



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:46 am BST

PDB ID : 3L2U  
Title : Crystal structure of the Prototype Foamy Virus (PFV) intasome in complex with magnesium and GS9137 (Elvitegravir)  
Authors : Hare, S.; Gupta, S.S.; Cherepanov, P.  
Deposited on : 2009-12-15  
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

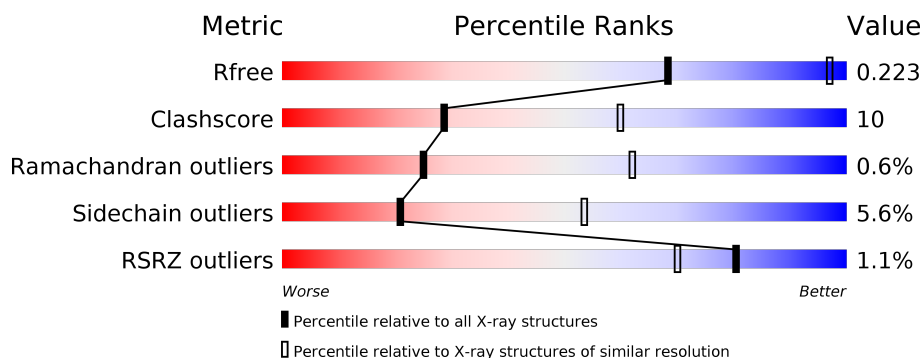
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	395	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 72%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>72%</span> <span>18%</span> <span>8%</span> </div> </div>
1	B	395	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 7%, green 34%, grey 59%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>34%</span> <span>7%</span> <span>59%</span> </div> </div>
2	C	19	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 37%, yellow 53%, orange 11%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>37%</span> <span>53%</span> <span>11%</span> </div> </div>
3	D	17	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 41%, yellow 53%, orange 6%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>41%</span> <span>53%</span> <span>6%</span> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NH4	A	396	-	-	-	X
7	ELV	A	397	-	-	X	-
8	GOL	A	802	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4944 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 Integrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2886	1852	506	524	4			
1	B	163	Total	C	N	O	S	0	0	0
			1266	830	203	232	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P14350
A	-1	PRO	-	EXPRESSION TAG	UNP P14350
A	0	GLY	-	EXPRESSION TAG	UNP P14350
A	217	SER	GLY	VARIANT	UNP P14350
A	218	GLY	SER	VARIANT	UNP P14350
B	-2	GLY	-	EXPRESSION TAG	UNP P14350
B	-1	PRO	-	EXPRESSION TAG	UNP P14350
B	0	GLY	-	EXPRESSION TAG	UNP P14350
B	217	SER	GLY	VARIANT	UNP P14350
B	218	GLY	SER	VARIANT	UNP P14350

- Molecule 2 is a DNA chain called 5'-D(\*AP\*TP\*TP\*GP\*TP\*CP\*AP\*TP\*GP\*GP\*AP\*A P\*TP\*TP\*TP\*TP\*GP\*TP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	19	Total	C	N	O	P	0	0	0
			389	189	66	116	18			

- Molecule 3 is a DNA chain called 5'-D(\*TP\*AP\*CP\*AP\*AP\*AP\*AP\*TP\*TP\*CP\*CP\*AP \*TP\*GP\*AP\*CP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	17	Total	C	N	O	P	0	0	0
			343	166	65	96	16			

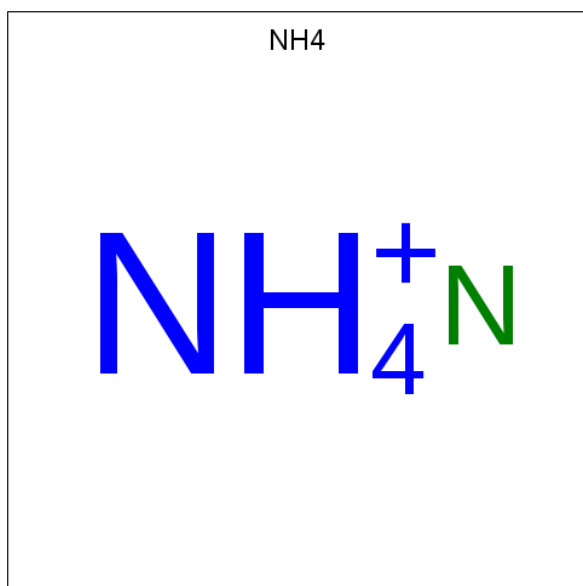
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

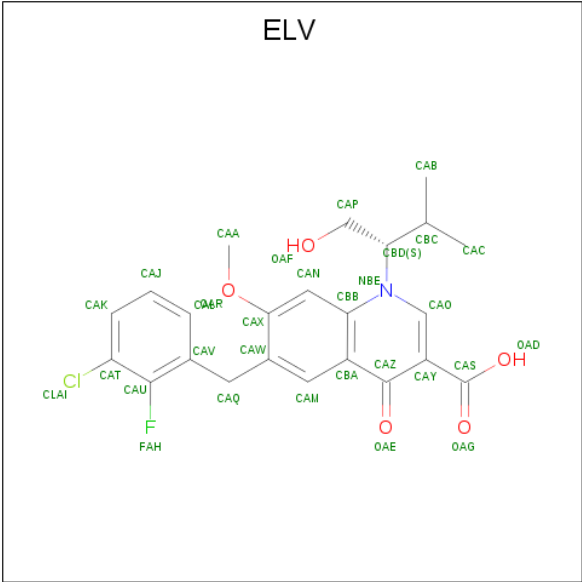
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is AMMONIUM ION (three-letter code: NH4) (formula: H<sub>4</sub>N).



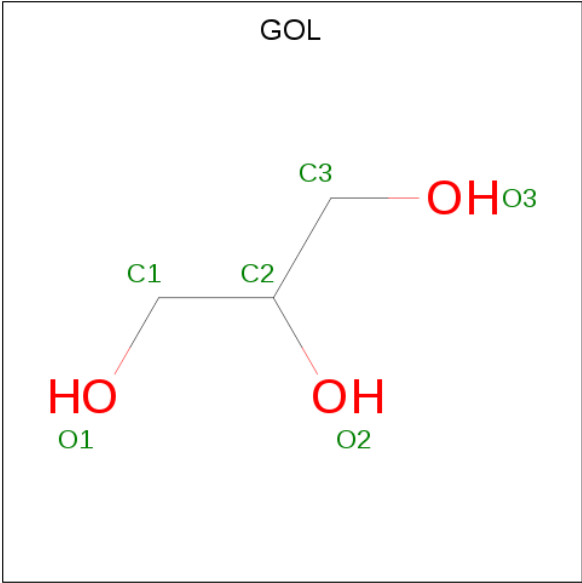
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	N	0	0
			1	1		

- Molecule 7 is 6-(3-chloro-2-fluorobenzyl)-1-[(1S)-1-(hydroxymethyl)-2-methylpropyl]-7-methoxy-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (three-letter code: ELV) (formula: C<sub>23</sub>H<sub>23</sub>ClFNO<sub>5</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	Cl	F	N	O	0	0
			31	23	1	1	1	5		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		
8	A	1	Total	C	O	0	0
			6	3	3		

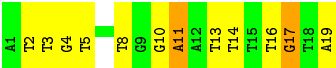
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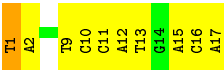
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			6	3	3		







● Molecule 3: 5'-D(\*TP\*AP\*CP\*AP\*AP\*AP\*AP\*TP\*TP\*CP\*CP\*AP\*TP\*GP\*AP\*CP\*A)-3',



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.10Å 157.10Å 124.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.44 – 3.15 36.44 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (36.44-3.15) 99.1 (36.44-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.193 , 0.218 0.200 , 0.223	Depositor DCC
$R_{free}$ test set	1391 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	114.3	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 66.0	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	0.95	EDS
Total number of atoms	4944	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, ELV, MG, NH4

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	0/2965	0.67	0/4051
1	B	0.53	0/1306	0.59	0/1792
2	C	1.01	0/435	1.81	11/671 (1.6%)
3	D	1.15	0/385	1.79	9/591 (1.5%)
All	All	0.65	0/5091	0.96	20/7105 (0.3%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2	DT	P-O3'-C3'	9.24	130.78	119.70
2	C	3	DT	O4'-C1'-N1	8.11	113.68	108.00
2	C	2	DT	C4-C5-C7	8.00	123.80	119.00
2	C	11	DA	P-O3'-C3'	7.02	128.12	119.70
2	C	14	DT	N3-C4-O4	6.41	123.75	119.90
2	C	2	DT	C6-C5-C7	-6.17	119.20	122.90
3	D	1	DT	O4'-C1'-N1	6.02	112.21	108.00
3	D	11	DC	O4'-C1'-N1	5.91	112.13	108.00
3	D	15	DA	O3'-P-O5'	-5.83	92.93	104.00
3	D	13	DT	O4'-C1'-N1	-5.81	103.93	108.00
2	C	14	DT	C5-C4-O4	-5.74	120.88	124.90
2	C	17	DG	O4'-C1'-N9	-5.42	104.20	108.00
2	C	2	DT	O4'-C1'-N1	-5.39	104.22	108.00
3	D	1	DT	C4-C5-C7	5.34	122.20	119.00
3	D	12	DA	O4'-C1'-N9	-5.26	104.32	108.00
2	C	13	DT	C5-C4-O4	-5.25	121.22	124.90
3	D	12	DA	N1-C6-N6	5.24	121.74	118.60
3	D	1	DT	P-O3'-C3'	5.10	125.82	119.70
2	C	8	DT	C5-C4-O4	-5.01	121.40	124.90
3	D	10	DC	O4'-C1'-N1	-5.00	104.50	108.00

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	2886	0	2905	58	0
1	B	1266	0	1244	20	0
2	C	389	0	220	6	0
3	D	343	0	193	6	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	31	0	22	15	0
8	A	24	0	32	3	0
All	All	4944	0	4616	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (93) 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)
7:A:397:ELV:CAL	7:A:397:ELV:HAM	1.63	1.17
7:A:397:ELV:HAL	7:A:397:ELV:HAM	1.10	1.07
7:A:397:ELV:HAJ	3:D:16:DC:H2'	1.47	0.97
7:A:397:ELV:CAL	7:A:397:ELV:CAM	2.34	0.94
7:A:397:ELV:CAJ	3:D:16:DC:H2'	1.98	0.94
1:A:357:HIS:HA	1:A:358:LEU:HB2	1.52	0.90
7:A:397:ELV:HAL	7:A:397:ELV:CAM	1.95	0.86
7:A:397:ELV:HAQA	7:A:397:ELV:HAAA	1.57	0.86
1:A:86:ARG:HH11	1:A:86:ARG:HG3	1.46	0.79
1:A:86:ARG:HH11	1:A:86:ARG:CG	1.99	0.76
1:A:126:PHE:CB	1:A:220:VAL:HG23	2.17	0.74
1:A:210:THR:HG21	1:A:365:SER:N	2.03	0.74
1:A:46:LYS:HE2	1:A:77:ALA:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:THR:HG21	1:A:365:SER:H	1.57	0.69
1:A:126:PHE:HB3	1:A:220:VAL:HG23	1.75	0.68
1:B:238:ARG:NH1	1:B:245:LEU:HD11	2.09	0.67
1:A:26:LYS:O	1:A:27:GLN:HB3	1.95	0.66
1:A:210:THR:HG23	1:A:211:PRO:HD2	1.76	0.66
1:A:126:PHE:HB2	1:A:220:VAL:HG23	1.81	0.62
1:A:230:LEU:HD23	1:A:249:VAL:HG13	1.82	0.61
1:A:162:SER:HB2	8:A:804:GOL:H2	1.83	0.60
1:B:234:LEU:HD23	1:B:234:LEU:C	2.21	0.60
1:A:292:LEU:HD22	1:B:271:GLY:HA3	1.83	0.60
1:A:341:SER:HB2	1:A:355:LEU:O	2.01	0.60
1:A:101:ILE:HD12	1:A:335:PRO:HG2	1.84	0.59
1:A:339:LYS:HG2	8:A:803:GOL:H31	1.86	0.57
1:A:339:LYS:NZ	1:A:358:LEU:HD13	2.19	0.57
7:A:397:ELV:HABA	7:A:397:ELV:HAN	1.87	0.56
1:A:137:GLN:H	8:A:801:GOL:H2	1.70	0.56
1:A:210:THR:HG23	1:A:364:VAL:HA	1.86	0.56
7:A:397:ELV:HAQA	7:A:397:ELV:CAA	2.34	0.56
1:B:139:TYR:CD1	1:B:157:PRO:HB2	2.42	0.55
7:A:397:ELV:HABA	7:A:397:ELV:CAN	2.36	0.55
2:C:10:DG:H2"	2:C:11:DA:C8	2.42	0.55
1:A:86:ARG:HG3	1:A:86:ARG:NH1	2.17	0.54
1:B:212:TYR:O	1:B:214:PRO:HD3	2.07	0.54
2:C:10:DG:H2"	2:C:11:DA:H8	1.73	0.54
1:A:73:LEU:HD22	1:A:86:ARG:CZ	2.39	0.53
1:A:337:TRP:CD2	1:A:370:LYS:HD3	2.44	0.52
1:A:108:ALA:O	1:A:314:SER:HA	2.10	0.51
1:A:212:TYR:HA	7:A:397:ELV:HACA	1.92	0.51
1:A:272:ILE:HD12	1:A:291:GLU:OE2	2.12	0.50
1:A:262:LYS:NZ	3:D:9:DT:OP2	2.39	0.50
1:A:26:LYS:O	1:A:27:GLN:CB	2.59	0.50
1:B:127:ILE:HA	1:B:144:VAL:O	2.12	0.50
3:D:16:DC:C5'	3:D:17:DA:OP2	2.60	0.49
7:A:397:ELV:CAB	7:A:397:ELV:HAN	2.42	0.48
7:A:397:ELV:HAAA	7:A:397:ELV:CAQ	2.36	0.48
3:D:1:DT:H2"	3:D:2:DA:OP2	2.13	0.48
1:A:186:GLN:HE22	1:A:211:PRO:HD3	1.78	0.48
7:A:397:ELV:HAN	7:A:397:ELV:HAPA	1.96	0.48
1:A:357:HIS:CD2	1:A:357:HIS:H	2.31	0.48
1:A:73:LEU:HD13	1:A:86:ARG:HG2	1.95	0.47
2:C:16:DT:H2"	2:C:17:DG:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:PHE:O	1:A:179:PRO:HA	2.14	0.47
1:B:234:LEU:HD23	1:B:235:LEU:N	2.29	0.47
1:A:274:SER:HB2	1:B:178:ILE:H	1.79	0.46
1:A:112:ILE:HA	1:A:350:ARG:CD	2.46	0.46
1:A:356:ASP:O	1:A:358:LEU:HA	2.16	0.45
1:A:337:TRP:CE2	1:A:370:LYS:HD3	2.52	0.45
1:A:178:ILE:HD12	1:B:276:THR:HG21	1.97	0.45
1:A:358:LEU:HA	1:A:359:GLY:HA2	1.57	0.45
1:A:209:SER:HB3	1:A:216:SER:HB2	1.99	0.44
1:B:234:LEU:HD21	1:B:242:TRP:HB3	2.00	0.44
1:B:211:PRO:O	1:B:212:TYR:HB2	2.18	0.44
1:B:238:ARG:HH12	1:B:245:LEU:HD11	1.81	0.44
1:A:155:LEU:HD13	1:A:246:LEU:HD22	2.00	0.44
1:A:210:THR:CG2	1:A:211:PRO:HD2	2.46	0.44
1:A:16:LEU:HD21	1:A:32:LEU:HB2	1.99	0.44
1:A:223:LYS:HB2	1:A:223:LYS:HE2	1.84	0.43
1:B:124:LYS:HA	1:B:181:VAL:O	2.19	0.43
1:A:261:LEU:O	1:A:262:LYS:HB2	2.18	0.43
1:A:112:ILE:O	1:A:307:THR:HB	2.19	0.43
1:A:214:PRO:HG3	7:A:397:ELV:HACB	2.01	0.43
1:A:357:HIS:HA	1:A:358:LEU:CB	2.28	0.42
1:A:141:TYR:CE2	1:A:161:PRO:HD3	2.54	0.42
1:A:127:ILE:HG22	1:A:145:VAL:HG13	2.02	0.42
1:B:158:THR:HB	1:B:165:ALA:HB1	2.02	0.42
1:A:180:LYS:HE3	1:B:275:ASN:OD1	2.19	0.42
1:B:183:HIS:HA	1:B:207:GLU:O	2.19	0.42
1:A:148:GLY:O	1:A:219:LYS:HE2	2.20	0.42
1:B:125:PHE:CD2	1:B:179:PRO:HG3	2.55	0.42
1:A:183:HIS:ND1	1:A:207:GLU:HG2	2.35	0.41
1:B:237:GLY:C	1:B:238:ARG:HG3	2.40	0.41
2:C:19:DA:H2	3:D:1:DT:H3	1.67	0.41
1:B:246:LEU:N	1:B:247:PRO:HD2	2.35	0.41
1:A:350:ARG:HE	2:C:4:DG:P	2.43	0.41
1:A:126:PHE:CB	1:A:220:VAL:CG2	2.95	0.41
2:C:4:DG:H2"	2:C:5:DT:O5'	2.21	0.41
1:A:292:LEU:HD22	1:B:271:GLY:CA	2.49	0.41
1:A:324:GLN:HG2	1:A:340:PRO:HA	2.03	0.41
1:A:86:ARG:CG	1:A:86:ARG:NH1	2.68	0.40
1:A:333:LEU:HA	1:A:333:LEU:HD23	1.89	0.40

There are no symmetry-related clashes.

## 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	363/395 (92%)	344 (95%)	17 (5%)	2 (1%)	25	62
1	B	161/395 (41%)	151 (94%)	9 (6%)	1 (1%)	25	62
All	All	524/790 (66%)	495 (94%)	26 (5%)	3 (1%)	25	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	328	ALA
1	B	212	TYR

### 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	322/354 (91%)	301 (94%)	21 (6%)	17	48
1	B	139/354 (39%)	134 (96%)	5 (4%)	35	67
All	All	461/708 (65%)	435 (94%)	26 (6%)	21	53

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	16	LEU
1	A	29	THR

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Mol	Chain	Res	Type
1	A	86	ARG
1	A	107	LYS
1	A	149	MET
1	A	169	SER
1	A	191	THR
1	A	207	GLU
1	A	251	LEU
1	A	260	VAL
1	A	262	LYS
1	A	297	GLU
1	A	307	THR
1	A	312	SER
1	A	316	SER
1	A	323	VAL
1	A	336	ARG
1	A	342	THR
1	A	358	LEU
1	A	374	HIS
1	B	230	LEU
1	B	234	LEU
1	B	238	ARG
1	B	260	VAL
1	B	274	SER

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

Mol	Chain	Res	Type
1	A	19	HIS
1	A	186	GLN
1	A	255	ASN
1	A	357	HIS

### 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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic and 1 is modelled with single atom - leaving 5 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
8	GOL	A	803	-	5,5,5	0.39	0	5,5,5	0.26	0
8	GOL	A	802	-	5,5,5	0.42	0	5,5,5	0.32	0
8	GOL	A	801	-	5,5,5	0.44	0	5,5,5	0.26	0
7	ELV	A	397	5	27,33,33	2.12	5 (18%)	33,48,48	5.48	16 (48%)
8	GOL	A	804	-	5,5,5	0.41	0	5,5,5	0.24	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	GOL	A	803	-	-	1/4/4/4	-
8	GOL	A	802	-	-	1/4/4/4	-
8	GOL	A	801	-	-	4/4/4/4	-
7	ELV	A	397	5	-	2/14/20/20	0/3/3/3
8	GOL	A	804	-	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	397	ELV	CAY-CAS	7.10	1.54	1.47
7	A	397	ELV	CAT-CAU	4.78	1.42	1.38
7	A	397	ELV	CBB-NBE	3.63	1.44	1.40
7	A	397	ELV	CAN-CAX	3.16	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	397	ELV	OAR-CAX	2.28	1.40	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	397	ELV	CAU-CAT-CLAI	23.94	128.70	119.50
7	A	397	ELV	CAK-CAT-CAU	10.76	125.21	119.29
7	A	397	ELV	CAQ-CAV-CAU	7.02	133.77	121.00
7	A	397	ELV	CAQ-CAV-CAL	-6.80	109.29	120.46
7	A	397	ELV	CAN-CAX-CAW	-6.61	118.39	121.23
7	A	397	ELV	CAK-CAT-CLAI	-6.14	106.09	118.41
7	A	397	ELV	CAW-CAQ-CAV	-4.73	99.61	112.67
7	A	397	ELV	CAZ-CBA-CBB	4.30	122.33	118.59
7	A	397	ELV	CAQ-CAW-CAM	-3.88	117.29	122.08
7	A	397	ELV	FAH-CAU-CAV	3.10	121.12	117.85
7	A	397	ELV	CAN-CBB-NBE	2.82	123.60	121.08
7	A	397	ELV	OAR-CAX-CAW	2.54	119.51	115.97
7	A	397	ELV	OAR-CAX-CAN	-2.43	122.10	125.24
7	A	397	ELV	CAQ-CAW-CAX	2.42	124.15	121.21
7	A	397	ELV	CAX-CAN-CBB	2.38	122.75	117.90
7	A	397	ELV	CAJ-CAL-CAV	2.22	124.22	120.89

There are no chirality outliers.

All (12) torsion outliers are listed below:

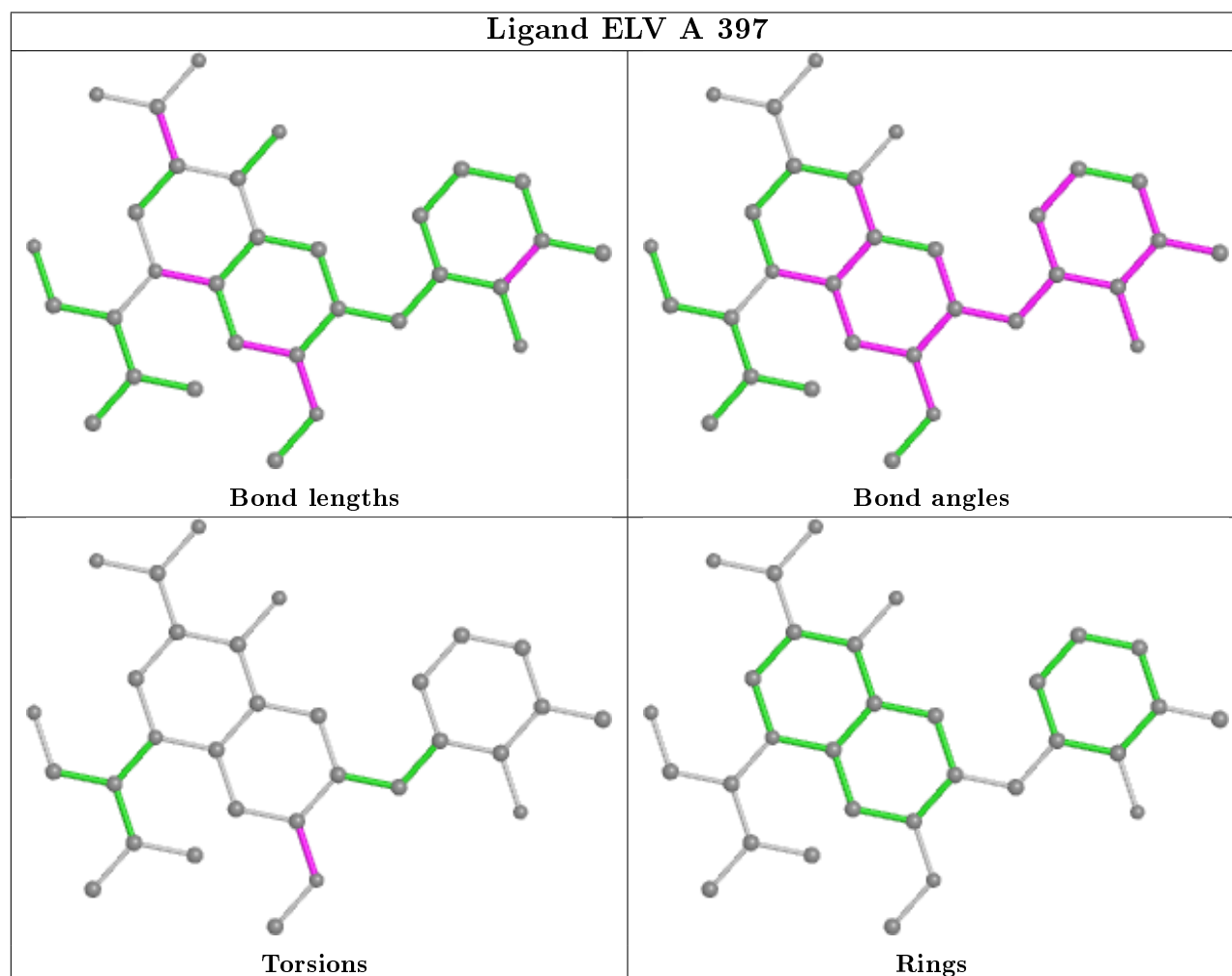
Mol	Chain	Res	Type	Atoms
8	A	804	GOL	O1-C1-C2-C3
8	A	804	GOL	C1-C2-C3-O3
8	A	801	GOL	O1-C1-C2-O2
8	A	801	GOL	O1-C1-C2-C3
7	A	397	ELV	CAW-CAX-OAR-CAA
7	A	397	ELV	CAN-CAX-OAR-CAA
8	A	803	GOL	O1-C1-C2-C3
8	A	801	GOL	C1-C2-C3-O3
8	A	804	GOL	O1-C1-C2-O2
8	A	804	GOL	O2-C2-C3-O3
8	A	801	GOL	O2-C2-C3-O3
8	A	802	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	803	GOL	1	0
8	A	801	GOL	1	0
7	A	397	ELV	15	0
8	A	804	GOL	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.



## 5.7 Other polymers

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	365/395 (92%)	-0.05	3 (0%) 86 78	81, 98, 145, 169	0
1	B	163/395 (41%)	-0.19	3 (1%) 68 55	88, 107, 143, 160	0
2	C	19/19 (100%)	-0.30	0 100 100	78, 98, 127, 148	0
3	D	17/17 (100%)	-0.42	0 100 100	84, 91, 129, 160	0
All	All	564/826 (68%)	-0.11	6 (1%) 80 70	78, 101, 145, 169	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	278	PHE	3.3
1	A	153	THR	2.5
1	A	254	ASN	2.4
1	A	11	GLU	2.2
1	B	237	GLY	2.2
1	B	116	ASP	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

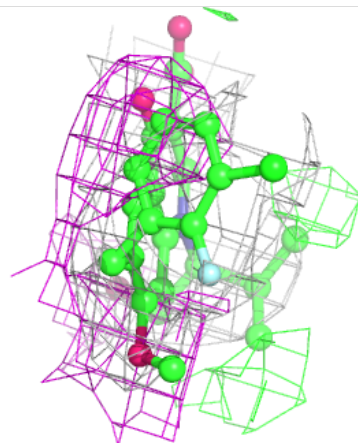
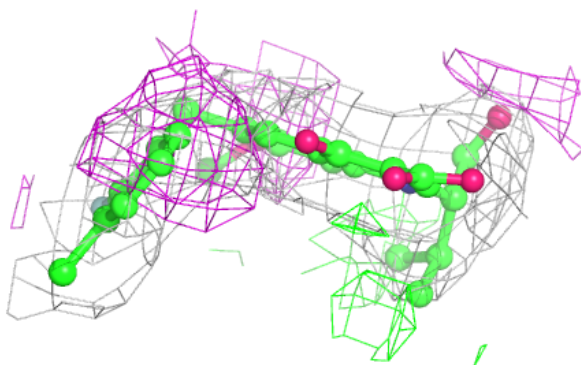
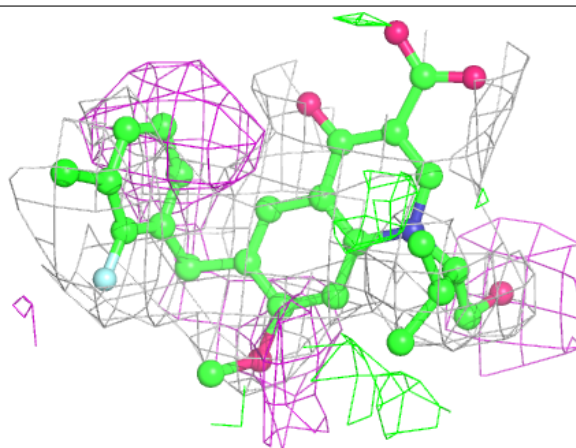
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	NH4	A	396	1/1	0.66	0.47	50,50,50,50	0
8	GOL	A	802	6/6	0.72	0.56	115,116,116,117	0
8	GOL	A	804	6/6	0.88	0.32	129,130,131,131	0
5	MG	B	393	1/1	0.90	0.21	123,123,123,123	0
8	GOL	A	801	6/6	0.92	0.24	119,121,122,122	0
7	ELV	A	397	31/31	0.93	0.20	69,75,80,88	0
8	GOL	A	803	6/6	0.94	0.12	107,112,113,114	0
5	MG	A	394	1/1	0.98	0.20	70,70,70,70	0
4	ZN	A	393	1/1	0.99	0.14	91,91,91,91	0
5	MG	A	395	1/1	0.99	0.16	79,79,79,79	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 ELV A 397:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.