



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2025 – 01:02 PM EDT

PDB ID : 9O0W / pdb\_00009o0w  
Title : Co-crystal structure of human TREX1 in complex with an inhibitor  
Authors : Dehghani-Tafti, S.; Dong, A.; Li, Y.; Ackloo, S.; Arrowsmith, C.H.; Edwards, A.M.; Halabelian, L.; Structural Genomics Consortium (SGC)  
Deposited on : 2025-04-03  
Resolution : 1.43 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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

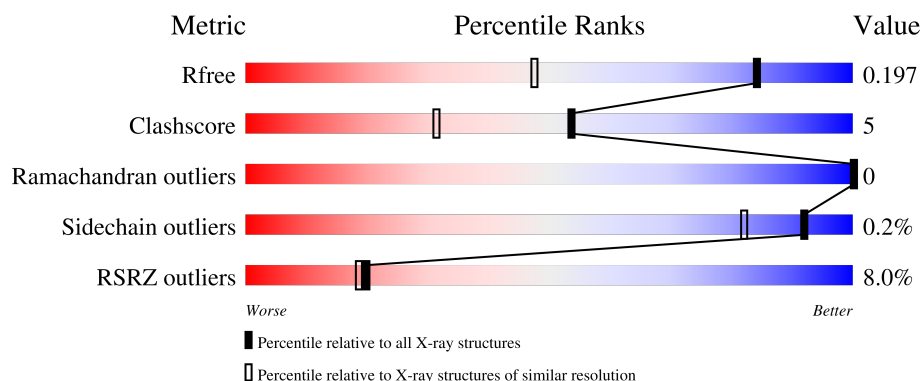
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


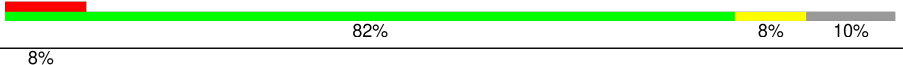
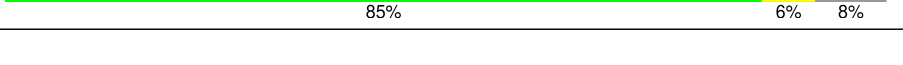
The reported resolution of this entry is 1.43 Å.

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))
$R_{free}$	164625	2809 (1.46-1.42)
Clashscore	180529	3008 (1.46-1.42)
Ramachandran outliers	177936	2971 (1.46-1.42)
Sidechain outliers	177891	2971 (1.46-1.42)
RSRZ outliers	164620	2809 (1.46-1.42)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	234	
1	B	234	
1	C	234	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	C	304	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5728 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.

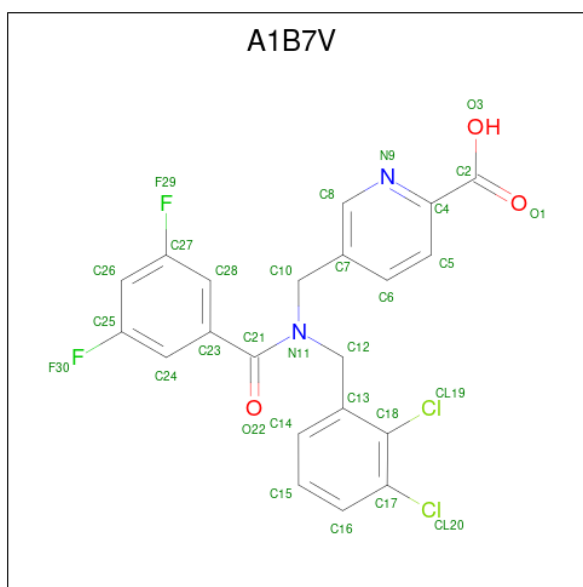
- Molecule 1 is a protein called Three-prime repair exonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	9	0
			1680	1078	285	304	13			
1	B	211	Total	C	N	O	S	0	12	0
			1678	1073	289	304	12			
1	C	215	Total	C	N	O	S	0	10	0
			1694	1081	294	306	13			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	PRO	conflict	UNP Q9NSU2
A	10	HIS	PRO	conflict	UNP Q9NSU2
A	26	SER	PHE	conflict	UNP Q9NSU2
A	28	ARG	GLN	conflict	UNP Q9NSU2
A	30	GLU	LYS	conflict	UNP Q9NSU2
B	8	HIS	PRO	conflict	UNP Q9NSU2
B	10	HIS	PRO	conflict	UNP Q9NSU2
B	26	SER	PHE	conflict	UNP Q9NSU2
B	28	ARG	GLN	conflict	UNP Q9NSU2
B	30	GLU	LYS	conflict	UNP Q9NSU2
C	8	HIS	PRO	conflict	UNP Q9NSU2
C	10	HIS	PRO	conflict	UNP Q9NSU2
C	26	SER	PHE	conflict	UNP Q9NSU2
C	28	ARG	GLN	conflict	UNP Q9NSU2
C	30	GLU	LYS	conflict	UNP Q9NSU2

- Molecule 2 is 5-({N-[(2,3-dichlorophenyl)methyl]-3,5-difluorobenzamido}methyl)pyridine-2-carboxylic acid (CCD ID: A1B7V) (formula: C<sub>21</sub>H<sub>14</sub>Cl<sub>2</sub>F<sub>2</sub>N<sub>2</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			30	21	2	2	2	3		
2	B	1	Total	C	Cl	F	N	O	0	0
			30	21	2	2	2	3		
2	C	1	Total	C	Cl	F	N	O	0	0
			30	21	2	2	2	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total X 5 5	0	0
5	B	3	Total X 3 3	0	0
5	C	1	Total X 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	186	Total O 187 187	0	1

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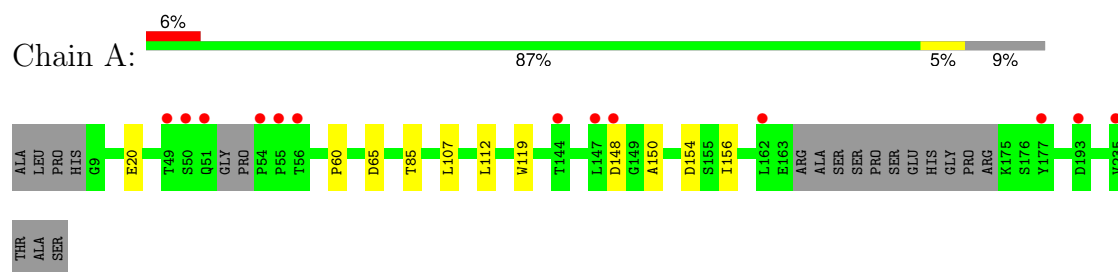
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	191	Total 195	O 195	0	4
6	C	170	Total 172	O 172	0	2

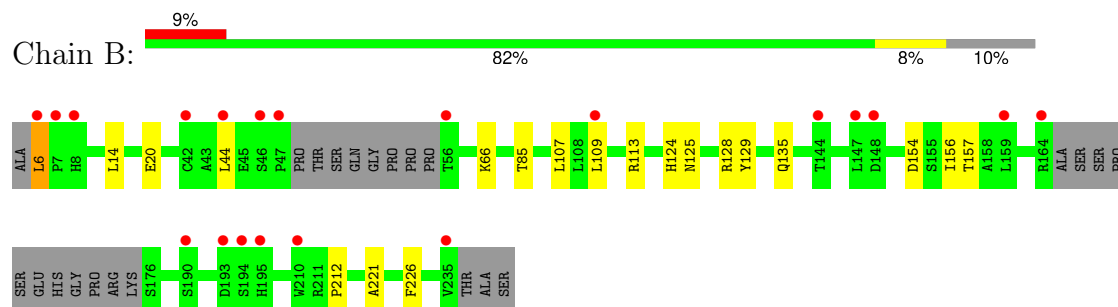
### 3 Residue-property plots [i](#)

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.

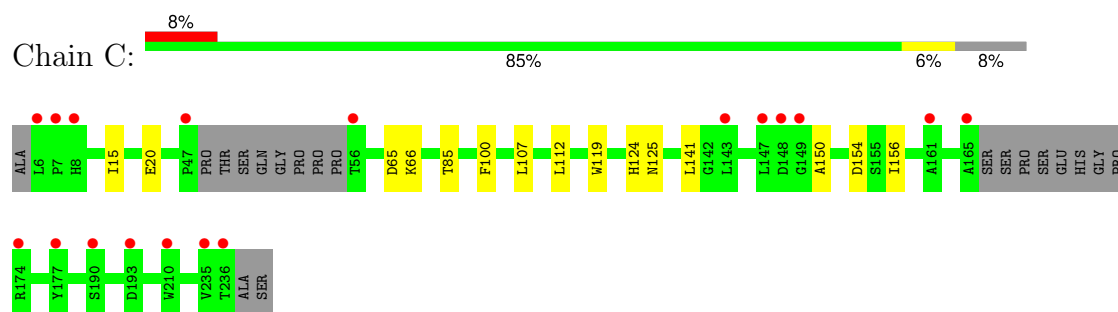
- Molecule 1: Three-prime repair exonuclease 1



- Molecule 1: Three-prime repair exonuclease 1



- Molecule 1: Three-prime repair exonuclease 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.70Å 153.69Å 137.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.11 – 1.43 49.11 – 1.43	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.11-1.43) 99.8 (49.11-1.43)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 1.43Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.162 , 0.181 0.180 , 0.197	Depositor DCC
$R_{free}$ test set	3074 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	14.1	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: A1B7V, UNX, EDO, MG

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	0.52	0/1726	0.81	2/2359 (0.1%)
1	B	0.51	0/1718	0.81	0/2346
1	C	0.52	0/1737	0.83	1/2373 (0.0%)
All	All	0.51	0/5181	0.82	3/7078 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	PRO	N-CA-CB	5.59	106.32	103.19
1	A	65	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	65	ASP	CA-CB-CG	5.07	117.67	112.60

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	1680	0	1655	8	0
1	B	1678	0	1652	16	0
1	C	1694	0	1648	22	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	30	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	1	0
4	C	12	0	18	7	0
5	A	5	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
6	A	187	0	0	1	0
6	B	195	0	0	3	0
6	C	172	0	0	4	1
All	All	5728	0	4985	49	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 5.

All (49) 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:C:119[B]:TRP:CH2	1:C:150:ALA:HB2	2.02	0.93
4:C:304:EDO:H21	6:C:468:HOH:O	1.77	0.85
1:C:15:ILE:HD11	1:C:119[B]:TRP:HB2	1.65	0.78
1:B:154:ASP:OD1	1:B:156[A]:ILE:HG12	1.86	0.75
1:A:119[B]:TRP:CH2	1:A:150:ALA:HB2	2.23	0.74
1:C:15:ILE:CD1	1:C:119[B]:TRP:HB2	2.23	0.68
1:C:112:LEU:HD13	1:C:119[B]:TRP:CH2	2.31	0.65
1:A:154:ASP:OD1	1:A:156:ILE:HG22	1.97	0.64
1:C:154:ASP:OD1	1:C:156[A]:ILE:HG22	1.98	0.64
1:C:124:HIS:CE1	1:C:156[B]:ILE:HG22	2.34	0.63
1:B:156[A]:ILE:CD1	6:B:467:HOH:O	2.47	0.62
1:C:100:PHE:O	4:C:304:EDO:H12	2.02	0.60
1:C:119[B]:TRP:CZ3	1:C:150:ALA:CB	2.85	0.58
1:A:20[B]:GLU:OE1	1:A:85:THR:HB	2.05	0.57
1:C:112:LEU:HD13	1:C:119[B]:TRP:CZ2	2.38	0.57
1:C:154:ASP:OD1	1:C:156[B]:ILE:HG12	2.05	0.57
1:C:119[B]:TRP:CZ3	1:C:150:ALA:HB2	2.38	0.57
1:B:6:LEU:HD21	1:B:221:ALA:O	2.06	0.55
4:C:304:EDO:H22	6:C:401:HOH:O	2.06	0.55
1:C:15:ILE:HD13	1:C:119[B]:TRP:CE3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20[A]:GLU:OE1	6:B:402:HOH:O	2.18	0.55
1:B:20[B]:GLU:OE1	1:B:85:THR:HB	2.08	0.54
1:A:107[B]:LEU:C	1:A:107[B]:LEU:HD23	2.35	0.52
1:A:112:LEU:HD13	1:A:119[B]:TRP:CH2	2.44	0.52
1:C:107:LEU:C	1:C:107:LEU:HD23	2.36	0.51
1:C:141:LEU:CD2	4:C:304:EDO:H11	2.41	0.50
1:C:119[B]:TRP:CH2	1:C:150:ALA:CB	2.87	0.50
1:C:119[B]:TRP:CZ3	1:C:150:ALA:HB1	2.48	0.49
1:B:125:ASN:OD1	1:B:156[A]:ILE:HD13	2.14	0.48
1:B:107:LEU:C	1:B:107:LEU:HD23	2.39	0.47
1:A:148:ASP:O	6:A:401:HOH:O	2.20	0.47
1:B:124:HIS:CE1	1:B:156[A]:ILE:HG22	2.50	0.47
1:B:44:LEU:O	1:B:212:PRO:HB2	2.15	0.46
1:C:66:LYS:CE	4:C:305:EDO:O1	2.63	0.46
1:C:66:LYS:HE3	4:C:305:EDO:O1	2.15	0.46
1:B:135[A]:GLN:CD	1:B:226:PHE:CE2	2.95	0.45
1:C:124:HIS:NE2	1:C:156[B]:ILE:HG22	2.32	0.45
1:B:109:LEU:HG	1:B:113:ARG:NH2	2.32	0.45
1:B:128:ARG:HD2	1:B:129:TYR:CZ	2.53	0.43
1:A:119[B]:TRP:CZ3	1:A:150:ALA:CB	3.02	0.43
1:C:20[B]:GLU:OE1	1:C:85:THR:HB	2.18	0.43
1:C:125:ASN:OD1	1:C:156[B]:ILE:HD13	2.19	0.43
4:C:303:EDO:H11	6:C:485:HOH:O	2.18	0.43
1:B:156[A]:ILE:HG13	1:B:157:THR:N	2.34	0.42
1:B:14[B]:LEU:HD12	1:B:44:LEU:HD13	2.02	0.41
1:B:156[A]:ILE:HD12	6:B:467:HOH:O	2.17	0.41
1:C:156[B]:ILE:CD1	6:C:480:HOH:O	2.68	0.41
1:B:66[A]:LYS:HE3	4:B:303:EDO:O2	2.19	0.41
1:A:119[B]:TRP:CZ3	1:A:150:ALA:HB1	2.55	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)
6:C:530:HOH:O	6:C:530:HOH:O[3_555]	2.01	0.19

## 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	217/234 (93%)	215 (99%)	2 (1%)	0	100	100
1	B	217/234 (93%)	214 (99%)	3 (1%)	0	100	100
1	C	219/234 (94%)	214 (98%)	5 (2%)	0	100	100
All	All	653/702 (93%)	643 (98%)	10 (2%)	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	178/192 (93%)	178 (100%)	0	100	100
1	B	176/192 (92%)	175 (99%)	1 (1%)	84	66
1	C	177/192 (92%)	177 (100%)	0	100	100
All	All	531/576 (92%)	530 (100%)	1 (0%)	92	82

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	HIS

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 3 are monoatomic and 9 are unknown - leaving 8 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	A1B7V	C	301	3	32,32,32	0.44	0	45,45,45	0.72	1 (2%)
4	EDO	A	303	-	3,3,3	0.13	0	2,2,2	0.01	0
4	EDO	C	304	-	3,3,3	0.35	0	2,2,2	0.18	0
4	EDO	C	305	-	3,3,3	0.12	0	2,2,2	0.14	0
4	EDO	B	303	-	3,3,3	0.19	0	2,2,2	0.07	0
4	EDO	C	303	-	3,3,3	0.12	0	2,2,2	0.51	0
2	A1B7V	B	301	3	32,32,32	0.47	0	45,45,45	0.74	1 (2%)
2	A1B7V	A	301	3	32,32,32	0.43	0	45,45,45	0.72	1 (2%)

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	A1B7V	C	301	3	-	0/20/20/20	0/3/3/3
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	C	304	-	-	1/1/1/1	-
4	EDO	C	305	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
4	EDO	C	303	-	-	1/1/1/1	-
2	A1B7V	B	301	3	-	0/20/20/20	0/3/3/3
2	A1B7V	A	301	3	-	0/20/20/20	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	A1B7V	O1-C2-C4	-2.84	115.58	121.30
2	A	301	A1B7V	O1-C2-C4	-2.79	115.68	121.30
2	B	301	A1B7V	O1-C2-C4	-2.53	116.21	121.30

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	303	EDO	O1-C1-C2-O2
4	C	304	EDO	O1-C1-C2-O2

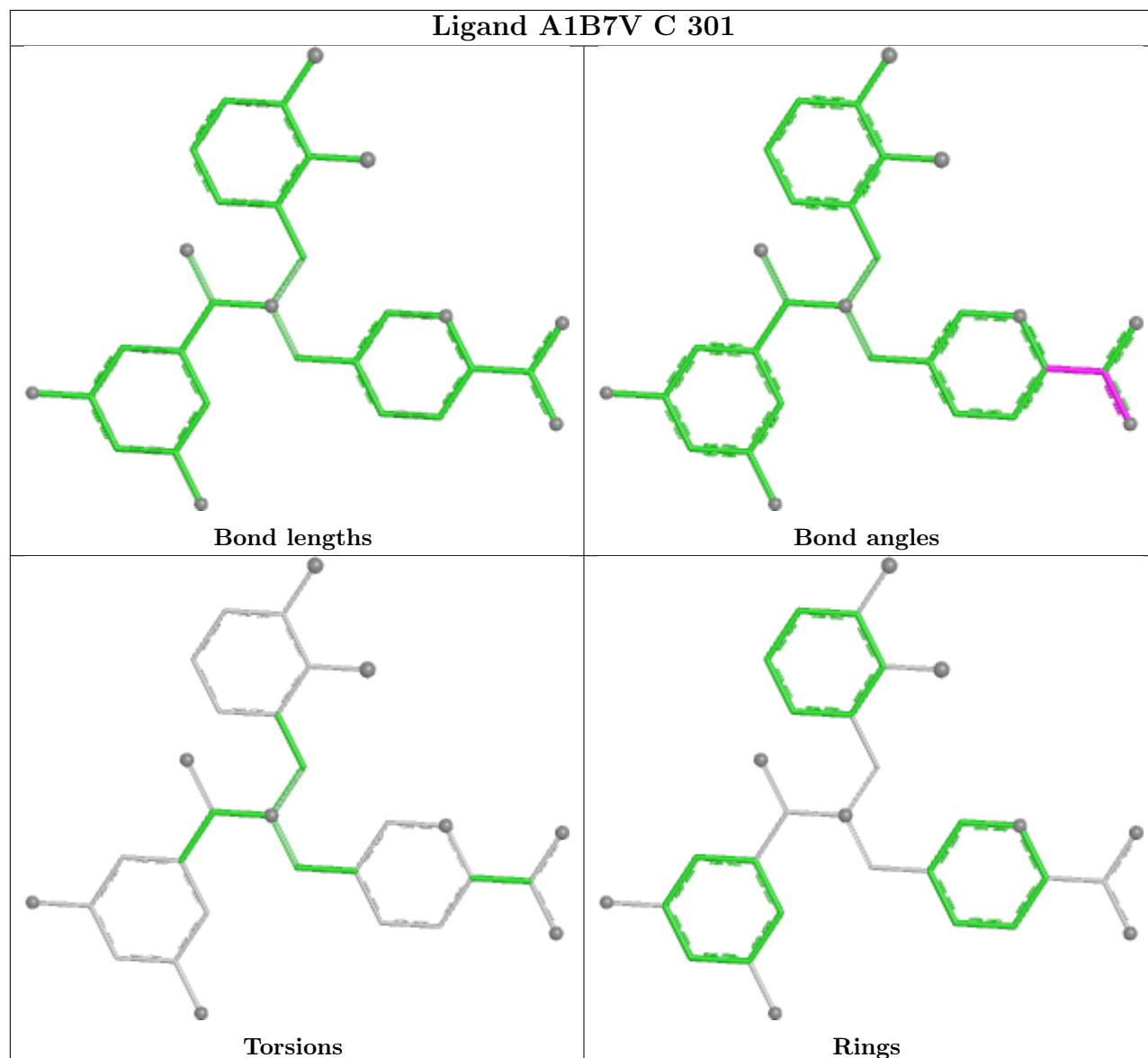
There are no ring outliers.

4 monomers are involved in 8 short contacts:

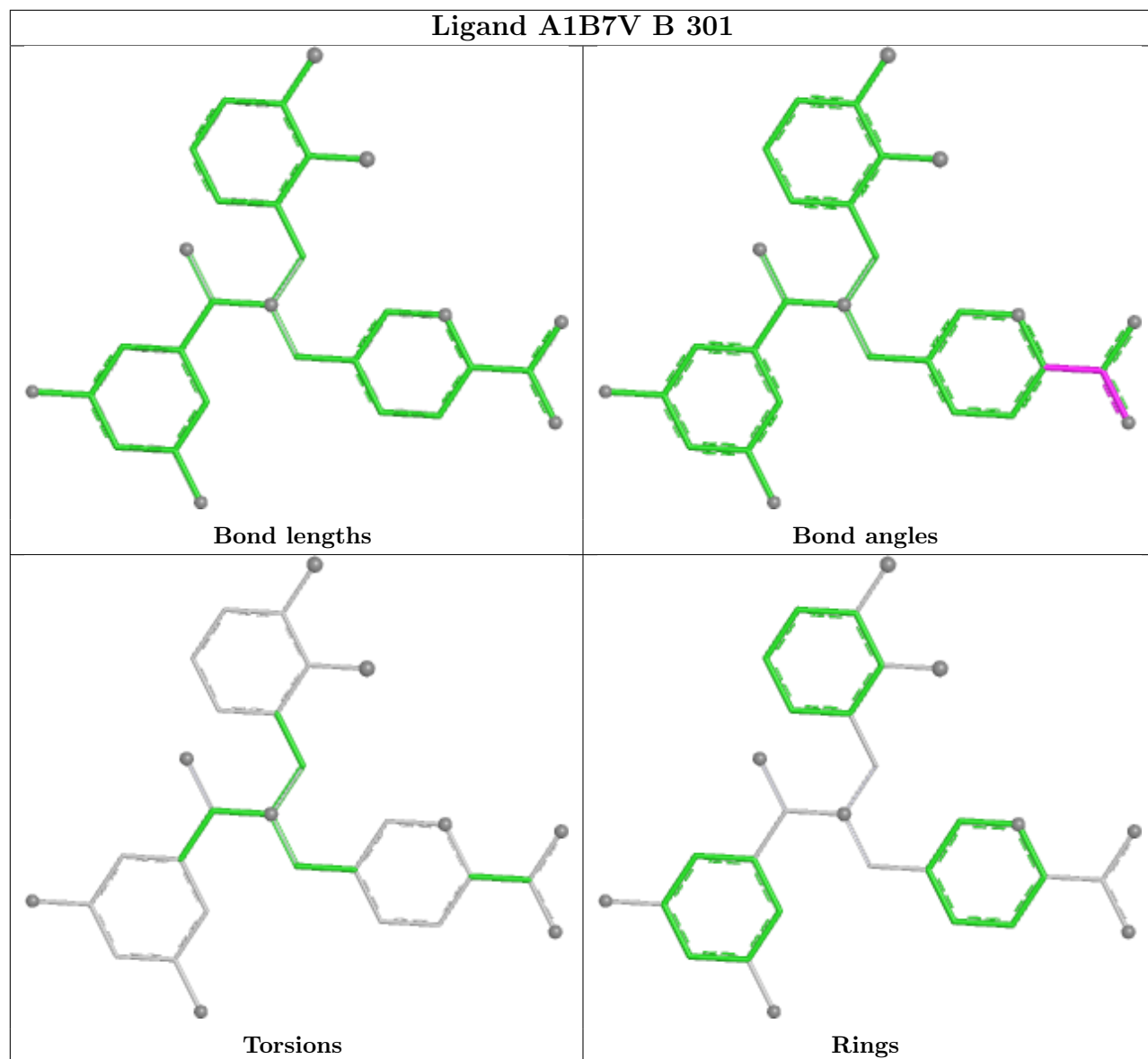
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	304	EDO	4	0
4	C	305	EDO	2	0
4	B	303	EDO	1	0
4	C	303	EDO	1	0

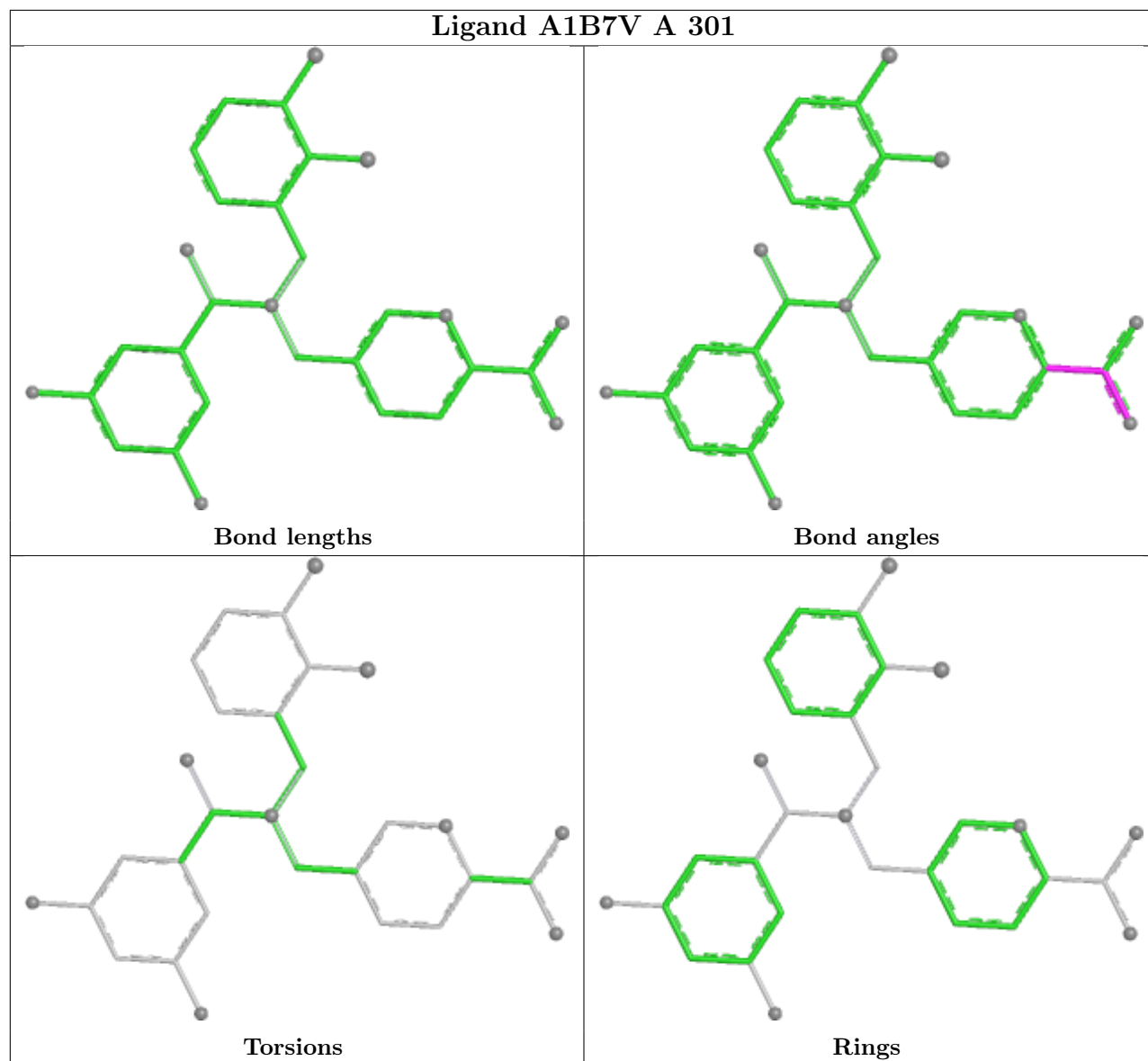
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



## Ligand A1B7V B 301





## 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	214/234 (91%)	0.07	13 (6%)	28 27	5, 15, 42, 61	9 (4%)
1	B	211/234 (90%)	0.15	20 (9%)	15 13	5, 15, 40, 52	12 (5%)
1	C	215/234 (91%)	0.24	18 (8%)	18 17	5, 16, 41, 56	10 (4%)
All	All	640/702 (91%)	0.15	51 (7%)	20 19	5, 16, 41, 61	31 (4%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	47	PRO	5.8
1	C	236	THR	5.5
1	A	235	VAL	5.4
1	A	54	PRO	5.3
1	B	6	LEU	4.9
1	B	235	VAL	4.6
1	A	51	GLN	4.6
1	C	165	ALA	4.4
1	A	50	SER	4.3
1	B	210	TRP	4.1
1	C	7	PRO	4.0
1	C	147	LEU	3.8
1	C	56	THR	3.6
1	C	235	VAL	3.6
1	C	174	ARG	3.6
1	A	49	THR	3.4
1	B	193	ASP	3.4
1	C	6	LEU	3.3
1	A	147	LEU	3.2
1	B	46	SER	3.2
1	C	8	HIS	3.1
1	B	194	SER	2.9
1	A	148	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	193	ASP	2.8
1	B	7	PRO	2.8
1	B	144	THR	2.8
1	B	8	HIS	2.7
1	B	56	THR	2.7
1	B	44	LEU	2.6
1	A	162	LEU	2.6
1	C	177	TYR	2.5
1	C	193	ASP	2.5
1	C	47	PRO	2.5
1	B	195	HIS	2.4
1	A	56	THR	2.4
1	C	148	ASP	2.4
1	C	210	TRP	2.4
1	C	190	SER	2.4
1	B	42	CYS	2.3
1	C	161	ALA	2.3
1	B	148[A]	ASP	2.3
1	A	177	TYR	2.3
1	B	164	ARG	2.2
1	A	55	PRO	2.2
1	C	143	LEU	2.2
1	C	149	GLY	2.1
1	B	190	SER	2.1
1	B	109	LEU	2.1
1	B	159	LEU	2.1
1	A	144	THR	2.0
1	B	147	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,

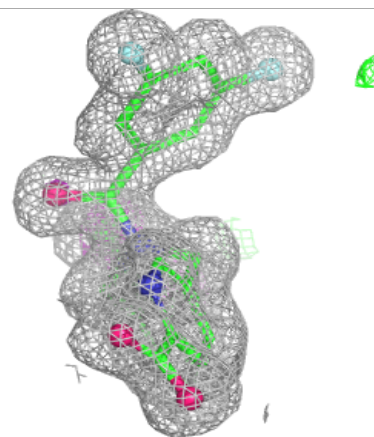
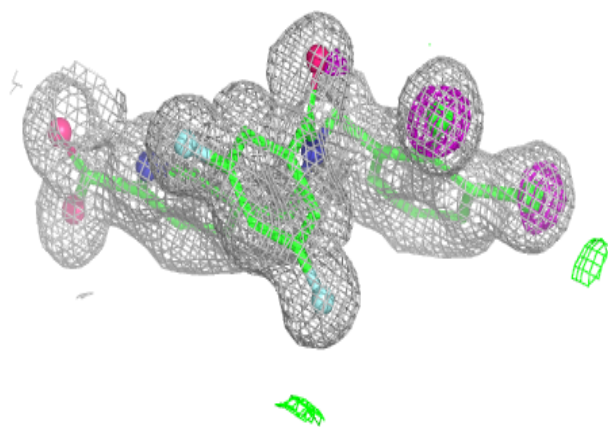
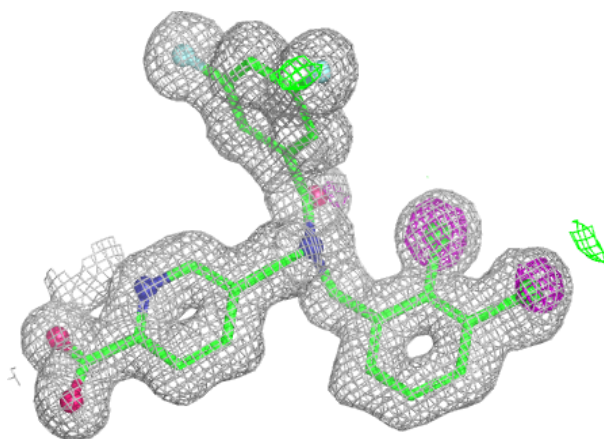
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	EDO	C	303	4/4	0.84	0.15	31,35,36,37	0
4	EDO	C	304	4/4	0.90	0.12	26,30,32,33	0
4	EDO	B	303	4/4	0.95	0.09	24,25,26,26	0
4	EDO	A	303	4/4	0.96	0.09	24,25,26,26	0
4	EDO	C	305	4/4	0.96	0.08	24,25,25,25	0
2	A1B7V	C	301	30/30	0.98	0.05	10,12,15,16	0
2	A1B7V	B	301	30/30	0.98	0.05	9,11,13,15	0
5	UNX	A	306	1/1	0.98	0.46	0,0,0,0	0
5	UNX	A	308	1/1	0.98	0.43	0,0,0,0	0
5	UNX	A	305	1/1	0.99	0.47	1,1,1,1	0
2	A1B7V	A	301	30/30	0.99	0.04	10,12,13,15	0
5	UNX	A	307	1/1	0.99	0.26	13,13,13,13	0
5	UNX	A	304	1/1	0.99	0.45	1,1,1,1	0
5	UNX	B	304	1/1	0.99	0.45	1,1,1,1	0
5	UNX	B	305	1/1	0.99	0.40	0,0,0,0	0
5	UNX	B	306	1/1	0.99	0.23	13,13,13,13	0
5	UNX	C	306	1/1	0.99	0.24	20,20,20,20	0
3	MG	C	302	1/1	1.00	0.01	12,12,12,12	0
3	MG	A	302	1/1	1.00	0.01	12,12,12,12	0
3	MG	B	302	1/1	1.00	0.01	11,11,11,11	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.

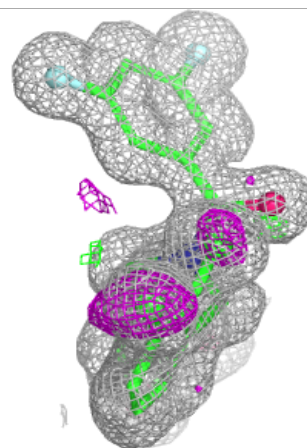
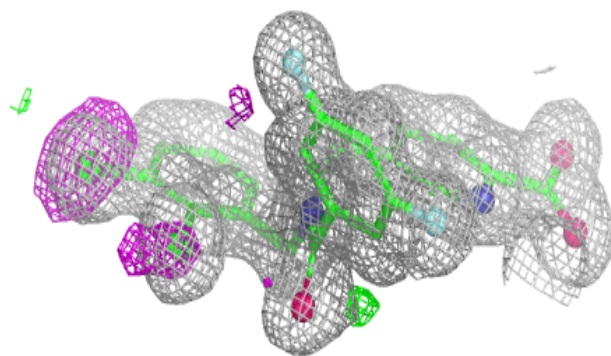
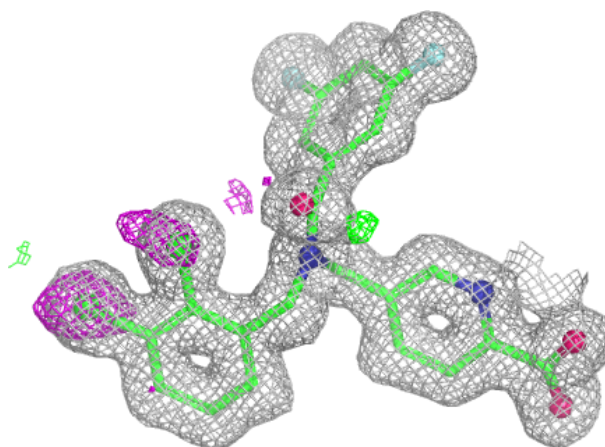
**Electron density around A1B7V C 301:**

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



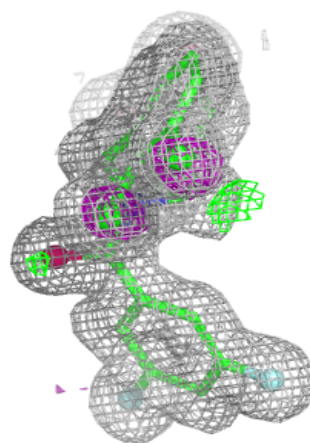
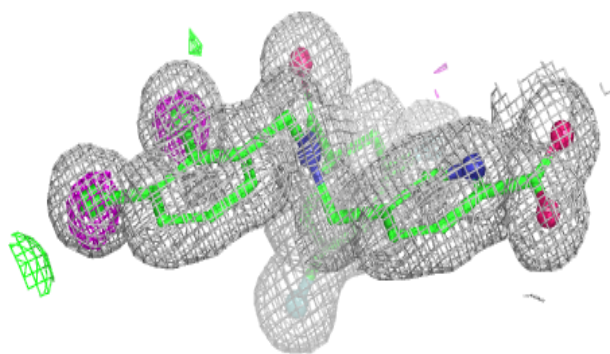
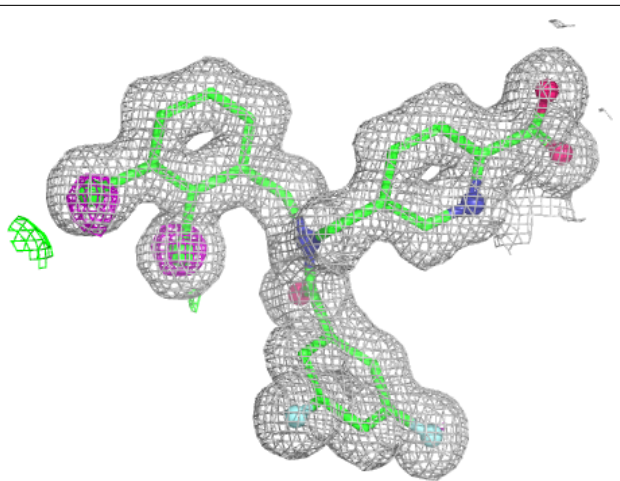
**Electron density around A1B7V B 301:**

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



**Electron density around A1B7V 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.