



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:32 PM BST

PDB ID : 6L50  
Title : Crystal structure of Zika NS2B-NS3 protease with compound 16  
Authors : Quek, J.P.  
Deposited on : 2019-10-21  
Resolution : 1.95 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 : 2.13.1  
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) : 2.13.1

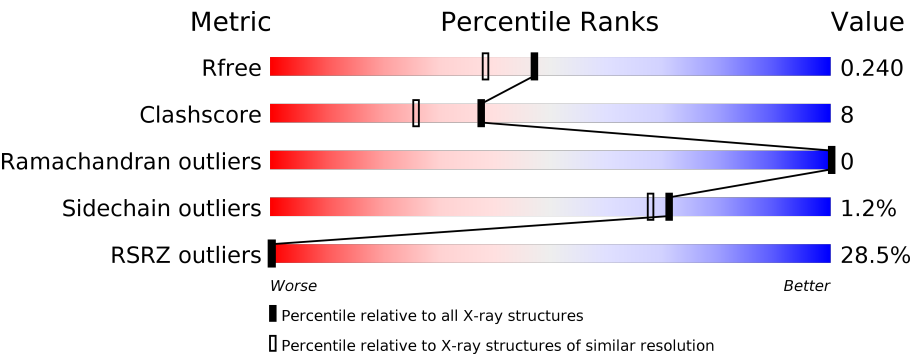
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	53	<div><div>28%</div><div><div></div><div>64%</div><div>8%</div><div>28%</div></div></div>
1	C	53	<div><div>26%</div><div><div></div><div>58%</div><div>11%</div><div>30%</div></div></div>
1	E	53	<div><div>23%</div><div><div></div><div>58%</div><div>11%</div><div>30%</div></div></div>
1	G	53	<div><div>13%</div><div><div></div><div>58%</div><div>13%</div><div>28%</div></div></div>
2	B	178	<div><div>25%</div><div><div></div><div>76%</div><div>11%</div><div>13%</div></div></div>
2	D	178	<div><div>27%</div><div><div></div><div>69%</div><div>17%</div><div>13%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	178	<div><div></div><div>22%</div><div>62%</div><div>22%</div><div>16%</div></div>
2	H	178	<div><div></div><div>21%</div><div>69%</div><div>15%</div><div>•</div><div>16%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5707 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 Serine protease subunit NS2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	38	Total	C	N	O	S	0	0	0
			292	181	47	63	1			
1	C	37	Total	C	N	O	S	0	0	0
			284	177	46	60	1			
1	E	37	Total	C	N	O	S	0	0	0
			284	177	46	60	1			
1	G	38	Total	C	N	O	S	0	0	0
			292	181	47	63	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	initiating methionine	UNP Q32ZE1
A	45	THR	-	expression tag	UNP Q32ZE1
C	44	MET	-	initiating methionine	UNP Q32ZE1
C	45	THR	-	expression tag	UNP Q32ZE1
E	44	MET	-	initiating methionine	UNP Q32ZE1
E	45	THR	-	expression tag	UNP Q32ZE1
G	44	MET	-	initiating methionine	UNP Q32ZE1
G	45	THR	-	expression tag	UNP Q32ZE1

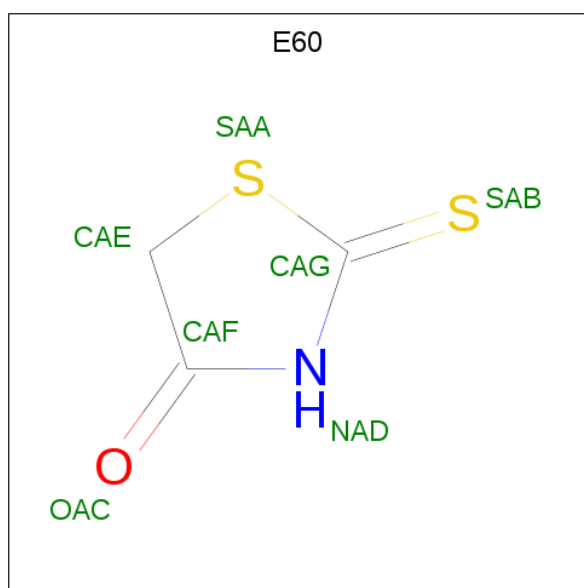
- Molecule 2 is a protein called NS3 protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	155	Total	C	N	O	S	0	0	0
			1138	720	199	214	5			
2	D	154	Total	C	N	O	S	0	0	0
			1133	717	198	213	5			
2	F	150	Total	C	N	O	S	0	0	0
			1101	696	191	209	5			
2	H	150	Total	C	N	O	S	0	0	0
			1105	698	194	208	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A142IX72
D	0	GLY	-	expression tag	UNP A0A142IX72
F	0	GLY	-	expression tag	UNP A0A142IX72
H	0	GLY	-	expression tag	UNP A0A142IX72

- Molecule 3 is 2-sulfanylidene-1,3-thiazolidin-4-one (three-letter code: E60) (formula:  $C_3H_3NOS_2$ ) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total	C	N	O	S	0	0
			7	3	1	1	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	13	Total	O	0	0
			13	13		
4	C	1	Total	O	0	0
			1	1		
4	D	6	Total	O	0	0
			6	6		
4	E	4	Total	O	0	0
			4	4		

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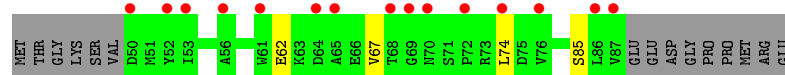
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	16	Total 16	O 16	0	0
4	G	5	Total 5	O 5	0	0
4	H	22	Total 22	O 22	0	0

### 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 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.

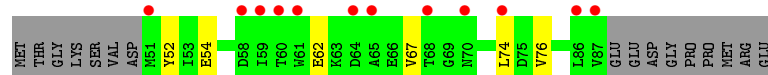
- Molecule 1: Serine protease subunit NS2B



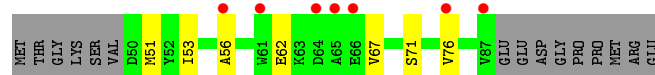
- Molecule 1: Serine protease subunit NS2B



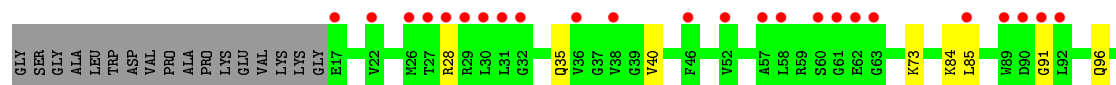
- Molecule 1: Serine protease subunit NS2B

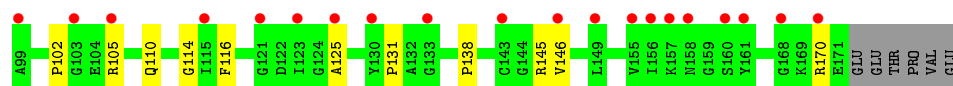


- Molecule 1: Serine protease subunit NS2B

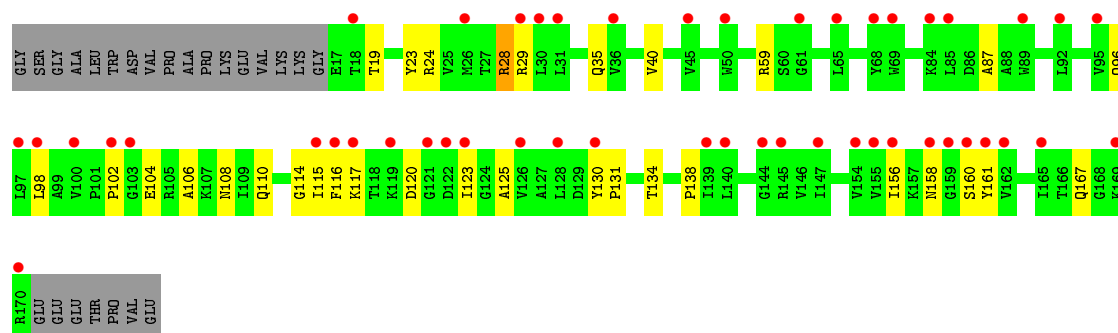


- Molecule 2: NS3 protease

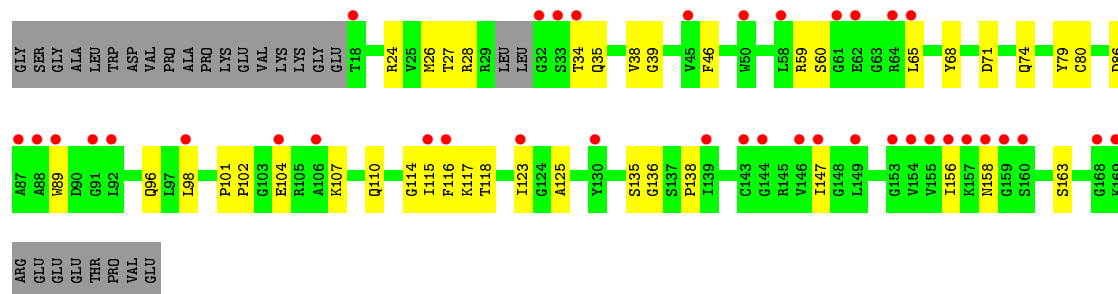




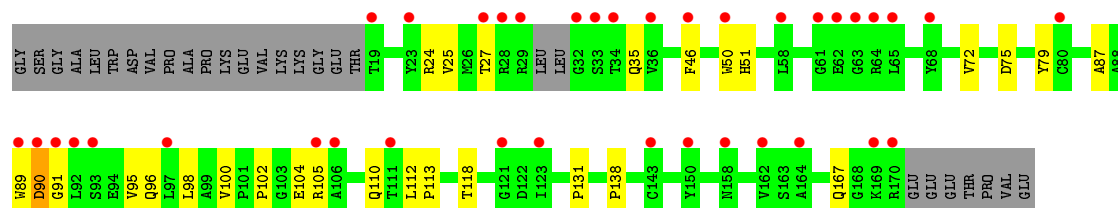
• Molecule 2: NS3 protease



• Molecule 2: NS3 protease



• Molecule 2: NS3 protease





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.74Å 59.91Å 214.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.30 – 1.95 42.30 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (42.30-1.95) 97.8 (42.30-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	15.09 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.215 , 0.235 0.218 , 0.240	Depositor DCC
$R_{free}$ test set	1999 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.6	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 31.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.357 for k,h,-l	Xtriage
Reported twinning fraction	0.430 for k,h,-l	Depositor
Outliers	0 of 56423 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0208e-03.*

<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: E60

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	0.24	0/296	0.46	0/401
1	C	0.26	0/288	0.48	0/390
1	E	0.24	0/288	0.46	0/390
1	G	0.26	0/296	0.48	0/401
2	B	0.29	0/1162	0.53	0/1582
2	D	0.32	0/1157	0.52	0/1575
2	F	0.26	0/1124	0.49	0/1529
2	H	0.35	1/1128 (0.1%)	0.58	2/1533 (0.1%)
All	All	0.29	1/5739 (0.0%)	0.52	2/7801 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	105	ARG	CZ-NH1	5.03	1.39	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	105	ARG	NE-CZ-NH2	-7.83	116.39	120.30
2	H	105	ARG	NE-CZ-NH1	5.62	123.11	120.30

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	292	0	269	3	0
1	C	284	0	265	5	0
1	E	284	0	265	6	0
1	G	292	0	269	7	0
2	B	1138	0	1111	10	1
2	D	1133	0	1109	21	0
2	F	1101	0	1071	30	0
2	H	1105	0	1077	24	0
3	H	7	0	0	0	0
4	A	4	0	0	0	0
4	B	13	0	0	0	0
4	C	1	0	0	0	0
4	D	6	0	0	0	0
4	E	4	0	0	0	0
4	F	16	0	0	0	0
4	G	5	0	0	0	0
4	H	22	0	0	0	0
All	All	5707	0	5436	85	1

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 (85) 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)
2:D:156:ILE:HG13	2:D:158:ASN:OD1	1.77	0.84
2:F:65:LEU:HD12	2:F:80:CYS:SG	2.27	0.74
2:D:160:SER:OG	2:D:161:TYR:N	2.23	0.71
1:G:51:MET:HG2	2:H:27:THR:HG22	1.73	0.70
2:F:28:ARG:HD2	2:F:59:ARG:HH12	1.56	0.69
2:H:90:ASP:OD1	2:H:91:GLY:N	2.25	0.69
1:G:67:VAL:HG22	2:H:110:GLN:HB3	1.76	0.68
2:D:35:GLN:HB3	2:D:102:PRO:HB3	1.76	0.67
2:F:28:ARG:HD2	2:F:59:ARG:NH1	2.10	0.67
1:E:67:VAL:HG22	2:F:110:GLN:HB3	1.75	0.66
2:B:35:GLN:HB3	2:B:102:PRO:HB3	1.82	0.61
2:B:114:GLY:N	2:B:125:ALA:O	2.33	0.60
2:F:35:GLN:HB3	2:F:102:PRO:HB3	1.84	0.60
2:F:116:PHE:HB2	2:F:123:ILE:HG13	1.84	0.59
2:F:27:THR:HG22	2:F:34:THR:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:GLN:HB3	2:H:102:PRO:HB3	1.85	0.59
2:D:131:PRO:O	2:D:134:THR:HG22	2.03	0.59
2:F:114:GLY:N	2:F:125:ALA:O	2.34	0.59
2:F:89:TRP:HB2	2:F:147:ILE:HD12	1.86	0.58
2:B:102:PRO:HD2	2:B:131:PRO:HG2	1.86	0.57
2:D:28:ARG:H	2:D:28:ARG:HD3	1.72	0.55
2:F:28:ARG:HH21	2:F:59:ARG:HH12	1.55	0.55
2:D:98:LEU:HD21	2:D:106:ALA:HB1	1.90	0.54
2:F:60:SER:HB2	2:F:65:LEU:HD21	1.89	0.54
2:H:89:TRP:NE1	2:H:91:GLY:HA2	2.23	0.53
1:G:76:VAL:HG23	2:H:118:THR:HG22	1.90	0.53
2:H:89:TRP:CE2	2:H:91:GLY:HA2	2.44	0.52
1:C:67:VAL:HG22	2:D:110:GLN:HB3	1.92	0.52
2:H:90:ASP:OD1	2:H:90:ASP:C	2.48	0.52
2:H:35:GLN:NE2	2:H:100:VAL:O	2.42	0.51
1:G:53:ILE:HG22	2:H:25:VAL:HG22	1.92	0.51
2:F:114:GLY:O	2:F:115:ILE:HD13	2.11	0.51
1:A:74:LEU:HD12	2:B:116:PHE:HE1	1.76	0.51
2:D:130:TYR:HB3	2:D:134:THR:HG21	1.93	0.51
1:C:76:VAL:HG11	1:C:84:PHE:HB3	1.93	0.50
1:E:74:LEU:HD12	2:F:116:PHE:HE1	1.76	0.50
2:D:116:PHE:HB2	2:D:123:ILE:HG13	1.93	0.49
2:F:46:PHE:HB3	2:F:79:TYR:HB2	1.94	0.49
2:H:98:LEU:HB3	2:H:138:PRO:HG2	1.94	0.49
1:E:76:VAL:HG23	2:F:118:THR:HG22	1.93	0.49
1:E:62:GLU:O	2:F:96:GLN:NE2	2.31	0.49
2:H:102:PRO:HD2	2:H:131:PRO:HG2	1.95	0.49
1:C:52:TYR:HB3	2:D:59:ARG:HB3	1.95	0.48
1:G:62:GLU:O	2:H:96:GLN:NE2	2.28	0.48
2:H:89:TRP:HE1	2:H:113:PRO:HG2	1.78	0.48
2:H:87:ALA:O	2:H:167:GLN:NE2	2.33	0.48
2:D:24:ARG:NH2	2:D:104:GLU:O	2.30	0.48
2:D:87:ALA:O	2:D:167:GLN:NE2	2.33	0.47
2:H:89:TRP:NE1	2:H:113:PRO:HG2	2.30	0.47
2:H:51:HIS:ND1	2:H:75:ASP:OD2	2.44	0.46
2:F:71:ASP:HB3	2:F:74:GLN:HB2	1.97	0.46
2:F:39:GLY:HA3	2:F:46:PHE:CZ	2.50	0.46
2:F:156:ILE:HG13	2:F:158:ASN:OD1	2.16	0.46
2:H:24:ARG:NH2	2:H:104:GLU:O	2.36	0.46
2:H:95:VAL:O	2:H:110:GLN:HA	2.16	0.46
2:D:130:TYR:CB	2:D:134:THR:HG21	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:ARG:HH21	2:F:59:ARG:NH1	2.13	0.45
1:E:52:TYR:HB3	2:F:59:ARG:HB3	1.97	0.45
2:B:84:LYS:HA	2:B:170:ARG:HD2	1.99	0.45
2:D:114:GLY:N	2:D:125:ALA:O	2.44	0.45
2:H:50:TRP:NE1	2:H:72:VAL:HG22	2.32	0.45
2:D:28:ARG:HH21	2:D:29:ARG:H	1.64	0.44
2:F:24:ARG:NH2	2:F:104:GLU:O	2.26	0.44
2:B:40:VAL:HG21	2:B:138:PRO:HB3	1.99	0.44
1:G:56:ALA:HB2	2:H:24:ARG:HG3	2.00	0.44
2:D:96:GLN:OE1	2:D:108:ASN:HB3	2.18	0.43
2:B:85:LEU:HD13	2:B:146:VAL:HG11	1.99	0.43
1:C:53:ILE:HA	2:D:24:ARG:O	2.19	0.42
2:D:19:THR:O	2:D:23:TYR:OH	2.30	0.42
2:F:98:LEU:HB3	2:F:138:PRO:HG2	2.01	0.42
2:D:40:VAL:HG21	2:D:138:PRO:HB3	2.00	0.42
2:F:38:VAL:O	2:F:136:GLY:HA3	2.19	0.42
2:F:86:ASP:OD1	2:F:86:ASP:N	2.52	0.42
2:F:38:VAL:N	2:F:135:SER:O	2.48	0.42
2:B:73:LYS:HB2	2:F:68:TYR:OH	2.20	0.41
2:D:115:ILE:HG22	2:D:117:LYS:HG3	2.01	0.41
1:C:86:LEU:HD21	2:D:156:ILE:HA	2.01	0.41
2:F:115:ILE:HG22	2:F:117:LYS:HG3	2.03	0.41
1:E:54:GLU:OE1	2:F:26:MET:HG3	2.19	0.41
2:F:101:PRO:HG2	2:F:107:LYS:HE3	2.02	0.41
1:A:62:GLU:O	2:B:96:GLN:NE2	2.33	0.41
1:A:67:VAL:HG22	2:B:110:GLN:HB3	2.03	0.41
2:H:89:TRP:CD1	2:H:91:GLY:HA2	2.56	0.40
2:H:46:PHE:HB3	2:H:79:TYR:HB2	2.03	0.40
1:G:71:SER:OG	2:H:112:LEU:HD23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:GLY:O	2:B:105:ARG:NH2[3_545]	2.10	0.10

## 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	36/53 (68%)	35 (97%)	1 (3%)	0	100	100
1	C	35/53 (66%)	34 (97%)	1 (3%)	0	100	100
1	E	35/53 (66%)	34 (97%)	1 (3%)	0	100	100
1	G	36/53 (68%)	35 (97%)	1 (3%)	0	100	100
2	B	153/178 (86%)	148 (97%)	5 (3%)	0	100	100
2	D	152/178 (85%)	148 (97%)	4 (3%)	0	100	100
2	F	146/178 (82%)	141 (97%)	5 (3%)	0	100	100
2	H	146/178 (82%)	140 (96%)	6 (4%)	0	100	100
All	All	739/924 (80%)	715 (97%)	24 (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	31/45 (69%)	30 (97%)	1 (3%)	39	27
1	C	30/45 (67%)	30 (100%)	0	100	100
1	E	30/45 (67%)	30 (100%)	0	100	100
1	G	31/45 (69%)	31 (100%)	0	100	100
2	B	115/140 (82%)	113 (98%)	2 (2%)	60	55
2	D	115/140 (82%)	113 (98%)	2 (2%)	60	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	112/140 (80%)	111 (99%)	1 (1%)	78	77
2	H	112/140 (80%)	111 (99%)	1 (1%)	78	77
All	All	576/740 (78%)	569 (99%)	7 (1%)	71	68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	SER
2	B	28	ARG
2	B	145	ARG
2	D	28	ARG
2	D	120	ASP
2	F	163	SER
2	H	90	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
3	E60	H	201	-	7,7,7	3.24	3 (42%)	9,9,9	2.51	5 (55%)

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
3	E60	H	201	-	-	-	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	201	E60	CAE-CAF	-6.50	1.40	1.51
3	H	201	E60	CAG-SAA	-3.93	1.66	1.74
3	H	201	E60	CAG-SAB	3.45	1.72	1.66

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	201	E60	CAE-CAF-NAD	4.21	116.86	111.76
3	H	201	E60	CAF-CAE-SAA	-3.92	102.80	107.11
3	H	201	E60	OAC-CAF-NAD	-2.73	121.33	125.00
3	H	201	E60	SAA-CAG-SAB	2.09	124.57	121.79
3	H	201	E60	CAG-NAD-CAF	-2.08	115.10	117.69

There are no chirality outliers.

There are no torsion outliers.

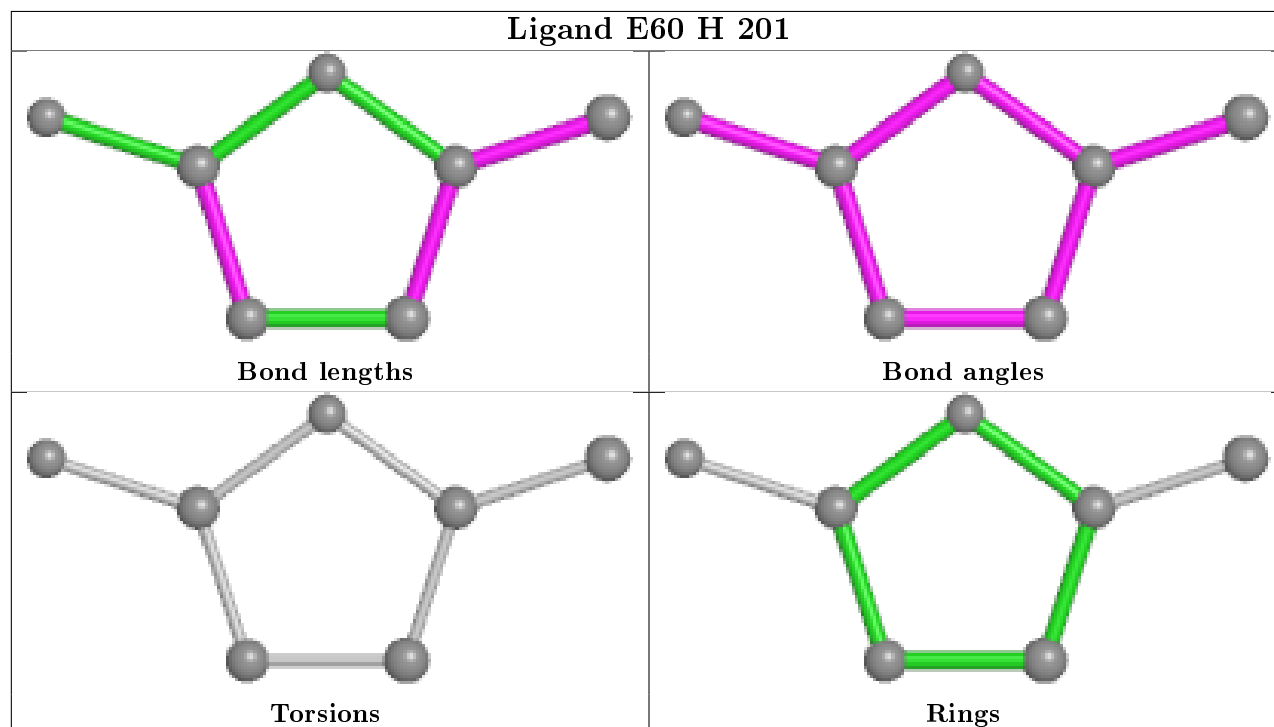
There are no ring outliers.

No monomer is involved in short contacts.

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	38/53 (71%)	1.87	15 (39%) 0 0	26, 35, 53, 54	0
1	C	37/53 (69%)	1.89	14 (37%) 0 0	23, 39, 45, 49	0
1	E	37/53 (69%)	1.71	12 (32%) 0 0	22, 29, 44, 52	0
1	G	38/53 (71%)	1.51	7 (18%) 1 1	23, 30, 44, 60	0
2	B	155/178 (87%)	1.71	44 (28%) 0 0	22, 31, 48, 73	0
2	D	154/178 (86%)	1.65	48 (31%) 0 0	20, 30, 49, 76	0
2	F	150/178 (84%)	1.56	39 (26%) 0 0	18, 26, 46, 64	0
2	H	150/178 (84%)	1.81	37 (24%) 0 0	18, 27, 48, 66	0
All	All	759/924 (82%)	1.69	216 (28%) 0 0	18, 29, 49, 76	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	91	GLY	24.4
2	H	33	SER	9.4
2	H	89	TRP	6.7
2	H	29	ARG	6.6
2	F	61	GLY	6.5
2	H	61	GLY	6.2
2	H	32	GLY	6.2
2	B	29	ARG	6.1
2	F	169	LYS	6.1
2	D	29	ARG	5.3
2	D	160	SER	5.3
2	D	158	ASN	5.1
2	D	31	LEU	5.1
1	A	50	ASP	4.8
1	G	64	ASP	4.8
1	C	87	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	158	ASN	4.7
2	D	30	LEU	4.7
2	D	170	ARG	4.6
2	D	169	LYS	4.5
1	E	65	ALA	4.4
2	H	92	LEU	4.4
2	D	161	TYR	4.4
1	C	68	THR	4.4
2	B	103	GLY	4.2
2	H	19	THR	4.2
2	H	158	ASN	4.1
2	B	146	VAL	4.0
1	E	64	ASP	4.0
2	B	91	GLY	4.0
2	H	93	SER	3.9
1	C	64	ASP	3.9
2	B	89	TRP	3.8
2	F	157	LYS	3.8
1	A	64	ASP	3.7
1	E	87	VAL	3.7
1	G	87	VAL	3.7
1	E	59	ILE	3.7
2	B	57	ALA	3.6
2	B	31	LEU	3.6
2	F	156	ILE	3.6
2	H	34	THR	3.6
2	B	62	GLU	3.6
2	D	130	TYR	3.5
2	F	158	ASN	3.5
2	F	34	THR	3.5
2	F	87	ALA	3.5
2	F	147	ILE	3.5
2	H	123	ILE	3.5
1	C	77	ALA	3.5
2	F	168	GLY	3.5
2	H	90	ASP	3.5
2	D	61	GLY	3.4
2	H	121	GLY	3.4
2	D	92	LEU	3.4
2	F	155	VAL	3.4
2	B	161	TYR	3.4
1	A	86	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	86	LEU	3.4
2	D	154	VAL	3.3
2	B	52	VAL	3.3
1	G	66	GLU	3.2
2	F	50	TRP	3.2
2	B	99	ALA	3.2
1	C	86	LEU	3.2
1	A	74	LEU	3.2
2	D	162	VAL	3.2
2	D	18	THR	3.1
2	B	63	GLY	3.1
2	F	154	VAL	3.1
2	D	103	GLY	3.1
2	B	155	VAL	3.1
2	B	61	GLY	3.1
1	A	68	THR	3.1
1	A	65	ALA	3.1
1	A	76	VAL	3.0
2	H	62	GLU	3.0
2	B	58	LEU	3.0
2	D	147	ILE	3.0
2	D	68	TYR	3.0
2	H	143	CYS	3.0
1	A	56	ALA	2.9
2	B	143	CYS	2.9
2	D	156	ILE	2.9
2	F	115	ILE	2.9
2	D	97	LEU	2.9
1	E	74	LEU	2.9
2	D	85	LEU	2.9
1	G	65	ALA	2.9
2	F	92	LEU	2.8
2	H	28	ARG	2.8
2	B	38	VAL	2.8
1	C	76	VAL	2.8
2	D	126	VAL	2.8
2	B	156	ILE	2.8
1	C	82	GLY	2.7
1	A	53	ILE	2.7
2	D	121	GLY	2.7
2	D	102	PRO	2.7
2	H	23	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	H	36	VAL	2.7
2	H	63	GLY	2.7
2	F	159	GLY	2.7
1	A	87	VAL	2.7
2	F	91	GLY	2.7
2	D	123	ILE	2.6
2	B	105	ARG	2.6
2	B	30	LEU	2.6
2	B	149	LEU	2.6
2	D	115	ILE	2.6
2	F	160	SER	2.6
2	D	155	VAL	2.6
1	C	67	VAL	2.6
1	G	61	TRP	2.6
2	F	33	SER	2.6
2	F	64	ARG	2.6
2	B	46	PHE	2.5
2	B	92	LEU	2.5
2	B	115	ILE	2.5
2	F	62	GLU	2.5
1	E	58	ASP	2.5
2	B	157	LYS	2.5
2	H	80	CYS	2.5
2	B	123	ILE	2.5
2	D	117	LYS	2.5
2	F	88	ALA	2.5
2	H	164	ALA	2.5
1	C	74	LEU	2.5
1	E	68	THR	2.5
2	H	105	ARG	2.5
2	F	144	GLY	2.4
2	F	45	VAL	2.4
2	D	140	LEU	2.4
2	B	27	THR	2.4
2	D	100	VAL	2.4
2	H	46	PHE	2.4
2	B	17	GLU	2.4
2	D	95	VAL	2.4
1	C	61	TRP	2.4
2	H	97	LEU	2.4
2	F	143	CYS	2.4
2	H	111	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	65	ALA	2.4
1	A	72	PRO	2.4
2	D	36	VAL	2.4
2	F	98	LEU	2.3
2	D	119	LYS	2.3
1	A	70	ASN	2.3
2	D	50	TRP	2.3
2	B	85	LEU	2.3
1	C	79	ASP	2.3
2	B	170	ARG	2.3
2	B	36	VAL	2.3
1	G	56	ALA	2.3
2	F	130	TYR	2.3
2	F	89	TRP	2.3
2	F	146	VAL	2.3
2	D	139	ILE	2.3
2	H	170	ARG	2.3
2	D	65	LEU	2.3
1	C	66	GLU	2.3
2	H	169	LYS	2.3
1	C	69	GLY	2.3
2	D	122	ASP	2.3
1	A	61	TRP	2.3
2	H	106	ALA	2.3
2	B	130	TYR	2.2
2	B	121	GLY	2.2
2	F	116	PHE	2.2
2	D	26	MET	2.2
2	B	22	VAL	2.2
2	B	125	ALA	2.2
2	B	168	GLY	2.2
2	B	90	ASP	2.2
2	H	150	TYR	2.2
1	E	60	THR	2.2
2	B	60	SER	2.2
2	D	116	PHE	2.2
1	G	76	VAL	2.2
2	D	69	TRP	2.2
2	H	65	LEU	2.2
2	B	160	SER	2.2
2	B	28	ARG	2.2
2	D	45	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	104	GLU	2.2
2	F	123	ILE	2.2
2	F	149	LEU	2.2
2	H	27	THR	2.2
1	A	69	GLY	2.2
2	D	145	ARG	2.2
2	F	106	ALA	2.2
2	H	68	TYR	2.2
1	E	51	MET	2.1
2	D	128	LEU	2.1
2	H	58	LEU	2.1
2	D	159	GLY	2.1
2	H	162	VAL	2.1
2	B	26	MET	2.1
2	B	32	GLY	2.1
2	D	144	GLY	2.1
2	F	18	THR	2.1
2	F	139	ILE	2.1
1	E	70	ASN	2.1
2	D	165	ILE	2.1
1	A	52	TYR	2.1
1	E	61	TRP	2.1
2	H	50	TRP	2.1
2	F	153	GLY	2.1
2	H	64	ARG	2.0
2	D	84	LYS	2.0
2	F	32	GLY	2.0
2	F	65	LEU	2.0
2	B	133	GLY	2.0
2	D	89	TRP	2.0
2	D	98	LEU	2.0
2	F	58	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](#)

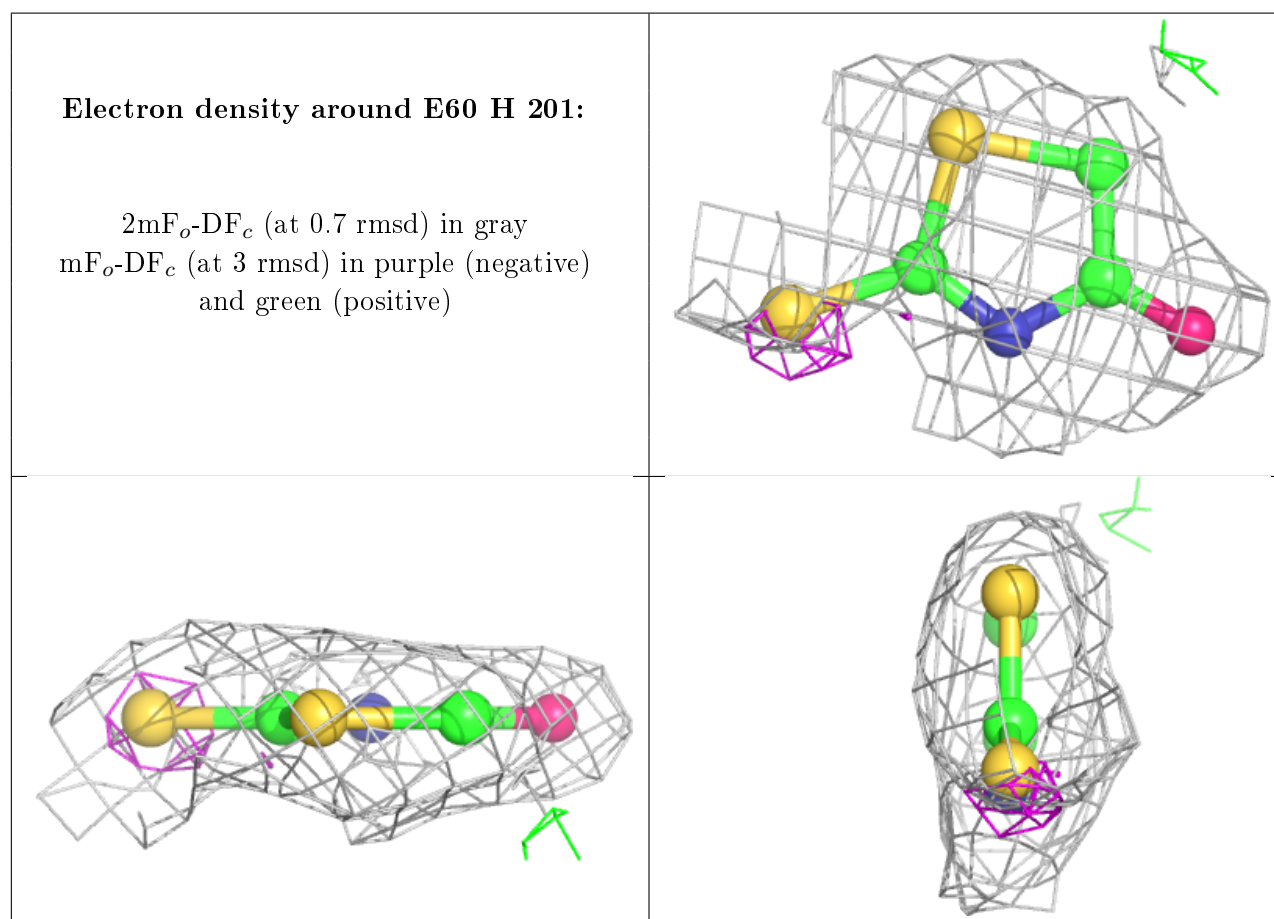
There are no monosaccharides in this entry.

## 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
3	E60	H	201	7/7	0.75	0.23	26,32,40,42	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.