



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:59 PM UTC

PDB ID : 1N1L / pdb_00001n1l
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

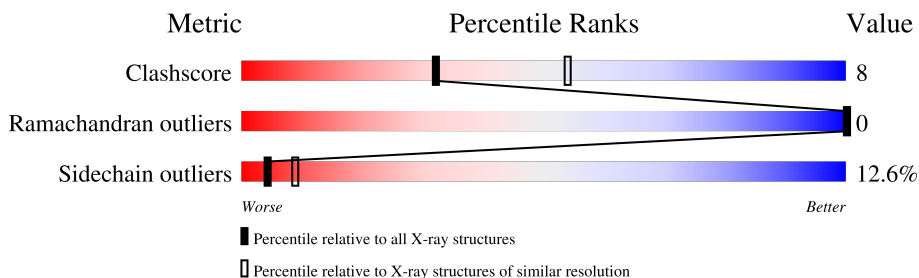
1 Overall quality at a glance

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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

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 mutation	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 mutation	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			

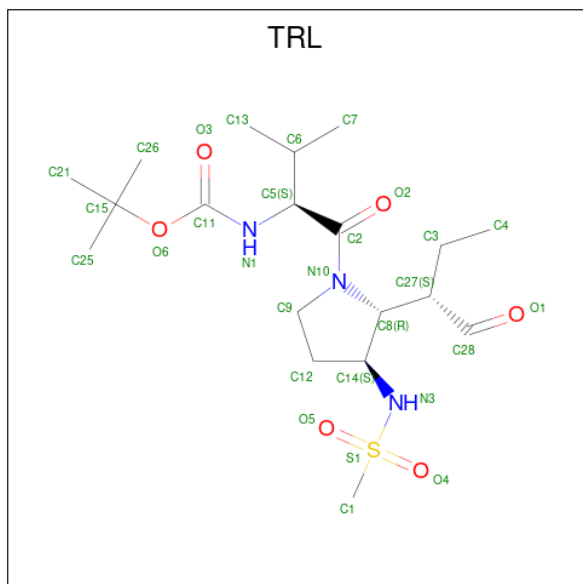
There are 8 discrepancies between the modelled and reference sequences:

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 (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	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 (CCD ID: TRL) (formula: C₁₉H₃₅N₃O₆S).



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		

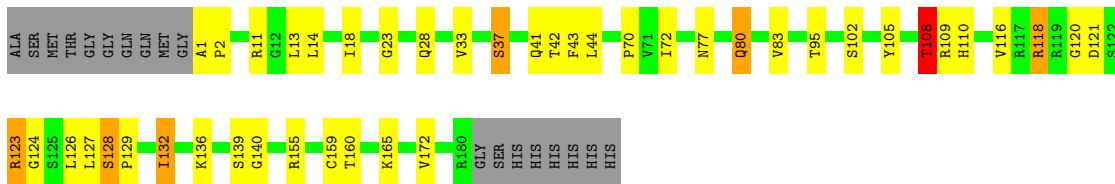
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.

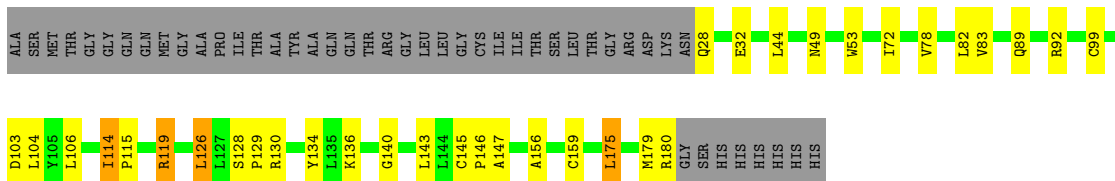
• Molecule 1: HCV NS3 SERINE PROTEASE

Chain A: 



• Molecule 1: HCV NS3 SERINE PROTEASE

Chain B: 



• Molecule 2: NS4A COFACTOR

Chain C: 



• Molecule 2: NS4A COFACTOR

Chain D: 



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, α , β , γ	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 ²)	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: TRL, ZN

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	0.91	0/1363	1.10	2/1859 (0.1%)
1	B	0.97	0/1162	1.12	2/1586 (0.1%)
2	C	1.11	0/150	1.13	0/201
2	D	1.09	0/108	1.08	0/145
All	All	0.96	0/2783	1.11	4/3791 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	THR	N-CA-CB	-6.22	100.51	110.46
1	A	41	GLN	N-CA-C	5.56	117.72	108.99
1	B	159	CYS	N-CA-C	5.18	118.19	109.95
1	B	156	ALA	N-CA-C	5.10	116.82	108.76

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	19	0
2	C	149	0	180	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	45	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 (45) 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:139:SER:HB2	4:A:200:TRL:HC13	1.53	0.88
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:B:53:TRP:HZ2	1:B:179:MET:HE2	1.67	0.60
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:43:PHE:CG	4:A:200:TRL:HC11	2.40	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:43:PHE:CB	4:A:200:TRL:HC11	2.37	0.53
1:A:43:PHE:HB3	4:A:200:TRL:HC11	1.89	0.53
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:106:LEU:C	1:B:106:LEU:HD23	2.35	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:ASN:HB2	1:B:179:MET:HE1	1.94	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: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:126:LEU:N	1:B:126:LEU:HD23	2.31	0.46
1:B:103:ASP:C	1:B:104:LEU:HD23	2.41	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:O	1:A:132:ILE:HD13	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: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 [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	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%)	126 (86%)	21 (14%)	3	6
1	B	126/160 (79%)	112 (89%)	14 (11%)	6	12
2	C	17/19 (90%)	15 (88%)	2 (12%)	5	10
2	D	12/19 (63%)	11 (92%)	1 (8%)	10	23
All	All	302/358 (84%)	264 (87%)	38 (13%)	4	9

All (38) 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	95	THR
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	136	LYS
1	A	155	ARG
1	A	159	CYS
1	A	160	THR
1	A	165	LYS
1	A	172	VAL
1	B	28	GLN

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Mol	Chain	Res	Type
1	B	32	GLU
1	B	72	ILE
1	B	78	VAL
1	B	83	VAL
1	B	89	GLN
1	B	92	ARG
1	B	114	ILE
1	B	119	ARG
1	B	126	LEU
1	B	136	LYS
1	B	143	LEU
1	B	175	LEU
1	B	180	ARG
2	C	22	SER
2	C	40	LYS
2	D	22	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	B	49	ASN
1	B	89	GLN
1	B	174	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	28,29,29	0.93	1 (3%)	35,43,43	2.74	13 (37%)

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	-	11/33/47/47	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	2.20	1.54	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	200	TRL	C15-O6-C11	9.04	134.68	120.97
4	A	200	TRL	C5-N1-C11	6.61	135.39	120.92
4	A	200	TRL	C6-C5-N1	-6.24	96.34	111.44
4	A	200	TRL	O4-S1-N3	-3.83	101.84	107.29
4	A	200	TRL	O4-S1-C1	3.62	113.98	108.26
4	A	200	TRL	O5-S1-O4	3.54	123.62	118.87
4	A	200	TRL	O1-C28-C27	2.93	131.76	125.19
4	A	200	TRL	O6-C11-N1	-2.88	105.31	110.03
4	A	200	TRL	O5-S1-C1	-2.47	104.36	108.26
4	A	200	TRL	C25-C15-C26	-2.36	105.25	111.13
4	A	200	TRL	O6-C11-O3	2.29	129.71	125.64
4	A	200	TRL	C26-C15-C21	-2.08	105.93	111.13
4	A	200	TRL	C13-C6-C5	2.04	116.75	111.16

There are no chirality outliers.

All (11) torsion outliers are listed below:

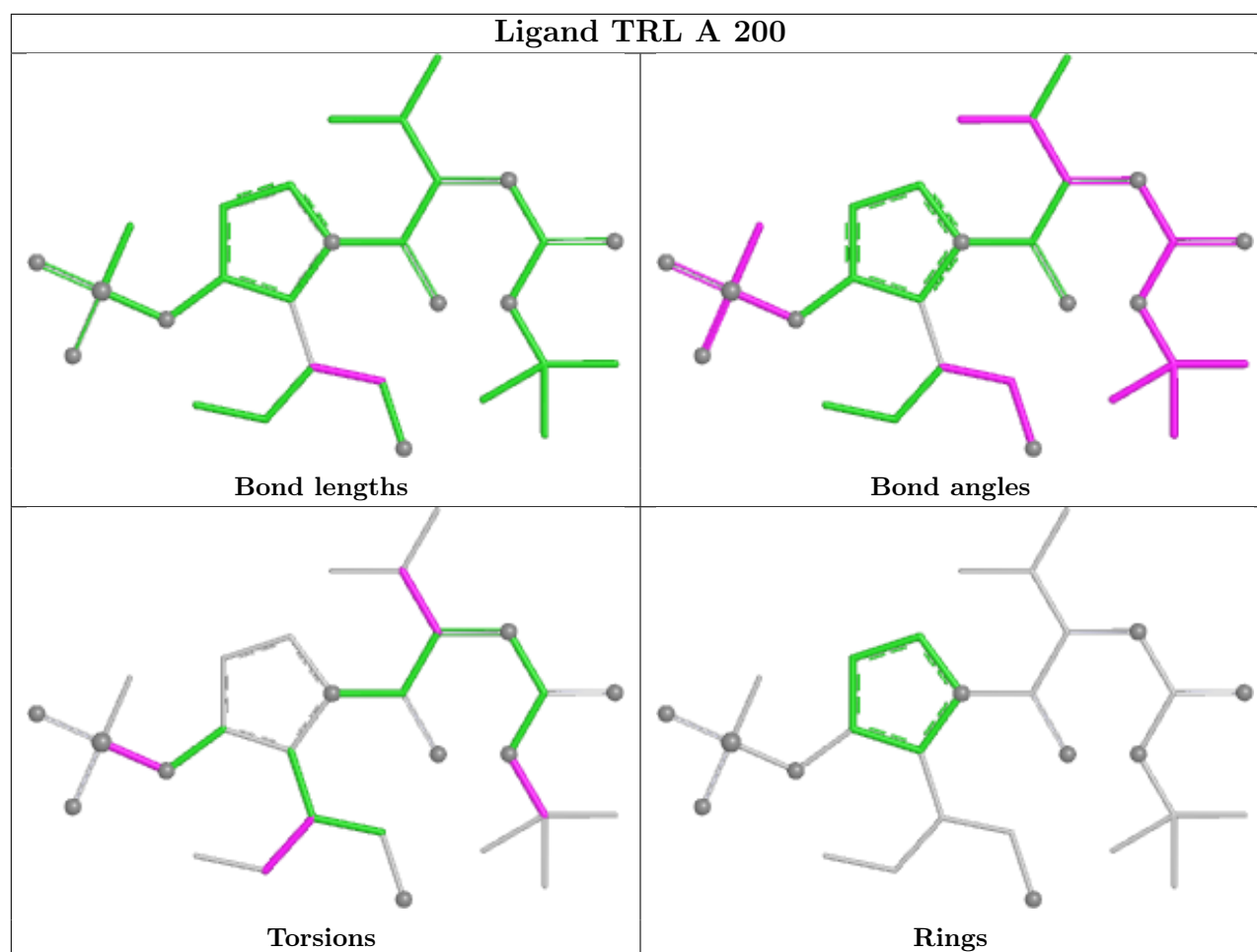
Mol	Chain	Res	Type	Atoms
4	A	200	TRL	C14-N3-S1-O5
4	A	200	TRL	C14-N3-S1-C1
4	A	200	TRL	N1-C5-C6-C13
4	A	200	TRL	C25-C15-O6-C11
4	A	200	TRL	C26-C15-O6-C11
4	A	200	TRL	C2-C5-C6-C13
4	A	200	TRL	C21-C15-O6-C11
4	A	200	TRL	N1-C5-C6-C7
4	A	200	TRL	C2-C5-C6-C7
4	A	200	TRL	C28-C27-C3-C4
4	A	200	TRL	C8-C27-C3-C4

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.