



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:52 am BST

PDB ID : 3L2V
Title : Crystal structure of the Prototype Foamy Virus (PFV) intasome in complex with manganese and MK0518 (Raltegravir)
Authors : Hare, S.; Gupta, S.S.; Cherepanov, P.
Deposited on : 2009-12-15
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

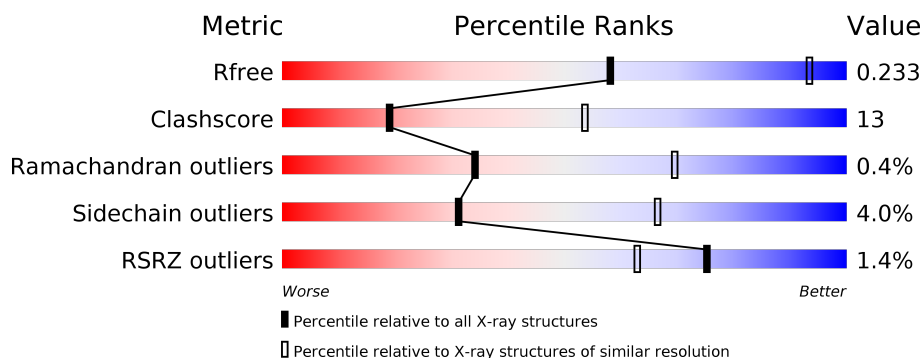
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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>2%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>8%</div> </div> </div>
1	B	395	<div> <div>34%</div> <div>7%</div> <div>59%</div> </div>
2	C	19	<div> <div>5%</div> <div> <div></div> <div>37%</div> <div>26%</div> <div>37%</div> </div> </div>
3	D	17	<div> <div>35%</div> <div>47%</div> <div>18%</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
8	GOL	A	801	-	-	X	-
8	GOL	A	802	-	-	X	-
8	GOL	A	804	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4919 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
			2878	1846	504	524	4			
1	B	163	Total	C	N	O	S	0	0	0
			1248	820	198	229	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			

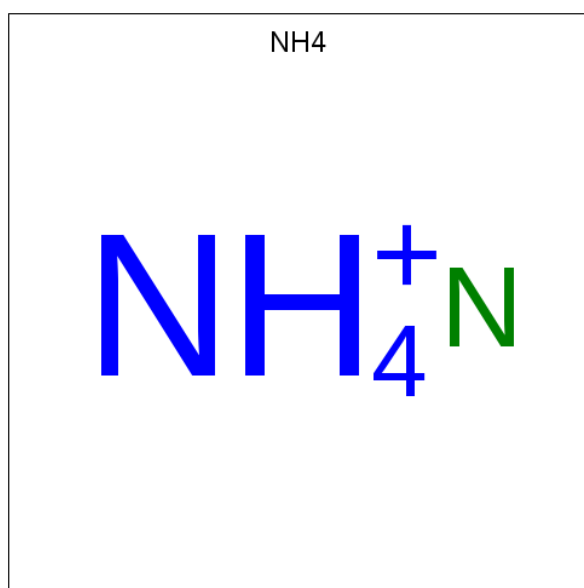
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

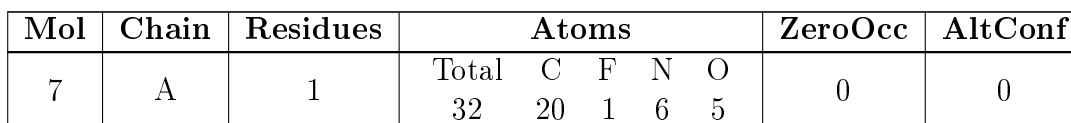
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mn	0	0
			1	1		
5	A	2	Total	Mn	0	0
			2	2		

- Molecule 6 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



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

- Molecule 7 is N-(4-fluorobenzyl)-5-hydroxy-1-methyl-2-(1-methyl-1-[(5-methyl-1,3,4-oxadiazol-2-yl)carbonyl]amino}ethyl)-6-oxo-1,6-dihydropyrimidine-4-carboxamide (three-letter code: RLT) (formula: C₂₀H₂₁FN₆O₅).



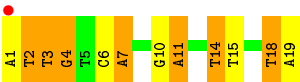
- GOL
-
- The diagram shows the skeletal structure of 1,2,3-propanetriol (glycerol). It consists of a three-carbon chain. The first carbon (left) is bonded to a hydroxyl group (HO) labeled O1. The second carbon (middle) is bonded to a hydroxyl group (OH) labeled O2. The third carbon (right) is bonded to a hydroxyl group (OH) labeled O3. The carbons are labeled C1, C2, and C3 in green. The hydroxyl groups are shown in red.

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



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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, α , β , γ	158.65Å 158.65Å 125.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.48 – 3.20 38.48 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (38.48-3.20) 99.5 (38.48-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.18Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.232 0.207 , 0.233	Depositor DCC
R_{free} test set	1356 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	111.6	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4919	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, ZN, MN, NH4, RLT

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	0.47	0/2957	0.64	0/4043
1	B	0.46	0/1288	0.57	0/1771
2	C	0.93	0/435	1.67	8/671 (1.2%)
3	D	0.96	0/385	1.90	14/591 (2.4%)
All	All	0.57	0/5065	0.94	22/7076 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1	DT	O4'-C1'-N1	14.19	117.94	108.00
3	D	11	DC	O4'-C1'-N1	8.66	114.06	108.00
2	C	3	DT	O4'-C1'-N1	8.08	113.66	108.00
2	C	2	DT	P-O3'-C3'	7.21	128.35	119.70
3	D	12	DA	O4'-C1'-N9	-6.85	103.21	108.00
2	C	18	DT	C1'-O4'-C4'	-6.61	103.50	110.10
3	D	5	DA	O4'-C1'-N9	6.54	112.58	108.00
3	D	8	DT	N3-C4-O4	6.39	123.73	119.90
2	C	18	DT	O4'-C4'-C3'	-6.29	101.98	104.50
3	D	13	DT	O4'-C1'-N1	-6.23	103.64	108.00
3	D	1	DT	O4'-C1'-C2'	-6.07	101.05	105.90
3	D	10	DC	O4'-C1'-N1	-6.05	103.77	108.00
2	C	4	DG	O4'-C1'-N9	5.69	111.98	108.00
3	D	5	DA	C3'-C2'-C1'	-5.57	95.82	102.50
3	D	7	DA	P-O3'-C3'	5.52	126.32	119.70
2	C	11	DA	P-O3'-C3'	5.36	126.13	119.70
3	D	1	DT	P-O3'-C3'	5.35	126.12	119.70
3	D	2	DA	O4'-C1'-N9	-5.31	104.28	108.00
3	D	4	DA	P-O3'-C3'	5.30	126.06	119.70
2	C	7	DA	O4'-C1'-N9	-5.25	104.32	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	14	DT	P-O3'-C3'	5.19	125.93	119.70
3	D	12	DA	P-O3'-C3'	5.18	125.92	119.70

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	2878	0	2883	86	0
1	B	1248	0	1212	27	0
2	C	389	0	220	14	0
3	D	343	0	193	7	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	32	0	20	5	0
8	A	24	0	32	13	0
All	All	4919	0	4560	123	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 13.

All (123) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ILE:HD11	1:B:122:PHE:HD1	1.26	0.95
1:A:202:ARG:HH11	1:A:202:ARG:HG3	1.31	0.92
1:B:202:ARG:HH11	1:B:202:ARG:CG	1.83	0.90
1:A:126:PHE:HB3	1:A:220:VAL:CG2	2.04	0.86
1:A:272:ILE:HD11	1:B:122:PHE:CD1	2.11	0.86
1:A:350:ARG:HA	1:A:366:ILE:HD11	1.58	0.85
1:B:127:ILE:HG22	1:B:145:VAL:HG22	1.62	0.79
1:A:357:HIS:HA	1:A:358:LEU:HB2	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ARG:HH11	1:B:202:ARG:HG2	1.49	0.77
1:A:202:ARG:CG	1:A:202:ARG:HH11	1.98	0.77
7:A:397:RLT:CAV	7:A:397:RLT:HABB	2.16	0.75
1:A:126:PHE:HB3	1:A:220:VAL:HG22	1.69	0.75
1:A:350:ARG:HA	1:A:366:ILE:CD1	2.19	0.72
1:A:292:LEU:HD22	1:B:271:GLY:HA3	1.70	0.71
2:C:19:DA:C2	3:D:2:DA:C2	2.79	0.71
1:A:338:HIS:ND1	8:A:802:GOL:O1	2.23	0.68
2:C:19:DA:C2	3:D:2:DA:N1	2.62	0.68
1:A:339:LYS:H	8:A:802:GOL:H31	1.59	0.67
1:B:202:ARG:HH11	1:B:202:ARG:HG3	1.59	0.66
1:A:324:GLN:HG2	1:A:340:PRO:HA	1.77	0.66
1:B:202:ARG:NH1	1:B:202:ARG:CG	2.54	0.64
1:A:46:LYS:HE2	1:A:77:ALA:O	1.97	0.64
2:C:18:DT:H2"	2:C:19:DA:O5'	1.98	0.64
1:A:137:GLN:H	8:A:801:GOL:C1	2.10	0.64
1:A:111:PRO:HG3	1:A:310:ALA:HA	1.80	0.64
1:A:136:SER:HA	8:A:801:GOL:H2	1.80	0.64
1:A:241:LYS:CG	8:A:801:GOL:O3	2.45	0.64
1:A:357:HIS:HA	1:A:358:LEU:CB	2.29	0.63
1:A:339:LYS:CB	8:A:802:GOL:O3	2.48	0.62
1:A:126:PHE:CB	1:A:220:VAL:HG22	2.29	0.62
1:A:357:HIS:CD2	1:A:357:HIS:H	2.18	0.61
1:A:186:GLN:HB2	7:A:397:RLT:HAA	1.82	0.61
1:A:209:SER:CB	1:A:216:SER:HB2	2.30	0.61
1:A:67:THR:HB	1:A:71:ALA:HB3	1.84	0.60
1:A:86:ARG:O	1:A:90:VAL:HG23	2.02	0.59
1:A:241:LYS:HG3	8:A:801:GOL:O3	2.01	0.59
1:B:202:ARG:HG2	1:B:202:ARG:NH1	2.18	0.59
1:A:349:PRO:O	1:A:366:ILE:HD11	2.03	0.58
1:A:82:TRP:HB2	1:A:83:PRO:HD2	1.86	0.58
1:A:338:HIS:HD1	8:A:802:GOL:HO1	1.50	0.57
2:C:19:DA:C2	3:D:2:DA:C6	2.93	0.56
7:A:397:RLT:NAS	7:A:397:RLT:CAB	2.68	0.56
1:A:241:LYS:HG2	8:A:801:GOL:O3	2.06	0.55
1:B:231:LEU:O	1:B:235:LEU:HB2	2.07	0.54
1:A:272:ILE:HD12	1:A:273:ASP:O	2.08	0.53
1:A:54:ARG:HD3	1:A:82:TRP:CD2	2.44	0.53
1:A:209:SER:HB3	1:A:216:SER:HB2	1.90	0.52
1:A:202:ARG:CG	1:A:202:ARG:NH1	2.64	0.52
1:A:347:LEU:HB3	2:C:2:DT:O2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:OD2	1:A:116:ASP:N	2.43	0.52
1:A:230:LEU:HD23	1:A:249:VAL:HG13	1.91	0.52
1:A:163:THR:HB	8:A:803:GOL:H31	1.91	0.52
1:B:163:THR:HG23	1:B:195:PHE:HB2	1.91	0.51
1:B:121:PRO:O	1:B:122:PHE:HB2	2.10	0.51
7:A:397:RLT:NAS	7:A:397:RLT:HABB	2.25	0.51
1:A:132:PRO:HG3	1:A:141:TYR:OH	2.11	0.51
1:A:332:SER:O	1:A:333:LEU:HB2	2.11	0.51
1:A:180:LYS:HE3	1:B:275:ASN:OD1	2.11	0.50
1:A:26:LYS:O	1:A:27:GLN:HB3	2.11	0.50
1:A:250:GLN:NE2	1:B:175:SER:HB3	2.27	0.50
1:A:350:ARG:HE	2:C:4:DG:P	2.34	0.49
1:A:73:LEU:HD22	1:A:86:ARG:CZ	2.42	0.49
1:A:348:ASN:OD1	1:A:351:THR:N	2.46	0.48
2:C:18:DT:C4	2:C:19:DA:C6	3.01	0.48
1:A:120:LYS:HD2	1:B:272:ILE:HG21	1.95	0.48
3:D:5:DA:H2'	3:D:5:DA:OP2	2.14	0.48
1:A:108:ALA:O	1:A:314:SER:HA	2.14	0.47
3:D:1:DT:H1'	3:D:2:DA:O5'	2.13	0.47
1:A:272:ILE:HD12	1:A:273:ASP:C	2.35	0.47
1:B:261:LEU:HD13	1:B:268:LEU:HD11	1.96	0.47
1:A:234:LEU:HD23	1:A:234:LEU:HA	1.78	0.46
1:A:323:VAL:HG11	1:A:369:LEU:HD13	1.98	0.46
1:A:358:LEU:HA	1:A:359:GLY:HA2	1.67	0.46
1:A:82:TRP:HB2	1:A:83:PRO:CD	2.46	0.46
1:A:184:SER:HB2	1:A:190:PHE:CD2	2.51	0.46
1:A:164:SER:HB3	8:A:803:GOL:H32	1.97	0.46
2:C:18:DT:O4	2:C:19:DA:N6	2.49	0.46
1:A:26:LYS:O	1:A:27:GLN:CB	2.64	0.45
1:A:209:SER:HB3	1:A:216:SER:CB	2.46	0.45
2:C:6:DC:H1'	2:C:7:DA:N7	2.31	0.45
1:A:209:SER:HB2	1:A:216:SER:HB2	1.97	0.45
1:A:216:SER:C	1:A:218:GLY:H	2.19	0.45
1:A:157:PRO:HG3	1:A:246:LEU:HD12	1.98	0.45
1:A:112:ILE:HA	1:A:350:ARG:CD	2.47	0.44
2:C:14:DT:H2''	2:C:15:DT:OP2	2.17	0.44
1:A:339:LYS:H	8:A:802:GOL:C3	2.28	0.44
1:A:163:THR:HG23	1:A:195:PHE:HB2	1.99	0.44
1:A:315:TRP:CD2	1:A:371:PRO:HG3	2.53	0.44
1:B:121:PRO:O	1:B:122:PHE:CB	2.65	0.44
1:A:112:ILE:HA	1:A:350:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.64	0.44
1:A:137:GLN:H	8:A:801:GOL:H11	1.79	0.43
1:A:266:HIS:C	1:A:266:HIS:CD2	2.92	0.43
1:A:276:THR:HG22	1:A:277:PRO:O	2.18	0.43
1:A:66:HIS:HB3	1:A:99:CYS:SG	2.59	0.43
2:C:19:DA:N3	3:D:2:DA:C2	2.86	0.43
1:A:295:LEU:HD21	1:A:299:ARG:NH2	2.35	0.42
1:B:238:ARG:O	1:B:238:ARG:CG	2.67	0.42
1:A:186:GLN:HB2	7:A:397:RLT:CAA	2.49	0.42
2:C:1:DA:H3'	2:C:2:DT:C5'	2.49	0.42
1:B:141:TYR:CE2	1:B:161:PRO:HD3	2.55	0.42
1:A:350:ARG:O	1:A:366:ILE:HG13	2.19	0.42
1:B:170:LEU:HA	1:B:170:LEU:HD23	1.83	0.42
1:A:272:ILE:HG22	1:A:291:GLU:OE2	2.20	0.42
1:A:120:LYS:HD2	1:B:272:ILE:CG2	2.50	0.42
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.79	0.41
1:A:348:ASN:C	1:A:350:ARG:H	2.23	0.41
2:C:2:DT:H2''	2:C:3:DT:O5'	2.20	0.41
1:A:178:ILE:O	1:B:275:ASN:ND2	2.53	0.41
1:A:111:PRO:HG3	1:A:310:ALA:CA	2.48	0.41
1:A:12:LEU:HD12	1:A:12:LEU:H	1.86	0.41
1:A:183:HIS:HA	1:A:207:GLU:O	2.20	0.41
1:A:55:GLN:HG3	1:A:92:GLN:NE2	2.35	0.41
2:C:10:DG:H2''	2:C:11:DA:C8	2.55	0.41
1:A:221:GLU:HA	1:A:221:GLU:OE1	2.21	0.41
1:B:126:PHE:CD2	1:B:220:VAL:HG21	2.55	0.41
1:A:40:SER:HA	1:A:45:VAL:HG22	2.03	0.41
1:A:266:HIS:NE2	1:A:272:ILE:O	2.53	0.41
1:B:131:GLY:HA3	1:B:141:TYR:CD1	2.56	0.41
1:B:132:PRO:HG3	1:B:141:TYR:OH	2.21	0.40
1:B:154:TRP:HB3	1:B:156:TYR:CE2	2.56	0.40
3:D:2:DA:H2''	3:D:3:DC:O5'	2.21	0.40
1:B:243:TYR:C	1:B:243:TYR:CD2	2.95	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%)	333 (92%)	28 (8%)	2 (1%)	25	64
1	B	161/395 (41%)	150 (93%)	11 (7%)	0	100	100
All	All	524/790 (66%)	483 (92%)	39 (7%)	2 (0%)	34	69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	ALA
1	A	27	GLN

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	320/354 (90%)	308 (96%)	12 (4%)	33	67
1	B	135/354 (38%)	129 (96%)	6 (4%)	28	64
All	All	455/708 (64%)	437 (96%)	18 (4%)	31	66

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	29	THR
1	A	116	ASP
1	A	149	MET

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Mol	Chain	Res	Type
1	A	202	ARG
1	A	223	LYS
1	A	238	ARG
1	A	248	VAL
1	A	251	LEU
1	A	281	GLN
1	A	358	LEU
1	A	360	ASN
1	B	149	MET
1	B	202	ARG
1	B	223	LYS
1	B	224	ASN
1	B	232	THR
1	B	275	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 1 is modelled with single atom and 4 are monoatomic - 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	801	-	5,5,5	0.47	0	5,5,5	0.89	0
8	GOL	A	802	-	5,5,5	0.43	0	5,5,5	0.81	0
7	RLT	A	397	5	29,34,34	2.25	7 (24%)	31,50,50	1.74	5 (16%)
8	GOL	A	803	-	5,5,5	0.31	0	5,5,5	0.48	0
8	GOL	A	804	-	5,5,5	0.41	0	5,5,5	0.52	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	801	-	-	4/4/4/4	-
8	GOL	A	802	-	-	2/4/4/4	-
7	RLT	A	397	5	-	0/17/24/24	0/3/3/3
8	GOL	A	803	-	-	2/4/4/4	-
8	GOL	A	804	-	-	3/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	397	RLT	NAP-NAO	-6.69	1.24	1.37
7	A	397	RLT	CBA-CAV	4.90	1.57	1.50
7	A	397	RLT	CAA-CAW	4.57	1.54	1.49
7	A	397	RLT	CBC-NBE	3.99	1.45	1.36
7	A	397	RLT	CBF-CBC	3.72	1.58	1.53
7	A	397	RLT	CBB-CAU	2.53	1.54	1.50
7	A	397	RLT	CBC-NAQ	2.34	1.34	1.31

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	397	RLT	CBB-CAU-NAR	-4.85	110.94	115.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	397	RLT	CAY-CAN-NAR	2.69	118.81	113.05
7	A	397	RLT	NAQ-CBC-NBE	-2.26	115.99	121.80
7	A	397	RLT	CAM-CAY-CAL	2.17	121.58	118.17
7	A	397	RLT	CBA-NAP-NAO	2.00	109.41	105.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

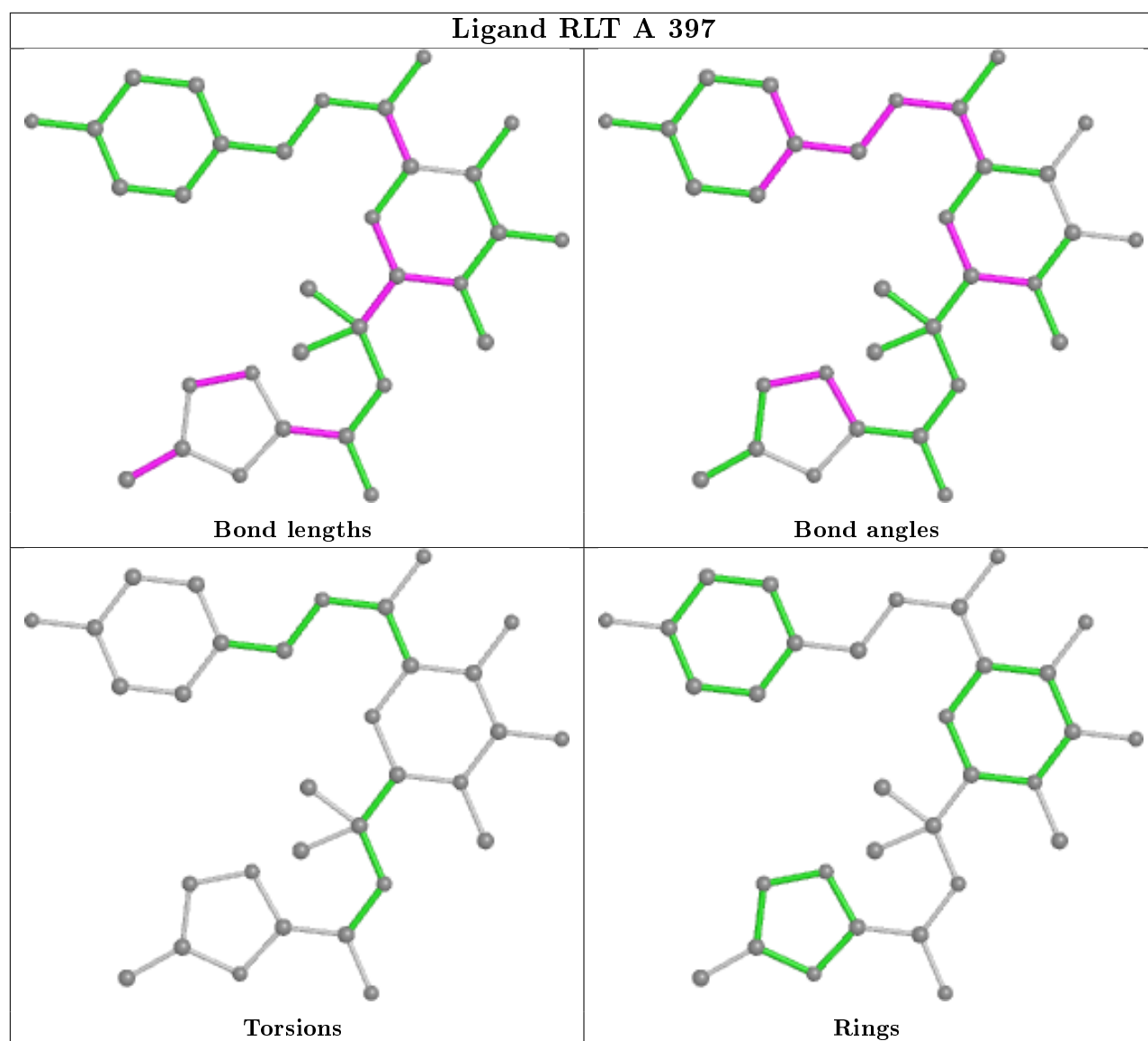
Mol	Chain	Res	Type	Atoms
8	A	802	GOL	O1-C1-C2-O2
8	A	802	GOL	O1-C1-C2-C3
8	A	803	GOL	C1-C2-C3-O3
8	A	801	GOL	O1-C1-C2-C3
8	A	801	GOL	C1-C2-C3-O3
8	A	804	GOL	O1-C1-C2-C3
8	A	801	GOL	O1-C1-C2-O2
8	A	803	GOL	O2-C2-C3-O3
8	A	804	GOL	O1-C1-C2-O2
8	A	801	GOL	O2-C2-C3-O3
8	A	804	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	801	GOL	6	0
8	A	802	GOL	5	0
7	A	397	RLT	5	0
8	A	803	GOL	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th 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 ²)	Q<0.9
1	A	365/395 (92%)	0.00	6 (1%) 72 59	82, 105, 160, 183	0
1	B	163/395 (41%)	-0.19	1 (0%) 89 83	89, 112, 142, 160	0
2	C	19/19 (100%)	-0.24	1 (5%) 26 14	84, 106, 138, 152	0
3	D	17/17 (100%)	-0.46	0 100 100	85, 99, 147, 173	0
All	All	564/826 (68%)	-0.07	8 (1%) 75 63	82, 107, 155, 183	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	VAL	2.9
1	A	254	ASN	2.8
1	A	30	TYR	2.8
1	A	16	LEU	2.6
1	A	15	LEU	2.5
1	B	257	TYR	2.3
1	A	21	ILE	2.1
2	C	1	DA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

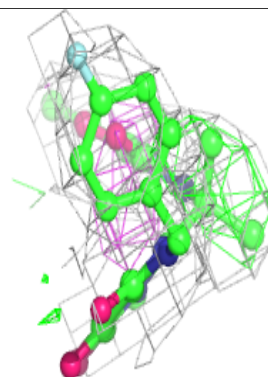
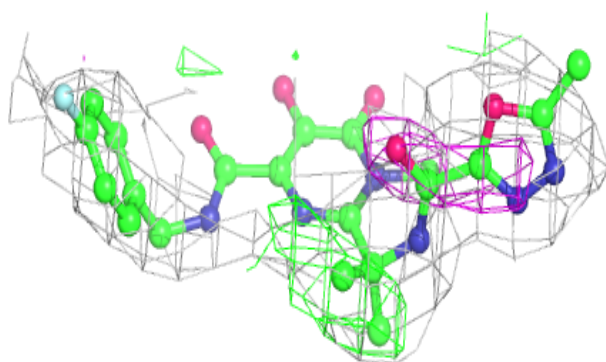
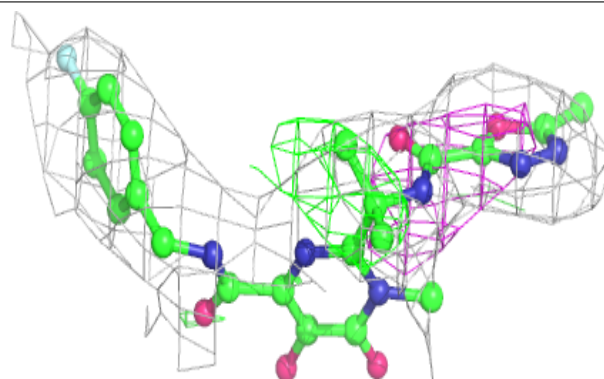
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	A	804	6/6	0.64	0.77	121,122,123,124	0
6	NH4	A	396	1/1	0.67	0.34	49,49,49,49	0
8	GOL	A	803	6/6	0.83	0.25	133,133,134,134	0
8	GOL	A	801	6/6	0.89	0.18	96,99,100,101	0
8	GOL	A	802	6/6	0.94	0.12	109,110,110,112	0
7	RLT	A	397	32/32	0.95	0.20	70,80,112,114	0
5	MN	B	393	1/1	0.98	0.20	101,101,101,101	0
5	MN	A	395	1/1	0.99	0.16	77,77,77,77	0
4	ZN	A	393	1/1	0.99	0.15	90,90,90,90	0
5	MN	A	394	1/1	1.00	0.15	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 RLT A 397:

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.