



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 09:17 AM BST

PDB ID : 6VH1
Title : 2.30 Å resolution structure of MERS 3CL protease in complex with inhibitor 6h
Authors : Lovell, S.; Battaile, K.P.; Kashipathy, M.M.; Rathnayake, A.D.; Zheng, J.; Kim, Y.; Nguyen, H.N.; Chang, K.O.; Groutas, W.C.
Deposited on : 2020-01-09
Resolution : 2.30 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 : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

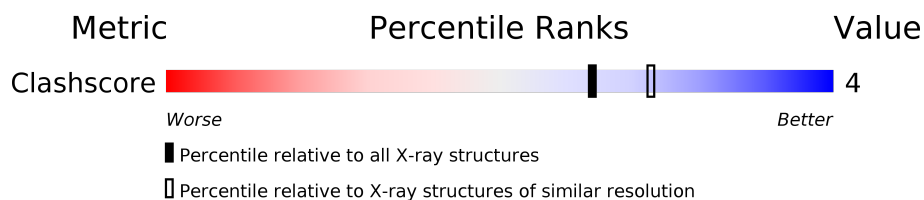
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	313	83% 12% 5%
1	B	313	89% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4601 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.

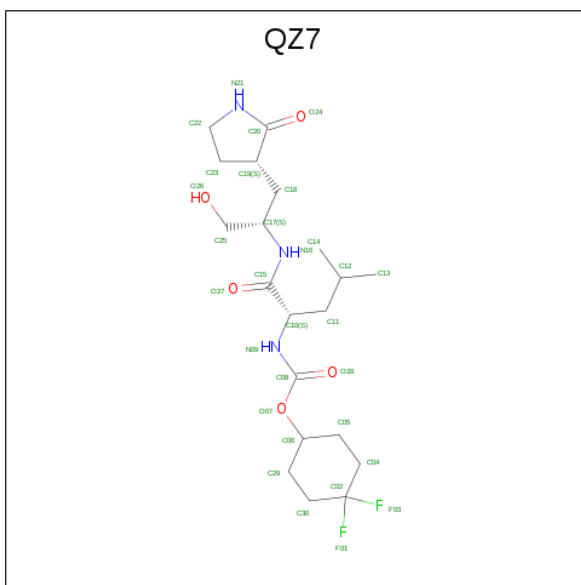
- Molecule 1 is a protein called Orf1a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2213	1413	362	416	22			
1	B	299	Total	C	N	O	S	0	0	0
			2248	1433	366	424	25			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP A0A1L2E0X0
A	-5	HIS	-	expression tag	UNP A0A1L2E0X0
A	-4	HIS	-	expression tag	UNP A0A1L2E0X0
A	-3	HIS	-	expression tag	UNP A0A1L2E0X0
A	-2	HIS	-	expression tag	UNP A0A1L2E0X0
A	-1	HIS	-	expression tag	UNP A0A1L2E0X0
A	0	HIS	-	expression tag	UNP A0A1L2E0X0
B	-6	MET	-	expression tag	UNP A0A1L2E0X0
B	-5	HIS	-	expression tag	UNP A0A1L2E0X0
B	-4	HIS	-	expression tag	UNP A0A1L2E0X0
B	-3	HIS	-	expression tag	UNP A0A1L2E0X0
B	-2	HIS	-	expression tag	UNP A0A1L2E0X0
B	-1	HIS	-	expression tag	UNP A0A1L2E0X0
B	0	HIS	-	expression tag	UNP A0A1L2E0X0

- Molecule 2 is N² -{[(4,4-difluorocyclohexyl)oxy]carbonyl}-N-{(2S)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propan-2-yl}-L-leucinamide (three-letter code: QZ7) (formula: C₂₀H₃₃F₂N₃O₅) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 30	C 20	F 2	N 3	O 5	0	0
2	B	1	Total 30	C 20	F 2	N 3	O 5	0	0

- Molecule 3 is water.


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	58	Total O 58 58	0	0

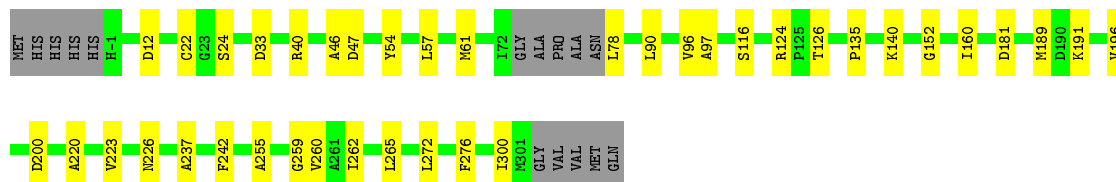
3 Residue-property plots

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. 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. 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.


Note EDS failed to run properly.

- Molecule 1: Orfla protein

Chain A: 



- Molecule 1: Orfla protein

Chain B: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.06Å 91.24Å 100.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.12 – 2.30	Depositor
% Data completeness (in resolution range)	99.9 (39.12-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.16_3544	Depositor
R, R_{free}	0.192 , 0.253	Depositor
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.535	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4601	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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: QZ7

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	0.58	0/2266	0.66	0/3095
1	B	0.64	0/2302	0.71	1/3139 (0.0%)
All	All	0.61	0/4568	0.69	1/6234 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	ARG	NE-CZ-NH2	-5.64	117.48	120.30

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	2213	0	2090	24	0
1	B	2248	0	2136	14	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
3	A	22	0	0	0	0
3	B	58	0	0	2	0
All	All	4601	0	4226	37	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 4.

All (37) 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:220:ALA:O	1:A:223:VAL:HG12	1.80	0.81
1:A:255:ALA:O	1:A:259:GLY:N	2.35	0.60
1:B:166:HIS:HE1	1:B:175:HIS:HB3	1.66	0.59
1:A:272:LEU:HD22	1:A:276:PHE:CE1	2.40	0.56
1:A:300:ILE:O	1:A:300:ILE:HG22	2.07	0.55
1:A:124:ARG:O	1:A:126:THR:HG23	2.07	0.54
1:A:226:ASN:N	1:A:226:ASN:OD1	2.40	0.53
1:B:57:LEU:O	1:B:61:MET:HG2	2.10	0.52
1:A:57:LEU:O	1:A:61:MET:HG2	2.10	0.52
1:B:8:HIS:HB3	3:B:527:HOH:O	2.09	0.51
1:B:51:ASP:HA	1:B:191:LYS:HD3	1.92	0.51
1:A:260:VAL:O	1:A:260:VAL:HG12	2.11	0.49
1:B:297:ASN:O	1:B:301:MET:HA	2.13	0.48
1:A:237:ALA:HB1	1:A:242:PHE:CB	2.44	0.48
1:A:33:ASP:O	1:A:97:ALA:HA	2.13	0.47
1:B:116:SER:O	1:B:152:GLY:HA2	2.14	0.47
1:A:40:ARG:HA	1:A:90:LEU:HG	1.96	0.47
1:A:135:PRO:HD2	1:A:200:ASP:OD1	2.15	0.47
1:B:134:ARG:HG2	1:B:138:THR:O	2.16	0.45
1:B:276:PHE:CD1	1:B:276:PHE:N	2.82	0.45
1:A:40:ARG:CZ	1:A:54:TYR:CD2	2.99	0.45
1:A:237:ALA:HB1	1:A:242:PHE:HB2	1.99	0.44
1:A:189:MET:HB3	1:A:191:LYS:HG3	2.00	0.44
1:B:51:ASP:CG	1:B:51:ASP:O	2.56	0.44
1:A:46:ALA:O	1:A:47:ASP:C	2.57	0.43
1:A:78:LEU:HD21	1:A:96:VAL:HB	2.00	0.43
1:A:22:CYS:O	1:A:24:SER:N	2.52	0.42
1:B:33:ASP:HB3	3:B:515:HOH:O	2.18	0.42
1:A:181:ASP:OD1	1:A:181:ASP:C	2.58	0.42
1:B:1:SER:HA	1:B:217:ASN:OD1	2.20	0.41
1:A:262:ILE:O	1:A:265:LEU:N	2.48	0.41
1:A:140:LYS:HB3	1:B:0:HIS:CE1	2.55	0.41
1:A:12:ASP:CB	1:A:160:ILE:HD11	2.52	0.40
1:A:116:SER:O	1:A:152:GLY:HA2	2.21	0.40
1:B:166:HIS:CE1	1:B:175:HIS:HB3	2.52	0.40
1:B:79:ARG:O	1:B:94:VAL:HA	2.21	0.40
1:A:196:VAL:HG13	1:A:196:VAL:O	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	QZ7	A	401	1	31,31,31	2.69	8 (25%)	39,43,43	2.20	9 (23%)
2	QZ7	B	401	1	31,31,31	3.06	11 (35%)	39,43,43	2.11	7 (17%)

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	QZ7	A	401	1	-	1/26/48/48	0/2/2/2
2	QZ7	B	401	1	-	1/26/48/48	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	QZ7	C30-C02	10.61	1.61	1.50
2	A	401	QZ7	C30-C02	9.19	1.59	1.50
2	A	401	QZ7	C04-C02	8.07	1.58	1.50
2	B	401	QZ7	C25-C17	7.49	1.64	1.52
2	B	401	QZ7	C20-N21	7.07	1.41	1.33
2	A	401	QZ7	C20-N21	4.51	1.38	1.33
2	B	401	QZ7	C04-C02	4.01	1.54	1.50
2	A	401	QZ7	O07-C06	-3.66	1.37	1.46
2	A	401	QZ7	C10-N09	-3.15	1.39	1.45
2	B	401	QZ7	O07-C06	-2.93	1.39	1.46
2	B	401	QZ7	C18-C19	2.73	1.60	1.53
2	A	401	QZ7	C19-C20	-2.68	1.48	1.52
2	B	401	QZ7	C29-C06	2.63	1.58	1.51
2	A	401	QZ7	C05-C06	2.58	1.58	1.51
2	B	401	QZ7	C23-C22	2.43	1.56	1.53
2	B	401	QZ7	C19-C20	2.40	1.55	1.52
2	B	401	QZ7	C04-C05	-2.07	1.49	1.53
2	B	401	QZ7	C15-N16	2.06	1.38	1.34
2	A	401	QZ7	C25-C17	2.01	1.55	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	QZ7	C29-C30-C02	7.43	115.34	110.93
2	B	401	QZ7	C29-C30-C02	7.28	115.25	110.93
2	A	401	QZ7	C05-C04-C02	5.84	114.40	110.93
2	B	401	QZ7	C30-C29-C06	4.79	118.49	110.33
2	B	401	QZ7	F03-C02-C30	4.45	112.27	109.37
2	A	401	QZ7	C30-C29-C06	4.26	117.59	110.33
2	B	401	QZ7	O07-C06-C29	3.87	117.66	108.33
2	A	401	QZ7	C04-C05-C06	3.57	116.41	110.33
2	B	401	QZ7	O24-C20-N21	-3.31	120.94	125.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	QZ7	F03-C02-C30	3.16	111.42	109.37
2	A	401	QZ7	O07-C08-N09	3.13	114.38	110.32
2	A	401	QZ7	O07-C06-C29	2.82	115.15	108.33
2	A	401	QZ7	O26-C25-C17	-2.79	104.74	111.95
2	B	401	QZ7	C18-C17-C25	2.71	115.41	111.65
2	A	401	QZ7	O24-C20-N21	-2.26	122.40	125.54
2	B	401	QZ7	C25-C17-N16	-2.01	105.08	109.60

There are no chirality outliers.

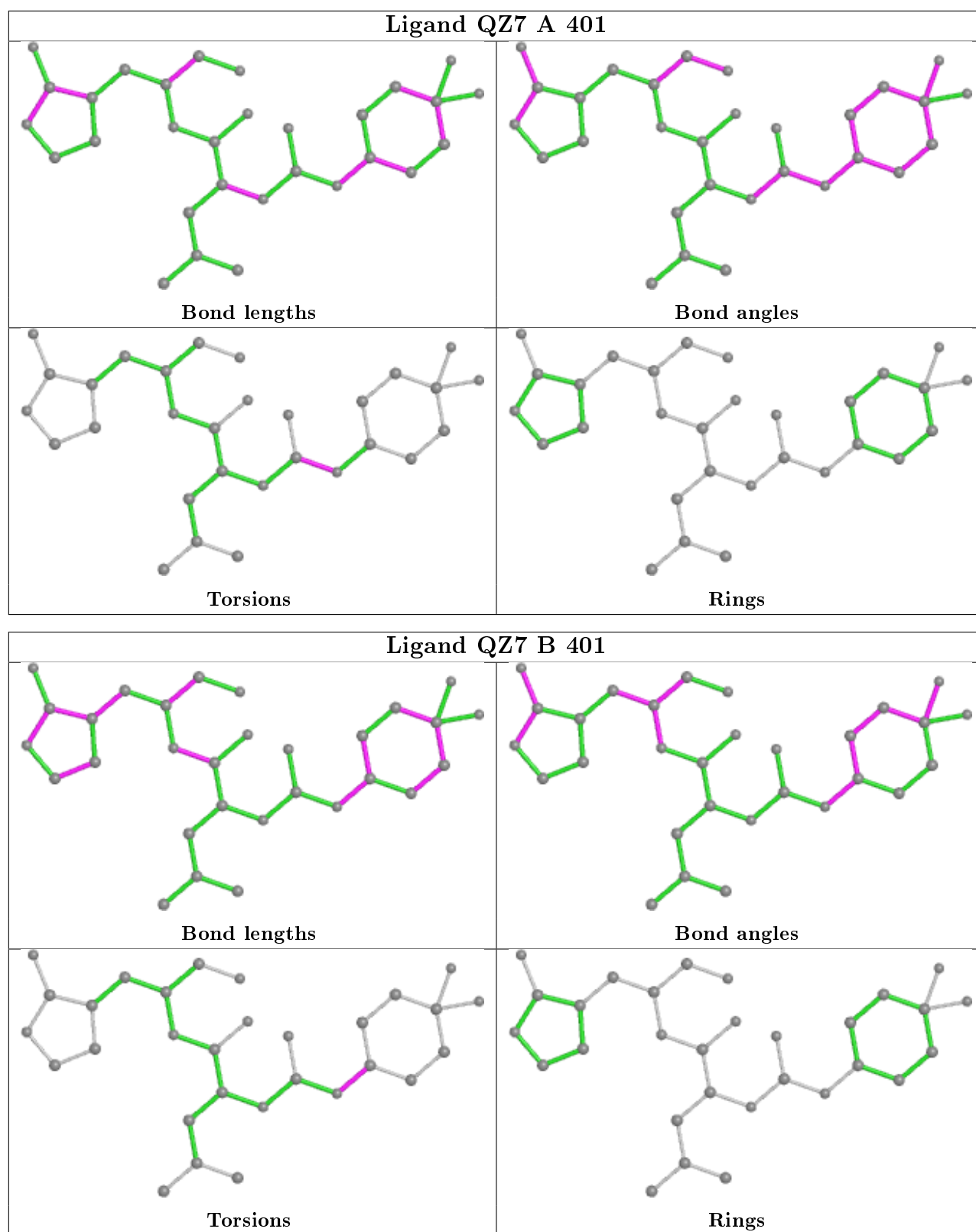
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	QZ7	C29-C06-O07-C08
2	A	401	QZ7	O28-C08-O07-C06

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

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](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.