



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 12:45 AM JST

PDB ID : 7CBT  
Title : The crystal structure of SARS-CoV-2 main protease in complex with GC376  
Authors : Shi, Y.; Peng, G.  
Deposited on : 2020-06-13  
Resolution : 2.35 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.

The types of validation reports are described at

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

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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 : 2.36  
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

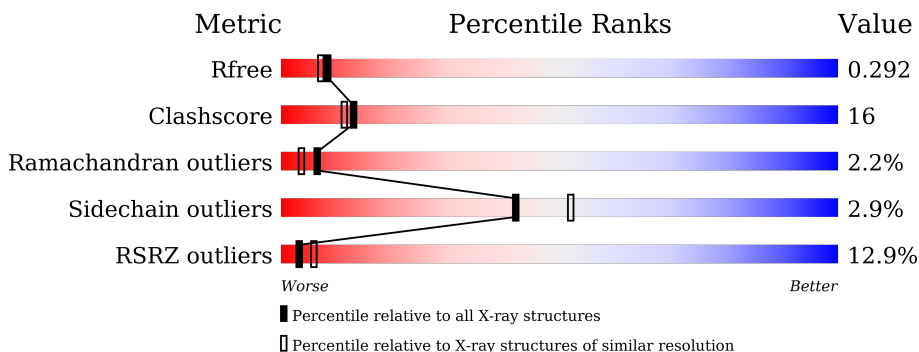
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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  $\geq 3$ , 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	333	
1	B	333	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9428 atoms, of which 4577 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
			Total	C	H	N	O	S			
1	A	298	4567	1460	2259	393	433	22	0	0	0
1	B	298	4566	1460	2258	393	433	22	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

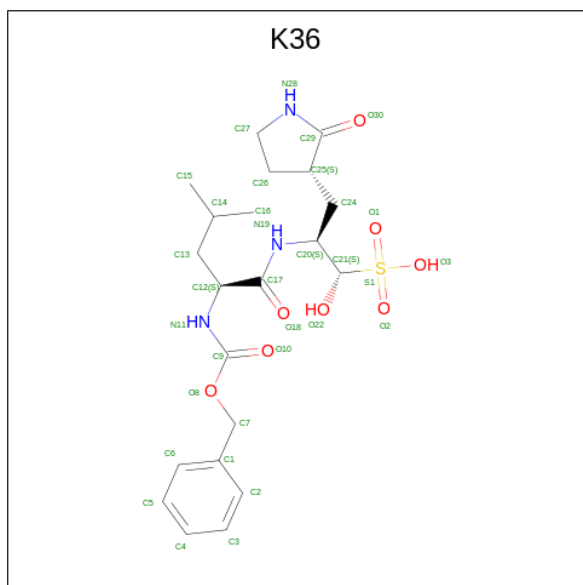
Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP P0DTD1
A	-25	HIS	-	expression tag	UNP P0DTD1
A	-24	HIS	-	expression tag	UNP P0DTD1
A	-23	HIS	-	expression tag	UNP P0DTD1
A	-22	HIS	-	expression tag	UNP P0DTD1
A	-21	HIS	-	expression tag	UNP P0DTD1
A	-20	HIS	-	expression tag	UNP P0DTD1
A	-19	GLY	-	expression tag	UNP P0DTD1
A	-18	LEU	-	expression tag	UNP P0DTD1
A	-17	ASN	-	expression tag	UNP P0DTD1
A	-16	ASP	-	expression tag	UNP P0DTD1
A	-15	ILE	-	expression tag	UNP P0DTD1
A	-14	PHE	-	expression tag	UNP P0DTD1
A	-13	GLU	-	expression tag	UNP P0DTD1
A	-12	ALA	-	expression tag	UNP P0DTD1
A	-11	GLN	-	expression tag	UNP P0DTD1
A	-10	LYS	-	expression tag	UNP P0DTD1
A	-9	ILE	-	expression tag	UNP P0DTD1
A	-8	GLU	-	expression tag	UNP P0DTD1
A	-7	TRP	-	expression tag	UNP P0DTD1
A	-6	HIS	-	expression tag	UNP P0DTD1
A	-5	GLU	-	expression tag	UNP P0DTD1
A	-4	GLY	-	expression tag	UNP P0DTD1
A	-3	GLY	-	expression tag	UNP P0DTD1
A	-2	GLY	-	expression tag	UNP P0DTD1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P0DTD1
A	0	SER	-	expression tag	UNP P0DTD1
B	-26	MET	-	initiating methionine	UNP P0DTD1
B	-25	HIS	-	expression tag	UNP P0DTD1
B	-24	HIS	-	expression tag	UNP P0DTD1
B	-23	HIS	-	expression tag	UNP P0DTD1
B	-22	HIS	-	expression tag	UNP P0DTD1
B	-21	HIS	-	expression tag	UNP P0DTD1
B	-20	HIS	-	expression tag	UNP P0DTD1
B	-19	GLY	-	expression tag	UNP P0DTD1
B	-18	LEU	-	expression tag	UNP P0DTD1
B	-17	ASN	-	expression tag	UNP P0DTD1
B	-16	ASP	-	expression tag	UNP P0DTD1
B	-15	ILE	-	expression tag	UNP P0DTD1
B	-14	PHE	-	expression tag	UNP P0DTD1
B	-13	GLU	-	expression tag	UNP P0DTD1
B	-12	ALA	-	expression tag	UNP P0DTD1
B	-11	GLN	-	expression tag	UNP P0DTD1
B	-10	LYS	-	expression tag	UNP P0DTD1
B	-9	ILE	-	expression tag	UNP P0DTD1
B	-8	GLU	-	expression tag	UNP P0DTD1
B	-7	TRP	-	expression tag	UNP P0DTD1
B	-6	HIS	-	expression tag	UNP P0DTD1
B	-5	GLU	-	expression tag	UNP P0DTD1
B	-4	GLY	-	expression tag	UNP P0DTD1
B	-3	GLY	-	expression tag	UNP P0DTD1
B	-2	GLY	-	expression tag	UNP P0DTD1
B	-1	GLY	-	expression tag	UNP P0DTD1
B	0	SER	-	expression tag	UNP P0DTD1

- Molecule 2 is (1S,2S)-2-({N-[(benzyloxy)carbonyl]-L-leucyl}amino)-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (three-letter code: K36) (formula: C<sub>21</sub>H<sub>31</sub>N<sub>3</sub>O<sub>8</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	59	21	30	3	5	0	0
2	B	1	59	21	30	3	5	0	0

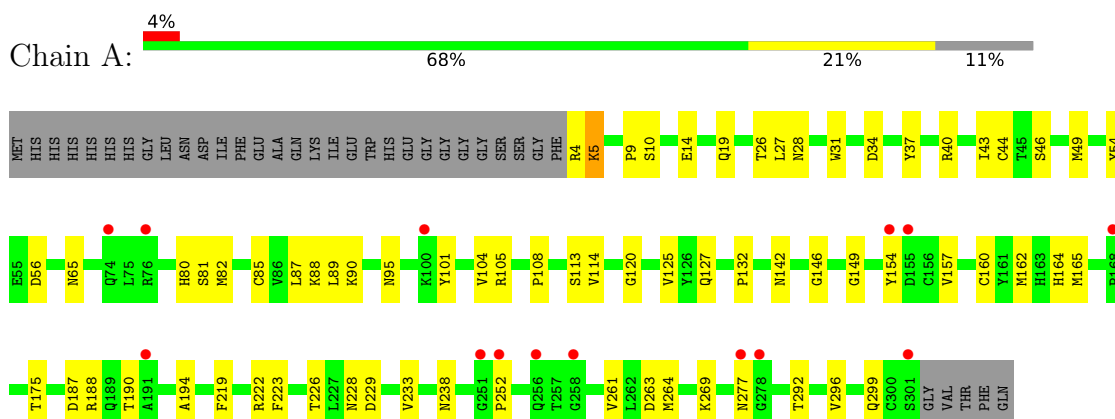
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	99	99	99	0	0
3	B	78	78	78	0	0

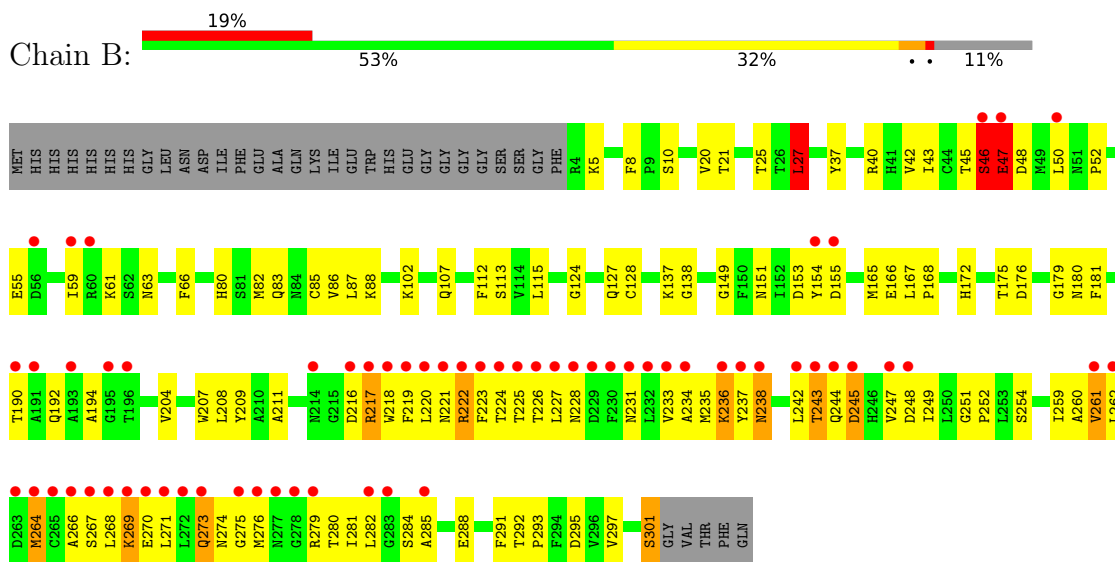
### 3 Residue-property plots [i](#)

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 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.12Å 99.75Å 60.36Å 90.00° 108.63° 90.00°	Depositor
Resolution (Å)	28.15 – 2.35 28.15 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.1 (28.15-2.35) 99.1 (28.15-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.209 , 0.292 0.209 , 0.292	Depositor DCC
$R_{free}$ test set	1991 reflections (7.74%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtrriage
Anisotropy	0.145	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 53.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K36

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	0.66	0/2359	0.84	4/3207 (0.1%)
1	B	0.74	4/2359 (0.2%)	0.87	7/3207 (0.2%)
All	All	0.70	4/4718 (0.1%)	0.85	11/6414 (0.2%)

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	B	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	236	LYS	CE-NZ	-10.94	1.21	1.49
1	B	47	GLU	CB-CG	10.42	1.72	1.52
1	B	128	CYS	CB-SG	-7.29	1.69	1.82
1	B	47	GLU	CD-OE1	-5.21	1.20	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	GLU	CG-CD-OE1	-7.21	103.88	118.30
1	A	187	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	105	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	B	176	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	194	ALA	C-N-CA	-5.36	111.05	122.30
1	B	27	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	B	46	SER	O-C-N	5.27	131.14	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	GLU	CA-CB-CG	5.06	124.53	113.40
1	B	47	GLU	CG-CD-OE2	5.06	128.42	118.30
1	B	242	LEU	CA-CB-CG	-5.05	103.69	115.30
1	A	162	MET	CG-SD-CE	5.04	108.27	100.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	245	ASP	Peptide
1	B	248	ASP	Peptide

## 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	2308	2259	2257	42	1
1	B	2308	2258	2257	112	0
2	A	29	30	29	1	0
2	B	29	30	28	2	0
3	A	99	0	0	7	0
3	B	78	0	0	12	0
All	All	4851	4577	4571	152	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 16.

All (152) 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:B:276:MET:SD	3:B:502:HOH:O	2.21	0.97
1:B:221:ASN:O	3:B:501:HOH:O	1.86	0.93
1:B:46:SER:O	1:B:47:GLU:HB2	1.72	0.87
1:B:285:ALA:O	3:B:502:HOH:O	1.96	0.81
1:B:27:LEU:HD21	1:B:42:VAL:HB	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:THR:OG1	1:B:295:ASP:N	2.17	0.78
1:A:226:THR:HG22	1:A:228:ASN:H	1.50	0.75
1:B:281:ILE:HG22	1:B:282:LEU:HG	1.69	0.74
1:A:229:ASP:OD1	3:A:501:HOH:O	2.07	0.71
1:B:102:LYS:NZ	3:B:505:HOH:O	2.24	0.70
1:B:217:ARG:HH21	1:B:220:LEU:HD22	1.57	0.70
1:B:218:TRP:CE2	1:B:279:ARG:HG2	2.26	0.69
1:B:244:GLN:HA	1:B:247:VAL:CG2	2.26	0.66
1:B:261:VAL:O	1:B:264:MET:HB3	1.98	0.63
1:A:219:PHE:HE2	1:A:264:MET:HE1	1.63	0.63
1:B:218:TRP:CZ2	1:B:279:ARG:CG	2.83	0.62
1:B:266:ALA:HA	1:B:269:LYS:HD3	1.80	0.62
1:B:271:LEU:HD22	1:B:276:MET:HG3	1.83	0.60
1:A:80:HIS:NE2	3:A:505:HOH:O	2.31	0.60
1:B:107:GLN:NE2	3:B:503:HOH:O	2.17	0.60
1:B:271:LEU:CD2	1:B:276:MET:HG3	2.31	0.60
1:B:180:ASN:ND2	3:B:511:HOH:O	2.34	0.59
1:A:188:ARG:HG2	1:A:190:THR:HG22	1.85	0.59
1:A:88:LYS:NZ	3:A:507:HOH:O	2.35	0.58
1:B:61:LYS:NZ	3:B:506:HOH:O	2.24	0.58
1:B:244:GLN:HA	1:B:247:VAL:HG23	1.85	0.58
1:B:261:VAL:HB	1:B:262:LEU:CD1	2.33	0.58
1:B:243:THR:OG1	1:B:244:GLN:N	2.36	0.58
1:B:218:TRP:CZ2	1:B:279:ARG:HG2	2.38	0.58
1:B:40:ARG:O	1:B:43:ILE:HG12	2.04	0.58
1:B:260:ALA:O	1:B:262:LEU:N	2.37	0.58
1:A:113:SER:HB3	1:A:127:GLN:OE1	2.04	0.57
1:A:299:GLN:O	1:A:299:GLN:HG2	2.06	0.56
1:B:217:ARG:NH2	1:B:220:LEU:HD22	2.19	0.56
1:B:261:VAL:HB	1:B:262:LEU:HD12	1.86	0.56
1:B:270:GLU:HA	1:B:273:GLN:HB3	1.89	0.55
1:B:219:PHE:HD1	1:B:267:SER:HB3	1.72	0.55
1:B:244:GLN:O	1:B:244:GLN:HG3	2.07	0.55
1:B:228:ASN:OD1	3:B:504:HOH:O	2.18	0.54
1:A:10:SER:OG	1:A:14:GLU:OE2	2.20	0.53
1:B:224:THR:HG22	1:B:225:THR:N	2.24	0.53
1:B:217:ARG:HG3	1:B:220:LEU:HD22	1.91	0.53
1:B:207:TRP:CH2	1:B:281:ILE:HB	2.44	0.53
1:B:249:ILE:HG23	1:B:293:PRO:HG2	1.90	0.53
1:A:226:THR:HG22	1:A:228:ASN:N	2.20	0.52
1:A:44:CYS:HB3	1:A:49:MET:HG3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:ND2	3:A:512:HOH:O	2.43	0.52
1:A:142:ASN:OD1	3:A:502:HOH:O	2.19	0.52
1:A:4:ARG:NH2	1:B:127:GLN:O	2.43	0.52
1:B:268:LEU:HB3	3:B:519:HOH:O	2.10	0.52
1:A:40:ARG:HD3	1:A:85:CYS:HA	1.91	0.51
1:B:55:GLU:O	1:B:59:ILE:HG12	2.10	0.51
1:B:209:TYR:CD1	1:B:264:MET:HE2	2.45	0.51
1:B:269:LYS:N	1:B:269:LYS:HD2	2.24	0.51
1:B:66:PHE:CE1	1:B:87:LEU:HD21	2.46	0.51
1:B:234:ALA:O	1:B:237:TYR:N	2.43	0.51
1:B:270:GLU:HA	1:B:273:GLN:CB	2.41	0.51
1:B:113:SER:O	1:B:149:GLY:HA2	2.10	0.50
1:B:231:ASN:O	1:B:235:MET:HB2	2.11	0.50
1:A:101:TYR:HA	1:A:157:VAL:O	2.11	0.50
1:B:175:THR:HG22	1:B:181:PHE:HA	1.92	0.50
1:B:218:TRP:CH2	1:B:281:ILE:HG13	2.46	0.50
1:B:279:ARG:HG3	1:B:280:THR:N	2.27	0.50
1:A:120:GLY:O	3:A:503:HOH:O	2.20	0.50
1:B:40:ARG:HD3	1:B:85:CYS:HA	1.93	0.50
1:B:279:ARG:HG3	1:B:280:THR:H	1.76	0.50
1:B:288:GLU:HG2	1:B:291:PHE:CE2	2.47	0.50
1:A:9:PRO:HD3	1:B:124:GLY:HA2	1.93	0.50
1:B:222:ARG:HA	1:B:222:ARG:HE	1.77	0.49
1:B:45:THR:O	1:B:47:GLU:N	2.45	0.49
1:B:204:VAL:HG11	1:B:268:LEU:CD1	2.42	0.49
1:B:218:TRP:CZ2	1:B:279:ARG:HG3	2.47	0.49
1:B:292:THR:HG23	1:B:295:ASP:OD2	2.12	0.49
1:B:48:ASP:O	1:B:52:PRO:HB3	2.12	0.49
1:A:108:PRO:HB3	1:A:132:PRO:HA	1.95	0.49
1:A:164:HIS:CD2	1:A:175:THR:HG23	2.48	0.49
1:A:104:VAL:HG23	1:A:160:CYS:HB3	1.95	0.49
1:B:165:MET:CG	2:B:401:K36:H10	2.43	0.49
1:B:233:VAL:O	1:B:237:TYR:CD2	2.66	0.49
1:A:40:ARG:O	1:A:43:ILE:HG12	2.13	0.48
1:B:208:LEU:O	1:B:211:ALA:HB3	2.13	0.48
1:B:262:LEU:N	1:B:262:LEU:HD12	2.28	0.48
1:A:299:GLN:O	1:A:299:GLN:CG	2.60	0.48
1:B:20:VAL:HB	1:B:27:LEU:HD12	1.94	0.48
1:A:219:PHE:CE2	1:A:264:MET:HE1	2.45	0.48
1:B:217:ARG:NH2	1:B:220:LEU:CD2	2.76	0.48
1:A:223:PHE:O	1:A:263:ASP:OD1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:C	1:B:236:LYS:N	2.66	0.48
1:B:151:ASN:ND2	3:B:518:HOH:O	2.45	0.48
1:B:112:PHE:CD2	1:B:149:GLY:HA3	2.49	0.47
1:A:40:ARG:HD2	1:A:82:MET:HE2	1.96	0.47
1:B:269:LYS:HD2	3:B:519:HOH:O	2.13	0.47
1:B:276:MET:SD	1:B:285:ALA:O	2.73	0.47
1:B:222:ARG:HA	1:B:222:ARG:NE	2.29	0.46
1:A:34:ASP:OD2	1:A:90:LYS:HE2	2.15	0.46
1:A:165:MET:HG2	2:A:401:K36:H11	1.97	0.46
1:B:244:GLN:HA	1:B:247:VAL:HG21	1.98	0.46
1:A:40:ARG:CD	1:A:85:CYS:HA	2.46	0.46
1:B:251:GLY:N	1:B:252:PRO:CD	2.79	0.46
1:A:31:TRP:CE2	1:A:95:ASN:HB2	2.51	0.45
1:A:292:THR:O	1:A:296:VAL:HG23	2.16	0.45
1:B:37:TYR:N	1:B:37:TYR:CD1	2.84	0.45
1:B:211:ALA:HA	1:B:282:LEU:HD21	1.98	0.45
1:B:226:THR:OG1	1:B:227:LEU:N	2.47	0.45
1:B:288:GLU:HG2	1:B:291:PHE:HE2	1.82	0.45
1:B:218:TRP:CE3	1:B:219:PHE:N	2.85	0.44
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.99	0.44
1:A:87:LEU:HD21	1:A:89:LEU:HD21	2.00	0.44
1:A:233:VAL:HG21	1:A:269:LYS:HE2	2.00	0.44
1:B:280:THR:OG1	1:B:284:SER:C	2.55	0.44
1:B:234:ALA:O	1:B:238:ASN:N	2.51	0.44
1:B:20:VAL:HB	1:B:27:LEU:CD1	2.48	0.43
1:B:40:ARG:HD2	1:B:82:MET:SD	2.57	0.43
1:A:46:SER:HA	1:A:49:MET:HE2	2.01	0.43
1:B:47:GLU:HA	1:B:50:LEU:CD1	2.48	0.43
1:B:83:GLN:OE1	1:B:88:LYS:NZ	2.47	0.43
1:B:243:THR:OG1	1:B:245:ASP:N	2.49	0.43
1:B:10:SER:HB2	1:B:115:LEU:HD13	2.00	0.43
1:B:5:LYS:NZ	1:B:288:GLU:OE1	2.49	0.43
1:B:231:ASN:O	1:B:235:MET:CB	2.67	0.42
1:A:31:TRP:CD2	1:A:95:ASN:HB2	2.55	0.42
1:B:21:THR:HG23	1:B:25:THR:O	2.18	0.42
1:B:138:GLY:H	1:B:172:HIS:HD2	1.66	0.42
1:B:204:VAL:CG1	1:B:268:LEU:HD13	2.49	0.42
1:B:218:TRP:CE2	1:B:279:ARG:CG	3.01	0.42
1:B:254:SER:HB2	1:B:259:ILE:O	2.19	0.42
1:B:8:PHE:HE2	1:B:151:ASN:HD22	1.67	0.42
1:B:209:TYR:HA	1:B:264:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:TRP:HZ2	1:B:280:THR:C	2.23	0.42
1:B:83:GLN:OE1	1:B:88:LYS:HE2	2.20	0.42
1:B:45:THR:HG23	1:B:48:ASP:H	1.85	0.42
1:B:224:THR:HG22	1:B:225:THR:H	1.83	0.42
1:B:233:VAL:O	1:B:237:TYR:HD2	2.03	0.42
1:B:228:ASN:HA	3:B:504:HOH:O	2.18	0.42
1:B:190:THR:O	1:B:192:GLN:HG3	2.20	0.42
1:B:218:TRP:CH2	1:B:281:ILE:CG1	3.02	0.42
1:B:166:GLU:HB2	2:B:401:K36:C29	2.50	0.41
1:B:297:VAL:O	1:B:301:SER:HB3	2.20	0.41
1:A:114:VAL:O	1:A:125:VAL:HA	2.20	0.41
1:B:167:LEU:HB3	1:B:168:PRO:CD	2.50	0.41
1:B:222:ARG:O	1:B:223:PHE:CG	2.74	0.41
1:A:238:ASN:ND2	3:A:521:HOH:O	2.52	0.41
1:A:28:ASN:O	1:A:146:GLY:HA3	2.21	0.41
1:A:54:TYR:HB3	1:A:82:MET:CE	2.51	0.41
1:A:113:SER:O	1:A:149:GLY:HA2	2.21	0.41
1:B:204:VAL:HG11	1:B:268:LEU:HD11	2.03	0.41
1:B:225:THR:HG21	1:B:269:LYS:NZ	2.36	0.41
1:B:63:ASN:OD1	1:B:80:HIS:ND1	2.47	0.41
1:B:270:GLU:O	1:B:270:GLU:HG3	2.21	0.41
1:A:5:LYS:HG2	1:A:127:GLN:HB2	2.02	0.40
1:B:204:VAL:HG11	1:B:268:LEU:HD13	2.03	0.40
1:A:19:GLN:HE21	1:A:26:THR:HG21	1.87	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)
1:A:56:ASP:OD1	1:A:222:ARG:NH2[1_656]	1.98	0.22

## 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	A	296/333 (89%)	279 (94%)	12 (4%)	5 (2%)	9	6
1	B	296/333 (89%)	265 (90%)	23 (8%)	8 (3%)	5	2
All	All	592/666 (89%)	544 (92%)	35 (6%)	13 (2%)	6	4

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	46	SER
1	B	243	THR
1	B	47	GLU
1	B	261	VAL
1	A	154	TYR
1	A	261	VAL
1	A	277	ASN
1	B	238	ASN
1	B	194	ALA
1	B	274	ASN
1	A	81	SER
1	A	252	PRO
1	B	275	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	A	257/284 (90%)	254 (99%)	3 (1%)	71	82
1	B	257/284 (90%)	245 (95%)	12 (5%)	26	33
All	All	514/568 (90%)	499 (97%)	15 (3%)	42	52

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS

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Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	TYR
1	B	27	LEU
1	B	137	LYS
1	B	153	ASP
1	B	154	TYR
1	B	155	ASP
1	B	216	ASP
1	B	217	ARG
1	B	222	ARG
1	B	264	MET
1	B	269	LYS
1	B	273	GLN
1	B	301	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	192	GLN

### 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	K36	B	401	1	30,30,34	3.67	10 (33%)	37,39,47	2.10	12 (32%)
2	K36	A	401	1	30,30,34	3.90	11 (36%)	37,39,47	2.03	11 (29%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	K36	B	401	1	-	3/27/37/45	0/2/2/2
2	K36	A	401	1	-	6/27/37/45	0/2/2/2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	K36	C29-N28	17.11	1.51	1.33
2	B	401	K36	C29-N28	16.39	1.51	1.33
2	A	401	K36	C17-N19	6.43	1.48	1.34
2	A	401	K36	C9-N11	5.60	1.48	1.34
2	B	401	K36	C17-N19	5.41	1.45	1.34
2	B	401	K36	C25-C29	-5.02	1.46	1.52
2	A	401	K36	C25-C29	-5.02	1.46	1.52
2	B	401	K36	C9-N11	4.26	1.45	1.34
2	B	401	K36	C26-C27	-3.47	1.47	1.53
2	A	401	K36	C26-C27	-3.45	1.47	1.53
2	A	401	K36	O8-C9	3.44	1.41	1.35
2	B	401	K36	O8-C9	3.20	1.41	1.35
2	B	401	K36	C27-N28	2.98	1.52	1.46
2	A	401	K36	C24-C25	2.77	1.60	1.53
2	B	401	K36	O30-C29	-2.73	1.18	1.23
2	A	401	K36	C27-N28	2.62	1.51	1.46
2	A	401	K36	O30-C29	-2.34	1.18	1.23
2	A	401	K36	O8-C7	-2.26	1.41	1.45
2	B	401	K36	O8-C7	-2.07	1.41	1.45
2	A	401	K36	O18-C17	-2.02	1.19	1.23
2	B	401	K36	C24-C25	2.01	1.58	1.53



All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	K36	O8-C9-N11	5.79	122.27	110.50
2	B	401	K36	C24-C20-C21	4.62	118.08	111.65
2	B	401	K36	O10-C9-N11	-4.53	117.42	124.85
2	B	401	K36	O8-C9-N11	4.46	119.57	110.50
2	A	401	K36	O8-C9-O10	-4.11	116.36	124.25
2	A	401	K36	C27-N28-C29	-3.86	106.25	113.84
2	A	401	K36	C7-O8-C9	-3.80	107.45	115.93
2	B	401	K36	C26-C25-C29	3.65	107.63	102.88
2	B	401	K36	O18-C17-N19	-3.43	116.57	122.93
2	B	401	K36	O18-C17-C12	3.37	127.54	120.45
2	B	401	K36	C21-C20-N19	-3.16	102.52	109.60
2	B	401	K36	C27-N28-C29	-3.08	107.78	113.84
2	B	401	K36	C26-C27-N28	2.99	107.81	103.43
2	A	401	K36	C24-C25-C26	-2.72	107.32	117.31
2	A	401	K36	C26-C25-C29	2.66	106.34	102.88
2	A	401	K36	C26-C27-N28	2.66	107.32	103.43
2	A	401	K36	C21-C20-N19	-2.59	103.79	109.60
2	B	401	K36	C20-N19-C17	-2.54	119.15	123.20
2	B	401	K36	C14-C13-C12	-2.36	108.94	115.43
2	A	401	K36	C14-C13-C12	-2.33	109.02	115.43
2	A	401	K36	C13-C12-N11	2.33	115.94	110.58
2	B	401	K36	C12-N11-C9	-2.19	115.55	120.90
2	A	401	K36	O10-C9-N11	-2.13	121.35	124.85

There are no chirality outliers.

All (9) torsion outliers are listed below:

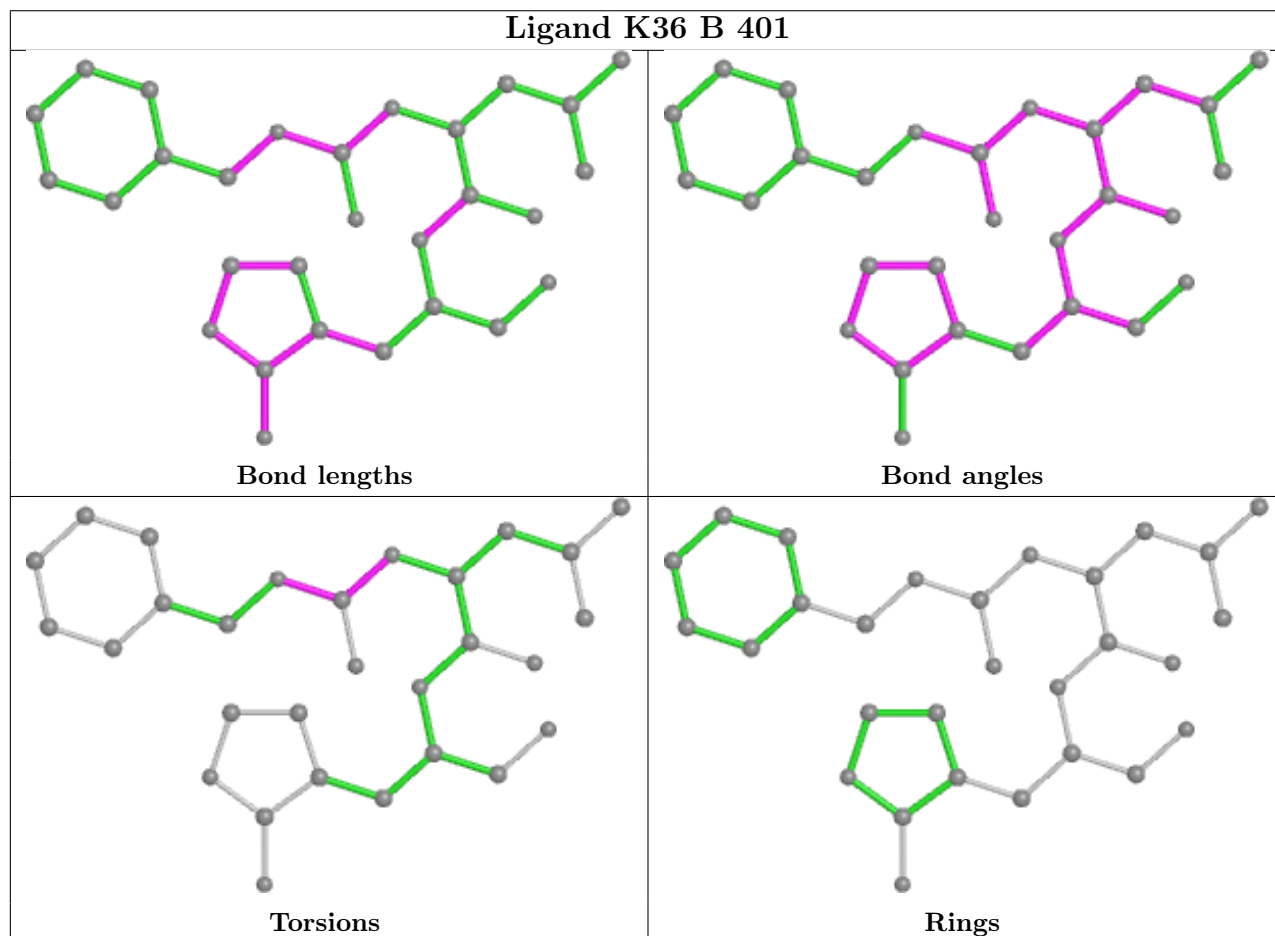
Mol	Chain	Res	Type	Atoms
2	A	401	K36	O10-C9-O8-C7
2	A	401	K36	N11-C9-O8-C7
2	B	401	K36	N11-C9-O8-C7
2	A	401	K36	N11-C12-C13-C14
2	A	401	K36	N19-C20-C21-O22
2	A	401	K36	C24-C20-C21-O22
2	B	401	K36	O10-C9-O8-C7
2	B	401	K36	O8-C9-N11-C12
2	A	401	K36	C17-C12-C13-C14

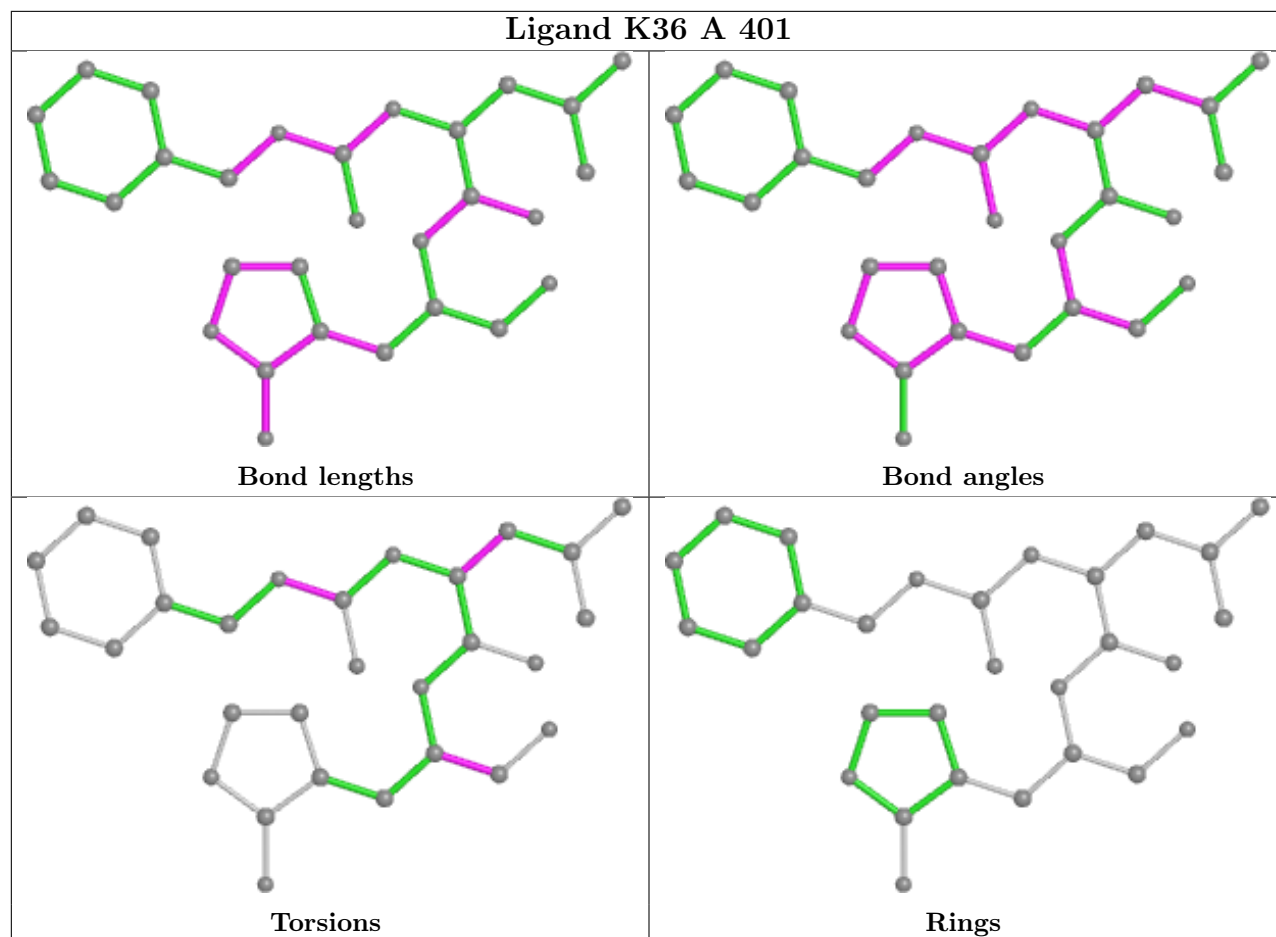
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	K36	2	0
2	A	401	K36	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 [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, 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	298/333 (89%)	0.44	14 (4%) 31 42	18, 37, 58, 91	0
1	B	298/333 (89%)	1.17	63 (21%) 1 1	22, 39, 121, 183	0
All	All	596/666 (89%)	0.81	77 (12%) 3 6	18, 38, 107, 183	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	PHE	9.6
1	B	283	GLY	9.1
1	B	232	LEU	8.8
1	B	223	PHE	8.5
1	B	272	LEU	7.8
1	B	271	LEU	7.7
1	B	277	ASN	7.7
1	A	278	GLY	7.3
1	B	224	THR	7.2
1	B	218	TRP	6.8
1	A	154	TYR	6.4
1	B	279	ARG	5.9
1	B	268	LEU	5.9
1	A	155	ASP	5.9
1	B	244	GLN	5.7
1	B	154	TYR	5.6
1	B	285	ALA	5.5
1	B	278	GLY	5.5
1	B	237	TYR	5.1
1	B	193	ALA	5.0
1	B	234	ALA	5.0
1	B	266	ALA	5.0
1	B	216	ASP	4.9
1	B	222	ARG	4.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	220	LEU	4.7
1	B	221	ASN	4.7
1	B	267	SER	4.7
1	B	270	GLU	4.5
1	B	233	VAL	4.3
1	B	276	MET	4.3
1	A	252	PRO	4.2
1	B	248	ASP	4.2
1	B	242	LEU	4.1
1	A	277	ASN	4.1
1	B	196	THR	4.1
1	B	226	THR	4.0
1	B	264	MET	3.9
1	B	229	ASP	3.9
1	B	275	GLY	3.8
1	B	227	LEU	3.8
1	B	47	GLU	3.8
1	B	214	ASN	3.7
1	A	251	GLY	3.6
1	B	262	LEU	3.6
1	B	219	PHE	3.4
1	B	225	THR	3.4
1	B	247	VAL	3.3
1	B	263	ASP	3.2
1	B	236	LYS	3.2
1	A	301	SER	3.0
1	B	190	THR	3.0
1	B	191	ALA	3.0
1	B	265	CYS	3.0
1	A	191	ALA	2.9
1	B	217	ARG	2.9
1	B	46	SER	2.9
1	B	243	THR	2.8
1	B	238	ASN	2.8
1	B	228	ASN	2.6
1	B	245	ASP	2.6
1	B	261	VAL	2.6
1	B	273	GLN	2.5
1	B	59	ILE	2.5
1	A	168	PRO	2.5
1	A	258	GLY	2.5
1	B	282	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	74	GLN	2.5
1	B	155	ASP	2.5
1	B	56	ASP	2.4
1	B	60	ARG	2.4
1	A	256	GLN	2.3
1	A	76	ARG	2.2
1	B	195	GLY	2.2
1	B	50	LEU	2.2
1	B	231	ASN	2.1
1	B	269	LYS	2.1
1	A	100	LYS	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](#)

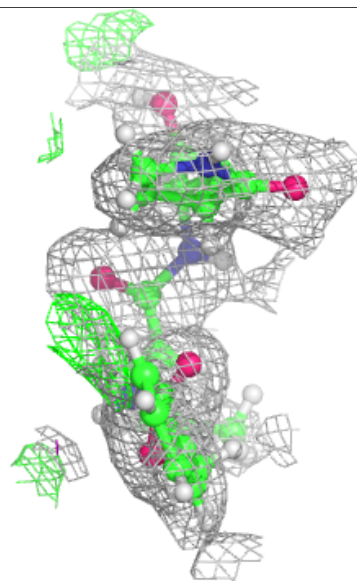
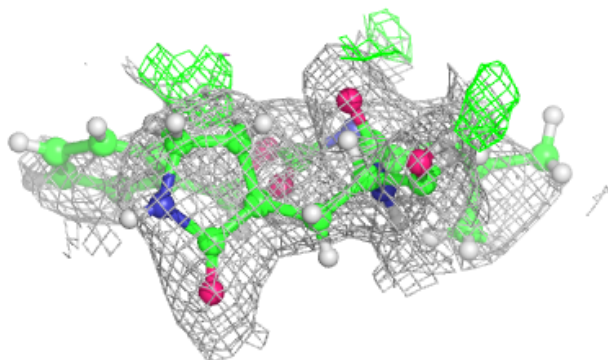
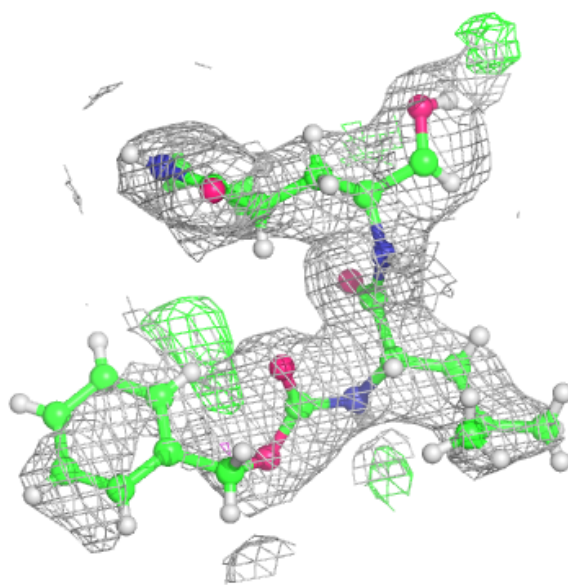
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

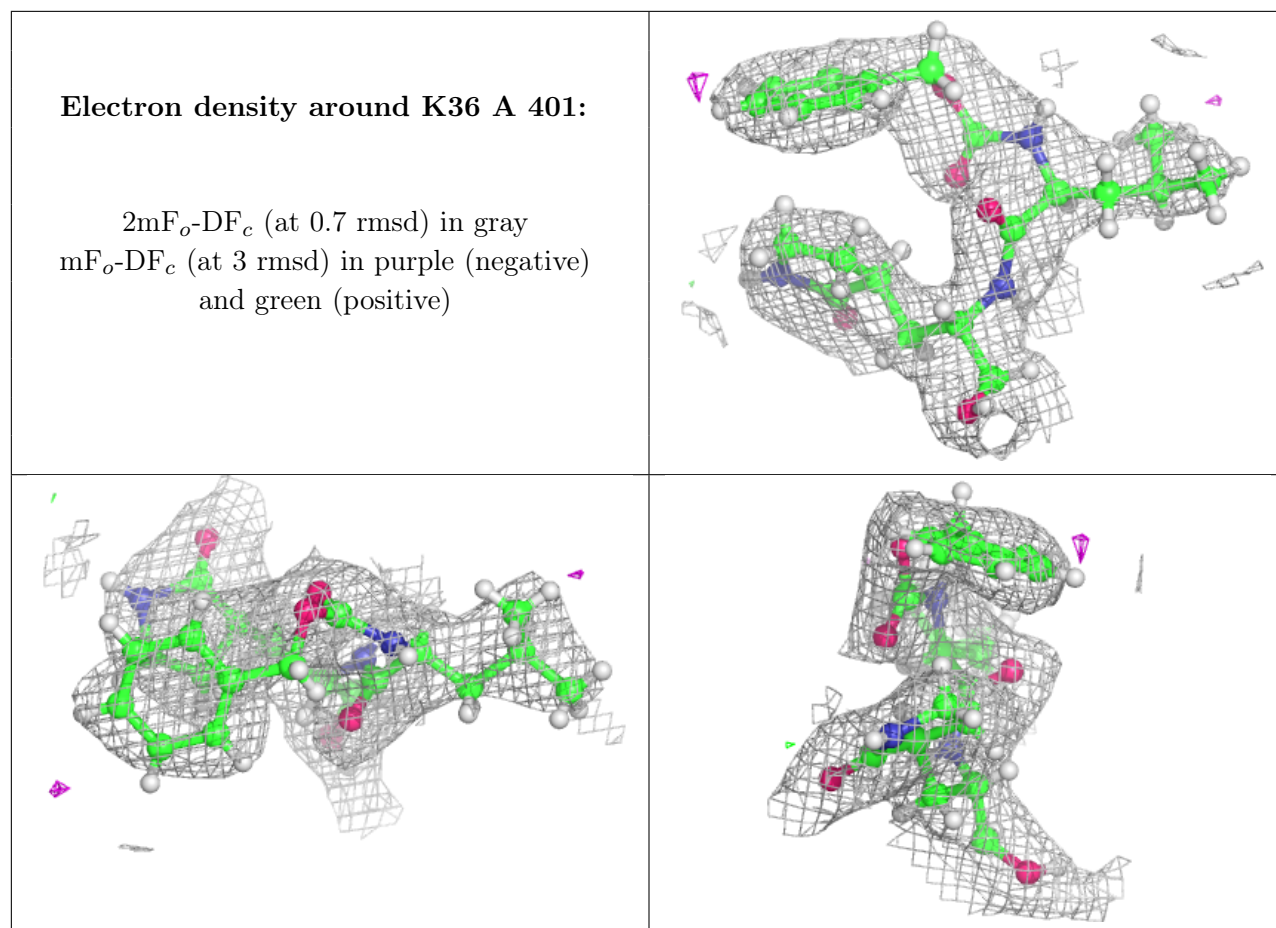
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	K36	B	401	29/33	0.88	0.21	25,46,77,88	0
2	K36	A	401	29/33	0.93	0.14	21,39,58,68	0

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 K36 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.