



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:07 PM GMT

PDB ID : 1D7X
Title : CRYSTAL STRUCTURE OF MMP3 COMPLEXED WITH A MODIFIED PROLINE SCAFFOLD BASED INHIBITOR.
Authors : Cheng, M.Y.; Natchus, M.G.; De, B.; Almstead, N.G.; Pikul, S.
Deposited on : 1999-10-20
Resolution : 2.00 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>

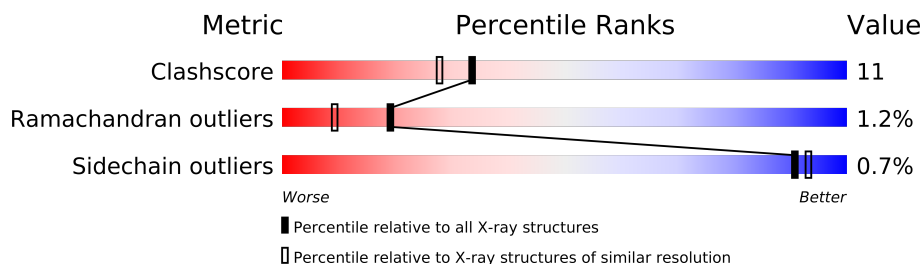
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (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. 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	173	
1	B	173	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2947 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 STROMELYSIN-1 PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1346	865	224	255	2			
1	B	173	Total	C	N	O	S	0	0	0
			1376	882	228	264	2			

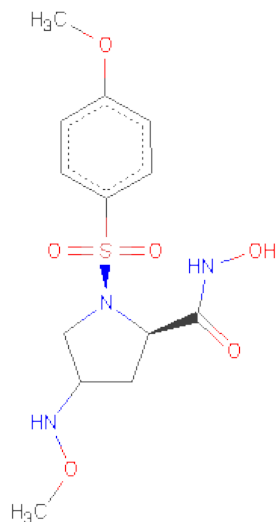
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		

- Molecule 4 is N-HYDROXY 1N(4-METHOXYPHENYL)SULFONYL-4-(Z,E-N-METHOXYIMINO)PYRROLIDINE-2R-CARBOXAMIDE (three-letter code: SPC) (formula: C₁₃H₁₉N₃O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			23	13	3	6	1		
4	B	1	Total	C	N	O	S	0	0
			23	13	3	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	65	Total	O	0	0
			65	65		

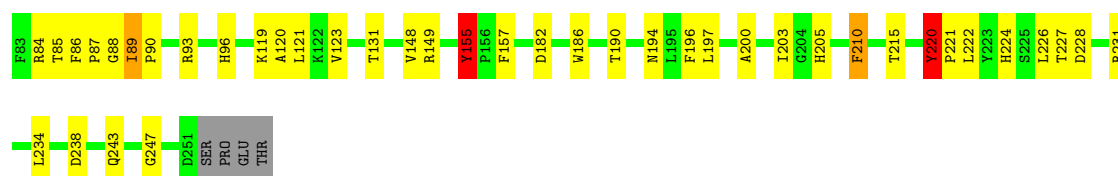
3 Residue-property plots

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.

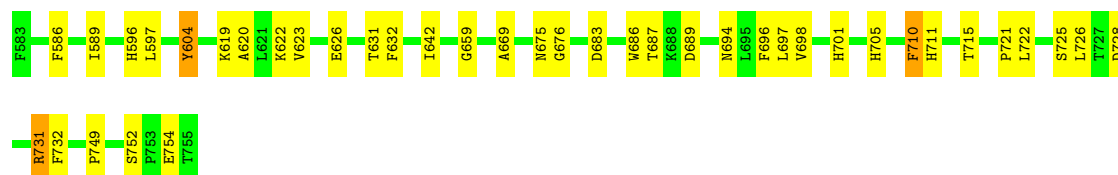
• Molecule 1: STROMELYSIN-1 PRECURSOR

Chain A: 



• Molecule 1: STROMELYSIN-1 PRECURSOR

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	37.85Å 78.22Å 104.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	100.0 (10.00-2.00)	Depositor
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.262 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2947	wwPDB-VP
Average B, all atoms (Å ²)	13.0	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: ZN, SPC, CA

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	0.58	1/1390 (0.1%)	1.36	8/1899 (0.4%)
1	B	0.50	0/1421	1.66	15/1941 (0.8%)
All	All	0.54	1/2811 (0.0%)	1.52	23/3840 (0.6%)

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	2
1	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	186	TRP	NE1-CE2	8.77	1.49	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	604	TYR	CB-CG-CD2	-28.51	103.89	121.00
1	A	210	PHE	CB-CG-CD2	-22.09	105.33	120.80
1	B	604	TYR	CB-CG-CD1	22.02	134.21	121.00
1	A	220	TYR	CB-CG-CD2	-21.47	108.12	121.00
1	B	710	PHE	CB-CG-CD2	-21.40	105.82	120.80
1	B	732	PHE	CB-CG-CD1	-20.87	106.19	120.80
1	B	731	ARG	NE-CZ-NH2	-19.40	110.60	120.30
1	A	210	PHE	CB-CG-CD1	18.70	133.89	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	710	PHE	CB-CG-CD1	18.58	133.81	120.80
1	A	155	TYR	CB-CG-CD2	-18.35	109.99	121.00
1	B	731	ARG	CD-NE-CZ	-17.47	99.14	123.60
1	B	732	PHE	CB-CG-CD2	16.05	132.03	120.80
1	A	220	TYR	CB-CG-CD1	15.38	130.23	121.00
1	B	731	ARG	NE-CZ-NH1	13.23	126.92	120.30
1	A	155	TYR	CB-CG-CD1	11.55	127.93	121.00
1	A	220	TYR	CA-CB-CG	-7.93	98.34	113.40
1	B	604	TYR	CA-CB-CG	-7.37	99.40	113.40
1	B	731	ARG	CG-CD-NE	6.83	126.15	111.80
1	B	701	HIS	CA-CB-CG	5.65	123.21	113.60
1	B	710	PHE	CA-CB-CG	-5.62	100.42	113.90
1	B	731	ARG	CB-CG-CD	5.53	125.97	111.60
1	A	84	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	731	ARG	CA-CB-CG	5.52	125.55	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	TYR	Sidechain
1	A	220	TYR	Sidechain
1	B	604	TYR	Sidechain
1	B	731	ARG	Sidechain

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	1346	0	1270	28	0
1	B	1376	0	1295	33	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	23	0	17	0	0
4	B	23	0	17	0	0
5	A	104	0	0	1	0
5	B	65	0	0	2	0
All	All	2947	0	2599	59	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 11.

All (59) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:686:TRP:CZ3	1:B:698:VAL:HG21	2.01	0.95
1:B:686:TRP:HZ3	1:B:698:VAL:HG21	1.30	0.92
1:B:586:PHE:CE1	1:B:710:PHE:HD1	1.92	0.87
1:A:120:ALA:O	1:A:123:VAL:HG22	1.80	0.80
1:B:586:PHE:CE1	1:B:710:PHE:CD1	2.78	0.72
1:B:589:ILE:HG22	1:B:589:ILE:O	1.90	0.72
1:A:96:HIS:HD2	1:A:131:THR:OG1	1.72	0.70
1:B:596:HIS:HD2	1:B:631:THR:OG1	1.75	0.69
1:A:194:ASN:HD22	1:A:197:LEU:H	1.40	0.69
1:B:711:HIS:CD2	1:B:721:PRO:HB3	2.34	0.62
1:B:749:PRO:HB2	1:B:752:SER:HB3	1.82	0.62
1:A:194:ASN:ND2	1:A:197:LEU:H	1.97	0.61
1:B:669:ALA:O	1:B:675:ASN:HB3	2.01	0.61
1:B:710:PHE:CD2	1:B:711:HIS:N	2.65	0.60
1:B:619:LYS:HG2	1:B:696:PHE:CE1	2.37	0.59
1:A:228:ASP:HB3	1:A:231:ARG:HG3	1.85	0.58
1:A:224:HIS:O	1:A:226:LEU:N	2.36	0.58
1:A:148:VAL:HG12	1:A:149:ARG:HG2	1.87	0.57
1:B:694:ASN:O	1:B:698:VAL:HG22	2.05	0.57
1:A:93:ARG:HG2	1:A:93:ARG:O	2.07	0.55
1:B:589:ILE:CG2	1:B:589:ILE:O	2.56	0.54
1:A:215:THR:HG22	1:A:215:THR:O	2.08	0.53
1:B:686:TRP:HZ3	1:B:698:VAL:CG2	2.13	0.53
1:B:687:THR:CG2	1:B:689:ASP:H	2.23	0.52
1:B:622:LYS:O	1:B:626:GLU:HG3	2.09	0.51
1:A:226:LEU:HG	1:A:226:LEU:O	2.10	0.51
1:B:659:GLY:HA2	1:B:683:ASP:OD1	2.09	0.51
1:A:85:THR:HA	1:A:210:PHE:HD1	1.75	0.51
1:A:194:ASN:HD21	1:A:196:PHE:HB3	1.77	0.50
1:B:687:THR:HG22	1:B:689:ASP:H	1.77	0.49
1:B:619:LYS:HA	1:B:622:LYS:HE3	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:226:LEU:O	1:A:227:THR:C	2.51	0.49
1:B:687:THR:HG22	1:B:689:ASP:O	2.14	0.48
1:A:119:LYS:O	1:A:123:VAL:HG13	2.13	0.48
1:B:687:THR:CG2	1:B:689:ASP:OD1	2.63	0.47
1:A:157:PHE:HA	5:A:476:HOH:O	2.15	0.46
1:A:89:ILE:HD12	1:A:90:PRO:O	2.16	0.46
1:B:620:ALA:O	1:B:623:VAL:HG22	2.15	0.46
1:A:222:LEU:HD23	1:A:224:HIS:CE1	2.51	0.45
1:B:687:THR:HG22	1:B:689:ASP:N	2.31	0.45
1:A:121:LEU:HD23	1:A:203:ILE:HD13	1.98	0.44
1:A:190:THR:HG21	1:A:227:THR:HA	2.00	0.44
1:B:697:LEU:HD11	1:B:726:LEU:HD23	1.98	0.43
1:B:705:HIS:CD2	5:B:48:HOH:O	2.72	0.42
1:A:96:HIS:CD2	1:A:131:THR:OG1	2.62	0.42
1:A:234:LEU:HG	1:A:238:ASP:HB2	2.01	0.42
1:B:711:HIS:CG	1:B:721:PRO:HB3	2.54	0.42
1:A:220:TYR:CG	1:A:221:PRO:HD2	2.55	0.42
1:A:89:ILE:HA	1:A:90:PRO:HD3	1.95	0.42
1:B:754:GLU:HB2	5:B:138:HOH:O	2.20	0.41
1:A:120:ALA:HB1	1:A:200:ALA:HA	2.02	0.41
1:B:687:THR:HG21	1:B:689:ASP:OD1	2.18	0.41
1:B:597:LEU:O	1:B:632:PHE:HA	2.20	0.41
1:B:642:ILE:HG23	1:B:676:GLY:O	2.21	0.41
1:B:722:LEU:HA	1:B:722:LEU:HD12	1.68	0.41
1:A:155:TYR:OH	1:B:752:SER:HB2	2.21	0.41
1:A:86:PHE:O	1:A:88:GLY:N	2.54	0.40
1:A:205:HIS:CE1	1:B:754:GLU:OE2	2.73	0.40
1:A:243:GLN:HG2	1:A:247:GLY:O	2.22	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	167/173 (96%)	157 (94%)	9 (5%)	1 (1%)	33 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	171/173 (99%)	161 (94%)	7 (4%)	3 (2%)	13	5
All	All	338/346 (98%)	318 (94%)	16 (5%)	4 (1%)	19	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	SER
1	B	728	ASP
1	B	715	THR
1	A	87	PRO

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	143/147 (97%)	141 (99%)	2 (1%)	78	81
1	B	147/147 (100%)	147 (100%)	0	100	100
All	All	290/294 (99%)	288 (99%)	2 (1%)	91	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ILE
1	A	182	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	194	ASN
1	A	224	HIS
1	B	596	HIS
1	B	724	HIS
1	B	736	GLN

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 ⓘ

Of 12 ligands modelled in this entry, 10 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	$\# Z > 2$
4	SPC	A	401	2	24,24,24	1.81	5 (20%)	34,34,34	3.01	15 (44%)
4	SPC	B	901	2	24,24,24	2.16	5 (20%)	34,34,34	3.34	18 (52%)

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
4	SPC	A	401	2	1/1/5/7	0/23/35/35	0/2/2/2
4	SPC	B	901	2	1/1/5/7	0/23/35/35	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	901	SPC	S11-N14	7.60	1.74	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	SPC	S11-N14	6.25	1.72	1.63
4	B	901	SPC	O33-N32	3.21	1.45	1.39
4	A	401	SPC	C15-C29	2.86	1.59	1.52
4	B	901	SPC	C18-N14	-2.66	1.46	1.48
4	B	901	SPC	C16-C17	2.39	1.57	1.53
4	A	401	SPC	C18-N14	-2.28	1.46	1.48
4	A	401	SPC	O33-N32	2.26	1.44	1.39
4	B	901	SPC	O24-N23	-2.25	1.38	1.44
4	A	401	SPC	O24-N23	-2.19	1.38	1.44

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	SPC	O24-N23-C17	11.49	132.46	107.83
4	B	901	SPC	C18-C17-N23	9.01	127.68	111.12
4	B	901	SPC	C25-O24-N23	7.64	118.64	109.27
4	B	901	SPC	O31-C29-N32	-5.34	116.78	123.25
4	A	401	SPC	C18-C17-N23	5.28	120.83	111.12
4	B	901	SPC	O12-S11-C1	5.24	114.89	107.94
4	B	901	SPC	O24-N23-C17	5.13	118.82	107.83
4	B	901	SPC	C1-S11-N14	4.84	115.54	107.44
4	B	901	SPC	C6-C1-S11	-4.61	114.68	119.80
4	B	901	SPC	C16-C17-C18	4.21	112.04	103.66
4	A	401	SPC	C16-C17-N23	4.16	127.81	112.60
4	A	401	SPC	O31-C29-N32	-4.07	118.33	123.25
4	B	901	SPC	C2-C1-S11	3.80	124.03	119.80
4	A	401	SPC	C6-C1-S11	-3.79	115.59	119.80
4	A	401	SPC	C16-C17-C18	3.70	111.03	103.66
4	B	901	SPC	C2-C3-C4	-3.68	114.84	119.76
4	B	901	SPC	O12-S11-N14	-3.50	99.05	106.96
4	A	401	SPC	O33-N32-C29	-3.11	115.62	119.80
4	A	401	SPC	C15-C16-C17	-3.10	99.64	103.83
4	A	401	SPC	O31-C29-C15	2.93	126.90	120.38
4	A	401	SPC	O13-S11-C1	2.81	111.67	107.94
4	A	401	SPC	C1-S11-N14	2.67	111.90	107.44
4	B	901	SPC	C6-C5-C4	2.47	123.06	119.76
4	A	401	SPC	C15-N14-S11	2.45	123.66	119.67
4	B	901	SPC	O13-S11-C1	-2.44	104.70	107.94
4	A	401	SPC	C2-C3-C4	-2.32	116.65	119.76
4	B	901	SPC	O35-C4-C5	-2.31	108.64	119.84
4	B	901	SPC	O13-S11-N14	-2.26	101.84	106.96
4	A	401	SPC	C2-C1-S11	2.26	122.31	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	901	SPC	C15-C16-C17	-2.20	100.85	103.83
4	A	401	SPC	O12-S11-N14	-2.09	102.23	106.96
4	B	901	SPC	C16-C17-N23	2.08	120.20	112.60
4	B	901	SPC	O35-C4-C3	2.03	129.65	119.84

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	401	SPC	C17
4	B	901	SPC	C17

There are no torsion outliers.

There are no ring outliers.

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.