



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2024 – 09:01 pm GMT

PDB ID : 8C9O
Title : Crystal structure of SARS-CoV-2 Mpro-S144A mutant in complex with 13b-K
Authors : Ibrahim, M.; El Kilani, H.; Hilgenfeld, R.
Deposited on : 2023-01-23
Resolution : 1.69 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 types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

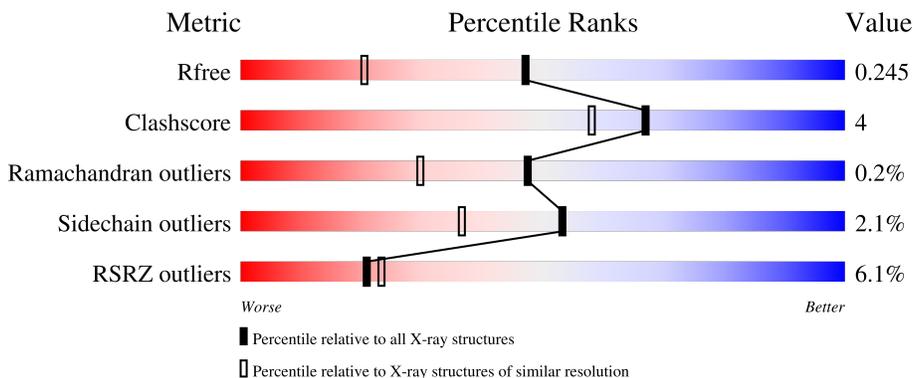
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	AAA	306	
1	BBB	306	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5104 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.

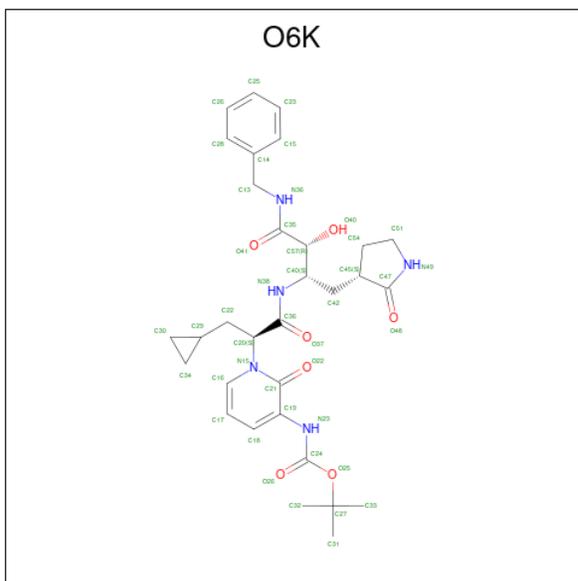
- Molecule 1 is a protein called 3C-like proteinase nsp5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	303	Total 2369	C 1499	N 402	O 444	S 24	0	4	0
1	BBB	306	Total 2388	C 1512	N 405	O 448	S 23	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	144	ALA	SER	engineered mutation	UNP P0DTC1
BBB	144	ALA	SER	engineered mutation	UNP P0DTC1

- Molecule 2 is {tert}-butyl {N}-[1-[(2 {S})-3-cyclopropyl-1-oxidanylidene-1-[[[(2 {S}),3 {R})-3-oxidanyl-4-oxidanylidene-1-[(3 {S})-2-oxidanylidene-pyrrolidin-3-yl]-4-[(phenylmethyl)amino]butan-2-yl]amino]propan-2-yl]-2-oxidanylidene-pyridin-3-yl]carbamate (three-letter code: O6K) (formula: C₃₁H₄₁N₅O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	N	O	0	0
			43	31	5	7		
2	BBB	1	Total	C	N	O	0	0
			43	31	5	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	171	Total	O	0	0
			171	171		
3	BBB	90	Total	O	0	0
			90	90		

3 Residue-property plots [i](#)

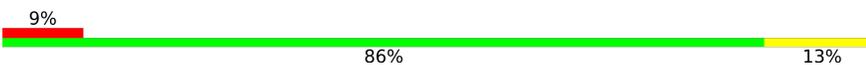
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

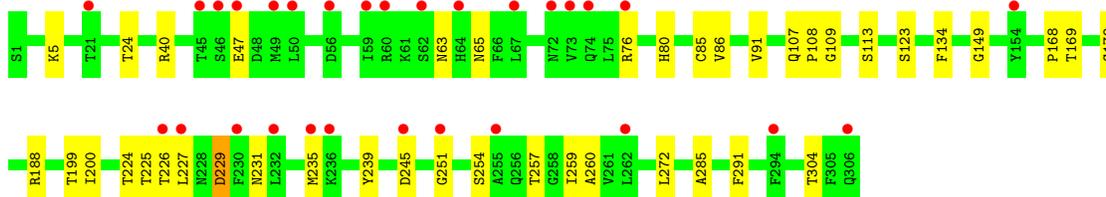
- Molecule 1: 3C-like proteinase nsp5

Chain AAA: 



- Molecule 1: 3C-like proteinase nsp5

Chain BBB: 



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.77Å 99.69Å 103.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.31 – 1.69 49.26 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.31-1.69) 99.9 (49.26-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 1.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.198 , 0.234 0.209 , 0.245	Depositor DCC
R_{free} test set	3819 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtrriage
Anisotropy	0.170	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.012 for -h,l,k	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5104	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage'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.*

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: O6K

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	AAA	0.72	0/2421	0.87	1/3290 (0.0%)
1	BBB	0.72	0/2441	0.87	0/3318
All	All	0.72	0/4862	0.87	1/6608 (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	AAA	153	ASP	CB-CA-C	5.61	121.62	110.40

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	AAA	2369	0	2314	17	0
1	BBB	2388	0	2330	23	0
2	AAA	43	0	0	0	0
2	BBB	43	0	0	0	0
3	AAA	171	0	0	2	0
3	BBB	90	0	0	2	0
All	All	5104	0	4644	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:BBB:226:THR:HB	1:BBB:229:ASP:OD1	1.85	0.76
1:BBB:168:PRO:O	1:BBB:169:THR:OG1	2.07	0.70
1:AAA:189:GLN:O	1:AAA:189:GLN:HG2	1.93	0.68
1:AAA:86[B]:VAL:HG23	1:AAA:179:GLY:HA2	1.82	0.62
1:BBB:254:SER:OG	1:BBB:260:ALA:HA	2.03	0.58
1:AAA:5:LYS:HD3	3:AAA:533:HOH:O	2.05	0.56
1:AAA:189:GLN:O	1:AAA:189:GLN:CG	2.55	0.54
1:AAA:288[A]:GLU:HG2	1:AAA:291:PHE:HE2	1.75	0.52
1:BBB:107:GLN:NE2	3:BBB:503:HOH:O	2.44	0.50
1:AAA:113:SER:O	1:AAA:149:GLY:HA2	2.13	0.48
1:BBB:224:THR:HG22	1:BBB:225:THR:N	2.28	0.48
1:AAA:288[A]:GLU:HG2	1:AAA:291:PHE:CE2	2.48	0.48
1:BBB:86[B]:VAL:HG23	1:BBB:179:GLY:HA2	1.96	0.47
1:BBB:76:ARG:O	1:BBB:91:VAL:HA	2.14	0.47
1:BBB:109:GLY:HA2	1:BBB:200:ILE:HD13	1.97	0.46
1:BBB:257:THR:O	1:BBB:259:ILE:HD12	2.14	0.46
1:AAA:47:GLU:O	1:AAA:48:ASP:HB3	2.16	0.46
1:AAA:95:ASN:HB3	1:AAA:98:THR:OG1	2.16	0.45
1:BBB:225:THR:OG1	1:BBB:226:THR:N	2.49	0.45
1:AAA:303:VAL:HG21	1:BBB:123:SER:HB2	1.98	0.44
1:AAA:188:ARG:HG3	3:AAA:598:HOH:O	2.18	0.44
1:AAA:285:ALA:HB3	1:BBB:285:ALA:HB3	1.98	0.44
1:BBB:5:LYS:HE3	1:BBB:291:PHE:CZ	2.53	0.44
1:BBB:40:ARG:HD3	1:BBB:85:CYS:HA	2.00	0.44
1:AAA:303:VAL:CG2	1:BBB:123:SER:HB2	2.49	0.43
1:BBB:231:ASN:O	1:BBB:235:MET:HG2	2.18	0.43
1:AAA:86[A]:VAL:HG13	1:AAA:179:GLY:HA2	2.00	0.43
1:BBB:199:THR:HG21	1:BBB:239:TYR:CZ	2.54	0.43
1:BBB:108:PRO:HG3	1:BBB:134:PHE:CE1	2.54	0.42
1:BBB:113:SER:O	1:BBB:149:GLY:HA2	2.20	0.42
1:BBB:63:ASN:OD1	1:BBB:80:HIS:CD2	2.72	0.42
1:AAA:86[B]:VAL:HG22	1:AAA:162[B]:MET:CE	2.51	0.41
1:AAA:231:ASN:O	1:AAA:235:MET:HG3	2.21	0.41
1:BBB:224:THR:HG22	1:BBB:225:THR:H	1.85	0.41
1:BBB:229:ASP:HB3	3:BBB:506:HOH:O	2.21	0.41
1:AAA:121:SER:HA	1:AAA:122:PRO:HD3	1.91	0.40
1:BBB:239:TYR:CZ	1:BBB:272:LEU:HD21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	AAA	305/306 (100%)	298 (98%)	7 (2%)	0	100	100
1	BBB	307/306 (100%)	297 (97%)	9 (3%)	1 (0%)	41	24
All	All	612/612 (100%)	595 (97%)	16 (3%)	1 (0%)	47	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	251	GLY

5.3.2 Protein sidechains [i](#)

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	AAA	263/262 (100%)	260 (99%)	3 (1%)	73	63
1	BBB	265/262 (101%)	257 (97%)	8 (3%)	41	22
All	All	528/524 (101%)	517 (98%)	11 (2%)	53	36

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	46	SER
1	AAA	47	GLU

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Mol	Chain	Res	Type
1	AAA	100	LYS
1	BBB	24	THR
1	BBB	47	GLU
1	BBB	65	ASN
1	BBB	188	ARG
1	BBB	227	LEU
1	BBB	229	ASP
1	BBB	245	ASP
1	BBB	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	O6K	BBB	401	1	46,46,46	0.74	1 (2%)	57,65,65	1.11	6 (10%)
2	O6K	AAA	401	1	46,46,46	0.84	1 (2%)	57,65,65	1.07	6 (10%)

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	O6K	BBB	401	1	-	5/42/54/54	0/4/4/4
2	O6K	AAA	401	1	-	3/42/54/54	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	401	O6K	C19-C21	-3.72	1.38	1.47
2	BBB	401	O6K	C19-C21	-3.17	1.40	1.47

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	401	O6K	C21-C19-N23	4.25	116.18	112.30
2	BBB	401	O6K	C18-C19-N23	-3.64	122.28	127.20
2	BBB	401	O6K	O22-C21-C19	2.95	125.73	122.29
2	AAA	401	O6K	C18-C19-C21	2.88	121.94	120.30
2	AAA	401	O6K	C36-C20-N15	-2.80	106.62	111.87
2	AAA	401	O6K	C18-C19-N23	-2.79	123.43	127.20
2	AAA	401	O6K	C21-C19-N23	2.54	114.61	112.30
2	BBB	401	O6K	C57-C40-N38	-2.39	105.53	110.03
2	BBB	401	O6K	C36-C20-N15	-2.20	107.75	111.87
2	BBB	401	O6K	C18-C19-C21	2.16	121.53	120.30
2	AAA	401	O6K	C57-C40-N38	-2.08	106.11	110.03
2	AAA	401	O6K	O40-C57-C35	-2.06	106.18	110.63

There are no chirality outliers.

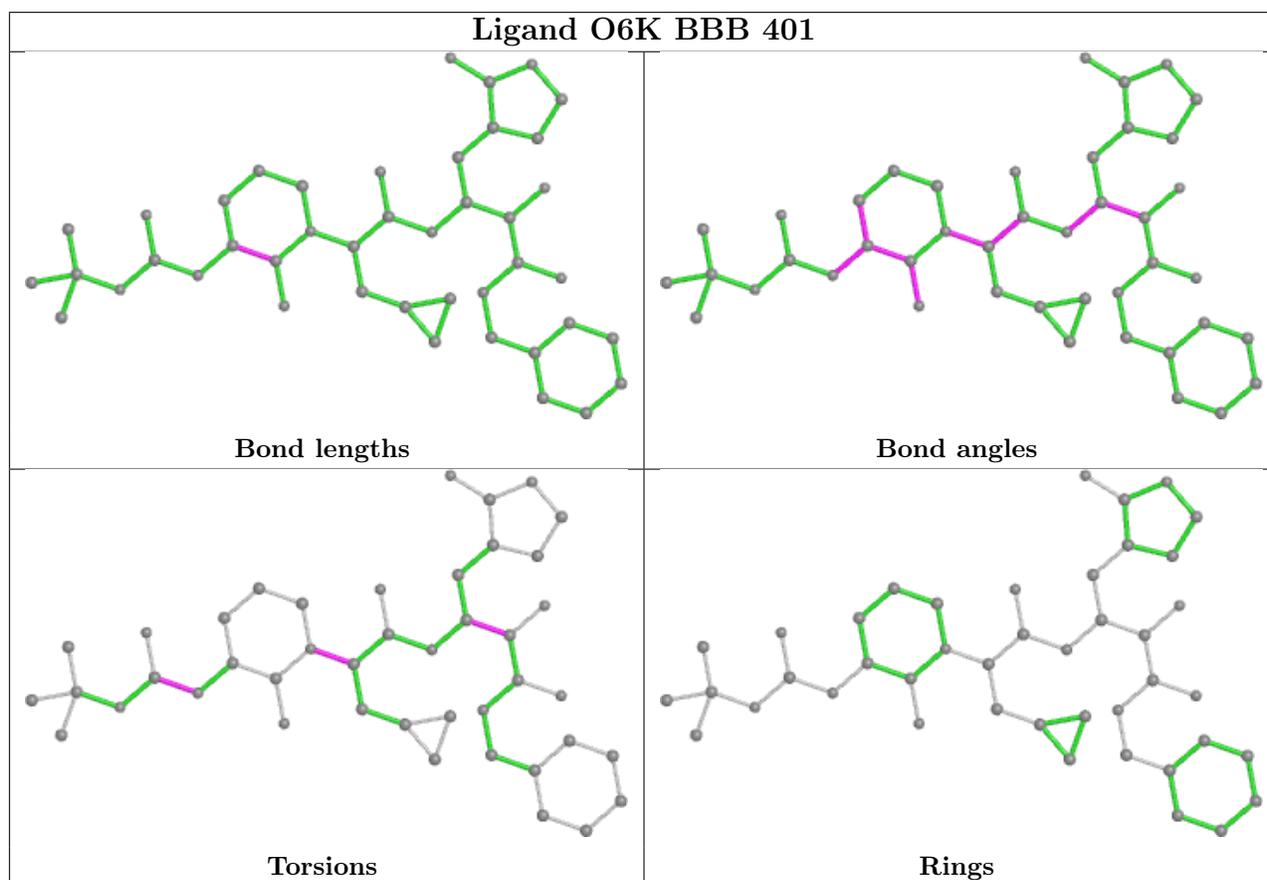
All (8) torsion outliers are listed below:

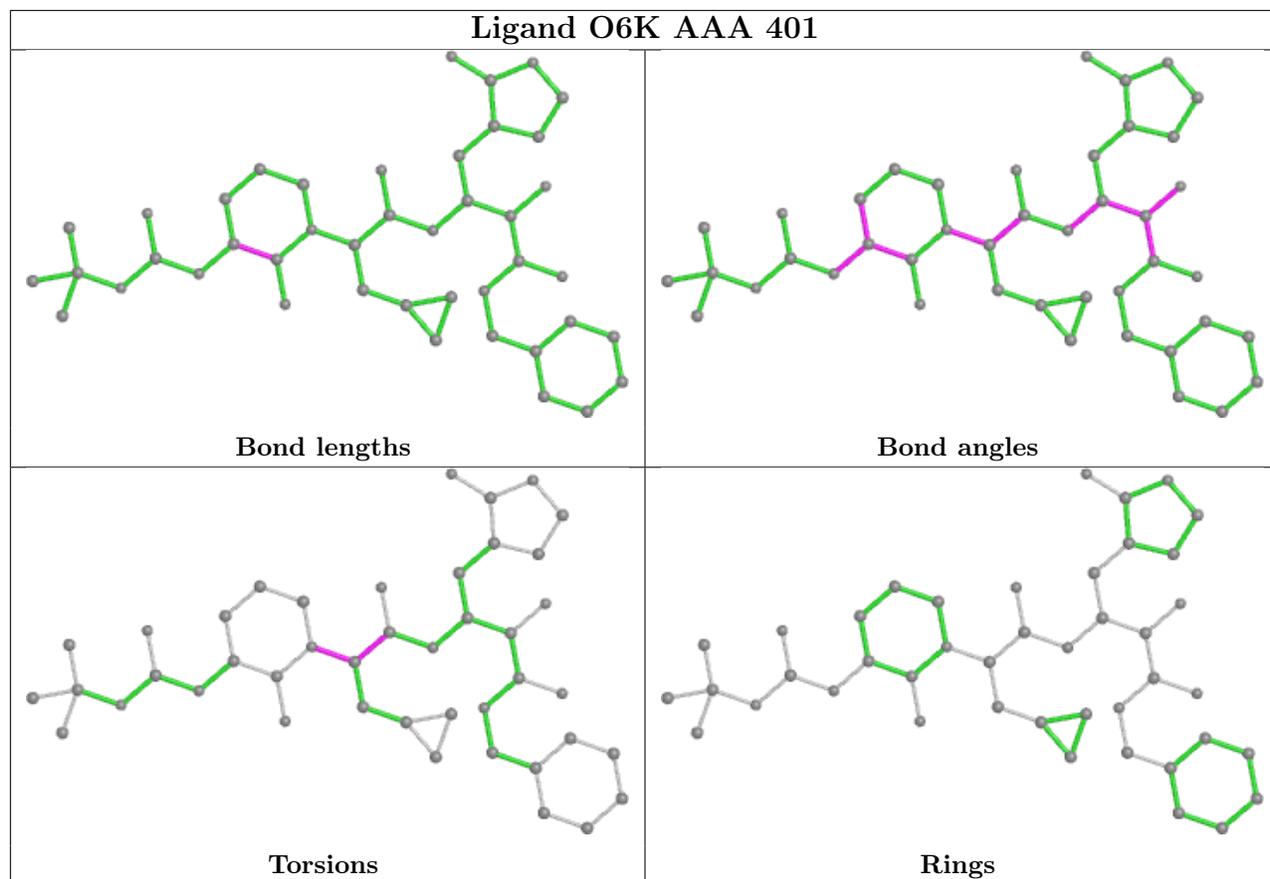
Mol	Chain	Res	Type	Atoms
2	AAA	401	O6K	C22-C20-N15-C21
2	AAA	401	O6K	C22-C20-N15-C16
2	BBB	401	O6K	C22-C20-N15-C16
2	BBB	401	O6K	C22-C20-N15-C21
2	BBB	401	O6K	O25-C24-N23-C19
2	BBB	401	O6K	O26-C24-N23-C19
2	BBB	401	O6K	N38-C40-C57-C35
2	AAA	401	O6K	N15-C20-C36-O37

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	AAA	303/306 (99%)	0.15	8 (2%) 56 60	24, 35, 57, 100	0
1	BBB	306/306 (100%)	0.37	29 (9%) 8 9	24, 40, 76, 111	0
All	All	609/612 (99%)	0.26	37 (6%) 21 23	24, 37, 70, 111	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	303	VAL	10.3
1	AAA	154	TYR	6.8
1	BBB	154	TYR	4.8
1	BBB	50	LEU	4.8
1	BBB	232	LEU	4.3
1	BBB	46	SER	3.8
1	BBB	72	ASN	3.8
1	BBB	45	THR	3.7
1	BBB	226	THR	3.7
1	BBB	235	MET	3.6
1	BBB	227	LEU	3.6
1	AAA	47	GLU	3.5
1	BBB	47	GLU	3.4
1	BBB	64	HIS	3.2
1	BBB	60	ARG	3.1
1	BBB	262	LEU	3.1
1	BBB	59	ILE	3.0
1	BBB	294	PHE	2.9
1	AAA	73	VAL	2.8
1	BBB	255	ALA	2.7
1	BBB	67	LEU	2.6
1	BBB	236	LYS	2.6
1	BBB	245	ASP	2.6
1	BBB	73	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	BBB	306	GLN	2.6
1	BBB	76	ARG	2.5
1	AAA	46	SER	2.5
1	AAA	302	GLY	2.4
1	BBB	251	GLY	2.4
1	BBB	62	SER	2.3
1	AAA	128[A]	CYS	2.2
1	BBB	49	MET	2.2
1	AAA	282	LEU	2.2
1	BBB	230	PHE	2.1
1	BBB	56	ASP	2.0
1	BBB	74	GLN	2.0
1	BBB	21	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

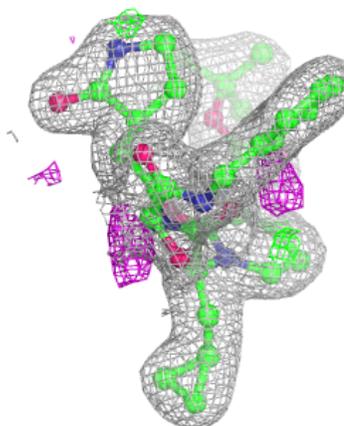
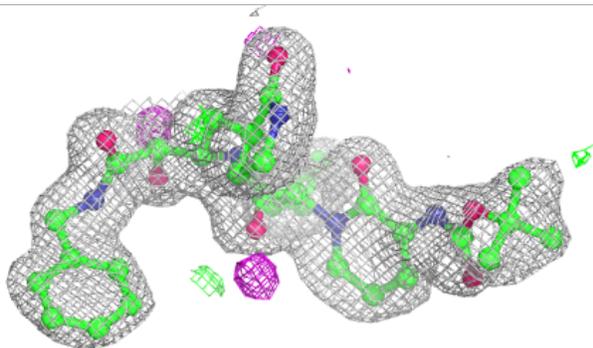
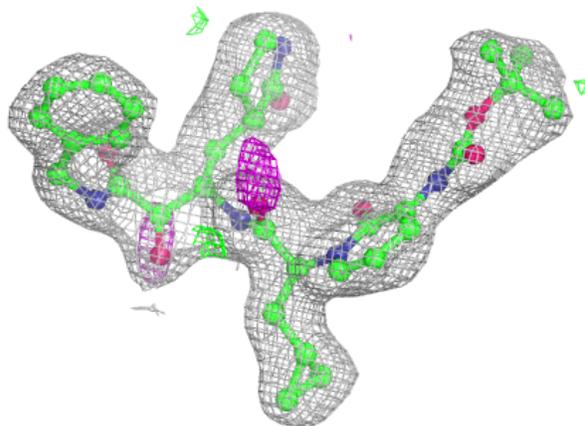
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

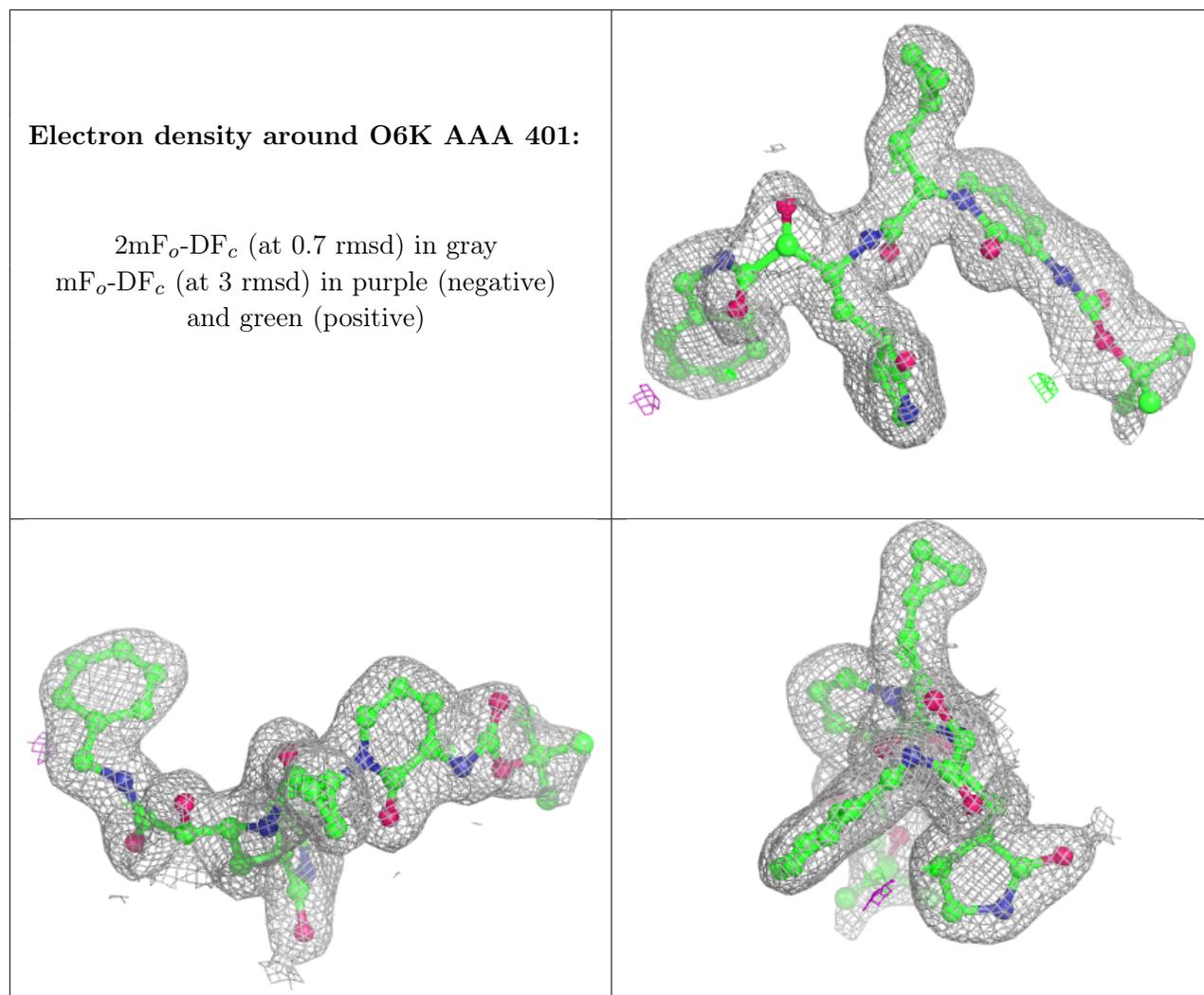
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	O6K	BBB	401	43/43	0.91	0.10	36,45,58,64	0
2	O6K	AAA	401	43/43	0.93	0.09	30,38,61,65	0

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 O6K BBB 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.