



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 1, 2021 – 02:03 PM EDT

PDB ID : 7LDL
Title : Improved Feline Drugs as SARS-CoV-2 Mpro Inhibitors: Structure-Activity Studies & Micellar Solubilization for Enhanced Bioavailability
Authors : Khan, M.B.; Lu, J.; Arutyunova, E.; Young, H.S.; Lemieux, M.J.
Deposited on : 2021-01-13
Resolution : 2.00 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 : 2.22
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) : 2.22

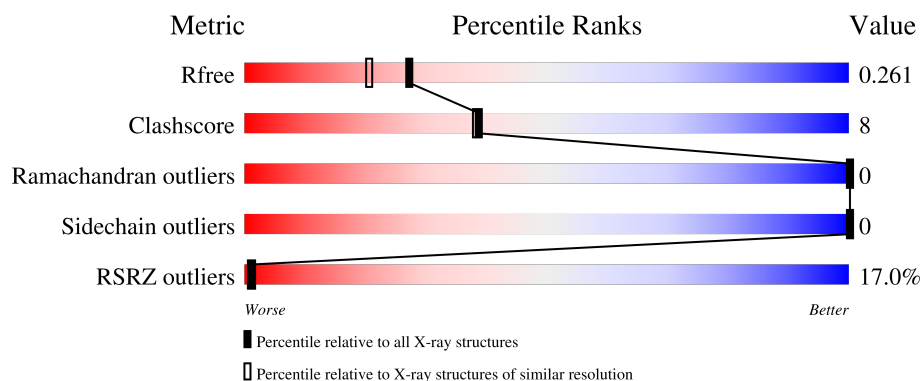
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 ≥ 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	306	<div> <div>18%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>
1	B	306	<div> <div>16%</div> <div>88%</div> <div>11%</div> </div>

2 Entry composition [i](#)

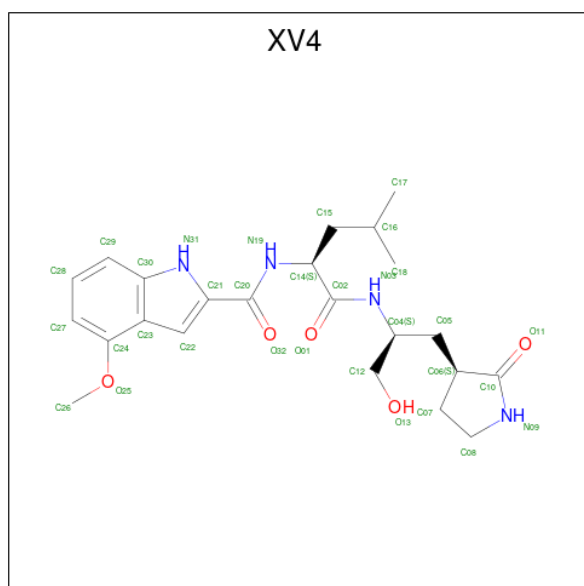
There are 3 unique types of molecules in this entry. The entry contains 9744 atoms, of which 4708 are hydrogens and 0 are deuteriums.

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 3C-like proteinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total	C	H	N	O	S	0	3	0
			4709	1508	2329	403	445	24			
1	B	306	Total	C	H	N	O	S	0	1	0
			4689	1501	2319	402	444	23			

- Molecule 2 is N-[(2S)-1-({(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}amino)-4-methyl-1-oxopentan-2-yl]-4-methoxy-1H-indole-2-carboxamide (three-letter code: XV4) (formula: C₂₃H₃₂N₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			62	23	30	4	5		
2	B	1	Total	C	H	N	O	0	0
			62	23	30	4	5		

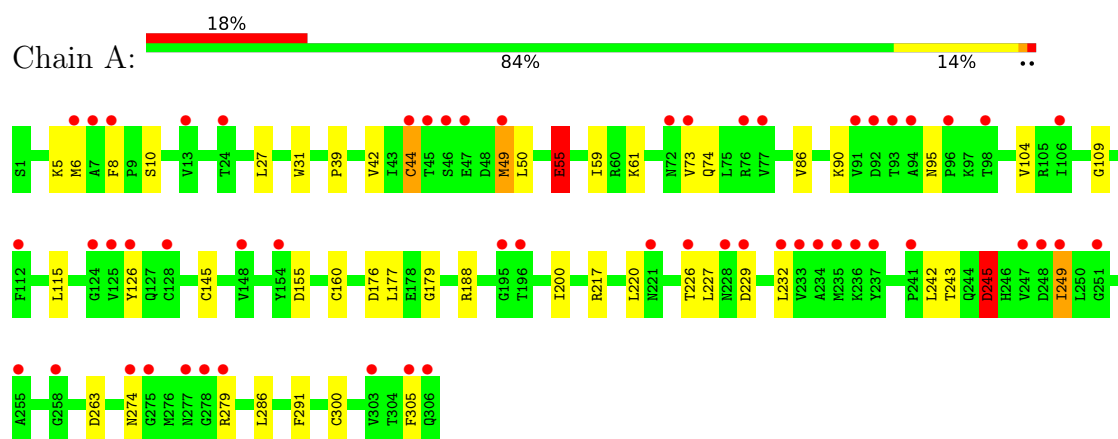
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total 107	O 107	0	0
3	B	115	Total 115	O 115	0	0

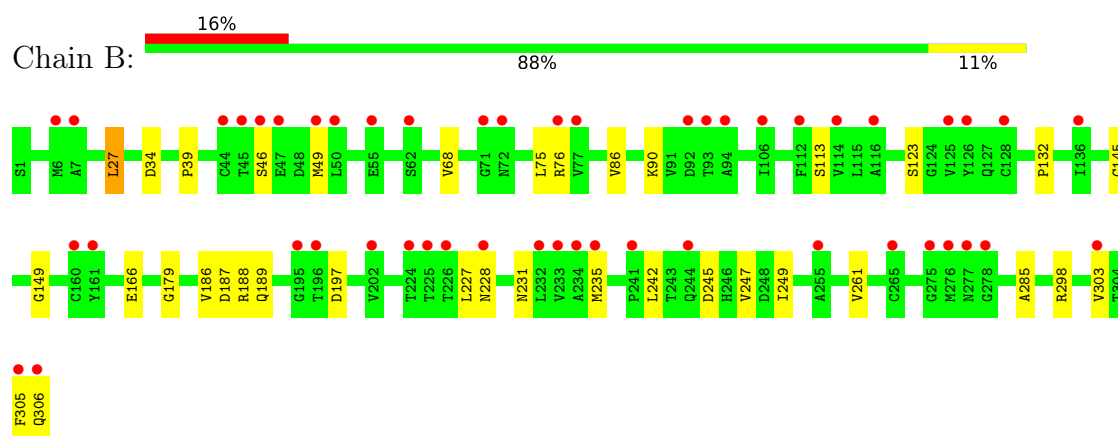
3 Residue-property plots [i](#)

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: 3C-like proteinase



• Molecule 1: 3C-like proteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.07Å 60.86Å 63.67Å 79.85° 68.24° 70.40°	Depositor
Resolution (Å)	39.92 – 2.00 39.92 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.1 (39.92-2.00) 94.1 (39.92-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.207 , 0.261 0.207 , 0.261	Depositor DCC
R_{free} test set	2332 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.128 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9744	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.39% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XV4

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	0.90	7/2442 (0.3%)	1.21	18/3318 (0.5%)
1	B	0.64	0/2426	0.84	2/3297 (0.1%)
All	All	0.78	7/4868 (0.1%)	1.04	20/6615 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	GLU	CB-CG	16.95	1.84	1.52
1	A	55	GLU	CG-CD	9.58	1.66	1.51
1	A	55	GLU	CD-OE2	9.39	1.35	1.25
1	A	55	GLU	CD-OE1	-8.15	1.16	1.25
1	A	249	ILE	CG1-CD1	5.89	1.91	1.50
1	A	44	CYS	CB-SG	-5.87	1.72	1.81
1	A	245	ASP	CB-CG	5.13	1.62	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	GLU	OE1-CD-OE2	-23.78	94.76	123.30
1	A	245	ASP	CB-CG-OD1	18.40	134.86	118.30
1	A	245	ASP	CB-CG-OD2	-17.96	102.14	118.30
1	A	55	GLU	CG-CD-OE2	-15.58	87.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ILE	CA-CB-CG1	-12.70	86.88	111.00
1	A	49	MET	CG-SD-CE	12.24	119.79	100.20
1	A	55	GLU	CG-CD-OE1	11.62	141.53	118.30
1	A	49	MET	CB-CA-C	8.62	127.65	110.40
1	A	245	ASP	OD1-CG-OD2	-8.38	107.37	123.30
1	A	249	ILE	CB-CA-C	7.85	127.29	111.60
1	A	55	GLU	CB-CA-C	-7.54	95.32	110.40
1	A	59	ILE	CG1-CB-CG2	7.02	126.84	111.40
1	A	90	LYS	CB-CG-CD	6.87	129.47	111.60
1	A	279	ARG	CG-CD-NE	6.73	125.94	111.80
1	B	27	LEU	CB-CG-CD2	-6.34	100.22	111.00
1	A	177	LEU	CA-CB-CG	-6.20	101.04	115.30
1	A	232	LEU	CB-CG-CD2	5.48	120.31	111.00
1	A	249	ILE	CG1-CB-CG2	5.44	123.37	111.40
1	A	55	GLU	CB-CG-CD	-5.24	100.06	114.20
1	B	187	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	ASP	Sidechain
1	A	274	ASN	Sidechain
1	A	55	GLU	Sidechain

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	2380	2329	2334	45	0
1	B	2370	2319	2319	27	0
2	A	32	30	0	5	0
2	B	32	30	0	4	0
3	A	107	0	0	13	1
3	B	115	0	0	4	1
All	All	5036	4708	4653	69	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (69) 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:55:GLU:CB	1:A:55:GLU:CG	1.84	1.52
1:A:249:ILE:CD1	1:A:249:ILE:CG1	1.91	1.49
1:A:286:LEU:HD21	1:B:285:ALA:HB2	1.53	0.90
1:A:145:CYS:SG	2:A:401:XV4:C04	2.67	0.82
1:B:123:SER:OG	3:B:501:HOH:O	2.02	0.78
1:A:249:ILE:CD1	1:A:249:ILE:CB	2.63	0.77
1:A:74:GLN:N	3:A:504:HOH:O	2.21	0.73
1:A:126:TYR:OH	3:A:501:HOH:O	1.97	0.72
1:A:44:CYS:HB3	1:A:49:MET:HB2	1.72	0.72
1:B:145:CYS:SG	2:B:401:XV4:C04	2.77	0.72
1:A:226:THR:HG23	1:A:229:ASP:H	1.55	0.72
1:A:300:CYS:O	3:A:502:HOH:O	2.09	0.70
1:A:74:GLN:NE2	3:A:508:HOH:O	2.24	0.69
1:A:10:SER:HB2	1:A:115:LEU:HD13	1.77	0.66
1:B:46:SER:O	3:B:502:HOH:O	2.12	0.66
1:A:243:THR:OG1	1:A:245:ASP:HB2	1.98	0.64
1:A:55:GLU:CG	1:A:55:GLU:CA	2.74	0.64
1:A:55:GLU:CB	1:A:55:GLU:CD	2.68	0.62
1:A:86:VAL:HG13	1:A:179:GLY:HA2	1.83	0.59
1:A:263:ASP:OD2	3:A:503:HOH:O	2.16	0.58
1:B:245:ASP:O	1:B:249:ILE:HG12	2.03	0.58
1:A:300:CYS:HB3	3:A:502:HOH:O	2.03	0.58
1:B:34:ASP:OD2	1:B:90:LYS:HE3	2.04	0.57
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.87	0.57
1:B:166:GLU:O	2:B:401:XV4:N31	2.38	0.56
1:B:228:ASN:ND2	3:B:509:HOH:O	2.37	0.56
1:B:113:SER:O	1:B:149:GLY:HA2	2.06	0.56
1:A:31:TRP:CD2	1:A:95:ASN:HB2	2.41	0.56
1:A:61:LYS:NZ	3:A:512:HOH:O	2.38	0.56
1:A:145:CYS:SG	2:A:401:XV4:N03	2.80	0.55
1:A:145:CYS:SG	2:A:401:XV4:C05	2.95	0.55
1:B:145:CYS:SG	2:B:401:XV4:C05	2.95	0.54
1:A:249:ILE:HG23	3:A:544:HOH:O	2.06	0.53
1:A:6[A]:MET:HE1	3:B:501:HOH:O	2.08	0.53
1:A:145:CYS:CB	2:A:401:XV4:C12	2.87	0.52
1:A:217:ARG:HB3	1:A:220:LEU:HD12	1.92	0.52
1:B:305:PHE:O	1:B:306:GLN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:VAL:HG23	1:B:188:ARG:HG2	1.94	0.49
1:B:145:CYS:CB	2:B:401:XV4:C12	2.89	0.49
1:A:249:ILE:CG2	3:A:544:HOH:O	2.61	0.49
1:B:227:LEU:CD1	1:B:242:LEU:HD23	2.43	0.49
1:A:27:LEU:HD13	1:A:39:PRO:HD2	1.95	0.48
1:A:8:PHE:HE1	1:A:305:PHE:CZ	2.33	0.47
1:A:286:LEU:HD21	1:B:285:ALA:CB	2.36	0.47
1:B:231:ASN:O	1:B:235:MET:HG2	2.16	0.46
1:A:49:MET:HG3	2:A:401:XV4:C17	2.45	0.46
1:A:27:LEU:HD21	1:A:42:VAL:HB	1.98	0.46
1:A:188:ARG:HD3	3:A:548:HOH:O	2.15	0.46
1:B:27:LEU:HD13	1:B:39:PRO:HD2	1.99	0.45
1:B:49:MET:HG3	1:B:189:GLN:HG3	1.98	0.45
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.51	0.45
1:A:86:VAL:HG13	1:A:179:GLY:CA	2.46	0.44
1:B:76:ARG:NH1	1:B:76:ARG:HG2	2.32	0.44
1:B:68:VAL:HG12	1:B:75:LEU:HD12	2.00	0.43
1:B:132:PRO:HD2	1:B:197:ASP:OD1	2.18	0.43
1:B:298:ARG:HG3	1:B:303:VAL:HB	2.01	0.43
1:A:286:LEU:CD2	1:B:285:ALA:HB2	2.37	0.43
1:B:247:VAL:HG22	1:B:261:VAL:HG11	2.01	0.43
1:A:73:VAL:HG13	3:A:504:HOH:O	2.19	0.42
1:A:5:LYS:HE3	1:A:291:PHE:CZ	2.55	0.42
1:A:176:ASP:HB2	3:A:523:HOH:O	2.18	0.42
1:A:109:GLY:HA2	1:A:200:ILE:HD13	2.01	0.41
1:A:155:ASP:OD1	1:A:155:ASP:N	2.42	0.41
1:B:27:LEU:C	1:B:27:LEU:HD12	2.41	0.41
1:A:50:LEU:HD23	1:A:50:LEU:O	2.21	0.41
1:A:115:LEU:O	3:A:505:HOH:O	2.22	0.41
1:A:104:VAL:O	1:A:160:CYS:HA	2.21	0.41
1:A:227:LEU:HD11	1:A:242:LEU:HB3	2.04	0.40
1:B:86:VAL:HG13	1:B:179:GLY:CA	2.51	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)
3:A:589:HOH:O	3:B:546:HOH:O[1_455]	2.06	0.14

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	307/306 (100%)	297 (97%)	10 (3%)	0	100	100
1	B	305/306 (100%)	295 (97%)	10 (3%)	0	100	100
All	All	612/612 (100%)	592 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	266/263 (101%)	266 (100%)	0	100	100
1	B	264/263 (100%)	264 (100%)	0	100	100
All	All	530/526 (101%)	530 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	244	GLN
1	A	274	ASN

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 ⓘ

2 ligands are 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	$\# Z > 2$
2	XV4	A	401	1	32,34,34	4.23	15 (46%)	41,47,47	1.91	9 (21%)
2	XV4	B	401	1	32,34,34	4.31	19 (59%)	41,47,47	1.89	8 (19%)

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	XV4	A	401	1	-	2/25/38/38	0/3/3/3
2	XV4	B	401	1	-	2/25/38/38	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	XV4	C10-N09	16.34	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	XV4	C10-N09	15.28	1.49	1.33
2	A	401	XV4	C28-C29	7.62	1.54	1.36
2	A	401	XV4	C20-N19	7.40	1.50	1.34
2	B	401	XV4	C28-C29	7.14	1.53	1.36
2	B	401	XV4	C02-N03	6.96	1.49	1.34
2	A	401	XV4	C02-N03	6.49	1.48	1.34
2	B	401	XV4	C20-N19	6.47	1.48	1.34
2	A	401	XV4	C27-C24	5.64	1.51	1.38
2	B	401	XV4	C27-C24	5.42	1.50	1.38
2	B	401	XV4	O13-C12	-5.33	1.19	1.42
2	A	401	XV4	O13-C12	-4.99	1.21	1.42
2	B	401	XV4	C08-N09	4.88	1.56	1.46
2	B	401	XV4	C29-C30	-4.64	1.33	1.41
2	A	401	XV4	C29-C30	-4.61	1.33	1.41
2	A	401	XV4	C08-N09	4.61	1.55	1.46
2	B	401	XV4	O11-C10	-3.80	1.15	1.23
2	B	401	XV4	C28-C27	-3.60	1.31	1.38
2	A	401	XV4	C23-C30	3.44	1.51	1.42
2	A	401	XV4	O25-C24	3.43	1.42	1.36
2	A	401	XV4	O11-C10	-3.24	1.17	1.23
2	A	401	XV4	C28-C27	-3.07	1.32	1.38
2	B	401	XV4	C24-C23	-2.76	1.35	1.42
2	A	401	XV4	C24-C23	-2.70	1.35	1.42
2	B	401	XV4	C21-C20	2.53	1.56	1.50
2	A	401	XV4	C22-C21	2.50	1.44	1.39
2	A	401	XV4	C21-C20	2.47	1.56	1.50
2	B	401	XV4	C23-C30	2.41	1.49	1.42
2	B	401	XV4	O25-C26	-2.33	1.35	1.42
2	B	401	XV4	C22-C21	2.26	1.43	1.39
2	B	401	XV4	C05-C06	2.15	1.58	1.53
2	B	401	XV4	O32-C20	-2.12	1.19	1.23
2	B	401	XV4	O25-C24	2.11	1.40	1.36
2	B	401	XV4	O01-C02	-2.01	1.19	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	XV4	C21-N31-C30	7.26	119.59	104.45
2	A	401	XV4	C21-N31-C30	6.85	118.74	104.45
2	B	401	XV4	O25-C24-C23	4.26	118.62	114.46
2	A	401	XV4	O25-C24-C23	4.22	118.58	114.46
2	B	401	XV4	C08-N09-C10	-3.95	106.09	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	XV4	O13-C12-C04	3.17	120.15	111.95
2	A	401	XV4	C21-C22-C23	-3.08	102.63	106.70
2	A	401	XV4	C16-C15-C14	-3.06	107.01	115.43
2	B	401	XV4	O13-C12-C04	2.99	119.69	111.95
2	A	401	XV4	C08-N09-C10	-2.84	108.27	113.84
2	A	401	XV4	C04-N03-C02	-2.80	118.74	123.20
2	B	401	XV4	O11-C10-N09	-2.38	122.24	125.54
2	B	401	XV4	C08-C07-C06	2.35	109.56	105.75
2	B	401	XV4	C05-C06-C07	-2.32	108.79	117.31
2	B	401	XV4	C21-C22-C23	-2.25	103.73	106.70
2	A	401	XV4	C05-C06-C07	-2.16	109.36	117.31
2	A	401	XV4	C26-O25-C24	-2.11	114.80	117.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

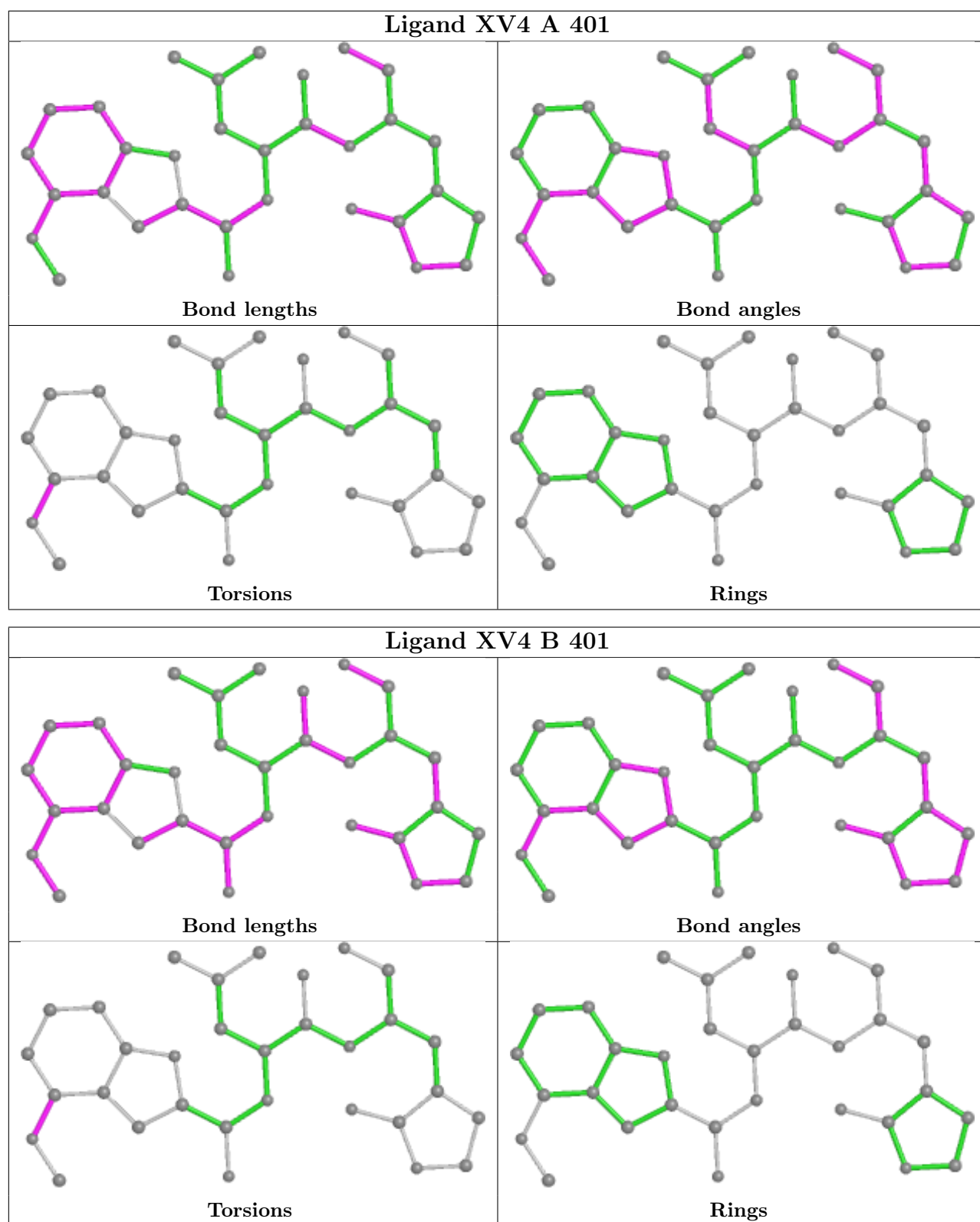
Mol	Chain	Res	Type	Atoms
2	B	401	XV4	C27-C24-O25-C26
2	B	401	XV4	C23-C24-O25-C26
2	A	401	XV4	C23-C24-O25-C26
2	A	401	XV4	C27-C24-O25-C26

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	XV4	5	0
2	B	401	XV4	4	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

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, 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	306/306 (100%)	1.12	55 (17%)  	27, 43, 66, 104	0
1	B	306/306 (100%)	1.11	49 (16%)  	29, 45, 69, 112	0
All	All	612/612 (100%)	1.11	104 (16%)  	27, 44, 68, 112	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	VAL	6.5
1	A	235	MET	6.4
1	B	45	THR	6.0
1	B	228	ASN	5.9
1	B	234	ALA	5.6
1	A	233	VAL	5.4
1	A	255	ALA	5.4
1	A	232	LEU	5.3
1	A	46	SER	5.2
1	A	196	THR	5.1
1	B	232	LEU	4.8
1	B	277	ASN	4.8
1	A	93	THR	4.7
1	A	277	ASN	4.7
1	A	154	TYR	4.6
1	A	72	ASN	4.6
1	B	235	MET	4.6
1	B	47	GLU	4.5
1	A	45	THR	4.3
1	B	306	GLN	4.2
1	B	72	ASN	4.2
1	A	234	ALA	4.2
1	B	49	MET	3.9
1	B	7	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	241	PRO	3.8
1	B	46	SER	3.7
1	B	76	ARG	3.6
1	A	274	ASN	3.6
1	A	7	ALA	3.4
1	A	47	GLU	3.4
1	A	228	ASN	3.4
1	B	265	CYS	3.4
1	A	195	GLY	3.3
1	A	249	ILE	3.2
1	B	128[A]	CYS	3.2
1	A	237	TYR	3.1
1	B	305	PHE	3.0
1	B	94	ALA	2.9
1	B	244	GLN	2.9
1	B	255	ALA	2.9
1	A	6[A]	MET	2.8
1	A	306	GLN	2.8
1	A	76	ARG	2.8
1	A	94	ALA	2.8
1	B	196	THR	2.7
1	B	62	SER	2.7
1	A	8	PHE	2.7
1	A	96	PRO	2.7
1	A	275	GLY	2.7
1	B	6	MET	2.7
1	A	91	VAL	2.7
1	A	128[A]	CYS	2.7
1	B	303	VAL	2.7
1	A	125	VAL	2.6
1	A	73	VAL	2.6
1	B	276	MET	2.6
1	B	44	CYS	2.6
1	A	303	VAL	2.6
1	B	71	GLY	2.6
1	B	50	LEU	2.5
1	A	278	GLY	2.5
1	A	241	PRO	2.5
1	A	248	ASP	2.5
1	B	92	ASP	2.5
1	B	225	THR	2.3
1	A	112	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	279	ARG	2.3
1	A	98	THR	2.3
1	B	226	THR	2.3
1	A	77	VAL	2.3
1	B	77	VAL	2.3
1	A	92	ASP	2.3
1	B	160	CYS	2.3
1	A	251	GLY	2.3
1	B	106	ILE	2.3
1	B	93	THR	2.2
1	B	112	PHE	2.2
1	B	224	THR	2.2
1	B	275	GLY	2.2
1	B	195	GLY	2.2
1	B	278	GLY	2.2
1	A	49	MET	2.2
1	B	116	ALA	2.2
1	A	44	CYS	2.1
1	A	221	ASN	2.1
1	A	258	GLY	2.1
1	A	24	THR	2.1
1	A	226	THR	2.1
1	B	136	ILE	2.1
1	A	229	ASP	2.1
1	A	247	VAL	2.1
1	B	114	VAL	2.1
1	A	126	TYR	2.1
1	B	126	TYR	2.1
1	A	124	GLY	2.1
1	A	148	VAL	2.1
1	A	13	VAL	2.1
1	B	202	VAL	2.1
1	B	55	GLU	2.1
1	B	125	VAL	2.0
1	A	305	PHE	2.0
1	A	236	LYS	2.0
1	B	161	TYR	2.0
1	A	106	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

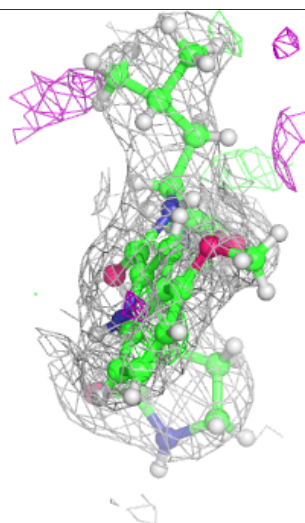
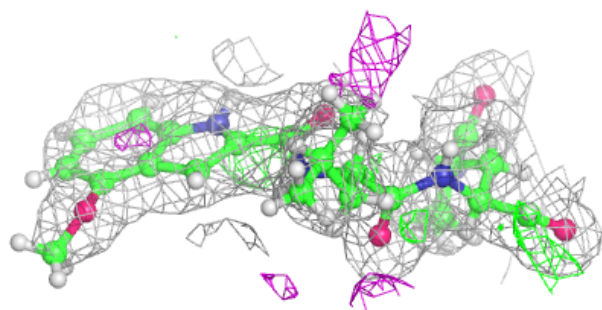
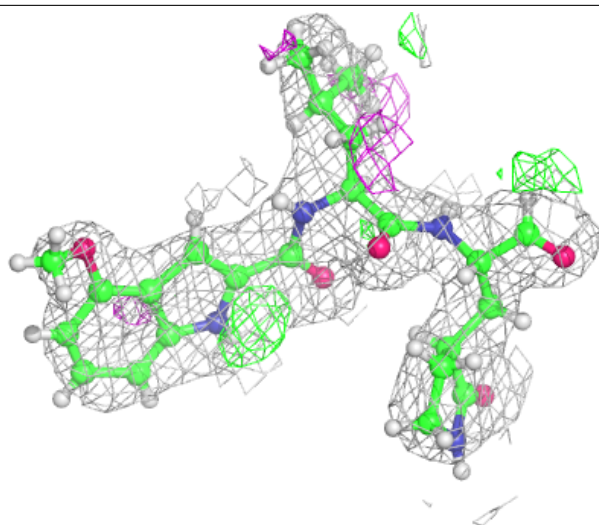
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	XV4	A	401	32/32	0.89	0.18	30,46,66,72	0
2	XV4	B	401	32/32	0.90	0.15	34,51,68,83	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.

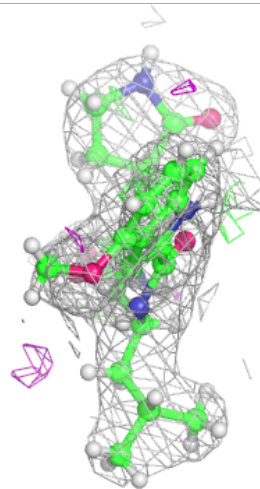
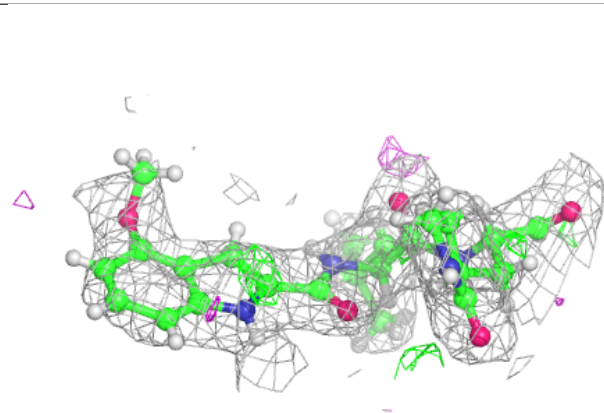
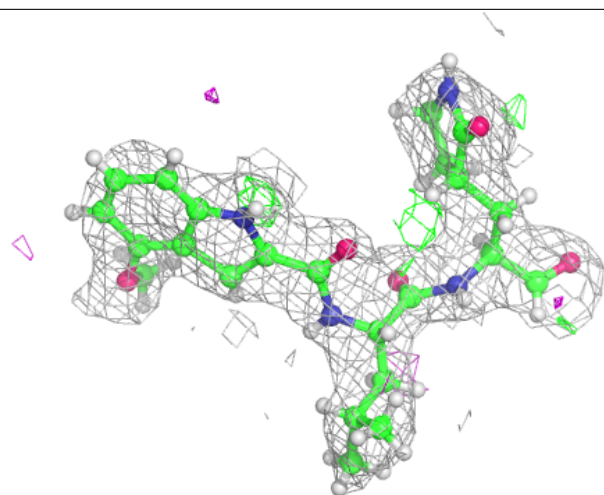
Electron density around XV4 A 401:

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



Electron density around XV4 B 401:

$2mF_o-DF_c$ (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.