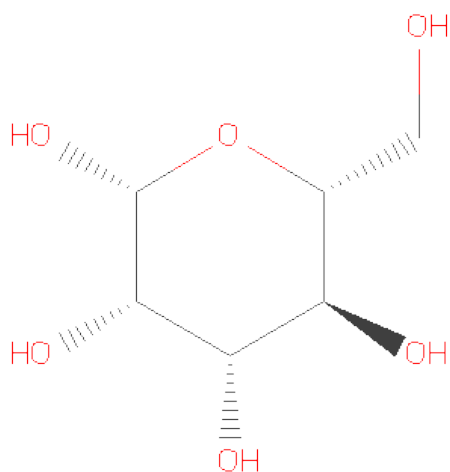
Chain	Residue	Modelled	Actual	Comment	Reference
A	183	SER	THR	CONFLICT	UNP Q94BW3
A	307	ARG	ASP	CONFLICT	UNP Q94BW3
B	183	SER	THR	CONFLICT	UNP Q94BW3
B	307	ARG	ASP	CONFLICT	UNP Q94BW3

- 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: C₁₆H₂₈N₂O₁₀).



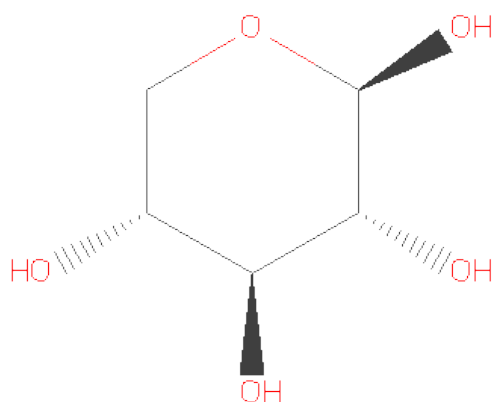
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	16	2	10		
2	A	1	Total	C	N	O	0	0
			28	16	2	10		
2	A	1	Total	C	N	O	0	0
			28	16	2	10		
2	B	1	Total	C	N	O	0	0
			28	16	2	10		
2	B	1	Total	C	N	O	0	0
			28	16	2	10		
2	B	1	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: C₆H₁₂O₆).



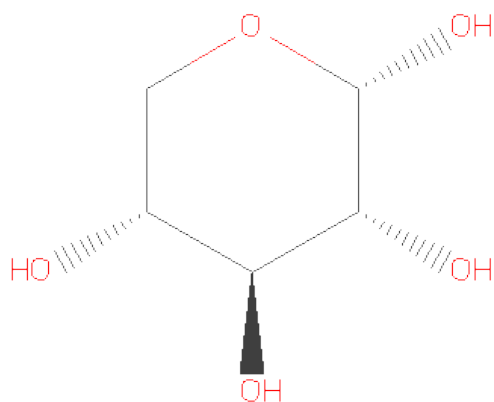
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is SUGAR (BETA-D-XYLOPYRANOSE) (three-letter code: XYP) (formula: C₅H₁₀O₅).



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: C₅H₁₀O₅).



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

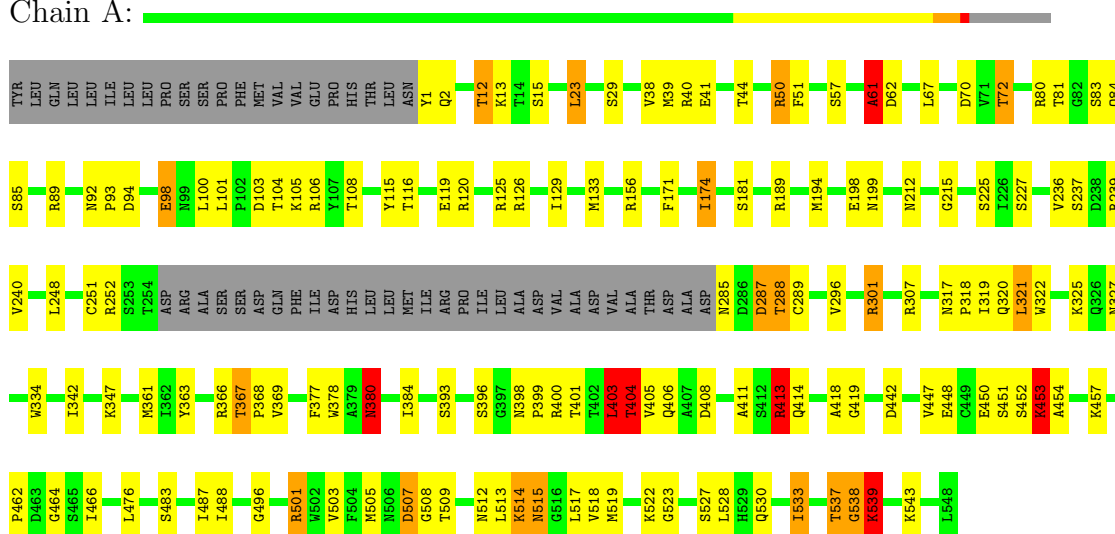
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

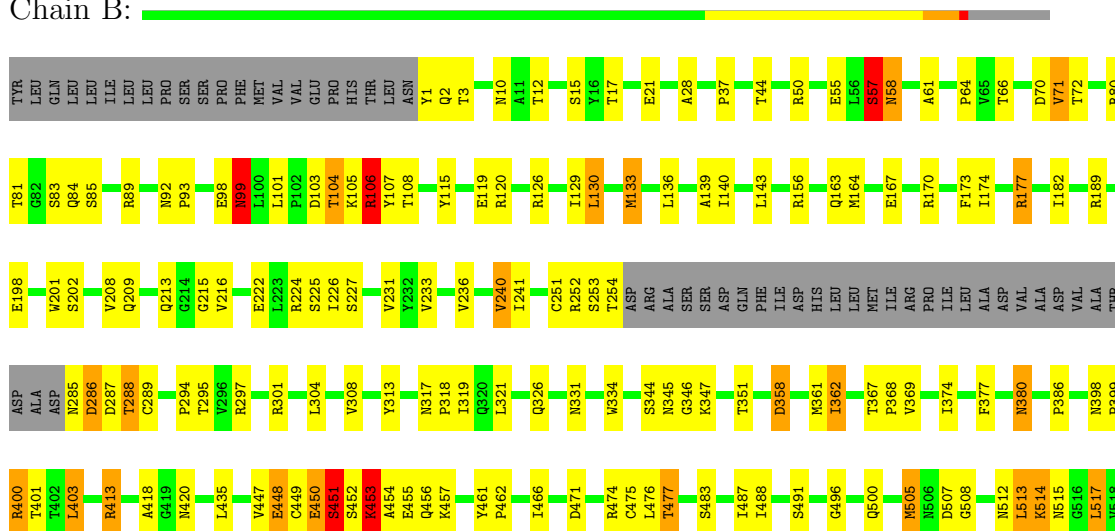
- Molecule 1: TYPE 2 RIBOSOME-INACTIVATINGPROTEIN CINNAMOMIN III

Chain A:



- Molecule 1: TYPE 2 RIBOSOME-INACTIVATINGPROTEIN CINNAMOMIN III

Chain B:





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

All (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
1	B	368	PRO	CB-CG	-10.06	0.99	1.50
1	A	368	PRO	CB-CG	-9.87	1.00	1.50
1	B	368	PRO	N-CD	-8.71	1.35	1.47

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	B	368	PRO	N-CD-CG	11.04	119.77	103.20
1	B	462	PRO	CA-CB-CG	9.11	122.11	104.80
1	A	462	PRO	CA-N-CD	-8.43	99.70	111.50
1	B	130	LEU	CA-CB-CG	7.92	133.52	115.30
1	B	543	LYS	CD-CE-NZ	-7.62	94.16	111.70
1	A	367	THR	C-N-CD	7.32	143.76	128.40
1	B	461	TYR	C-N-CD	7.09	143.29	128.40
1	A	380	ASN	CB-CA-C	-6.70	96.99	110.40
1	A	50	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	451	SER	N-CA-C	-6.55	93.31	111.00
1	B	539	LYS	N-CA-C	6.49	128.52	111.00
1	A	403	LEU	C-N-CA	6.43	137.78	121.70
1	B	368	PRO	CA-CB-CG	6.29	116.75	104.80
1	A	23	LEU	CB-CG-CD2	-6.04	100.72	111.00
1	B	177	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	413	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	368	PRO	CA-CB-CG	-5.44	93.66	104.00
1	A	396	SER	N-CA-CB	-5.40	102.40	110.50
1	A	404	THR	N-CA-CB	5.32	120.41	110.30
1	A	368	PRO	N-CD-CG	5.30	111.14	103.20
1	B	505	MET	CG-SD-CE	5.27	108.63	100.20
1	A	50	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	525	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	408	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	367	THR	Peptide
1	A	403	LEU	Peptide
1	A	450	GLU	Peptide
1	A	453	LYS	Peptide
1	A	537	THR	Peptide
1	A	539	LYS	Peptide
1	A	57	SER	Peptide
1	A	61	ALA	Peptide
1	A	98	GLU	Peptide
1	B	358	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	B	450	GLU	Peptide
1	B	453	LYS	Peptide
1	B	539	LYS	Peptide
1	B	57	SER	Peptide
1	B	61	ALA	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (239) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:1549:AS5:HA	3:A:1552:BMA:O3	1.27	1.26
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
3:B:1549:BMA:O6	2:B:1550:AS5:H1B	1.49	1.11
3:B:1549:BMA:H62	2:B:1550:AS5:H1B	1.33	1.07
3:B:1549:BMA:O6	2:B:1550:AS5:C5B	2.03	1.07

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:1549:AS5:C2B	3:A:1552:BMA:O3	2.03	1.05
1:B:420:ASN:OD1	2:B:1550:AS5:H1A1	1.59	1.01
1:A:61:ALA:HB1	1:A:62:ASP:HA	1.44	1.00
1:B:251:CYS:HB2	1:B:288:THR:O	1.61	0.98
3:B:1549:BMA:O6	2:B:1550:AS5:C6B	2.14	0.94
1:A:251:CYS:HB2	1:A:288:THR:O	1.67	0.94
3:B:1549:BMA:O6	2:B:1550:AS5:C1B	2.17	0.92
2:A:1549:AS5:O3B	4:A:1553:XYP:O4A	1.86	0.92
1:A:380:ASN:CG	1:A:380:ASN:O	2.08	0.91
2:A:1549:AS5:HA	3:A:1552:BMA:C3	2.03	0.89
1:A:517:LEU:HD23	1:A:533:ILE:HG23	1.58	0.85
3:B:1549:BMA:C6	2:B:1550:AS5:C1B	2.53	0.84
1:A:194:MET:O	1:A:198:GLU:HG3	1.80	0.82
3:B:1549:BMA:O6	3:B:1549:BMA:O4	1.92	0.81
1:B:225:SER:O	1:B:227:SER:O	1.99	0.81
1:B:477:THR:HB	1:B:500:GLN:HG2	1.61	0.81
1:B:380:ASN:OD1	2:B:1552:AS5:O6A	1.97	0.81
1:B:254:THR:HA	6:B:2027:HOH:O	1.81	0.80
3:B:1549:BMA:HO6	2:B:1550:AS5:C6B	1.92	0.80
1:A:61:ALA:CB	1:A:62:ASP:HA	2.11	0.80
3:B:1549:BMA:H62	2:B:1550:AS5:C1B	2.13	0.79
1:B:515:ASN:HB3	1:B:517:LEU:H	1.48	0.79
1:B:453:LYS:HE3	1:B:457:LYS:HE3	1.65	0.78
1:A:517:LEU:HD23	1:A:533:ILE:CG2	2.15	0.77
1:A:380:ASN:CG	1:A:513:LEU:HD11	2.05	0.76
1:A:380:ASN:OD1	1:A:501:ARG:NH1	2.17	0.76
1:B:98:GLU:O	1:B:99:ASN:HB2	1.85	0.76
1:A:513:LEU:O	1:A:514:LYS:CB	2.34	0.74
2:A:1549:AS5:N2B	3:A:1552:BMA:O3	2.21	0.74
1:A:453:LYS:HB2	1:A:454:ALA:HA	1.68	0.74
1:A:515:ASN:HB3	1:A:517:LEU:H	1.53	0.73
1:B:420:ASN:OD1	2:B:1550:AS5:C1A	2.36	0.72
1:B:513:LEU:O	1:B:514:LYS:HB3	1.87	0.72
1:B:449:CYS:O	1:B:450:GLU:HB3	1.88	0.72
1:B:513:LEU:O	1:B:514:LYS:CB	2.37	0.72
1:A:453:LYS:HD2	1:A:457:LYS:HG2	1.72	0.71
1:A:398:ASN:O	1:A:401:THR:HG23	1.90	0.71
2:A:1551:AS5:H1B	2:A:1551:AS5:H2A	1.73	0.70
1:A:451:SER:O	1:A:453:LYS:HG2	1.91	0.70
1:B:12:THR:HG23	1:B:15:SER:H	1.56	0.70
2:A:1549:AS5:HA	3:A:1552:BMA:C4	2.24	0.68
1:A:508:GLY:HA3	1:A:543:LYS:HE3	1.75	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:285:ASN:CG	1:B:285:ASN:O	2.32	0.68
1:A:287:ASP:O	1:A:289:CYS:N	2.27	0.68
1:B:451:SER:O	1:B:453:LYS:HG2	1.93	0.68
1:A:380:ASN:ND2	1:A:513:LEU:CD1	2.47	0.67
1:B:453:LYS:HE3	1:B:457:LYS:CE	2.25	0.67
1:B:28:ALA:HB1	6:B:2003:HOH:O	1.93	0.67
2:A:1551:AS5:O3B	2:A:1551:AS5:C7B	2.43	0.67
1:B:119:GLU:OE2	1:B:126:ARG:HG3	1.94	0.67
1:A:85:SER:H	1:A:105:LYS:HB3	1.59	0.66
1:B:287:ASP:O	1:B:289:CYS:N	2.29	0.66
1:A:442:ASP:OD2	1:B:538:GLY:HA2	1.96	0.66
1:B:285:ASN:CA	1:B:286:ASP:HB2	2.27	0.64
1:A:513:LEU:O	1:A:514:LYS:HB3	1.97	0.64
2:B:1552:AS5:O4B	2:B:1552:AS5:N2A	2.30	0.64
1:A:453:LYS:HD2	1:A:457:LYS:CG	2.27	0.63
3:B:1549:BMA:O6	2:B:1550:AS5:O5B	2.17	0.62
1:B:285:ASN:HA	1:B:286:ASP:HB2	1.79	0.62
1:A:84:GLN:HA	1:A:105:LYS:CB	2.31	0.61
1:A:70:ASP:OD1	1:A:72:THR:HB	2.00	0.61
1:A:84:GLN:HA	1:A:105:LYS:HB3	1.80	0.61
1:B:10:ASN:OD1	2:B:1551:AS5:O4A	2.19	0.61
1:A:321:LEU:HD13	1:A:403:LEU:HD21	1.83	0.60
1:B:477:THR:CG2	1:B:491:SER:HB3	2.32	0.60
1:B:101:LEU:O	1:B:104:THR:HG22	2.02	0.60
1:A:119:GLU:OE2	1:A:126:ARG:HG3	2.01	0.60
1:A:451:SER:O	1:A:453:LYS:CG	2.51	0.59
1:A:513:LEU:HD22	2:A:1551:AS5:H6A1	1.85	0.59
1:A:512:ASN:HB3	1:A:515:ASN:HB2	1.85	0.58
1:A:285:ASN:O	1:A:285:ASN:CG	2.42	0.58
1:B:453:LYS:HD2	1:B:457:LYS:HG3	1.84	0.58
2:B:1550:AS5:O5B	2:B:1550:AS5:H6A2	2.04	0.58
1:A:81:THR:O	1:A:81:THR:HG23	2.03	0.58
1:A:515:ASN:HB3	1:A:517:LEU:HB2	1.85	0.57
1:B:216:VAL:HG12	1:B:294:PRO:HG2	1.86	0.57
1:B:488:ILE:HD13	1:B:519:MET:HE2	1.86	0.57
1:B:101:LEU:O	1:B:104:THR:CG2	2.53	0.57
1:A:101:LEU:O	1:A:104:THR:HG22	2.05	0.57
2:A:1551:AS5:H1A1	6:A:2068:HOH:O	2.03	0.57
1:A:12:THR:HG23	1:A:15:SER:H	1.70	0.56
1:A:380:ASN:O	1:A:380:ASN:OD1	2.23	0.56
1:A:50:ARG:HG3	1:A:50:ARG:O	2.05	0.56
1:B:295:THR:O	2:B:1550:AS5:H2A	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:404:THR:HG22	1:A:406:GLN:HG2	1.88	0.56
1:A:466:ILE:HB	1:A:476:LEU:HB2	1.88	0.56
1:B:477:THR:HG21	1:B:491:SER:HB3	1.87	0.56
1:A:380:ASN:O	1:A:380:ASN:ND2	2.39	0.56
2:A:1550:AS5:O3A	2:A:1550:AS5:H1B	2.05	0.56
1:B:136:LEU:O	1:B:140:ILE:HG13	2.06	0.55
1:A:347:LYS:HB3	1:A:363:TYR:O	2.06	0.55
1:B:170:ARG:HD3	1:B:201:TRP:CD2	2.42	0.55
1:A:51:PHE:CD2	1:A:100:LEU:HD13	2.41	0.55
1:B:215:GLY:HA3	1:B:236:VAL:HG22	1.88	0.54
1:B:466:ILE:HB	1:B:476:LEU:HB2	1.90	0.54
1:B:50:ARG:O	1:B:71:VAL:HG23	2.09	0.54
1:A:225:SER:O	1:A:227:SER:O	2.26	0.53
1:B:471:ASP:CG	1:B:474:ARG:HD3	2.29	0.53
1:B:285:ASN:ND2	1:B:285:ASN:O	2.41	0.53
3:B:1549:BMA:O6	2:B:1550:AS5:O6B	2.26	0.53
1:A:488:ILE:HD13	1:A:519:MET:HE3	1.91	0.53
1:B:55:GLU:HG2	1:B:64:PRO:HG2	1.91	0.52
1:B:517:LEU:HD23	1:B:533:ILE:HG23	1.92	0.52
1:B:453:LYS:CB	1:B:456:GLN:HB2	2.40	0.52
1:B:216:VAL:HG22	1:B:418:ALA:HB3	1.90	0.52
1:B:105:LYS:HE3	1:B:107:TYR:HB2	1.90	0.52
1:A:378:TRP:CE3	2:A:1551:AS5:H3A	2.44	0.52
1:A:380:ASN:C	1:A:380:ASN:OD1	2.40	0.52
1:B:399:PRO:O	1:B:400:ARG:HB2	2.09	0.52
1:B:515:ASN:HB3	1:B:517:LEU:HB2	1.93	0.51
1:A:319:ILE:HG22	1:A:403:LEU:HD12	1.92	0.51
1:B:543:LYS:HA	1:B:543:LYS:HE2	1.92	0.51
1:B:285:ASN:N	1:B:286:ASP:HB2	2.25	0.51
1:B:222:GLU:OE2	1:B:224:ARG:NH2	2.44	0.51
1:B:539:LYS:HB2	1:B:540:PRO:HD3	1.93	0.51
1:B:231:VAL:HG21	1:B:548:LEU:HD11	1.93	0.51
1:B:508:GLY:HA3	1:B:543:LYS:NZ	2.26	0.51
1:A:307:ARG:HD2	1:A:322:TRP:CG	2.47	0.50
1:B:453:LYS:HB3	1:B:456:GLN:HB2	1.93	0.50
1:A:411:ALA:HB1	1:A:496:GLY:O	2.12	0.50
1:A:508:GLY:HA3	1:A:543:LYS:CE	2.42	0.49
1:A:380:ASN:HD22	1:A:503:VAL:HG21	1.77	0.49
1:A:393:SER:OG	1:A:414:GLN:HG2	2.12	0.49
1:A:537:THR:C	1:A:538:GLY:O	2.49	0.49
1:A:287:ASP:O	1:A:288:THR:C	2.50	0.49
1:B:313:TYR:OH	1:B:331:ASN:HA	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:380:ASN:HB3	2:A:1551:AS5:O3A	2.13	0.49
1:B:488:ILE:HG21	1:B:519:MET:HE3	1.93	0.49
1:A:126:ARG:NH1	1:A:199:ASN:OD1	2.46	0.49
1:A:129:ILE:HG23	1:A:156:ARG:CZ	2.43	0.49
1:B:115:TYR:CD2	1:B:126:ARG:HD3	2.48	0.49
1:A:453:LYS:HB2	1:A:454:ALA:CA	2.41	0.48
1:A:307:ARG:HD2	1:A:322:TRP:CB	2.43	0.48
1:B:297:ARG:H	1:B:420:ASN:ND2	2.12	0.48
1:B:233:VAL:HG11	1:B:241:ILE:HD11	1.95	0.48
1:A:116:THR:O	1:A:120:ARG:HB2	2.14	0.48
1:A:399:PRO:O	1:A:400:ARG:HB2	2.14	0.48
1:B:163:GLN:O	1:B:167:GLU:HB2	2.14	0.48
1:A:101:LEU:O	1:A:104:THR:CG2	2.60	0.48
1:B:471:ASP:OD2	1:B:474:ARG:HD3	2.13	0.48
1:B:81:THR:O	1:B:81:THR:HG23	2.14	0.48
1:A:171:PHE:HB2	1:A:174:ILE:HG23	1.96	0.48
1:A:29:SER:HB3	1:A:40:ARG:HG2	1.96	0.48
1:A:518:VAL:HG12	1:A:519:MET:O	2.13	0.47
1:B:66:THR:O	1:B:80:ARG:N	2.39	0.47
1:A:115:TYR:CD2	1:A:126:ARG:HD3	2.48	0.47
1:B:453:LYS:CD	1:B:457:LYS:HG3	2.44	0.47
1:B:347:LYS:HB3	1:B:362:ILE:HD12	1.96	0.47
2:B:1550:AS5:O3B	5:B:1553:XYS:O3	2.30	0.46
1:B:475:CYS:O	1:B:477:THR:HG22	2.16	0.46
1:B:129:ILE:HG23	1:B:156:ARG:CZ	2.45	0.46
1:B:374:ILE:O	1:B:386:PRO:HD2	2.16	0.46
1:B:57:SER:HA	1:B:58:ASN:HB2	1.96	0.46
1:B:85:SER:H	1:B:105:LYS:HB3	1.80	0.46
1:B:139:ALA:O	1:B:143:LEU:HG	2.15	0.46
2:A:1549:AS5:C3B	4:A:1553:XYP:O4A	2.61	0.46
1:B:170:ARG:HD3	1:B:201:TRP:CE2	2.49	0.46
1:B:507:ASP:O	1:B:543:LYS:HE3	2.16	0.46
1:A:133:MET:HA	1:A:133:MET:CE	2.45	0.46
2:A:1551:AS5:C1B	2:A:1551:AS5:H2A	2.44	0.46
1:B:345:ASN:HB3	1:B:346:GLY:H	1.60	0.46
1:B:84:GLN:HA	1:B:105:LYS:CB	2.45	0.46
1:B:512:ASN:HB3	1:B:515:ASN:HB2	1.98	0.46
1:A:301:ARG:NH2	1:A:413:ARG:HG3	2.31	0.45
1:A:507:ASP:HB3	1:A:509:THR:HG23	1.97	0.45
3:B:1549:BMA:H62	2:B:1550:AS5:O4A	2.17	0.45
1:A:513:LEU:O	1:A:514:LYS:HB2	2.12	0.45
1:A:404:THR:CG2	1:A:406:GLN:HG2	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:208:VAL:HG22	1:B:236:VAL:HG12	1.98	0.45
1:B:84:GLN:HA	1:B:105:LYS:HB2	1.98	0.45
1:B:413:ARG:HB2	1:B:496:GLY:O	2.17	0.45
1:A:378:TRP:CZ2	1:A:384:ILE:HG21	2.52	0.44
1:B:136:LEU:HD22	1:B:164:MET:HE1	1.99	0.44
1:A:307:ARG:HD3	1:A:320:GLN:HE21	1.81	0.44
2:B:1550:AS5:C3B	5:B:1553:XYS:HO3	2.25	0.44
1:A:322:TRP:HH2	6:A:2039:HOH:O	2.00	0.44
2:B:1550:AS5:H8B1	2:B:1550:AS5:HA	1.60	0.44
1:B:50:ARG:C	1:B:71:VAL:HG23	2.38	0.44
1:A:522:LYS:HE2	1:A:530:GLN:OE1	2.17	0.44
1:B:130:LEU:HD22	1:B:189:ARG:NH2	2.32	0.44
2:B:1552:AS5:O3A	2:B:1552:AS5:H1B	2.07	0.44
1:B:301:ARG:HD2	1:B:413:ARG:HA	1.99	0.44
1:A:378:TRP:CD2	2:A:1551:AS5:H3A	2.53	0.44
1:A:296:VAL:HG21	1:A:418:ALA:HB1	2.00	0.44
1:B:435:LEU:HD22	1:B:448:GLU:HA	2.00	0.44
1:A:41:GLU:O	1:A:44:THR:HB	2.18	0.44
1:B:453:LYS:O	1:B:455:GLU:N	2.50	0.43
1:B:92:ASN:O	1:B:93:PRO:C	2.55	0.43
1:A:537:THR:O	1:A:538:GLY:O	2.36	0.43
1:B:334:TRP:CZ3	1:B:344:SER:HB2	2.54	0.43
1:A:38:VAL:HG22	1:A:39:MET:N	2.33	0.43
1:B:476:LEU:HD12	1:B:476:LEU:HA	1.72	0.43
1:A:464:GLY:HA3	1:A:501:ARG:HG2	2.01	0.43
1:B:37:PRO:HB3	6:B:2003:HOH:O	2.16	0.43
1:A:413:ARG:HB2	1:A:496:GLY:O	2.18	0.43
1:A:212:ASN:OD1	1:A:212:ASN:C	2.57	0.43
1:B:420:ASN:OD1	2:B:1550:AS5:C2A	2.66	0.43
1:B:216:VAL:CG1	1:B:294:PRO:HG2	2.48	0.43
1:B:163:GLN:HE21	1:B:198:GLU:CD	2.22	0.43
1:A:84:GLN:HA	1:A:105:LYS:HB2	1.99	0.42
1:B:362:ILE:HD13	1:B:362:ILE:HA	1.95	0.42
1:A:215:GLY:HA3	1:A:236:VAL:HG22	2.01	0.42
1:A:29:SER:HB3	1:A:40:ARG:CG	2.49	0.42
1:B:308:VAL:HA	1:B:319:ILE:HD13	2.00	0.42
1:B:321:LEU:HD13	1:B:403:LEU:HD11	2.00	0.42
1:B:17:THR:O	1:B:21:GLU:HB2	2.18	0.42
1:B:252:ARG:O	1:B:288:THR:HG22	2.20	0.42
1:B:133:MET:HE2	1:B:182:ILE:HG12	2.00	0.42
1:B:420:ASN:OD1	2:B:1550:AS5:N2A	2.52	0.42
1:B:173:PHE:O	1:B:177:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:488:ILE:HD11	1:B:533:ILE:HG12	2.00	0.42
1:B:533:ILE:HD13	1:B:533:ILE:HA	1.82	0.42
1:A:92:ASN:O	1:A:93:PRO:C	2.57	0.42
1:B:517:LEU:HD23	1:B:533:ILE:CG2	2.50	0.42
1:B:380:ASN:HB2	1:B:513:LEU:HD21	2.00	0.41
1:B:477:THR:HG23	1:B:491:SER:HB3	2.02	0.41
1:A:61:ALA:HB1	1:A:62:ASP:CA	2.32	0.41
1:B:398:ASN:O	1:B:401:THR:HG23	2.19	0.41
1:B:317:ASN:HA	1:B:318:PRO:HD3	1.95	0.41
1:B:50:ARG:HH21	1:B:70:ASP:CG	2.24	0.41
1:B:304:LEU:HB2	1:B:321:LEU:HG	2.02	0.41
1:A:334:TRP:CE3	1:A:342:ILE:HG22	2.56	0.41
1:B:10:ASN:HD21	2:B:1551:AS5:C7B	2.34	0.41
1:B:319:ILE:HD11	1:B:362:ILE:HG12	2.03	0.40
1:A:505:MET:HE2	1:A:505:MET:HA	2.03	0.40
1:A:453:LYS:HD2	1:A:457:LYS:HG3	2.03	0.40
1:B:240:VAL:HG21	1:B:548:LEU:HD13	2.02	0.40
1:A:317:ASN:HA	1:A:318:PRO:HD3	1.84	0.40
1:B:106:ARG:HG3	1:B:106:ARG:HH11	1.86	0.40
1:A:419:GLY:HA3	6:A:2040:HOH:O	2.21	0.40
1:A:325:LYS:C	1:A:327:ASN:H	2.24	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	514/570 (90%)	467 (91%)	33 (6%)	14 (3%)	8	36
1	B	514/570 (90%)	469 (91%)	31 (6%)	14 (3%)	8	36
All	All	1028/1140 (90%)	936 (91%)	64 (6%)	28 (3%)	8	36

All (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
1	A	539	LYS
1	B	58	ASN
1	B	99	ASN
1	B	286	ASP
1	B	288	THR
1	B	453	LYS
1	B	454	ALA
1	B	514	LYS
1	B	539	LYS
1	A	61	ALA
1	A	413	ARG
1	B	413	ARG
1	B	538	GLY
1	A	507	ASP
1	A	523	GLY
1	B	452	SER
1	A	106	ARG
1	A	301	ARG
1	A	453	LYS
1	B	106	ARG
1	B	326	GLN
1	A	369	VAL
1	B	369	VAL

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	446/496 (90%)	406 (91%)	40 (9%)	14	45
1	B	446/496 (90%)	402 (90%)	44 (10%)	11	39
All	All	892/992 (90%)	808 (91%)	84 (9%)	13	42

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	TYR
1	A	2	GLN
1	A	12	THR
1	A	13	LYS
1	A	23	LEU
1	A	67	LEU
1	A	72	THR
1	A	80	ARG
1	A	83	SER
1	A	89	ARG
1	A	94	ASP
1	A	98	GLU
1	A	103	ASP
1	A	108	THR
1	A	125	ARG
1	A	174	ILE
1	A	181	SER
1	A	189	ARG
1	A	237	SER
1	A	239	ARG
1	A	240	VAL
1	A	248	LEU
1	A	252	ARG
1	A	321	LEU
1	A	361	MET
1	A	366	ARG
1	A	377	PHE
1	A	380	ASN
1	A	405	VAL
1	A	447	VAL
1	A	448	GLU
1	A	452	SER
1	A	483	SER
1	A	487	ILE
1	A	501	ARG
1	A	515	ASN
1	A	527	SER
1	A	528	LEU
1	A	533	ILE
1	A	539	LYS
1	B	1	TYR
1	B	2	GLN
1	B	3	THR

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Mol	Chain	Res	Type
1	B	44	THR
1	B	57	SER
1	B	71	VAL
1	B	72	THR
1	B	83	SER
1	B	89	ARG
1	B	99	ASN
1	B	103	ASP
1	B	104	THR
1	B	106	ARG
1	B	108	THR
1	B	120	ARG
1	B	133	MET
1	B	174	ILE
1	B	202	SER
1	B	209	GLN
1	B	213	GLN
1	B	226	ILE
1	B	240	VAL
1	B	253	SER
1	B	351	THR
1	B	361	MET
1	B	362	ILE
1	B	367	THR
1	B	377	PHE
1	B	380	ASN
1	B	400	ARG
1	B	403	LEU
1	B	447	VAL
1	B	448	GLU
1	B	451	SER
1	B	477	THR
1	B	483	SER
1	B	487	ILE
1	B	505	MET
1	B	513	LEU
1	B	517	LEU
1	B	524	SER
1	B	527	SER
1	B	533	ILE
1	B	543	LYS

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 ⓘ

There are no RNA chains 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 ⓘ

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	1.72	4 (13%)	41,41,41	4.80	17 (41%)
2	AS5	A	1550	-	29,29,29	1.02	1 (3%)	41,41,41	2.26	9 (21%)
2	AS5	A	1551	-	29,29,29	1.78	2 (6%)	41,41,41	2.64	17 (41%)
3	BMA	A	1552	-	12,12,12	0.69	0	17,17,17	2.33	7 (41%)
4	XYP	A	1553	-	10,10,10	1.25	1 (10%)	14,14,14	1.50	4 (28%)
3	BMA	B	1549	-	12,12,12	0.77	0	17,17,17	1.93	5 (29%)
2	AS5	B	1550	-	29,29,29	1.84	1 (3%)	41,41,41	2.48	12 (29%)
2	AS5	B	1551	-	29,29,29	0.73	1 (3%)	41,41,41	6.19	8 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	AS5	B	1552	-	29,29,29	1.01	2 (6%)	41,41,41	2.28	14 (34%)
5	XYS	B	1553	-	10,10,10	1.30	1 (10%)	14,14,14	1.54	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	2/2/2/2
2	AS5	A	1551	-	2/2/11/13	0/16/53/53	1/2/2/2
3	BMA	A	1552	-	-	0/2/22/22	1/1/1/1
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	1/2/2/2
2	AS5	B	1552	-	6/6/11/13	0/16/53/53	1/2/2/2
5	XYS	B	1553	-	-	0/0/17/17	1/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1550	AS5	O3B-C3B	-9.39	1.20	1.43
2	A	1551	AS5	O3B-C3B	-8.50	1.22	1.43
2	A	1549	AS5	O6B-C6B	4.74	1.63	1.42
2	A	1549	AS5	O3B-C3B	-4.16	1.32	1.43
2	A	1550	AS5	O3B-C3B	4.11	1.52	1.43
4	A	1553	XYP	O5B-C1B	-3.57	1.37	1.43
2	A	1549	AS5	C8B-C7B	3.43	1.57	1.50
5	B	1553	XYS	O5-C1	-3.31	1.37	1.43
2	B	1552	AS5	C4B-C5B	2.36	1.58	1.53
2	B	1551	AS5	O3B-C3B	2.28	1.48	1.43
2	A	1549	AS5	O4A-C1B	2.27	1.47	1.41
2	A	1551	AS5	C1B-C2B	2.10	1.56	1.53
2	B	1552	AS5	C3A-C4A	2.03	1.58	1.52

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1549	AS5	O3B-C3B-C2B	25.21	161.35	109.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1551	AS5	C8B-C7B-N2B	22.24	159.59	116.11
2	B	1551	AS5	O7B-C7B-C8B	-21.30	80.46	122.04
2	B	1551	AS5	O7B-C7B-N2B	-20.42	79.26	121.90
2	B	1551	AS5	O3B-C3B-C2B	11.44	133.09	109.61
2	A	1549	AS5	O3B-C3B-C4B	-10.03	87.86	110.35
2	B	1550	AS5	O6B-C6B-C5B	7.74	137.99	111.36
2	A	1551	AS5	C1A-C2A-N2A	6.99	122.59	110.62
2	A	1550	AS5	C1A-O5A-C5A	6.48	120.38	112.13
2	A	1550	AS5	O3B-C3B-C2B	6.35	122.65	109.61
2	A	1550	AS5	O3B-C3B-C4B	6.09	124.00	110.35
2	A	1551	AS5	O5A-C1A-C2A	-5.77	104.15	111.34
2	B	1552	AS5	O4A-C1B-C2B	5.75	120.17	108.06
2	B	1552	AS5	O3A-C3A-C4A	5.71	123.16	109.85
2	B	1550	AS5	O3B-C3B-C2B	5.69	121.28	109.61
2	B	1550	AS5	C2A-N2A-C7A	5.40	131.19	122.95
2	B	1550	AS5	O3B-C3B-C4B	5.36	122.37	110.35
2	A	1550	AS5	O4B-C4B-C5B	5.15	122.85	109.28
2	B	1552	AS5	O4A-C4A-C3A	5.12	120.30	107.16
2	A	1549	AS5	O5B-C5B-C6B	5.07	118.81	106.34
2	A	1551	AS5	O3B-C3B-C2B	4.73	119.32	109.61
2	A	1550	AS5	O4B-C4B-C3B	4.63	120.72	110.35
3	A	1552	BMA	O6-C6-C5	-4.51	95.82	111.36
2	A	1551	AS5	O4B-C4B-C5B	4.42	120.92	109.28
2	A	1551	AS5	O5B-C5B-C4B	4.29	117.70	109.76
2	A	1549	AS5	C1B-O5B-C5B	4.28	122.06	113.73
3	A	1552	BMA	C4-C3-C2	-4.19	103.08	110.82
2	B	1550	AS5	O4B-C4B-C5B	4.18	120.31	109.28
2	B	1552	AS5	O4A-C1B-O5B	4.12	120.97	110.69
3	B	1549	BMA	O6-C6-C5	-4.02	97.51	111.36
2	B	1551	AS5	O3B-C3B-C4B	-4.00	101.39	110.35
2	A	1551	AS5	C4A-C3A-C2A	-3.97	99.32	109.82
2	A	1549	AS5	O4A-C1B-C2B	3.93	116.33	108.06
2	A	1551	AS5	C1B-C2B-N2B	3.92	118.44	111.02
2	B	1552	AS5	O5B-C5B-C6B	3.80	115.67	106.34
2	A	1549	AS5	O5B-C5B-C4B	3.78	116.76	109.76
2	A	1551	AS5	C1A-C2A-C3A	-3.77	102.25	109.09
3	A	1552	BMA	O4-C4-C5	3.70	119.04	109.28
2	A	1551	AS5	O4A-C1B-C2B	3.62	115.68	108.06
2	A	1549	AS5	O6B-C6B-C5B	-3.53	99.22	111.36
2	A	1551	AS5	O4A-C4A-C5A	3.49	118.41	109.33
2	A	1549	AS5	C4A-C3A-C2A	3.44	118.92	109.82
2	B	1551	AS5	C1A-O5A-C5A	3.44	116.51	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1553	XYS	C1-C2-C3	-3.34	105.23	110.53
2	A	1549	AS5	O5A-C5A-C4A	3.34	115.98	110.09
2	A	1551	AS5	O3B-C3B-C4B	3.33	117.81	110.35
2	A	1551	AS5	C1B-O4A-C4A	3.31	126.44	117.99
2	A	1549	AS5	O5A-C1A-C2A	-3.30	107.22	111.34
3	A	1552	BMA	O4-C4-C3	3.29	117.73	110.35
2	B	1550	AS5	O4A-C1B-O5B	3.25	118.79	110.69
3	B	1549	BMA	O5-C5-C6	3.24	114.31	106.34
3	A	1552	BMA	O5-C5-C4	-3.21	103.81	109.76
2	B	1552	AS5	C1B-O4A-C4A	-3.16	109.92	117.99
2	A	1549	AS5	O4B-C4B-C3B	3.14	117.39	110.35
2	A	1549	AS5	O4A-C4A-C3A	3.07	115.03	107.16
2	B	1552	AS5	O5B-C1B-C2B	-3.06	104.20	110.78
2	B	1550	AS5	O4A-C1B-C2B	3.06	114.50	108.06
2	B	1552	AS5	C1A-C2A-N2A	3.06	115.85	110.62
2	A	1549	AS5	C2A-N2A-C7A	3.05	127.61	122.95
2	A	1551	AS5	C1B-O5B-C5B	3.03	119.62	113.73
2	B	1552	AS5	C3B-C2B-N2B	2.94	116.79	110.56
3	B	1549	BMA	O4-C4-C5	2.93	117.00	109.28
2	B	1550	AS5	C1A-C2A-N2A	-2.92	105.62	110.62
2	A	1550	AS5	O4A-C1B-C2B	2.89	114.14	108.06
5	B	1553	XYS	O5-C5-C4	-2.84	106.30	110.83
3	B	1549	BMA	C3-C4-C5	-2.83	105.15	110.20
2	B	1552	AS5	O6A-C6A-C5A	-2.80	101.71	111.36
3	A	1552	BMA	C6-C5-C4	-2.65	106.61	113.00
3	B	1549	BMA	C1-C2-C3	2.64	114.72	110.53
2	B	1552	AS5	O5B-C5B-C4B	2.62	114.61	109.76
2	A	1550	AS5	O4A-C4A-C3A	2.60	113.84	107.16
4	A	1553	XYP	O5B-C1B-C2B	2.47	112.77	109.24
2	B	1550	AS5	C4A-C3A-C2A	2.45	116.28	109.82
2	B	1550	AS5	O5A-C5A-C4A	2.43	114.39	110.09
2	A	1549	AS5	C3B-C2B-N2B	2.43	115.72	110.56
4	A	1553	XYP	C5B-C4B-C3B	-2.43	106.65	109.71
2	B	1552	AS5	C1B-C2B-C3B	-2.38	101.69	109.61
2	B	1552	AS5	O4B-C4B-C5B	2.37	115.54	109.28
4	A	1553	XYP	C5B-O5B-C1B	2.37	117.23	112.86
5	B	1553	XYS	O3-C3-C2	-2.36	105.06	110.35
2	A	1550	AS5	C1A-C2A-N2A	2.34	114.63	110.62
2	B	1550	AS5	C1B-O4A-C4A	2.34	123.95	117.99
2	B	1550	AS5	C1A-O5A-C5A	2.32	115.08	112.13
2	B	1551	AS5	C4B-C3B-C2B	2.31	113.73	110.44
2	A	1551	AS5	C3A-C2A-N2A	2.30	116.51	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1551	AS5	C2A-N2A-C7A	2.30	126.45	122.95
4	A	1553	XYP	C4B-C3B-C2B	-2.28	106.84	110.89
2	A	1549	AS5	O4A-C4A-C5A	2.27	115.23	109.33
2	A	1549	AS5	O7B-C7B-C8B	2.27	126.47	122.04
2	A	1551	AS5	C3A-C4A-C5A	-2.24	105.83	110.85
2	A	1550	AS5	O5A-C1A-C2A	2.18	114.06	111.34
2	A	1551	AS5	O4A-C4A-C3A	2.15	112.68	107.16
2	A	1549	AS5	C1A-O5A-C5A	2.15	114.87	112.13
2	B	1552	AS5	C1A-O5A-C5A	2.10	114.80	112.13
3	A	1552	BMA	C3-C4-C5	-2.06	106.52	110.20
2	A	1551	AS5	O4A-C1B-O5B	-2.05	105.59	110.69

All (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
2	A	1550	AS5	C5B
2	A	1550	AS5	C3A
2	B	1552	AS5	C1B
2	B	1552	AS5	C2A
2	B	1552	AS5	C5B
2	B	1552	AS5	C5A
2	B	1552	AS5	C4B
2	B	1552	AS5	C4A
2	B	1551	AS5	C4B
2	B	1551	AS5	C5A

There are no torsion outliers.

All (7) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1551	AS5	C1A-C2A-C3A-C4A-C5A-O5A
3	A	1552	BMA	C1-C2-C3-C4-C5-O5
2	A	1550	AS5	C1B-C2B-C3B-C4B-C5B-O5B
2	B	1552	AS5	C1A-C2A-C3A-C4A-C5A-O5A
2	B	1551	AS5	C1A-C2A-C3A-C4A-C5A-O5A
5	B	1553	XYS	C1-C2-C3-C4-C5-O5
2	A	1550	AS5	C1A-C2A-C3A-C4A-C5A-O5A

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.