



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:49 PM BST

PDB ID : 6L4Z  
Title : Crystal structure of Zika NS2B-NS3 protease with compound 6  
Authors : Quek, J.P.  
Deposited on : 2019-10-21  
Resolution : 1.90 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

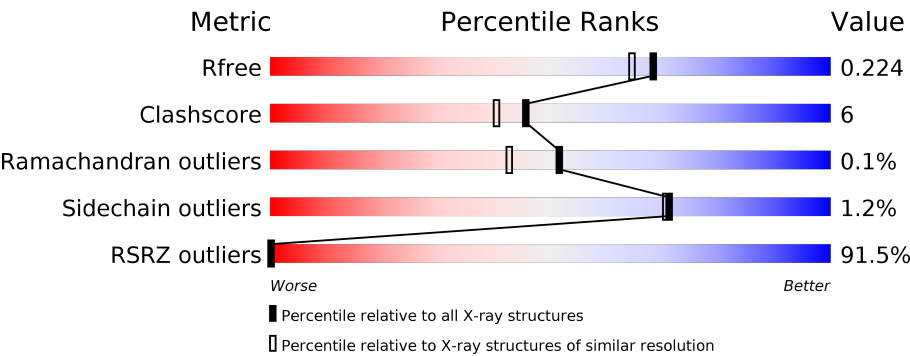
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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 <sub>free</sub>	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	38	<div><div>95%</div><div><div></div><div></div><div></div><div></div></div><div>92%</div><div>8%</div></div>
1	E	38	<div><div>87%</div><div><div></div><div></div><div></div><div></div></div><div>84%</div><div>16%</div></div>
2	B	155	<div><div>92%</div><div><div></div><div></div><div></div><div></div></div><div>89%</div><div>11%</div></div>
3	C	37	<div><div>95%</div><div><div></div><div></div><div></div><div></div></div><div>81%</div><div>16%</div><div>.</div></div>
4	D	153	<div><div>88%</div><div><div></div><div></div><div></div><div></div></div><div>83%</div><div>14%</div><div>.</div></div>
5	F	152	<div><div>95%</div><div><div></div><div></div><div></div><div></div></div><div>81%</div><div>18%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
6	G	40	85% 
			88%  10% .
7	H	159	86% 
			77%  18% . .

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5807 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	38	Total	C	N	O	S	0	0	0
			280	174	46	59	1			
1	E	38	Total	C	N	O	S	0	0	0
			282	177	47	57	1			

- Molecule 2 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	155	Total	C	N	O	S	0	1	0
			1141	725	196	215	5			

- Molecule 3 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	37	Total	C	N	O	S	0	0	0
			280	175	46	58	1			

- Molecule 4 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	148	Total	C	N	O	S	0	1	0
			1092	693	186	208	5			

- Molecule 5 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	152	Total	C	N	O	S	0	0	0
			1113	709	195	204	5			

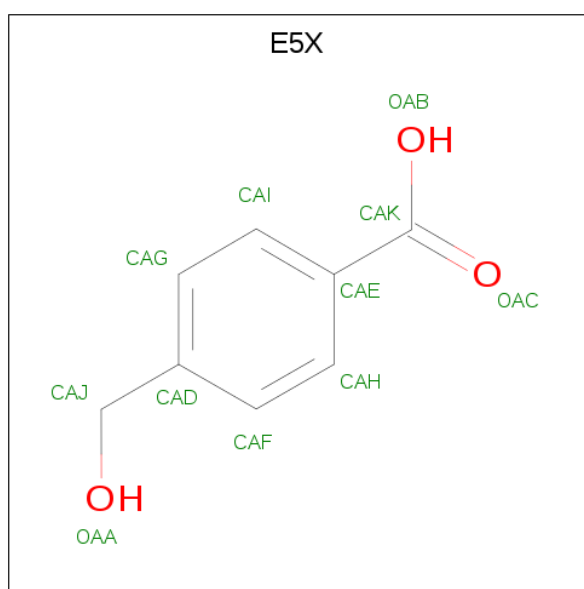
- Molecule 6 is a protein called Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	40	Total	C	N	O	S	0	0	0
			295	183	48	63	1			

- Molecule 7 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	153	Total	C	N	O	S	0	0	0
			1139	722	199	213	5			

- Molecule 8 is 4-(hydroxymethyl)benzoic acid (three-letter code: E5X) (formula: C<sub>8</sub>H<sub>8</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	H	1	Total	C	O	0	0
			11	8	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	11	Total	O	0	0
			11	11		
9	B	29	Total	O	0	0
			29	29		
9	C	11	Total	O	0	0
			11	11		
9	D	30	Total	O	0	0
			30	30		

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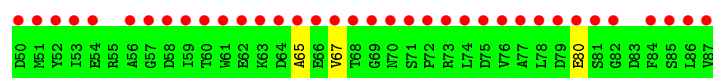
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	6	Total 6	O 6	0	0
9	F	17	Total 17	O 17	0	0
9	G	20	Total 20	O 20	0	0
9	H	50	Total 50	O 50	0	0

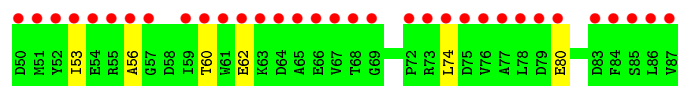
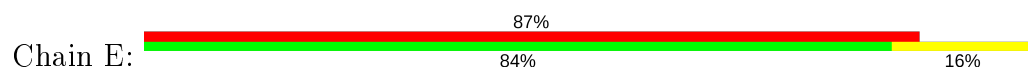
### 3 Residue-property plots [i](#)

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.

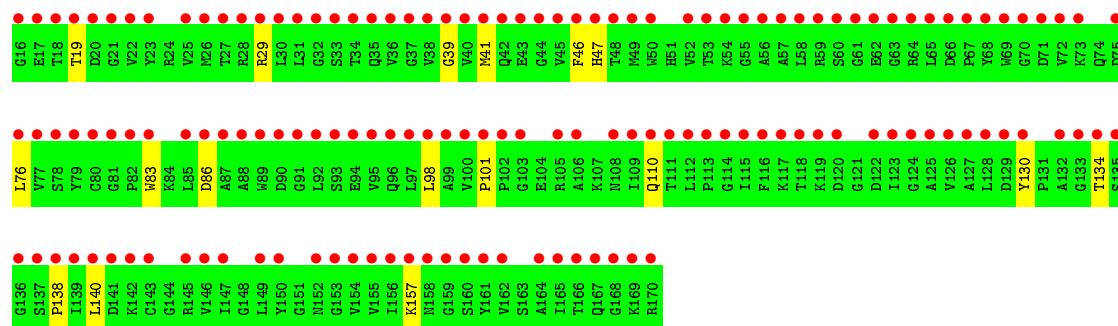
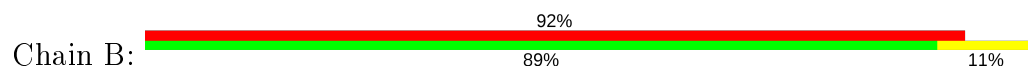
- Molecule 1: Genome polyprotein



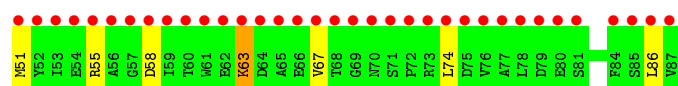
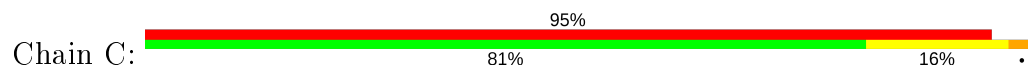
- Molecule 1: Genome polyprotein




- Molecule 2: Genome polyprotein

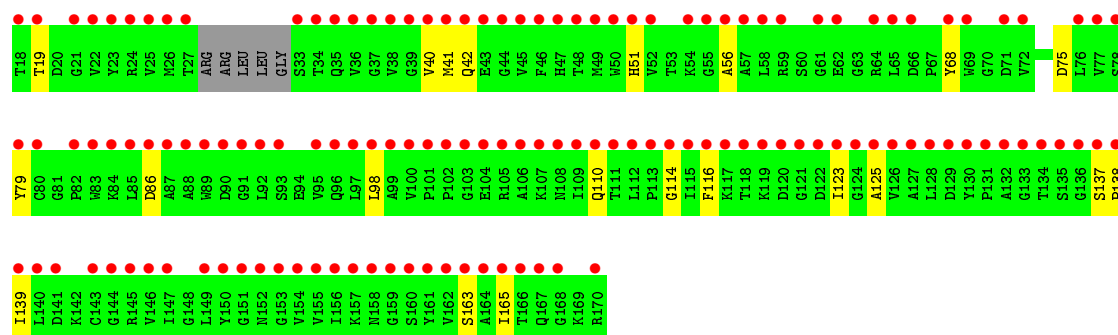


- Molecule 3: Genome polyprotein

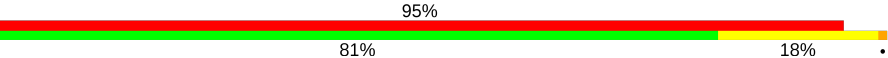


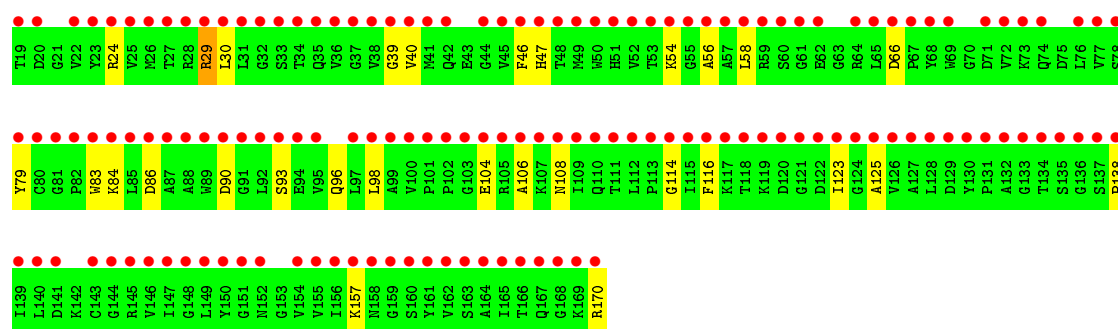
- Molecule 4: Genome polyprotein

Chain D: 




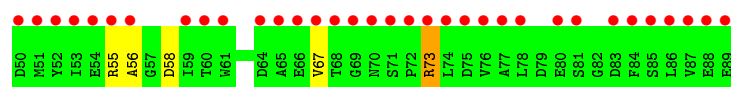
• Molecule 5: Genome polyprotein

Chain F: 




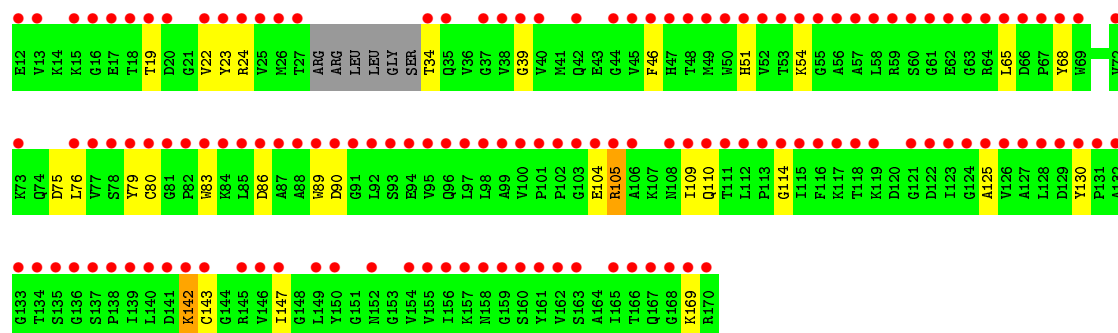
• Molecule 6: Genome polyprotein

Chain G: 



• Molecule 7: Genome polyprotein

Chain H: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	59.55Å 59.52Å 214.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.76 – 1.90 45.76 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.76-1.90) 99.9 (45.76-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	19.34 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.180 , 0.226 0.184 , 0.224	Depositor DCC
$R_{free}$ test set	3012 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 44.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.34$ , $\langle L^2 \rangle = 0.16$	Xtriage
Estimated twinning fraction	0.407 for k,h,-l	Xtriage
Reported twinning fraction	0.440 for k,h,-l	Depositor
Outliers	0 of 61146 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.04% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: E5X

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	0.29	0/284	0.50	0/387
1	E	0.27	0/286	0.49	0/388
2	B	0.32	0/1168	0.51	0/1589
3	C	0.27	0/284	0.47	0/385
4	D	0.29	0/1115	0.48	0/1516
5	F	0.30	0/1137	0.51	0/1546
6	G	0.30	0/299	0.55	0/407
7	H	0.36	0/1162	0.58	0/1574
All	All	0.31	0/5735	0.52	0/7792

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 [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	280	0	250	3	0
1	E	282	0	261	5	1
2	B	1141	0	1123	11	0
3	C	280	0	261	6	0
4	D	1092	0	1065	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	1113	0	1103	20	0
6	G	295	0	260	5	0
7	H	1139	0	1133	20	2
8	H	11	0	0	0	0
9	A	11	0	0	1	0
9	B	29	0	0	1	0
9	C	11	0	0	1	0
9	D	30	0	0	1	0
9	E	6	0	0	0	0
9	F	17	0	0	0	0
9	G	20	0	0	1	0
9	H	50	0	0	2	0
All	All	5807	0	5456	71	2

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 6.

All (71) 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)
6:G:73:ARG:NH1	9:G:101:HOH:O	2.17	0.76
1:A:67:VAL:HG22	2:B:110:GLN:HB3	1.69	0.72
7:H:169:LYS:NZ	9:H:303:HOH:O	2.27	0.67
4:D:42:GLN:NE2	9:D:202:HOH:O	2.29	0.66
5:F:90:ASP:OD2	5:F:93:SER:OG	2.12	0.66
4:D:51:HIS:ND1	4:D:75:ASP:OD2	2.29	0.63
6:G:55:ARG:NH2	6:G:58:ASP:OD1	2.29	0.61
6:G:56:ALA:HB2	7:H:24:ARG:HG3	1.84	0.60
5:F:84:LYS:O	5:F:170:ARG:NH2	2.34	0.59
1:E:62:GLU:O	5:F:96:GLN:NE2	2.30	0.59
3:C:74:LEU:HD12	4:D:116:PHE:HE1	1.67	0.59
7:H:34:THR:N	9:H:306:HOH:O	2.37	0.58
6:G:56:ALA:HB3	7:H:22:VAL:HG13	1.85	0.58
4:D:114:GLY:N	4:D:125:ALA:O	2.35	0.56
3:C:67:VAL:HG22	4:D:110:GLN:HB3	1.88	0.55
7:H:46:PHE:HB3	7:H:79:TYR:HB2	1.87	0.55
1:A:80:GLU:O	4:D:68:TYR:OH	2.20	0.55
7:H:65:LEU:HD22	7:H:80:CYS:SG	2.47	0.54
7:H:142:LYS:H	7:H:142:LYS:HD3	1.72	0.54
7:H:19:THR:HG21	7:H:23:TYR:OH	2.08	0.54
4:D:86:ASP:N	4:D:86:ASP:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ALA:N	9:A:101:HOH:O	2.39	0.54
3:C:55:ARG:NH2	3:C:58:ASP:OD1	2.21	0.53
7:H:39:GLY:HA3	7:H:46:PHE:CZ	2.44	0.53
3:C:51:MET:N	9:C:101:HOH:O	2.42	0.52
1:E:74:LEU:HD12	5:F:116:PHE:HE1	1.75	0.52
2:B:86:ASP:OD1	2:B:86:ASP:N	2.42	0.52
5:F:86:ASP:N	5:F:86:ASP:OD2	2.42	0.52
1:E:56:ALA:HB2	5:F:24:ARG:HG3	1.92	0.51
2:B:98:LEU:HD12	2:B:140:LEU:HD11	1.92	0.51
2:B:157:LYS:O	9:B:201:HOH:O	2.19	0.51
7:H:109:ILE:HD12	7:H:130:TYR:OH	2.11	0.50
5:F:114:GLY:N	5:F:125:ALA:O	2.40	0.50
5:F:116:PHE:HB2	5:F:123:ILE:HG13	1.93	0.50
2:B:39:GLY:HA3	2:B:46:PHE:CZ	2.47	0.49
3:C:86:LEU:H	3:C:86:LEU:HD12	1.78	0.49
1:E:60:THR:O	5:F:108:ASN:ND2	2.46	0.49
5:F:39:GLY:HA3	5:F:46:PHE:CZ	2.47	0.49
7:H:51:HIS:HA	7:H:54:LYS:HE3	1.94	0.48
2:B:101:PRO:HA	2:B:134:THR:HG22	1.95	0.48
4:D:19:THR:O	4:D:41:MET:HG2	2.13	0.48
2:B:47:HIS:HB3	2:B:83:TRP:CH2	2.48	0.48
4:D:56:ALA:O	4:D:79:TYR:OH	2.25	0.48
3:C:63:LYS:H	3:C:63:LYS:HD2	1.79	0.47
2:B:130:TYR:HB3	2:B:134:THR:HG21	1.95	0.47
7:H:89:TRP:HB2	7:H:147:ILE:HD12	1.97	0.47
7:H:114:GLY:N	7:H:125:ALA:O	2.44	0.45
1:E:53:ILE:HG23	5:F:58:LEU:HD22	1.99	0.45
5:F:29:ARG:HD3	5:F:30:LEU:N	2.33	0.44
7:H:51:HIS:ND1	7:H:75:ASP:OD2	2.39	0.44
5:F:54:LYS:HE3	5:F:54:LYS:HB3	1.65	0.44
4:D:139:ILE:HD13	4:D:165:ILE:HG12	2.00	0.44
2:B:19:THR:O	2:B:41:MET:HG2	2.18	0.43
5:F:56:ALA:O	5:F:79:TYR:OH	2.28	0.43
7:H:24:ARG:NH2	7:H:104:GLU:O	2.35	0.43
5:F:40:VAL:HG21	5:F:138:PRO:HB3	2.01	0.43
7:H:105:ARG:HA	7:H:105:ARG:HD3	1.75	0.43
7:H:86:ASP:OD1	7:H:86:ASP:N	2.52	0.43
5:F:24:ARG:NH2	5:F:104:GLU:O	2.37	0.42
4:D:116:PHE:HB2	4:D:123:ILE:HG13	2.02	0.42
4:D:98:LEU:O	4:D:137:SER:HB3	2.19	0.42
2:B:98:LEU:HB3	2:B:138:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:40:VAL:HG21	4:D:138:PRO:HB3	2.02	0.42
6:G:67:VAL:HG22	7:H:110:GLN:HB3	2.02	0.41
5:F:157:LYS:HB3	5:F:157:LYS:HE3	1.89	0.41
2:B:76:LEU:HD22	2:B:83:TRP:CH2	2.55	0.41
5:F:46:PHE:HB3	5:F:79:TYR:HB2	2.02	0.41
5:F:98:LEU:CD2	5:F:106:ALA:HB1	2.51	0.40
7:H:142:LYS:HG2	7:H:143:CYS:SG	2.60	0.40
5:F:47:HIS:HB3	5:F:83:TRP:CZ3	2.57	0.40
7:H:76:LEU:HD22	7:H:83:TRP:CH2	2.57	0.40

All (2) 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)
7:H:90:ASP:O	7:H:105:ARG:NH1[3_555]	2.12	0.08
1:E:80:GLU:O	7:H:68:TYR:OH[4_565]	2.19	0.01

## 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	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
1	E	36/38 (95%)	36 (100%)	0	0	100	100
2	B	154/155 (99%)	145 (94%)	8 (5%)	1 (1%)	25	15
3	C	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
4	D	145/153 (95%)	138 (95%)	7 (5%)	0	100	100
5	F	150/152 (99%)	143 (95%)	7 (5%)	0	100	100
6	G	38/40 (95%)	36 (95%)	2 (5%)	0	100	100
7	H	149/159 (94%)	144 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	743/772 (96%)	710 (96%)	32 (4%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	29	ARG

### 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	28/32 (88%)	28 (100%)	0	100	100
1	E	28/32 (88%)	28 (100%)	0	100	100
2	B	116/121 (96%)	116 (100%)	0	100	100
3	C	29/31 (94%)	28 (97%)	1 (3%)	37	28
4	D	112/120 (93%)	111 (99%)	1 (1%)	78	79
5	F	112/119 (94%)	110 (98%)	2 (2%)	59	55
6	G	29/34 (85%)	28 (97%)	1 (3%)	37	28
7	H	117/125 (94%)	115 (98%)	2 (2%)	60	57
All	All	571/614 (93%)	564 (99%)	7 (1%)	71	70

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

Mol	Chain	Res	Type
3	C	63	LYS
4	D	163	SER
5	F	29	ARG
5	F	66	ASP
6	G	73	ARG
7	H	105	ARG
7	H	142	LYS

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

such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	$\# Z  > 2$
8	E5X	H	201	-	9,11,11	3.29	2 (22%)	11,14,14	0.75	0

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
8	E5X	H	201	-	-	0/2/6/6	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	201	E5X	CAE-CAK	-9.20	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	201	E5X	CAJ-CAD	-3.39	1.39	1.51

There are no bond angle outliers.

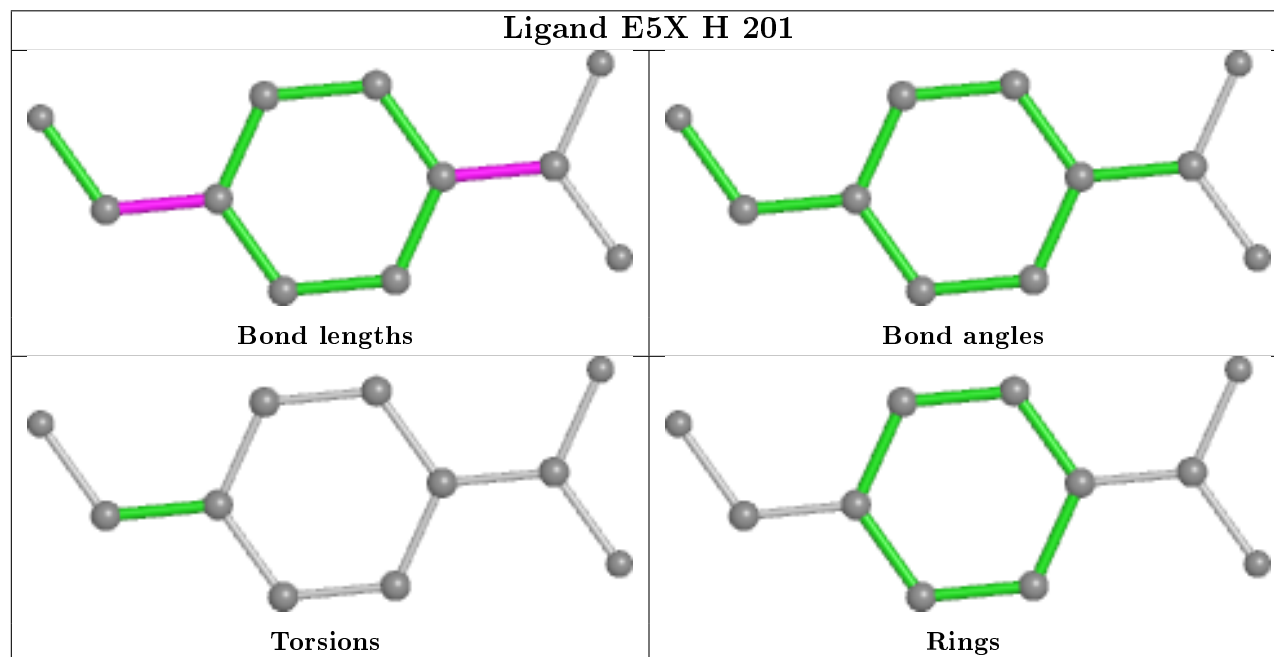
There are no chirality outliers.

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 ⓘ

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	38/38 (100%)	4.60	36 (94%) 0 0	18, 27, 43, 54	0
1	E	38/38 (100%)	5.47	33 (86%) 0 0	29, 38, 48, 58	0
2	B	155/155 (100%)	4.57	143 (92%) 0 0	15, 24, 48, 63	0
3	C	37/37 (100%)	4.88	35 (94%) 0 0	34, 43, 60, 60	0
4	D	148/153 (96%)	4.46	134 (90%) 0 0	24, 37, 54, 63	0
5	F	152/152 (100%)	4.54	144 (94%) 0 0	20, 31, 51, 60	0
6	G	40/40 (100%)	4.17	34 (85%) 0 0	22, 29, 44, 56	0
7	H	153/159 (96%)	4.08	137 (89%) 0 0	16, 24, 41, 85	0
All	All	761/772 (98%)	4.48	696 (91%) 0 0	15, 31, 51, 85	0

All (696) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	16	GLY	23.3
5	F	159	GLY	21.5
2	B	61	GLY	18.8
2	B	31	LEU	18.5
4	D	156	ILE	15.2
7	H	34	THR	15.0
1	E	57	GLY	14.6
1	E	86	LEU	13.1
1	A	87	VAL	12.4
4	D	161	TYR	12.3
2	B	112	LEU	11.9
4	D	85	LEU	11.5
2	B	63	GLY	11.4
4	D	165	ILE	11.3
7	H	63	GLY	11.3
1	A	50	ASP	10.8

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Mol	Chain	Res	Type	RSRZ
4	D	44	GLY	10.7
3	C	64	ASP	10.7
5	F	160	SER	10.6
5	F	156	ILE	10.0
2	B	92	LEU	10.0
7	H	62	GLU	9.9
5	F	50	TRP	9.8
3	C	52	TYR	9.7
4	D	123	ILE	9.7
2	B	18	THR	9.4
5	F	46	PHE	9.4
4	D	46	PHE	9.1
1	A	77	ALA	9.0
2	B	65	LEU	9.0
2	B	58	LEU	8.9
3	C	87	VAL	8.8
1	E	62	GLU	8.8
7	H	65	LEU	8.8
2	B	157	LYS	8.7
2	B	52	VAL	8.7
1	E	85	SER	8.6
1	E	68	THR	8.5
5	F	32	GLY	8.5
4	D	18	THR	8.4
1	E	65	ALA	8.4
4	D	157	LYS	8.4
7	H	89	TRP	8.3
7	H	69	TRP	8.3
1	A	61	TRP	8.2
5	F	134	THR	8.2
2	B	89	TRP	8.1
7	H	19	THR	8.1
2	B	27	THR	7.9
5	F	98	LEU	7.8
1	E	84	PHE	7.8
7	H	23	TYR	7.8
7	H	25	VAL	7.8
5	F	165	ILE	7.8
2	B	23	TYR	7.8
3	C	69	GLY	7.7
6	G	51	MET	7.7
2	B	33	SER	7.7

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Mol	Chain	Res	Type	RSRZ
5	F	105	ARG	7.7
1	E	50	ASP	7.6
4	D	102	PRO	7.6
1	A	60	THR	7.6
5	F	25	VAL	7.6
4	D	95	VAL	7.5
7	H	52	VAL	7.5
6	G	89	GLU	7.5
1	E	74	LEU	7.5
2	B	139	ILE	7.4
4	D	150	TYR	7.3
7	H	72	VAL	7.3
3	C	68	THR	7.3
5	F	85	LEU	7.3
4	D	115	ILE	7.3
5	F	61	GLY	7.2
2	B	59	ARG	7.2
4	D	130	TYR	7.2
7	H	58	LEU	7.2
3	C	74	LEU	7.2
5	F	97	LEU	7.2
2	B	88	ALA	7.2
5	F	62	GLU	7.1
3	C	86	LEU	7.1
1	E	60	THR	7.1
7	H	66	ASP	7.1
6	G	60	THR	7.1
4	D	58	LEU	7.0
7	H	60	SER	7.0
4	D	79	TYR	7.0
4	D	80	CYS	7.0
2	B	113	PRO	6.9
6	G	88	GLU	6.9
1	A	85	SER	6.9
1	E	51	MET	6.9
5	F	19	THR	6.9
7	H	130	TYR	6.9
4	D	133	GLY	6.9
5	F	88	ALA	6.8
5	F	127	ALA	6.8
4	D	116	PHE	6.8
7	H	118	THR	6.8

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Mol	Chain	Res	Type	RSRZ
7	H	99	ALA	6.8
5	F	161	TYR	6.7
7	H	142	LYS	6.7
7	H	13	VAL	6.6
7	H	140	LEU	6.6
4	D	19	THR	6.6
7	H	87	ALA	6.6
2	B	149	LEU	6.6
1	E	54	GLU	6.6
6	G	65	ALA	6.6
7	H	146	VAL	6.6
5	F	86	ASP	6.5
5	F	67	PRO	6.5
7	H	16	GLY	6.5
5	F	158	ASN	6.5
3	C	59	ILE	6.5
5	F	95	VAL	6.5
4	D	50	TRP	6.5
4	D	159	GLY	6.5
6	G	61	TRP	6.5
6	G	64	ASP	6.5
7	H	88	ALA	6.5
2	B	62	GLU	6.5
2	B	117	LYS	6.4
3	C	51	MET	6.4
5	F	38	VAL	6.4
4	D	119	LYS	6.4
5	F	118	THR	6.4
2	B	140	LEU	6.4
4	D	97	LEU	6.4
1	E	87	VAL	6.4
5	F	83	TRP	6.3
7	H	82	PRO	6.3
5	F	119	LYS	6.3
5	F	125	ALA	6.3
1	A	51	MET	6.3
2	B	67	PRO	6.3
4	D	56	ALA	6.2
5	F	143	CYS	6.2
5	F	162	VAL	6.2
2	B	30	LEU	6.2
6	G	53	ILE	6.1

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Mol	Chain	Res	Type	RSRZ
7	H	27	THR	6.1
1	E	59	ILE	6.1
1	E	52	TYR	6.1
7	H	18	THR	6.1
5	F	151	GLY	6.1
3	C	73	ARG	6.0
5	F	130	TYR	6.0
7	H	17	GLU	6.0
1	E	61	TRP	6.0
5	F	29	ARG	6.0
6	G	72	PRO	6.0
1	E	78	LEU	5.9
4	D	25	VAL	5.9
7	H	61	GLY	5.9
2	B	147	ILE	5.9
2	B	29	ARG	5.9
7	H	92	LEU	5.9
4	D	90	ASP	5.9
6	G	54	GLU	5.9
5	F	150	TYR	5.9
4	D	147	ILE	5.9
5	F	68	TYR	5.9
3	C	53	ILE	5.8
4	D	151	GLY	5.8
3	C	78	LEU	5.8
7	H	165	ILE	5.8
6	G	70	ASN	5.8
7	H	147	ILE	5.8
4	D	83	TRP	5.7
4	D	89	TRP	5.7
3	C	66	GLU	5.7
5	F	33	SER	5.7
7	H	162	VAL	5.7
4	D	62	GLU	5.7
4	D	128	LEU	5.7
4	D	26	MET	5.7
1	A	56	ALA	5.7
3	C	76	VAL	5.7
2	B	150	TYR	5.6
4	D	126	VAL	5.6
2	B	44	GLY	5.6
4	D	92	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	76	VAL	5.6
2	B	36	VAL	5.6
5	F	139	ILE	5.6
7	H	166	THR	5.6
5	F	147	ILE	5.5
4	D	140	LEU	5.5
5	F	126	VAL	5.5
1	A	66	GLU	5.5
2	B	73	LYS	5.5
7	H	145	ARG	5.5
1	A	78	LEU	5.5
1	A	73	ARG	5.4
1	A	62	GLU	5.4
2	B	85	LEU	5.4
2	B	97	LEU	5.4
5	F	120	ASP	5.4
1	E	64	ASP	5.4
2	B	28	ARG	5.4
4	D	86	ASP	5.4
2	B	19	THR	5.4
5	F	157	LYS	5.3
4	D	52	VAL	5.3
4	D	168	GLY	5.3
2	B	105	ARG	5.3
2	B	130	TYR	5.3
1	A	63	LYS	5.3
5	F	26	MET	5.3
2	B	60	SER	5.3
1	E	79	ASP	5.3
6	G	59	ILE	5.3
4	D	143	CYS	5.3
1	E	76	VAL	5.3
4	D	72	VAL	5.2
4	D	48	THR	5.2
6	G	78	LEU	5.2
5	F	115	ILE	5.2
2	B	102	PRO	5.2
4	D	118	THR	5.2
7	H	103	GLY	5.2
5	F	89	TRP	5.2
3	C	63	LYS	5.2
5	F	169	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	53	ILE	5.2
5	F	166	THR	5.2
7	H	91	GLY	5.1
6	G	50	ASP	5.1
5	F	116	PHE	5.1
7	H	12	GLU	5.1
6	G	68	THR	5.1
4	D	154	VAL	5.1
5	F	36	VAL	5.1
5	F	40	VAL	5.1
6	G	77	ALA	5.1
1	A	67	VAL	5.1
5	F	30	LEU	5.1
2	B	103	GLY	5.1
2	B	161	TYR	5.0
2	B	83	TRP	5.0
4	D	134	THR	5.0
2	B	168	GLY	5.0
4	D	135[A]	SER	5.0
2	B	46	PHE	5.0
5	F	168	GLY	5.0
2	B	155	VAL	5.0
2	B	142	LYS	5.0
4	D	145	ARG	4.9
5	F	144	GLY	4.9
6	G	85	SER	4.9
2	B	134	THR	4.9
7	H	169	LYS	4.9
4	D	170	ARG	4.9
2	B	77	VAL	4.9
5	F	66	ASP	4.9
2	B	50	TRP	4.9
5	F	149	LEU	4.9
4	D	109	ILE	4.9
7	H	38	VAL	4.9
4	D	27	THR	4.9
5	F	51	HIS	4.9
5	F	90	ASP	4.9
2	B	98	LEU	4.9
7	H	102	PRO	4.9
2	B	17	GLU	4.9
3	C	65	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
7	H	57	ALA	4.8
7	H	46	PHE	4.8
2	B	158	ASN	4.8
2	B	137	SER	4.8
2	B	100	VAL	4.8
4	D	155	VAL	4.8
2	B	123	ILE	4.8
2	B	116	PHE	4.8
2	B	72	VAL	4.8
6	G	76	VAL	4.8
3	C	56	ALA	4.8
7	H	76	LEU	4.8
2	B	56	ALA	4.7
2	B	22	VAL	4.7
7	H	50	TRP	4.7
5	F	64	ARG	4.7
4	D	36	VAL	4.7
4	D	99	ALA	4.7
5	F	101	PRO	4.7
5	F	92	LEU	4.7
2	B	169	LYS	4.7
1	E	77	ALA	4.7
5	F	131	PRO	4.7
5	F	148	GLY	4.7
5	F	41	MET	4.7
1	A	86	LEU	4.6
4	D	22	VAL	4.6
5	F	133	GLY	4.6
3	C	84	PHE	4.6
5	F	48	THR	4.6
4	D	152	ASN	4.6
7	H	116	PHE	4.6
4	D	139	ILE	4.6
4	D	160	SER	4.6
4	D	137	SER	4.6
7	H	163	SER	4.6
7	H	143	CYS	4.6
7	H	141	ASP	4.6
5	F	45	VAL	4.6
1	A	70	ASN	4.5
4	D	112	LEU	4.5
6	G	67	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
4	D	113	PRO	4.5
4	D	23	TYR	4.5
4	D	77	VAL	4.5
7	H	54	LYS	4.5
3	C	61	TRP	4.5
5	F	146	VAL	4.5
7	H	45	VAL	4.5
7	H	49	MET	4.5
5	F	113	PRO	4.5
2	B	133	GLY	4.4
7	H	77	VAL	4.4
3	C	72	PRO	4.4
7	H	35	GLN	4.4
4	D	88	ALA	4.4
2	B	153	GLY	4.4
7	H	149	LEU	4.4
2	B	156	ILE	4.4
5	F	123	ILE	4.4
7	H	98	LEU	4.4
4	D	61	GLY	4.4
7	H	22	VAL	4.4
5	F	138	PRO	4.3
5	F	73	LYS	4.3
5	F	135	SER	4.3
5	F	34	THR	4.3
2	B	45	VAL	4.3
2	B	132	ALA	4.3
2	B	109[A]	ILE	4.3
7	H	113	PRO	4.3
4	D	111	THR	4.3
7	H	15	LYS	4.2
1	E	80	GLU	4.2
5	F	163	SER	4.2
1	E	73	ARG	4.2
4	D	68	TYR	4.2
1	A	54	GLU	4.2
4	D	124	GLY	4.2
2	B	43	GLU	4.2
4	D	54	LYS	4.2
3	C	60	THR	4.2
5	F	53	THR	4.2
2	B	154	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
3	C	67	VAL	4.2
4	D	38	VAL	4.2
4	D	87	ALA	4.2
3	C	70	ASN	4.2
5	F	108	ASN	4.2
5	F	109	ILE	4.2
7	H	73	LYS	4.2
1	A	84	PHE	4.2
4	D	100	VAL	4.2
7	H	110	GLN	4.2
4	D	69	TRP	4.2
6	G	69	GLY	4.2
2	B	76	LEU	4.2
4	D	40	VAL	4.2
5	F	80	CYS	4.1
5	F	99	ALA	4.1
5	F	22	VAL	4.1
4	D	107	LYS	4.1
4	D	103	GLY	4.1
1	E	63	LYS	4.1
1	A	71	SER	4.1
2	B	145	ARG	4.1
5	F	55	GLY	4.1
4	D	45	VAL	4.1
2	B	96	GLN	4.1
2	B	87	ALA	4.1
4	D	120	ASP	4.1
4	D	98	LEU	4.0
4	D	106	ALA	4.0
7	H	101	PRO	4.0
2	B	81	GLY	4.0
5	F	128	LEU	4.0
7	H	109	ILE	4.0
2	B	143	CYS	4.0
2	B	167	GLN	4.0
7	H	128	LEU	4.0
6	G	87	VAL	4.0
2	B	120	ASP	4.0
5	F	31	LEU	4.0
7	H	123	ILE	3.9
5	F	91	GLY	3.9
5	F	129	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	56	ALA	3.9
5	F	145	ARG	3.9
2	B	115	ILE	3.9
7	H	105	ARG	3.9
7	H	161	TYR	3.9
2	B	49	MET	3.8
2	B	64	ARG	3.8
7	H	59	ARG	3.8
5	F	65	LEU	3.8
5	F	154	VAL	3.8
7	H	117	LYS	3.8
7	H	150	TYR	3.8
7	H	56	ALA	3.8
2	B	160	SER	3.8
2	B	95	VAL	3.8
5	F	49	MET	3.8
1	A	68	THR	3.8
2	B	68	TYR	3.8
1	E	75	ASP	3.8
5	F	58	LEU	3.8
7	H	154	VAL	3.8
2	B	135	SER	3.8
4	D	131	PRO	3.8
4	D	117	LYS	3.8
2	B	90	ASP	3.7
7	H	37	GLY	3.7
6	G	81	SER	3.7
4	D	57	ALA	3.7
5	F	79	TYR	3.7
5	F	39	GLY	3.7
7	H	81	GLY	3.7
5	F	76	LEU	3.7
3	C	71	SER	3.7
4	D	39	GLY	3.7
2	B	40	VAL	3.7
7	H	115	ILE	3.7
5	F	164	ALA	3.7
1	A	57	GLY	3.7
5	F	78	SER	3.7
1	A	59	ILE	3.7
4	D	21	GLY	3.6
5	F	69	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	66	ASP	3.6
4	D	129	ASP	3.6
4	D	34	THR	3.6
4	D	64	ARG	3.6
5	F	57	ALA	3.6
6	G	52	TYR	3.6
4	D	122	ASP	3.6
2	B	69	TRP	3.6
4	D	141	ASP	3.6
5	F	72	VAL	3.6
5	F	94	GLU	3.6
2	B	54	LYS	3.6
5	F	56	ALA	3.6
5	F	132	ALA	3.6
1	A	64	ASP	3.6
2	B	79	TYR	3.6
2	B	38	VAL	3.6
2	B	39	GLY	3.6
4	D	55	GLY	3.6
7	H	97	LEU	3.6
5	F	100	VAL	3.6
4	D	127	ALA	3.5
7	H	20	ASP	3.5
2	B	165	ILE	3.5
2	B	21	GLY	3.5
3	C	62	GLU	3.5
2	B	91	GLY	3.5
2	B	57	ALA	3.5
3	C	85	SER	3.5
2	B	127	ALA	3.5
7	H	132	ALA	3.5
2	B	119	LYS	3.5
3	C	55	ARG	3.5
6	G	56	ALA	3.5
2	B	82	PRO	3.5
4	D	105	ARG	3.5
2	B	118	THR	3.5
2	B	37	GLY	3.4
5	F	124	GLY	3.4
2	B	125	ALA	3.4
7	H	106	ALA	3.4
2	B	25	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
4	D	78	SER	3.4
1	A	65	ALA	3.4
7	H	85	LEU	3.4
4	D	164	ALA	3.4
5	F	170	ARG	3.4
2	B	111	THR	3.4
4	D	76	LEU	3.4
4	D	149	LEU	3.4
5	F	122	ASP	3.4
4	D	96	GLN	3.3
3	C	57	GLY	3.3
4	D	121	GLY	3.3
5	F	141	ASP	3.3
5	F	54	LYS	3.3
7	H	79	TYR	3.3
4	D	43	GLU	3.3
7	H	156	ILE	3.3
4	D	110	GLN	3.3
7	H	111	THR	3.3
7	H	83	TRP	3.3
5	F	103	GLY	3.3
7	H	55	GLY	3.3
4	D	24	ARG	3.3
5	F	24	ARG	3.3
2	B	20	ASP	3.3
5	F	74	GLN	3.3
4	D	144	GLY	3.3
5	F	52	VAL	3.3
4	D	166	THR	3.3
5	F	47	HIS	3.3
5	F	60	SER	3.2
7	H	114	GLY	3.2
7	H	137	SER	3.2
7	H	139	ILE	3.2
7	H	112	LEU	3.2
1	E	83	ASP	3.2
4	D	42	GLN	3.2
7	H	68	TYR	3.2
1	E	66	GLU	3.2
2	B	34	THR	3.2
2	B	53	THR	3.2
2	B	106	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
4	D	101	PRO	3.2
2	B	42	GLN	3.2
6	G	83	ASP	3.2
3	C	54	GLU	3.2
5	F	155	VAL	3.2
7	H	40	VAL	3.2
5	F	27	THR	3.2
7	H	155	VAL	3.2
4	D	66	ASP	3.1
7	H	44	GLY	3.1
1	E	55	ARG	3.1
7	H	80	CYS	3.1
7	H	167	GLN	3.1
4	D	37	GLY	3.1
5	F	121	GLY	3.1
2	B	99	ALA	3.1
4	D	41	MET	3.1
7	H	133	GLY	3.1
2	B	152	ASN	3.1
4	D	91	GLY	3.1
7	H	159	GLY	3.1
6	G	75	ASP	3.1
7	H	86	ASP	3.1
2	B	41	MET	3.1
2	B	122	ASP	3.0
5	F	93	SER	3.0
7	H	47	HIS	3.0
7	H	119	LYS	3.0
7	H	39	GLY	3.0
4	D	47	HIS	3.0
4	D	65	LEU	3.0
4	D	59	ARG	3.0
2	B	94	GLU	3.0
1	E	67	VAL	3.0
4	D	162	VAL	3.0
7	H	100	VAL	3.0
2	B	138	PRO	3.0
5	F	28	ARG	3.0
7	H	64	ARG	3.0
2	B	26	MET	3.0
2	B	166	THR	3.0
4	D	104	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
5	F	37	GLY	2.9
2	B	47	HIS	2.9
3	C	80	GLU	2.9
6	G	66	GLU	2.9
2	B	110	GLN	2.9
2	B	48	THR	2.9
4	D	82	PRO	2.9
4	D	132	ALA	2.9
5	F	107	LYS	2.9
5	F	77	VAL	2.9
5	F	102	PRO	2.9
7	H	24	ARG	2.9
2	B	80	CYS	2.9
7	H	94	GLU	2.9
2	B	162	VAL	2.9
7	H	126	VAL	2.9
4	D	33	SER	2.8
1	E	72	PRO	2.8
7	H	67	PRO	2.8
7	H	48	THR	2.8
6	G	73	ARG	2.8
1	E	69	GLY	2.8
7	H	42	GLN	2.8
1	A	58	ASP	2.8
7	H	122	ASP	2.8
5	F	44	GLY	2.8
2	B	78	SER	2.8
4	D	84	LYS	2.8
6	G	86	LEU	2.8
2	B	136	GLY	2.8
1	A	81	SER	2.8
3	C	81	SER	2.8
5	F	106	ALA	2.8
3	C	75	ASP	2.8
3	C	77	ALA	2.7
5	F	117	LYS	2.7
6	G	80	GLU	2.8
5	F	140	LEU	2.7
2	B	141	ASP	2.7
2	B	159	GLY	2.7
4	D	136	GLY	2.7
7	H	90	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	129	ASP	2.7
7	H	124	GLY	2.7
6	G	84	PHE	2.7
7	H	95	VAL	2.7
7	H	84	LYS	2.7
2	B	86	ASP	2.7
5	F	71	ASP	2.7
2	B	126	VAL	2.7
1	A	74	LEU	2.7
5	F	59	ARG	2.6
7	H	158	ASN	2.6
5	F	111	THR	2.6
7	H	170	ARG	2.6
5	F	35	GLN	2.6
1	A	79	ASP	2.6
2	B	75	ASP	2.6
2	B	146	VAL	2.6
7	H	134	THR	2.6
5	F	152	ASN	2.6
1	A	75	ASP	2.6
1	A	80	GLU	2.6
1	A	82	GLY	2.6
4	D	114	GLY	2.6
7	H	131	PRO	2.6
5	F	82	PRO	2.5
4	D	146	VAL	2.5
6	G	74	LEU	2.5
4	D	35	GLN	2.5
5	F	81	GLY	2.5
5	F	114	GLY	2.5
2	B	108	ASN	2.5
4	D	153	GLY	2.4
4	D	158	ASN	2.4
7	H	93	SER	2.4
7	H	104	GLU	2.4
7	H	152	ASN	2.4
3	C	79	ASP	2.4
2	B	101	PRO	2.4
7	H	121	GLY	2.4
7	H	157	LYS	2.4
2	B	128	LEU	2.4
4	D	93	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	55	GLY	2.4
4	D	138	PRO	2.4
2	B	170	ARG	2.3
5	F	87	ALA	2.3
2	B	35	GLN	2.3
5	F	136	GLY	2.3
7	H	78	SER	2.3
2	B	164	ALA	2.3
7	H	127	ALA	2.3
5	F	23	TYR	2.3
4	D	49	MET	2.3
2	B	114	GLY	2.3
7	H	26	MET	2.3
7	H	129	ASP	2.3
1	A	72	PRO	2.3
7	H	53	THR	2.3
4	D	163	SER	2.3
4	D	108	ASN	2.3
5	F	104	GLU	2.3
5	F	20	ASP	2.3
7	H	108	ASN	2.2
7	H	125	ALA	2.2
1	A	69	GLY	2.2
1	A	52	TYR	2.2
3	C	58	ASP	2.2
2	B	70	GLY	2.2
7	H	138	PRO	2.2
5	F	137	SER	2.2
2	B	32	GLY	2.2
7	H	168	GLY	2.2
7	H	160	SER	2.2
5	F	110	GLN	2.2
5	F	167	GLN	2.2
2	B	124	GLY	2.2
1	A	53	ILE	2.2
4	D	167	GLN	2.2
7	H	96	GLN	2.2
6	G	55	ARG	2.2
7	H	51	HIS	2.1
7	H	136	GLY	2.1
4	D	125	ALA	2.1
5	F	42	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
5	F	112	LEU	2.1
4	D	71	ASP	2.0
4	D	51	HIS	2.0
2	B	71	ASP	2.0
2	B	93	SER	2.0
5	F	84	LYS	2.0
6	G	71	SER	2.0
7	H	135	SER	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](#)

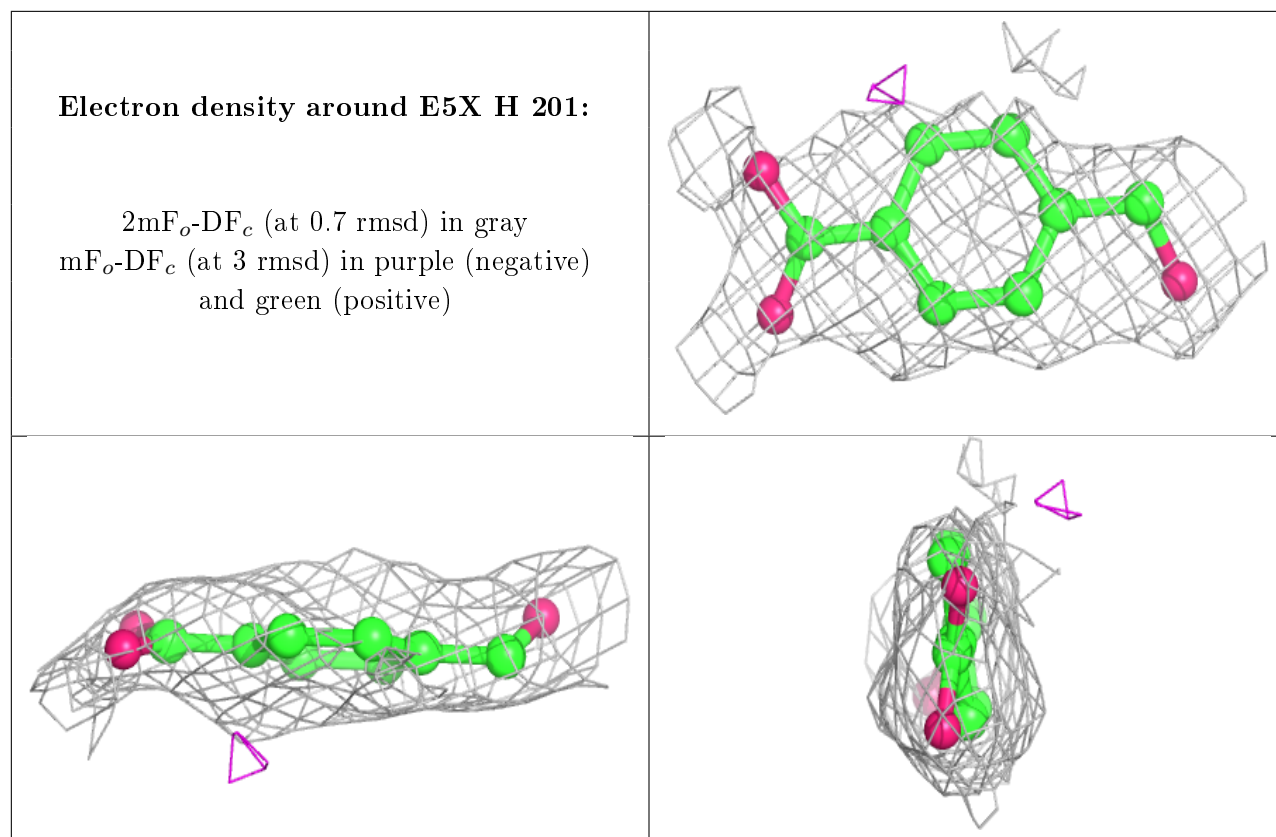
There are no monosaccharides in this entry.

## 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(Å <sup>2</sup> )	Q<0.9
8	E5X	H	201	11/11	0.59	0.26	29,31,35,35	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.