



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:30 am GMT

PDB ID : 1N1L  
Title : CRYSTAL STRUCTURE OF HCV NS3 PROTEASE DOMAIN:NS4A PEPTIDE COMPLEX WITH COVALENTLY BOUND INHIBITOR (GW472467X)  
Authors : Andrews, D.M.; Chaignot, H.; Coomber, B.A.; Good, A.C.; Hind, S.L.; Jones, P.S.; Mill, G.; Robinson, J.E.; Skarzynski, T.; Slater, M.J.; Somers, D.O.N.  
Deposited on : 2002-10-18  
Resolution : 2.60 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](mailto: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.

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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

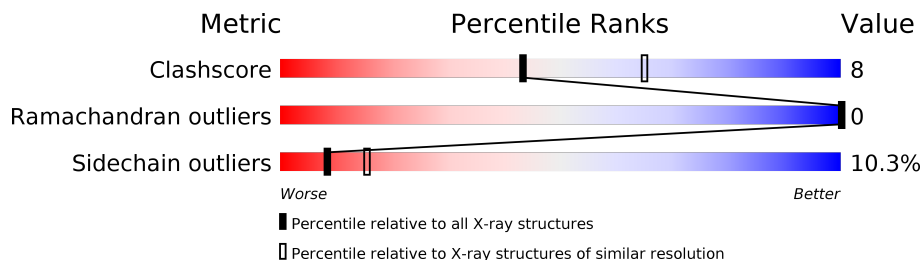
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)

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  $\geq 3$ , 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	198	
1	B	198	
2	C	23	
2	D	23	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2870 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 HCV NS3 SERINE PROTEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1337	834	243	251	9			
1	B	153	Total	C	N	O	S	0	0	0
			1138	711	206	213	8			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ALA	-	CLONING ARTIFACT	UNP P27958
A	-8	SER	-	CLONING ARTIFACT	UNP P27958
A	-7	MET	-	CLONING ARTIFACT	UNP P27958
A	-6	THR	-	CLONING ARTIFACT	UNP P27958
A	-5	GLY	-	CLONING ARTIFACT	UNP P27958
A	-4	GLY	-	CLONING ARTIFACT	UNP P27958
A	-3	GLN	-	CLONING ARTIFACT	UNP P27958
A	-2	GLN	-	CLONING ARTIFACT	UNP P27958
A	-1	MET	-	CLONING ARTIFACT	UNP P27958
A	0	GLY	-	CLONING ARTIFACT	UNP P27958
A	164	THR	ALA	ENGINEERED	UNP P27958
A	181	GLY	-	EXPRESSION TAG	UNP P27958
A	182	SER	-	EXPRESSION TAG	UNP P27958
A	183	HIS	-	EXPRESSION TAG	UNP P27958
A	184	HIS	-	EXPRESSION TAG	UNP P27958
A	185	HIS	-	EXPRESSION TAG	UNP P27958
A	186	HIS	-	EXPRESSION TAG	UNP P27958
A	187	HIS	-	EXPRESSION TAG	UNP P27958
A	188	HIS	-	EXPRESSION TAG	UNP P27958
B	-9	ALA	-	CLONING ARTIFACT	UNP P27958
B	-8	SER	-	CLONING ARTIFACT	UNP P27958
B	-7	MET	-	CLONING ARTIFACT	UNP P27958
B	-6	THR	-	CLONING ARTIFACT	UNP P27958
B	-5	GLY	-	CLONING ARTIFACT	UNP P27958
B	-4	GLY	-	CLONING ARTIFACT	UNP P27958

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLN	-	CLONING ARTIFACT	UNP P27958
B	-2	GLN	-	CLONING ARTIFACT	UNP P27958
B	-1	MET	-	CLONING ARTIFACT	UNP P27958
B	0	GLY	-	CLONING ARTIFACT	UNP P27958
B	164	THR	ALA	ENGINEERED	UNP P27958
B	181	GLY	-	EXPRESSION TAG	UNP P27958
B	182	SER	-	EXPRESSION TAG	UNP P27958
B	183	HIS	-	EXPRESSION TAG	UNP P27958
B	184	HIS	-	EXPRESSION TAG	UNP P27958
B	185	HIS	-	EXPRESSION TAG	UNP P27958
B	186	HIS	-	EXPRESSION TAG	UNP P27958
B	187	HIS	-	EXPRESSION TAG	UNP P27958
B	188	HIS	-	EXPRESSION TAG	UNP P27958

- Molecule 2 is a protein called NS4A COFACTOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	0	0	0
			149	99	27	23			
2	D	16	Total	C	N	O	0	0	0
			108	70	20	18			

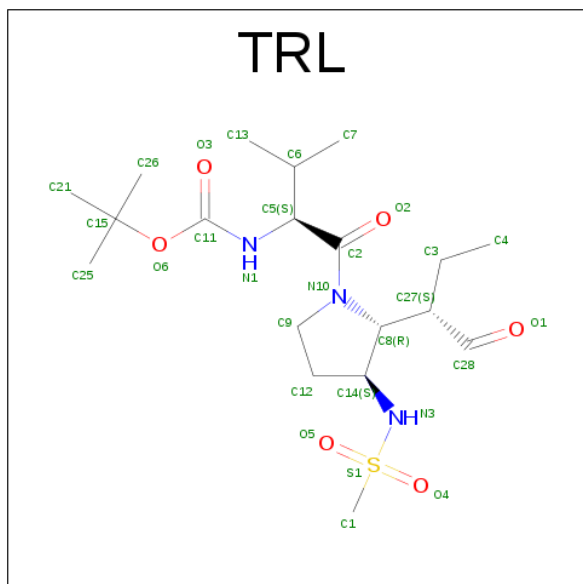
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	LYS	-	CLONING ARTIFACT	GB 5748511
C	20	LYS	-	CLONING ARTIFACT	GB 5748511
C	40	LYS	-	CLONING ARTIFACT	GB 5748511
C	41	LYS	-	CLONING ARTIFACT	GB 5748511
D	19	LYS	-	CLONING ARTIFACT	GB 5748511
D	20	LYS	-	CLONING ARTIFACT	GB 5748511
D	40	LYS	-	CLONING ARTIFACT	GB 5748511
D	41	LYS	-	CLONING ARTIFACT	GB 5748511

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is {1-[2-(1-FORMYL-PROPYL)-3-METHANESULFONYLAMINO-PYRROLIDINE-1-CARBONYL]-2-METHYL-PROPYL}-CARBAMIC ACID TERT-BUTYL ESTER (three-letter code: TRL) (formula: C<sub>19</sub>H<sub>35</sub>N<sub>3</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			29	19	3	6	1		

- Molecule 5 is water.

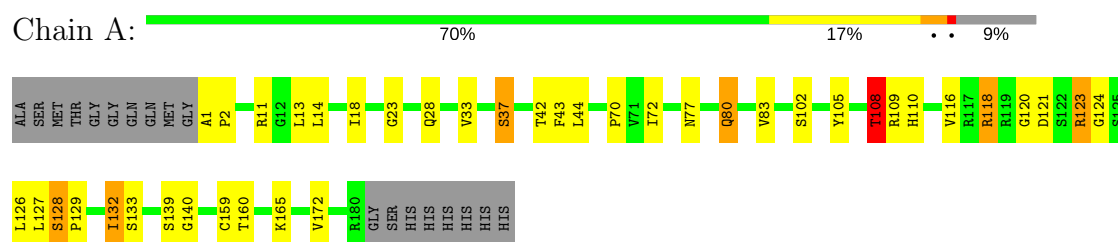
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	46	Total	O	0	0
			46	46		
5	B	43	Total	O	0	0
			43	43		
5	C	5	Total	O	0	0
			5	5		
5	D	13	Total	O	0	0
			13	13		

### 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: HCV NS3 SERINE PROTEASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	225.45 Å   225.45 Å   75.89 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.60)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.183 , 0.220	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	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: ZN, TRL

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	0.70	0/1363	0.93	1/1859 (0.1%)
1	B	0.75	0/1162	0.93	4/1586 (0.3%)
2	C	0.88	0/150	0.83	0/201
2	D	0.88	0/108	0.79	0/145
All	All	0.74	0/2783	0.92	5/3791 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	81	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	121	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	92	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	108	THR	N-CA-CB	-5.15	100.51	110.30

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	1337	0	1353	26	0
1	B	1138	0	1142	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	149	0	180	2	0
2	D	108	0	125	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	29	0	34	5	0
5	A	46	0	0	1	0
5	B	43	0	0	0	0
5	C	5	0	0	1	0
5	D	13	0	0	0	0
All	All	2870	0	2834	43	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 8.

All (43) 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:1:ALA:HB1	1:A:2:PRO:HD2	1.55	0.89
1:A:1:ALA:HB1	1:A:2:PRO:CD	2.02	0.89
1:A:14:LEU:O	1:A:18:ILE:HD12	1.77	0.83
1:A:1:ALA:CB	1:A:2:PRO:HD2	2.10	0.82
1:A:1:ALA:CB	1:A:2:PRO:CD	2.65	0.75
1:B:82:LEU:HD21	1:B:175:LEU:HD22	1.78	0.64
1:A:118:ARG:HD2	1:A:120:GLY:O	1.99	0.63
1:A:109:ARG:HG2	5:A:325:HOH:O	2.02	0.60
1:A:77:ASN:ND2	1:A:80:GLN:HB2	2.18	0.58
1:B:145:CYS:HB2	1:B:146:PRO:HD2	1.85	0.56
1:A:23:GLY:HA3	1:A:70:PRO:HG3	1.86	0.56
1:A:108:THR:HG22	1:A:110:HIS:H	1.70	0.55
1:A:139:SER:HB2	4:A:200:TRL:HC12	1.89	0.54
1:A:123:ARG:HG3	1:A:124:GLY:N	2.23	0.52
1:B:145:CYS:HB2	1:B:146:PRO:CD	2.39	0.52
1:B:114:ILE:HG21	1:B:134:TYR:HE1	1.75	0.51
1:B:82:LEU:CD2	1:B:175:LEU:HD22	2.42	0.50
1:A:108:THR:HG22	1:A:110:HIS:N	2.26	0.50
1:A:108:THR:CG2	1:A:110:HIS:H	2.25	0.49
1:B:119:ARG:HD3	1:B:119:ARG:HA	1.56	0.48
1:A:43:PHE:HB3	4:A:200:TRL:HC12	1.95	0.48
1:B:53:TRP:CE2	1:B:175:LEU:HD13	2.49	0.48
1:A:127:LEU:HD12	1:B:99:CYS:HA	1.96	0.48
1:A:139:SER:HB2	4:A:200:TRL:C1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:TRP:CD2	1:B:175:LEU:HD13	2.48	0.47
1:A:1:ALA:HB1	1:A:2:PRO:HD3	1.91	0.47
1:A:116:VAL:HG22	1:A:126:LEU:HD23	1.96	0.47
1:B:130:ARG:HD2	1:B:134:TYR:CD1	2.50	0.47
1:A:44:LEU:O	1:A:140:GLY:HA3	2.15	0.47
1:B:106:LEU:HD23	1:B:106:LEU:C	2.35	0.47
1:B:126:LEU:HD23	1:B:126:LEU:N	2.31	0.46
1:A:43:PHE:CB	4:A:200:TRL:HC12	2.46	0.45
1:A:33:VAL:HB	2:C:29:ILE:HB	2.00	0.44
1:B:114:ILE:HA	1:B:115:PRO:HD3	1.93	0.42
1:B:128:SER:HA	1:B:129:PRO:HD3	1.75	0.42
1:B:44:LEU:O	1:B:140:GLY:HA3	2.20	0.41
1:A:105:TYR:CD2	1:B:147:ALA:HB2	2.56	0.41
1:A:132:ILE:HD13	1:A:132:ILE:O	2.20	0.41
2:C:34:LYS:HG2	5:C:46:HOH:O	2.20	0.41
1:A:37:SER:OG	1:A:42:THR:HB	2.20	0.41
1:B:103:ASP:C	1:B:104:LEU:HD23	2.41	0.41
1:A:128:SER:HA	1:A:129:PRO:HD2	1.76	0.41
4:A:200:TRL:HC92	4:A:200:TRL:HC5	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	178/198 (90%)	175 (98%)	3 (2%)	0	100	100
1	B	151/198 (76%)	144 (95%)	7 (5%)	0	100	100
2	C	19/23 (83%)	19 (100%)	0	0	100	100
2	D	14/23 (61%)	14 (100%)	0	0	100	100
All	All	362/442 (82%)	352 (97%)	10 (3%)	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	147/160 (92%)	128 (87%)	19 (13%)	5	9
1	B	126/160 (79%)	117 (93%)	9 (7%)	17	34
2	C	17/19 (90%)	15 (88%)	2 (12%)	6	11
2	D	12/19 (63%)	11 (92%)	1 (8%)	13	25
All	All	302/358 (84%)	271 (90%)	31 (10%)	8	15

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	13	LEU
1	A	28	GLN
1	A	37	SER
1	A	72	ILE
1	A	80	GLN
1	A	83	VAL
1	A	102	SER
1	A	108	THR
1	A	118	ARG
1	A	121	ASP
1	A	123	ARG
1	A	128	SER
1	A	132	ILE
1	A	133	SER
1	A	159	CYS
1	A	160	THR
1	A	165	LYS
1	A	172	VAL
1	B	28	GLN
1	B	32	GLU
1	B	72	ILE

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Mol	Chain	Res	Type
1	B	89	GLN
1	B	92	ARG
1	B	119	ARG
1	B	136	LYS
1	B	143	LEU
1	B	180	ARG
2	C	22	SER
2	C	40	LYS
2	D	22	SER

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	49	ASN
1	B	89	GLN
1	B	174	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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	TRL	A	200	1	27,29,29	0.93	1 (3%)	33,43,43	2.65	11 (33%)

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	TRL	A	200	1	-	0/32/47/47	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	200	TRL	C27-C28	2.29	1.54	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	200	TRL	C6-C5-N1	-6.00	96.34	111.42
4	A	200	TRL	O4-S1-N3	-3.50	101.84	107.26
4	A	200	TRL	O6-C11-N1	-2.65	105.31	110.06
4	A	200	TRL	O5-S1-C1	-2.34	104.36	108.35
4	A	200	TRL	C25-C15-C26	-2.19	105.25	111.16
4	A	200	TRL	O6-C11-O3	2.13	129.71	125.56
4	A	200	TRL	O1-C28-C27	2.71	131.76	125.29
4	A	200	TRL	O5-S1-O4	3.19	123.62	118.78
4	A	200	TRL	O4-S1-C1	3.29	113.98	108.35
4	A	200	TRL	C5-N1-C11	6.45	135.39	120.80
4	A	200	TRL	C15-O6-C11	8.40	134.68	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	200	TRL	5	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.