



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 04:24 am BST

PDB ID : 4NWL  
Title : Crystal structure of hepatitis c virus protease (ns3) complexed with bms-650032  
aka n-(tert-butoxycarbonyl)-3-methyl-L-valyl-(4R)-4-((7-chloro-4-methoxy-1-isoquinolinyl)oxy)-N-((1R,2S)-1-((cyclopropylsulfonyl)carbamoyl)-2-vinylcyclopropyl)-L-prolinamide  
Authors : Muckelbauer, J.K.; Klei, H.E.  
Deposited on : 2013-12-06  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

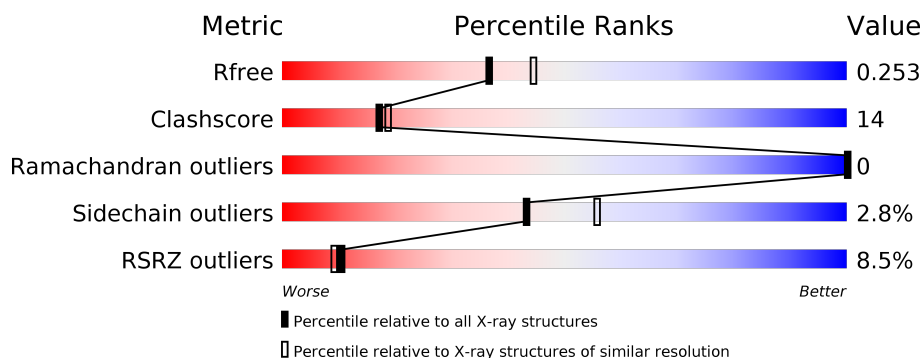
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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  $\leq 5\%$ . 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.

Mol	Chain	Length	Quality of chain
1	A	219	<div> <div>7%</div> <div>68%</div> <div>19%</div> <div>•</div> <div>11%</div> </div>
1	B	219	<div> <div>8%</div> <div>68%</div> <div>20%</div> <div>11%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3092 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 1a Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1438	888	264	279	7			
1	B	194	Total	C	N	O	S	0	0	0
			1438	888	264	279	7			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	EXPRESSION TAG	UNP A8DG50
A	-13	LYS	-	EXPRESSION TAG	UNP A8DG50
A	-12	LYS	-	EXPRESSION TAG	UNP A8DG50
A	-11	LYS	-	EXPRESSION TAG	UNP A8DG50
A	-9	SER	CYS	SEE REMARK 999	UNP A8DG50
A	-2	ILE	VAL	SEE REMARK 999	UNP A8DG50
A	-1	ASN	ILE	SEE REMARK 999	UNP A8DG50
A	1	SER	-	LINKER	UNP A8DG50
A	2	GLY	-	LINKER	UNP A8DG50
A	3	ASP	-	LINKER	UNP A8DG50
A	4	THR	-	LINKER	UNP A8DG50
A	13	GLU	LEU	ENGINEERED MUTATION	UNP A8DG50
A	14	GLU	LEU	ENGINEERED MUTATION	UNP A8DG50
A	17	GLN	ILE	ENGINEERED MUTATION	UNP A8DG50
A	18	GLU	ILE	ENGINEERED MUTATION	UNP A8DG50
A	21	GLN	LEU	ENGINEERED MUTATION	UNP A8DG50
A	40	THR	ALA	ENGINEERED MUTATION	UNP A8DG50
A	47	SER	CYS	ENGINEERED MUTATION	UNP A8DG50
A	52	LEU	CYS	ENGINEERED MUTATION	UNP A8DG50
A	72	THR	ILE	ENGINEERED MUTATION	UNP A8DG50
A	86	GLN	PRO	ENGINEERED MUTATION	UNP A8DG50
A	183	ALA	-	EXPRESSION TAG	UNP A8DG50
A	184	ILE	-	EXPRESSION TAG	UNP A8DG50
A	185	ARG	-	EXPRESSION TAG	UNP A8DG50
A	186	ALA	-	EXPRESSION TAG	UNP A8DG50

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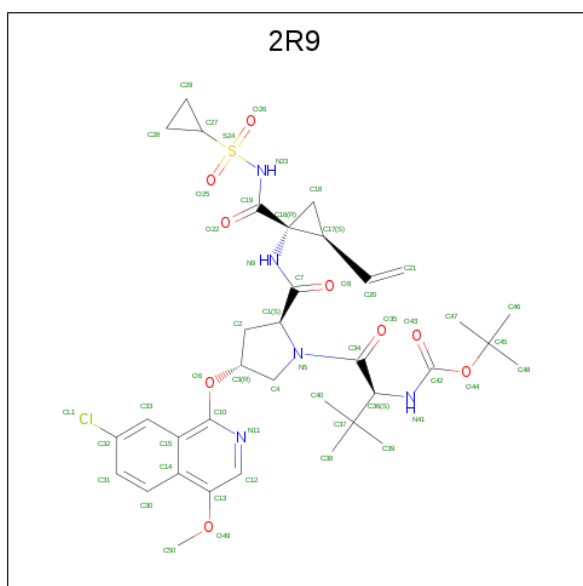
Chain	Residue	Modelled	Actual	Comment	Reference
A	187	PRO	-	EXPRESSION TAG	UNP A8DG50
A	188	SER	-	EXPRESSION TAG	UNP A8DG50
A	189	THR	-	EXPRESSION TAG	UNP A8DG50
A	190	SER	-	EXPRESSION TAG	UNP A8DG50
A	191	LEU	-	EXPRESSION TAG	UNP A8DG50
A	192	ARG	-	EXPRESSION TAG	UNP A8DG50
A	193	PRO	-	EXPRESSION TAG	UNP A8DG50
A	194	HIS	-	EXPRESSION TAG	UNP A8DG50
A	195	SER	-	EXPRESSION TAG	UNP A8DG50
A	196	SER	-	EXPRESSION TAG	UNP A8DG50
A	197	THR	-	EXPRESSION TAG	UNP A8DG50
A	198	THR	-	EXPRESSION TAG	UNP A8DG50
A	199	THR	-	EXPRESSION TAG	UNP A8DG50
A	200	THR	-	EXPRESSION TAG	UNP A8DG50
A	201	THR	-	EXPRESSION TAG	UNP A8DG50
A	202	THR	-	EXPRESSION TAG	UNP A8DG50
A	203	GLU	-	EXPRESSION TAG	UNP A8DG50
A	204	ILE	-	EXPRESSION TAG	UNP A8DG50
B	-14	MET	-	EXPRESSION TAG	UNP A8DG50
B	-13	LYS	-	EXPRESSION TAG	UNP A8DG50
B	-12	LYS	-	EXPRESSION TAG	UNP A8DG50
B	-11	LYS	-	EXPRESSION TAG	UNP A8DG50
B	-9	SER	CYS	SEE REMARK 999	UNP A8DG50
B	-2	ILE	VAL	SEE REMARK 999	UNP A8DG50
B	-1	ASN	ILE	SEE REMARK 999	UNP A8DG50
B	1	SER	-	LINKER	UNP A8DG50
B	2	GLY	-	LINKER	UNP A8DG50
B	3	ASP	-	LINKER	UNP A8DG50
B	4	THR	-	LINKER	UNP A8DG50
B	13	GLU	LEU	ENGINEERED MUTATION	UNP A8DG50
B	14	GLU	LEU	ENGINEERED MUTATION	UNP A8DG50
B	17	GLN	ILE	ENGINEERED MUTATION	UNP A8DG50
B	18	GLU	ILE	ENGINEERED MUTATION	UNP A8DG50
B	21	GLN	LEU	ENGINEERED MUTATION	UNP A8DG50
B	40	THR	ALA	ENGINEERED MUTATION	UNP A8DG50
B	47	SER	CYS	ENGINEERED MUTATION	UNP A8DG50
B	52	LEU	CYS	ENGINEERED MUTATION	UNP A8DG50
B	72	THR	ILE	ENGINEERED MUTATION	UNP A8DG50
B	86	GLN	PRO	ENGINEERED MUTATION	UNP A8DG50
B	183	ALA	-	EXPRESSION TAG	UNP A8DG50
B	184	ILE	-	EXPRESSION TAG	UNP A8DG50
B	185	ARG	-	EXPRESSION TAG	UNP A8DG50

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Chain	Residue	Modelled	Actual	Comment	Reference
B	186	ALA	-	EXPRESSION TAG	UNP A8DG50
B	187	PRO	-	EXPRESSION TAG	UNP A8DG50
B	188	SER	-	EXPRESSION TAG	UNP A8DG50
B	189	THR	-	EXPRESSION TAG	UNP A8DG50
B	190	SER	-	EXPRESSION TAG	UNP A8DG50
B	191	LEU	-	EXPRESSION TAG	UNP A8DG50
B	192	ARG	-	EXPRESSION TAG	UNP A8DG50
B	193	PRO	-	EXPRESSION TAG	UNP A8DG50
B	194	HIS	-	EXPRESSION TAG	UNP A8DG50
B	195	SER	-	EXPRESSION TAG	UNP A8DG50
B	196	SER	-	EXPRESSION TAG	UNP A8DG50
B	197	THR	-	EXPRESSION TAG	UNP A8DG50
B	198	THR	-	EXPRESSION TAG	UNP A8DG50
B	199	THR	-	EXPRESSION TAG	UNP A8DG50
B	200	THR	-	EXPRESSION TAG	UNP A8DG50
B	201	THR	-	EXPRESSION TAG	UNP A8DG50
B	202	THR	-	EXPRESSION TAG	UNP A8DG50
B	203	GLU	-	EXPRESSION TAG	UNP A8DG50
B	204	ILE	-	EXPRESSION TAG	UNP A8DG50

- Molecule 2 is N-(tert-butoxycarbonyl)-3-methyl-L-valyl-(4R)-4-[(7-chloro-4-methoxyisoquinolin-1-yl)oxy]-N-[(1R,2S)-1-[(cyclopropylsulfonyl)carbamoyl]-2-ethenylcyclopropyl]-L-prolinamide (three-letter code: 2R9) (formula: C<sub>35</sub>H<sub>46</sub>ClN<sub>5</sub>O<sub>9</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			51	35	1	5	9		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Cl	N	O	S	
			51	35	1	5	9	1	0

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

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

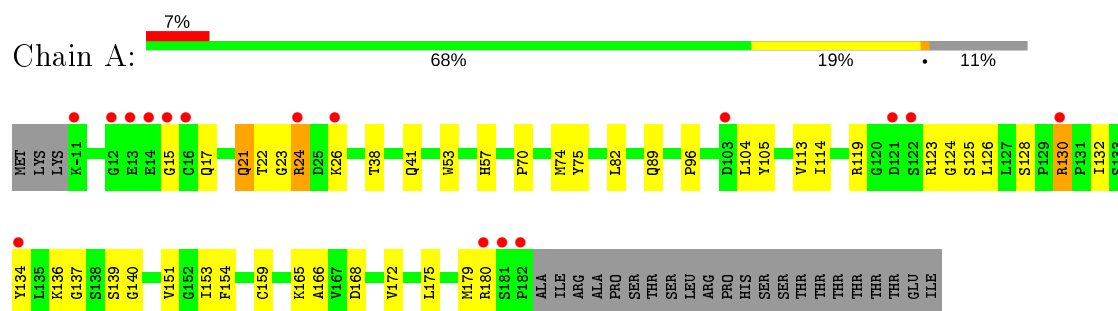
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O		
			57	57	0	0
4	B	55	Total	O		
			55	55	0	0

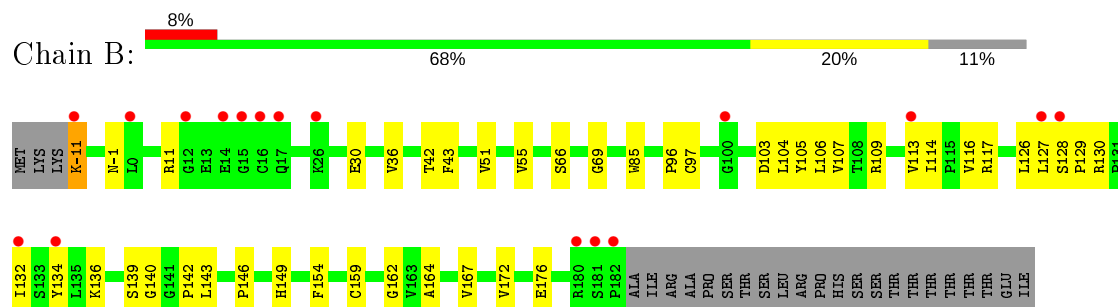
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

- Molecule 1: HCV NS3 1a Protease



- Molecule 1: HCV NS3 1a Protease



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.41Å 67.76Å 61.31Å 90.00° 108.46° 90.00°	Depositor
Resolution (Å)	36.35 – 2.20 36.35 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (36.35-2.20) 99.1 (36.35-2.20)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.03 (at 2.20Å)	Xtriage
Refinement program	CNS, CNX 2005	Depositor
R, $R_{free}$	0.246 , 0.289 0.245 , 0.253	Depositor DCC
$R_{free}$ test set	654 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.3	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3092	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 2R9

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	0.32	0/1463	0.53	0/1989
1	B	0.32	0/1463	0.53	0/1989
All	All	0.32	0/2926	0.53	0/3978

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	1438	0	1442	39	0
1	B	1438	0	1442	43	0
2	A	51	0	45	3	0
2	B	51	0	45	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	57	0	0	7	0
4	B	55	0	0	10	0
All	All	3092	0	2974	83	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 14.

All (83) 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:132:ILE:HD11	1:A:159:CYS:HB3	1.31	1.06
1:A:132:ILE:HD11	1:A:159:CYS:CB	2.08	0.82
1:B:114:ILE:HD11	1:B:134:TYR:HE2	1.42	0.81
1:A:57:HIS:CD2	2:A:301:2R9:H21	2.20	0.76
1:A:119:ARG:HH21	1:A:125:SER:HB3	1.51	0.75
1:B:55:VAL:HG22	4:B:440:HOH:O	1.89	0.73
1:B:42:THR:HG22	1:B:109:ARG:HH12	1.55	0.72
1:B:132:ILE:HD12	1:B:162:GLY:HA2	1.72	0.71
1:B:114:ILE:HD11	1:B:134:TYR:CE2	2.26	0.70
1:A:180:ARG:HD2	4:A:408:HOH:O	1.91	0.69
1:A:130:ARG:HG2	1:A:130:ARG:HH11	1.60	0.67
1:A:53:TRP:CE3	1:A:82:LEU:HD11	2.31	0.65
1:B:105:TYR:HB3	1:B:113:VAL:CG1	2.27	0.65
1:B:136:LYS:HD2	4:B:438:HOH:O	1.98	0.63
1:B:164:ALA:HB3	4:B:442:HOH:O	1.98	0.63
1:B:106:LEU:HG	4:B:441:HOH:O	1.98	0.63
1:A:154:PHE:N	4:A:442:HOH:O	2.31	0.63
1:B:114:ILE:HG23	1:B:130:ARG:NH2	2.13	0.63
1:B:126:LEU:HD21	1:B:167:VAL:HG13	1.81	0.63
1:A:96:PRO:HB3	1:A:172:VAL:HG21	1.82	0.61
1:B:42:THR:HG21	1:B:109:ARG:HH22	1.67	0.60
1:A:168:ASP:HB2	4:A:436:HOH:O	2.02	0.59
1:B:130:ARG:HB2	4:B:442:HOH:O	2.04	0.58
1:B:132:ILE:HD11	1:B:159:CYS:HB2	1.85	0.58
1:A:165:LYS:HE2	1:A:165:LYS:HA	1.86	0.58
1:A:38:THR:OG1	1:A:41:GLN:HG2	2.04	0.57
1:A:15:GLY:HA3	4:A:422:HOH:O	2.05	0.57
1:B:114:ILE:HG23	1:B:130:ARG:CZ	2.36	0.56
1:A:153:ILE:HD11	1:A:175:LEU:HD11	1.87	0.56
1:B:36:VAL:O	1:B:42:THR:HG23	2.06	0.56
1:B:143:LEU:HD22	4:B:441:HOH:O	2.05	0.55
1:A:105:TYR:HB3	1:A:113:VAL:HG12	1.86	0.55
1:B:97:CYS:HB2	1:B:149:HIS:HB2	1.90	0.54
1:A:136:LYS:HE2	1:A:137:GLY:N	2.23	0.54
1:A:53:TRP:HE3	1:A:82:LEU:HD11	1.72	0.53
1:B:139:SER:HB3	2:B:301:2R9:C19	2.39	0.53
1:B:66:SER:HB2	1:B:69:GLY:O	2.09	0.52
1:A:119:ARG:HH21	1:A:125:SER:CB	2.22	0.52
1:A:105:TYR:HB3	1:A:113:VAL:CG1	2.39	0.52
1:B:132:ILE:HG22	1:B:136:LYS:HZ2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLY:N	4:A:442:HOH:O	2.43	0.51
1:B:154:PHE:HB2	4:B:441:HOH:O	2.11	0.50
1:A:123:ARG:HG3	1:B:117:ARG:HH12	1.77	0.50
1:B:140:GLY:HA3	4:B:440:HOH:O	2.12	0.49
1:B:128:SER:O	1:B:130:ARG:CZ	2.61	0.49
1:B:51:VAL:HG13	1:B:85:TRP:O	2.13	0.49
1:A:175:LEU:O	1:A:179:MET:HG3	2.13	0.48
1:A:130:ARG:CG	1:A:130:ARG:HH11	2.27	0.48
1:B:43:PHE:HB3	2:B:301:2R9:H22	1.96	0.48
1:A:22:THR:HB	1:A:24:ARG:HD2	1.96	0.47
1:B:106:LEU:HD23	1:B:106:LEU:C	2.35	0.47
1:B:106:LEU:HD11	1:B:154:PHE:CD2	2.50	0.47
1:A:23:GLY:HA3	1:A:70:PRO:HG3	1.97	0.46
1:A:104:LEU:HD22	1:A:151:VAL:HG21	1.98	0.46
1:A:41:GLN:HB2	4:A:446:HOH:O	2.16	0.45
1:B:104:LEU:HB2	1:B:116:VAL:HB	1.98	0.45
1:B:-11:LYS:N	1:B:-11:LYS:HD2	2.32	0.45
1:B:114:ILE:CD1	1:B:134:TYR:HE2	2.21	0.45
2:A:301:2R9:O35	2:A:301:2R9:H26	2.16	0.45
1:B:159:CYS:SG	2:B:301:2R9:H27	2.56	0.44
1:A:136:LYS:HE2	1:A:137:GLY:CA	2.48	0.44
1:A:17:GLN:O	1:A:21:GLN:HG3	2.18	0.43
1:B:132:ILE:HG22	1:B:136:LYS:NZ	2.33	0.43
1:B:96:PRO:HB3	1:B:172:VAL:HG21	2.00	0.43
1:A:114:ILE:HD11	1:A:134:TYR:HE2	1.83	0.43
1:A:128:SER:O	1:A:130:ARG:NE	2.51	0.42
1:B:127:LEU:HD12	1:B:127:LEU:N	2.33	0.42
1:A:53:TRP:CE2	1:A:175:LEU:HD13	2.55	0.42
1:B:132:ILE:CD1	1:B:162:GLY:HA2	2.46	0.41
1:A:139:SER:HB3	2:A:301:2R9:C18	2.50	0.41
1:A:114:ILE:HD11	1:A:134:TYR:CE2	2.56	0.41
1:A:124:GLY:O	1:A:166:ALA:HB1	2.21	0.41
1:A:74:MET:SD	1:A:75:TYR:CZ	3.14	0.41
1:A:126:LEU:HD13	1:A:130:ARG:HD2	2.02	0.41
1:A:136:LYS:C	1:A:136:LYS:HD3	2.41	0.41
1:B:43:PHE:HD2	4:B:440:HOH:O	2.03	0.41
1:A:180:ARG:NH1	4:A:408:HOH:O	2.51	0.41
1:B:42:THR:CG2	1:B:109:ARG:HH22	2.33	0.41
1:B:103:ASP:O	1:B:146:PRO:HD3	2.20	0.40
1:B:107:VAL:HB	1:B:142:PRO:HD2	2.02	0.40
1:B:127:LEU:O	1:B:129:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-1:ASN:CG	4:B:407:HOH:O	2.59	0.40
2:B:301:2R9:H26	2:B:301:2R9:O35	2.21	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	192/219 (88%)	185 (96%)	7 (4%)	0	100	100
1	B	192/219 (88%)	188 (98%)	4 (2%)	0	100	100
All	All	384/438 (88%)	373 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	158/181 (87%)	153 (97%)	5 (3%)	39	50
1	B	158/181 (87%)	154 (98%)	4 (2%)	47	60
All	All	316/362 (87%)	307 (97%)	9 (3%)	43	56

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	24	ARG
1	A	26	LYS
1	A	89	GLN
1	A	130	ARG
1	B	-11	LYS
1	B	11	ARG
1	B	30	GLU
1	B	176	GLU

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	17	GLN
1	A	21	GLN
1	A	27	ASN
1	A	86	GLN
1	A	89	GLN
1	B	27	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 4 ligands modelled in this entry, 2 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	$\# Z  > 2$
2	2R9	B	301	-	49,55,55	2.28	15 (30%)	72,86,86	2.83	27 (37%)
2	2R9	A	301	-	49,55,55	2.23	16 (32%)	72,86,86	2.44	21 (29%)

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	2R9	B	301	-	-	3/55/79/79	0/5/5/5
2	2R9	A	301	-	-	3/55/79/79	0/5/5/5

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	2R9	C29-C28	-8.03	1.18	1.48
2	B	301	2R9	C29-C28	-7.66	1.19	1.48
2	B	301	2R9	C30-C31	5.15	1.47	1.36
2	B	301	2R9	C15-C14	4.89	1.52	1.43
2	B	301	2R9	C18-C16	4.85	1.56	1.51
2	A	301	2R9	C30-C31	4.64	1.46	1.36
2	A	301	2R9	C15-C14	4.62	1.52	1.43
2	A	301	2R9	C33-C32	4.29	1.45	1.36
2	A	301	2R9	C12-C13	4.27	1.45	1.38
2	B	301	2R9	C16-C19	-3.90	1.46	1.53
2	B	301	2R9	C31-C32	3.86	1.45	1.38
2	B	301	2R9	C33-C32	3.77	1.44	1.36
2	A	301	2R9	C31-C32	3.53	1.44	1.38
2	A	301	2R9	C18-C16	3.38	1.54	1.51
2	B	301	2R9	C12-C13	3.05	1.43	1.38
2	B	301	2R9	C4-N5	2.83	1.51	1.47
2	A	301	2R9	O44-C45	-2.54	1.43	1.48
2	B	301	2R9	C38-C37	2.46	1.58	1.53
2	A	301	2R9	S24-N23	2.45	1.67	1.63
2	B	301	2R9	C30-C14	2.39	1.47	1.42
2	A	301	2R9	C38-C37	2.35	1.58	1.53
2	B	301	2R9	C39-C37	2.33	1.58	1.53
2	A	301	2R9	C39-C37	2.32	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	2R9	S24-N23	2.30	1.67	1.63
2	A	301	2R9	C30-C14	2.22	1.46	1.42
2	B	301	2R9	O49-C13	2.19	1.40	1.36
2	A	301	2R9	C40-C37	2.12	1.58	1.53
2	A	301	2R9	C12-N11	2.11	1.38	1.34
2	A	301	2R9	C16-C19	-2.10	1.50	1.53
2	A	301	2R9	O25-S24	2.06	1.46	1.43
2	B	301	2R9	O25-S24	2.06	1.46	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	2R9	C33-C32-CL1	-9.37	107.91	119.64
2	A	301	2R9	C18-C16-N9	-8.15	106.85	117.80
2	B	301	2R9	C18-C16-N9	-7.86	107.25	117.80
2	B	301	2R9	C2-C3-C4	-7.27	97.34	103.66
2	A	301	2R9	C33-C32-CL1	-6.03	112.09	119.64
2	A	301	2R9	C2-C3-C4	-5.91	98.53	103.66
2	A	301	2R9	C10-O6-C3	-5.65	110.43	118.56
2	A	301	2R9	C29-C27-C28	-5.27	43.64	60.21
2	B	301	2R9	C34-C36-N41	5.16	112.96	107.34
2	B	301	2R9	C29-C27-C28	-5.10	44.18	60.21
2	B	301	2R9	C45-O44-C42	4.98	128.66	120.99
2	B	301	2R9	C15-C10-N11	-4.75	120.37	124.37
2	A	301	2R9	C16-C19-N23	4.57	123.61	115.70
2	B	301	2R9	C10-O6-C3	-4.47	112.14	118.56
2	A	301	2R9	O22-C19-C16	-4.35	115.56	120.74
2	B	301	2R9	O26-S24-O25	4.33	122.49	119.24
2	A	301	2R9	C37-C36-N41	-4.24	106.53	111.84
2	A	301	2R9	C28-C29-C27	4.17	68.39	59.90
2	B	301	2R9	C31-C32-CL1	4.13	125.81	119.35
2	B	301	2R9	C28-C29-C27	4.06	68.16	59.90
2	A	301	2R9	C29-C28-C27	3.97	67.97	59.90
2	B	301	2R9	C36-C34-N5	-3.82	113.93	118.52
2	B	301	2R9	C29-C28-C27	3.82	67.66	59.90
2	B	301	2R9	C18-C17-C16	3.76	61.36	59.09
2	B	301	2R9	C16-C19-N23	3.67	122.04	115.70
2	B	301	2R9	O6-C10-N11	3.51	124.78	118.89
2	B	301	2R9	C12-N11-C10	3.51	124.99	116.33
2	B	301	2R9	O22-C19-C16	-3.41	116.68	120.74
2	B	301	2R9	C31-C32-C33	3.38	125.98	121.99
2	B	301	2R9	O49-C13-C14	3.24	117.63	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	2R9	C13-C12-N11	-3.22	117.89	122.73
2	A	301	2R9	C13-C12-N11	-3.13	118.02	122.73
2	A	301	2R9	O49-C13-C14	3.11	117.50	114.46
2	A	301	2R9	C31-C32-C33	2.99	125.52	121.99
2	A	301	2R9	C12-N11-C10	2.79	123.21	116.33
2	A	301	2R9	C18-C17-C16	2.73	60.74	59.09
2	B	301	2R9	C39-C37-C38	2.67	113.98	108.80
2	A	301	2R9	O44-C42-N41	2.58	114.36	110.02
2	A	301	2R9	C38-C37-C36	-2.36	104.93	109.70
2	B	301	2R9	C37-C36-C34	-2.34	110.39	113.40
2	A	301	2R9	C15-C10-N11	-2.26	122.46	124.37
2	A	301	2R9	C39-C37-C38	2.23	113.13	108.80
2	B	301	2R9	O35-C34-N5	2.23	125.35	121.38
2	B	301	2R9	C17-C16-C19	2.19	121.46	116.80
2	B	301	2R9	C19-C16-N9	2.11	118.33	116.06
2	A	301	2R9	C17-C16-C19	2.10	121.25	116.80
2	B	301	2R9	C16-C18-C17	-2.07	59.64	61.56
2	A	301	2R9	C39-C37-C36	2.04	113.84	109.70

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	2R9	C19-N23-S24-C27
2	B	301	2R9	C19-N23-S24-O25
2	A	301	2R9	C19-N23-S24-C27
2	A	301	2R9	C19-N23-S24-O25
2	B	301	2R9	C2-C3-O6-C10
2	A	301	2R9	C2-C3-O6-C10

There are no ring outliers.

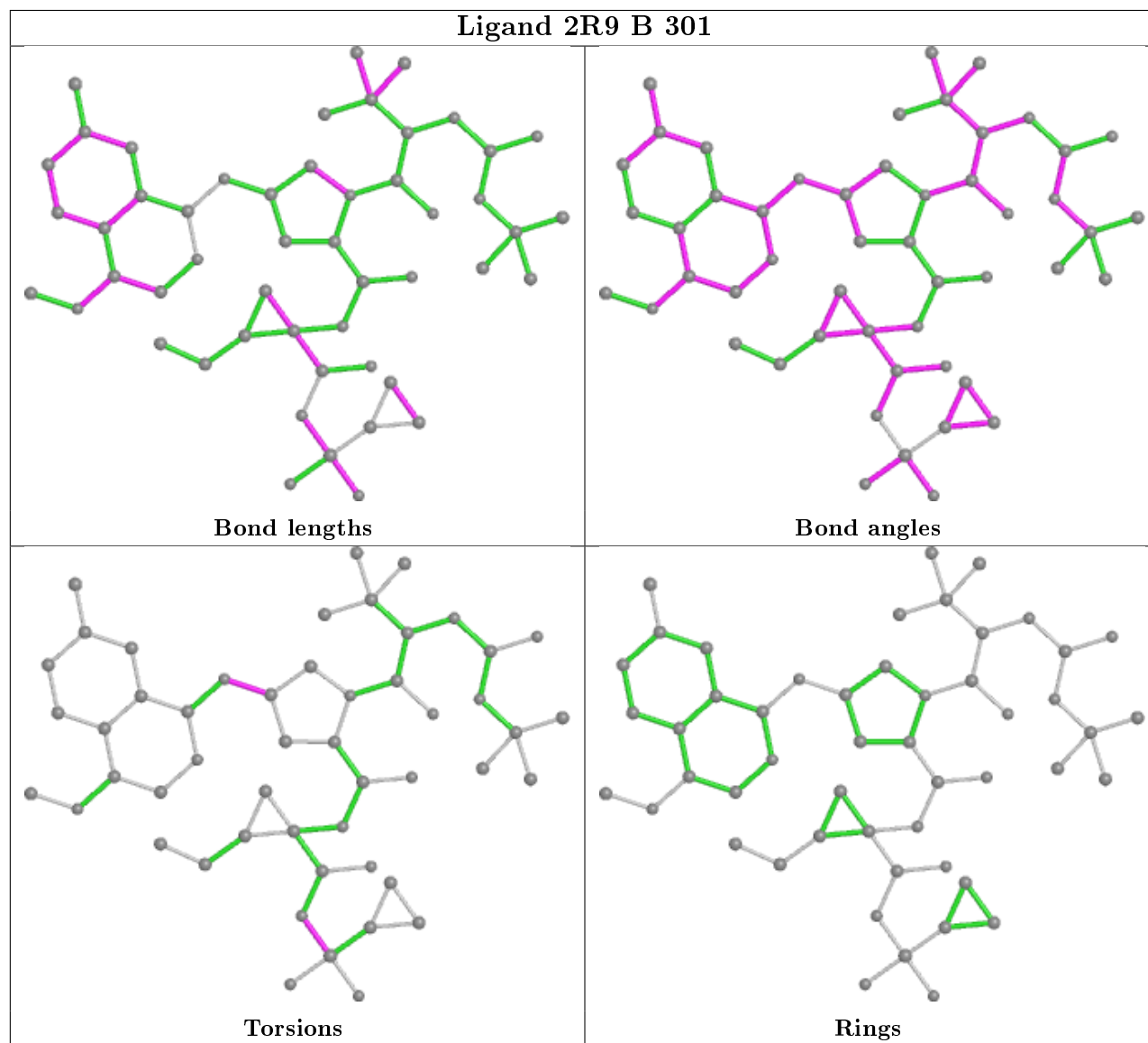
2 monomers are involved in 7 short contacts:

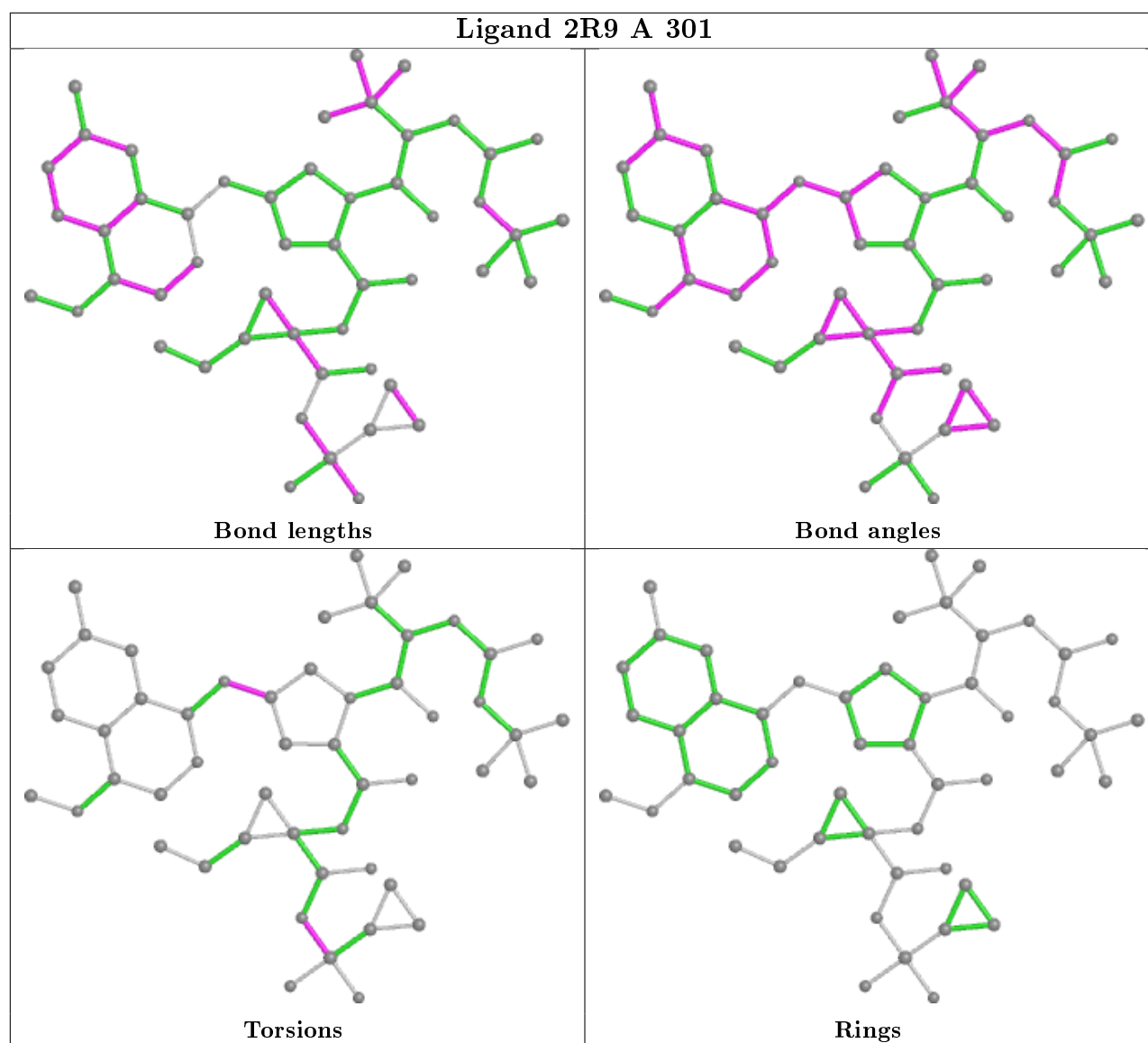
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	2R9	4	0
2	A	301	2R9	3	0

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	194/219 (88%)	0.66	16 (8%) 11 10	10, 20, 40, 56	0
1	B	194/219 (88%)	0.71	17 (8%) 10 8	11, 21, 42, 58	0
All	All	388/438 (88%)	0.69	33 (8%) 10 9	10, 21, 42, 58	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-11	LYS	5.5
1	B	182	PRO	5.0
1	A	14	GLU	4.7
1	B	15	GLY	4.1
1	A	15	GLY	4.0
1	B	134	TYR	4.0
1	A	180	ARG	3.9
1	A	182	PRO	3.9
1	A	-11	LYS	3.8
1	B	181	SER	3.5
1	A	13	GLU	3.5
1	B	14	GLU	3.1
1	A	134	TYR	3.0
1	B	0	LEU	2.8
1	A	12	GLY	2.7
1	B	12	GLY	2.7
1	B	113	VAL	2.7
1	B	132	ILE	2.6
1	A	26	LYS	2.5
1	B	16	CYS	2.5
1	A	16	CYS	2.4
1	A	122	SER	2.4
1	A	130	ARG	2.3
1	B	26	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	24	ARG	2.3
1	A	121	ASP	2.3
1	B	180	ARG	2.2
1	A	103	ASP	2.2
1	B	17	GLN	2.2
1	B	128	SER	2.2
1	A	181	SER	2.1
1	B	100	GLY	2.1
1	B	127	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

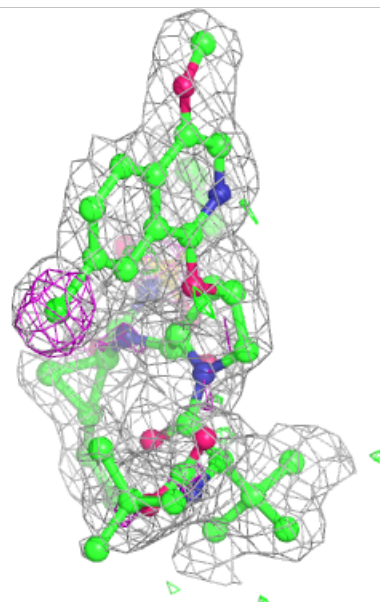
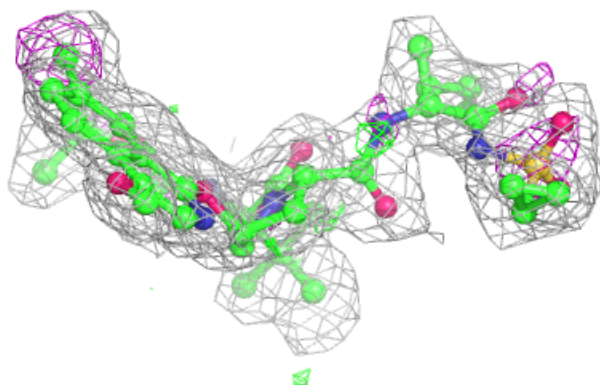
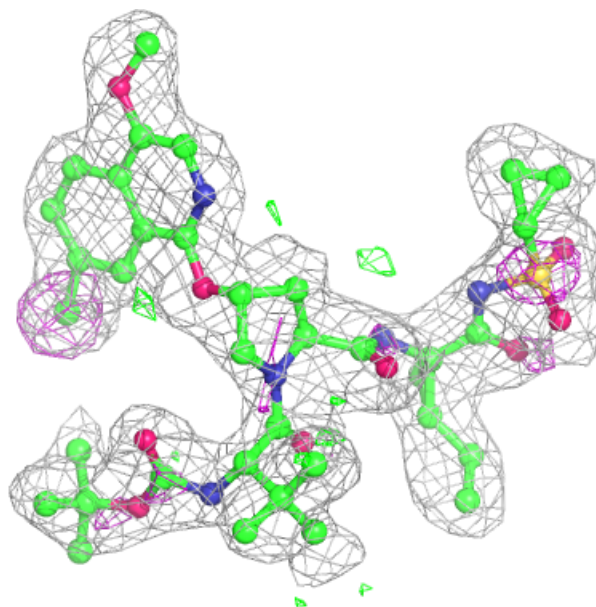
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	2R9	B	301	51/51	0.92	0.15	5,7,10,11	0
2	2R9	A	301	51/51	0.92	0.15	5,7,10,11	0
3	ZN	A	302	1/1	0.98	0.04	26,26,26,26	0
3	ZN	B	302	1/1	0.99	0.03	25,25,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

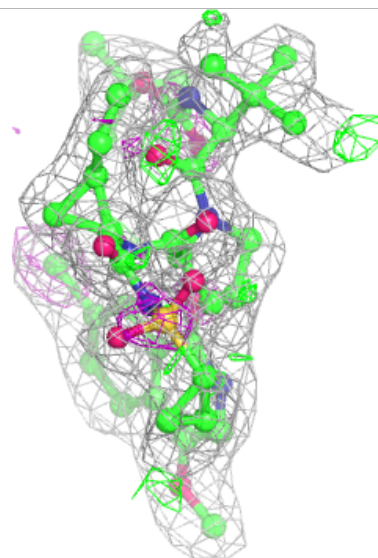
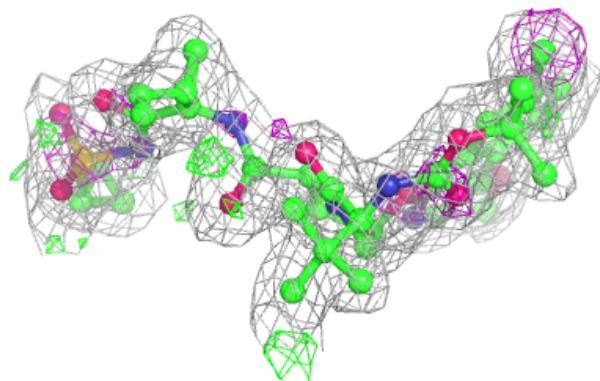
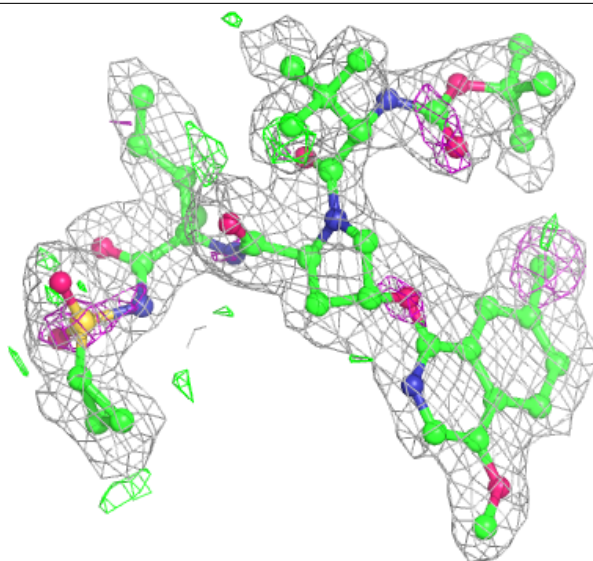
**Electron density around 2R9 B 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 2R9 A 301:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.