



# Full wwPDB X-ray Structure Validation Report i

Jan 23, 2024 – 04:28 pm GMT

PDB ID : 8Q71  
Title : Crystal structure of SARS-CoV-2 main protease (MPro) in complex with the inhibitor GC-67  
Authors : Strater, N.; Muller, C.E.; Sylvester, K.; Weisse, R.H.; Useini, A.; Gao, S.; Song, L.; Liu, Z.; Zhan, P.  
Deposited on : 2023-08-15  
Resolution : 2.32 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 i 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](#) ①) 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

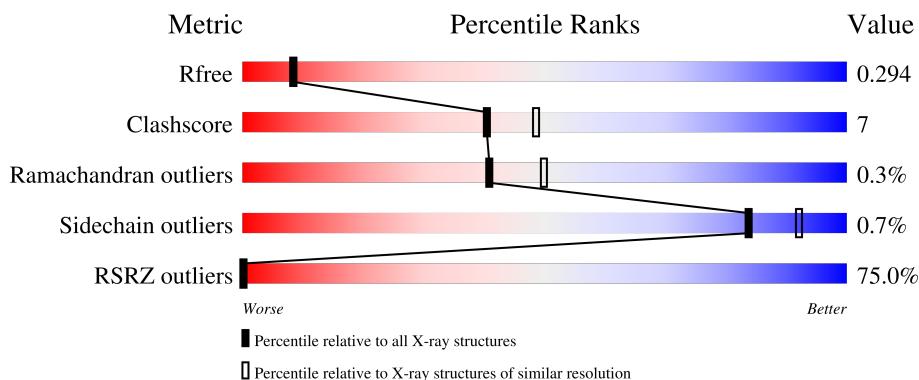
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

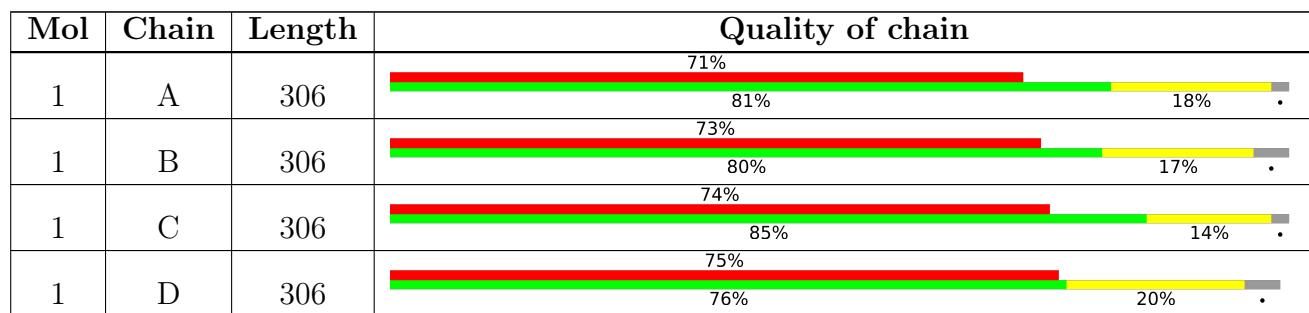
The reported resolution of this entry is 2.32 Å.

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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 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.



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	KKO	D	401	-	-	-	X

## 2 Entry composition [\(i\)](#)

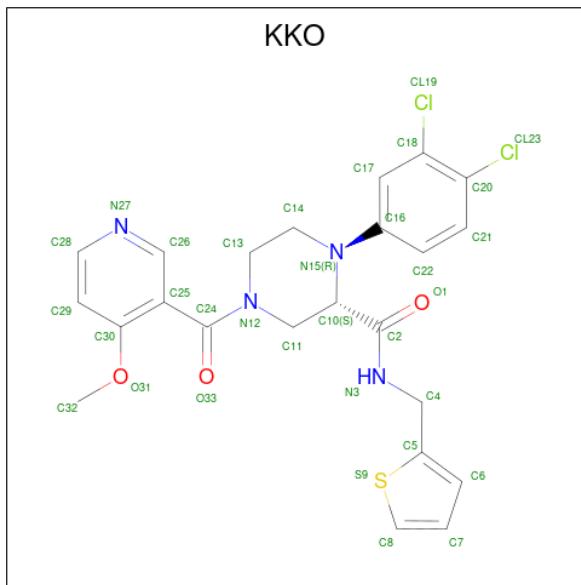
There are 3 unique types of molecules in this entry. The entry contains 18767 atoms, of which 9190 are hydrogens and 0 are deuteriums.

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
1	A	301	Total 4627	C 1488	H 2277	N 398	O 441	S 23	0	12	0
1	B	295	Total 4554	C 1456	H 2254	N 393	O 430	S 21	0	11	0
1	C	301	Total 4659	C 1498	H 2295	N 400	O 444	S 22	0	13	0
1	D	293	Total 4594	C 1467	H 2276	N 395	O 435	S 21	0	15	0

- Molecule 2 is (2 {S})-1-(3,4-dichlorophenyl)-4-(4-methoxypyridin-3-yl)carbonyl- {N }-(thiophen-2-ylmethyl)piperazine-2-carboxamide (three-letter code: KKO) (formula: C<sub>23</sub>H<sub>22</sub>Cl<sub>2</sub>N<sub>4</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
2	A	1	Total 55	C 23	Cl 2	H 22	N 4	O 3	S 1	0	0

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Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	B	1	Total	C	Cl	H	N	O	S	0	0
			55	23	2	22	4	3	1		
2	C	1	Total	C	Cl	H	N	O	S	0	0
			55	23	2	22	4	3	1		
2	D	1	Total	C	Cl	H	N	O	S	0	0
			55	23	2	22	4	3	1		

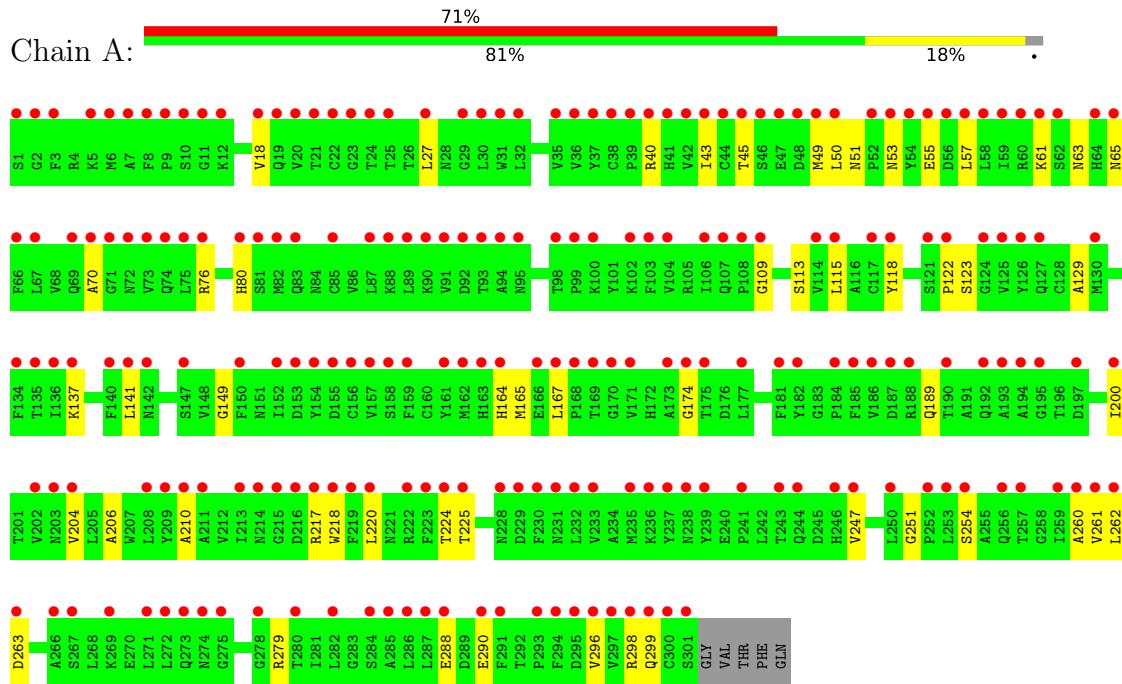
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		
3	B	27	Total	O	0	0
			27	27		
3	C	35	Total	O	0	0
			35	35		
3	D	24	Total	O	0	0
			24	24		

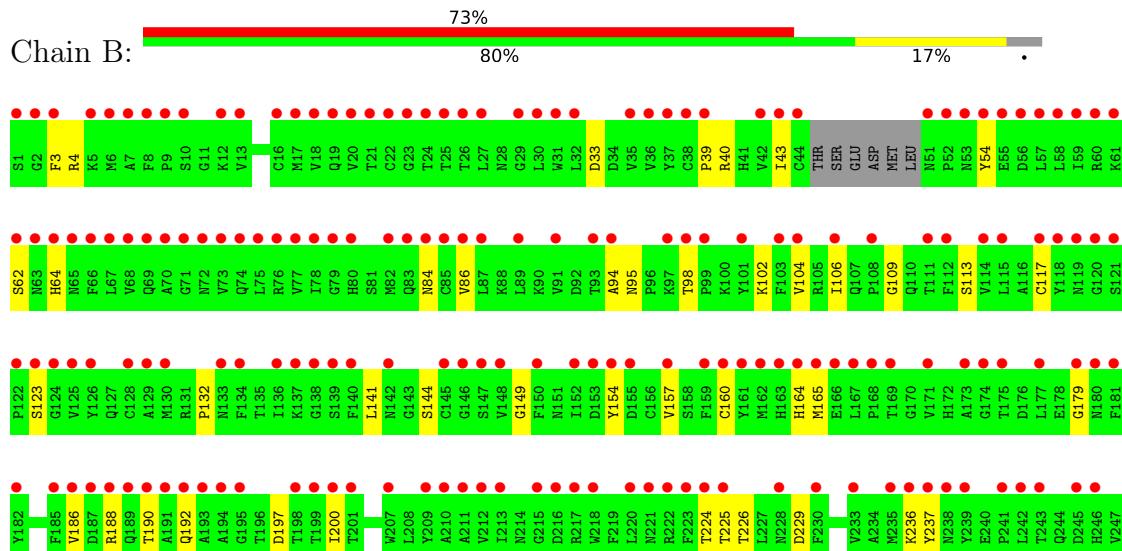
### 3 Residue-property plots

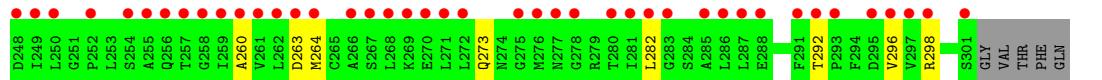
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

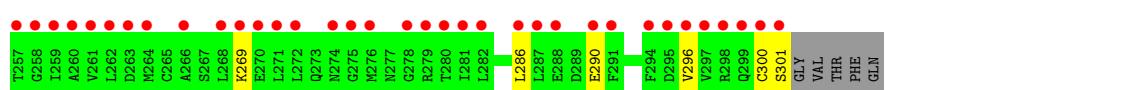
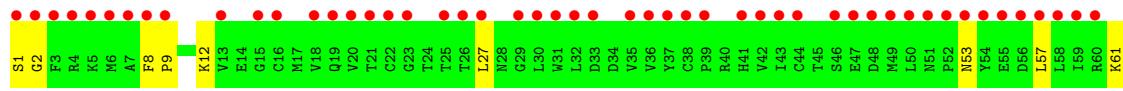
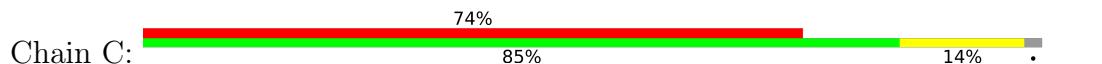


- Molecule 1: 3C-like proteinase nsp5

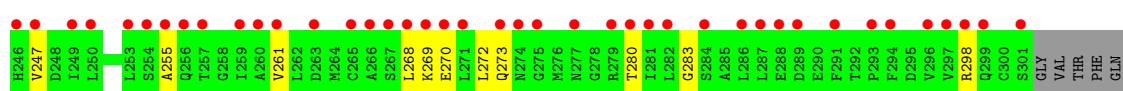
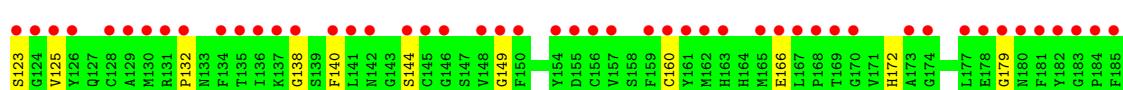




- Molecule 1: 3C-like proteinase nsp5



- Molecule 1: 3C-like proteinase nsp5



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.30 Å    211.63 Å    62.95 Å 90.00°    110.67°    90.00°	Depositor
Resolution (Å)	105.80 – 2.32 105.82 – 2.32	Depositor EDS
% Data completeness (in resolution range)	67.5 (105.80-2.32) 67.4 (105.82-2.32)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	15.12 (at 2.32 Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ????)	Depositor
$R$ , $R_{free}$	0.227 , 0.290 0.232 , 0.294	Depositor DCC
$R_{free}$ test set	1609 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 19.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.369 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	18767	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.85% 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: KKO

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	0.29	0/2479	0.58	0/3369
1	B	0.30	0/2425	0.58	0/3295
1	C	0.29	0/2494	0.55	0/3390
1	D	0.29	0/2442	0.56	0/3317
All	All	0.29	0/9840	0.57	0/13371

There are no bond length outliers.

There are no bond angle outliers.

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	2350	2277	2226	40	2
1	B	2300	2254	2171	33	2
1	C	2364	2295	2236	31	2
1	D	2318	2276	2190	43	2
2	A	33	22	0	0	0
2	B	33	22	0	1	0
2	C	33	22	0	1	0
2	D	33	22	0	0	0
3	A	27	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	0	2	0
3	C	35	0	0	3	0
3	D	24	0	0	2	0
All	All	9577	9190	8823	133	4

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 7.

All (133) 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:264:MET:SD	3:B:508:HOH:O	2.22	0.97
1:A:55:GLU:OE2	3:A:501:HOH:O	1.97	0.82
1:C:300:CYS:O	1:C:301:SER:OG	1.96	0.82
1:A:53:ASN:OD1	3:A:501:HOH:O	1.98	0.81
1:A:51:ASN:O	1:A:51:ASN:ND2	2.15	0.79
1:C:86:VAL:HG23	1:C:179:GLY:HA2	1.69	0.74
1:D:221:ASN:ND2	1:D:270[B]:GLU:OE1	2.21	0.74
1:C:166:GLU:OE2	1:D:1:SER:N	2.15	0.73
1:A:288[B]:GLU:OE1	3:A:502:HOH:O	2.06	0.73
1:C:269:LYS:NZ	3:C:501:HOH:O	2.19	0.70
1:C:256:GLN:NE2	3:C:502:HOH:O	2.28	0.66
1:C:188:ARG:HG3	1:C:190:THR:HG23	1.77	0.65
1:C:123:SER:O	1:D:298:ARG:NH2	2.28	0.64
1:A:298:ARG:NH2	1:B:123:SER:O	2.29	0.64
1:B:188:ARG:HG3	1:B:190:THR:HG23	1.82	0.61
1:A:118:TYR:OH	1:A:141:LEU:N	2.34	0.60
1:A:50:LEU:HA	1:A:189:GLN:HB3	1.83	0.59
1:C:286[A]:LEU:HD11	1:D:280:THR:HG22	1.83	0.58
1:D:33:ASP:OD1	1:D:98:THR:HG21	2.02	0.58
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.85	0.58
1:A:260:ALA:HB3	1:A:263:ASP:HB2	1.86	0.57
1:C:286[A]:LEU:HD11	1:D:280:THR:CG2	2.37	0.55
1:B:113:SER:O	1:B:149:GLY:HA2	2.06	0.54
1:A:204:VAL:HG22	1:A:288[B]:GLU:O	2.08	0.54
1:D:86:VAL:HG13	1:D:179:GLY:HA2	1.89	0.53
1:D:63:ASN:OD1	1:D:80:HIS:ND1	2.40	0.53
1:B:224:THR:HG22	1:B:225:THR:N	2.24	0.53
1:A:115:LEU:HD11	1:A:122:PRO:HB3	1.91	0.53
1:D:114:VAL:HG11	1:D:140:PHE:HZ	1.74	0.53
1:A:137:LYS:O	1:B:4:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLY:HA2	1:A:200:ILE:HD13	1.90	0.52
1:C:106:ILE:HG23	1:C:160:CYS:HB2	1.91	0.52
1:B:3:PHE:HB3	1:B:282:LEU:HD22	1.91	0.52
1:B:106:ILE:HG23	1:B:160:CYS:HB2	1.91	0.52
1:D:106:ILE:HG23	1:D:160:CYS:HB2	1.92	0.52
1:D:166:GLU:OE2	1:D:172:HIS:NE2	2.43	0.51
1:A:217:ARG:HB3	1:A:220:LEU:HD12	1.93	0.51
1:D:224:THR:HG22	1:D:225:THR:N	2.26	0.51
1:B:236:LYS:NZ	3:B:502:HOH:O	2.44	0.50
1:A:251:GLY:O	1:A:254:SER:N	2.45	0.50
1:A:224:THR:HG22	1:A:225:THR:N	2.27	0.50
1:A:247:VAL:HG22	1:A:261:VAL:HG11	1.94	0.50
1:B:226:THR:HG1	1:B:229:ASP:H	1.59	0.50
1:A:165:MET:CE	1:A:167:LEU:HD21	2.41	0.50
1:D:225:THR:OG1	1:D:269:LYS:NZ	2.41	0.49
1:A:137:LYS:O	1:B:4:ARG:NE	2.44	0.49
1:A:260:ALA:HB3	1:A:263:ASP:CB	2.42	0.49
1:B:186:VAL:N	1:B:192:GLN:OE1	2.39	0.49
1:A:63:ASN:OD1	1:A:80:HIS:ND1	2.38	0.48
1:A:204:VAL:HG22	1:A:288[A]:GLU:O	2.13	0.48
1:A:299:GLN:O	1:B:141:LEU:HD11	2.12	0.48
1:C:300:CYS:O	1:C:301:SER:CB	2.61	0.48
1:B:260:ALA:HB3	1:B:263:ASP:HB2	1.97	0.47
1:C:8:PHE:HB3	1:C:152:ILE:HD12	1.96	0.47
1:B:292:THR:O	1:B:296:VAL:HG23	2.15	0.47
1:C:57:LEU:O	1:C:61:LYS:HG2	2.14	0.47
1:A:45:THR:O	1:A:49[A]:MET:HG3	2.15	0.47
1:A:210:ALA:HB2	1:A:296:VAL:CG1	2.45	0.47
1:C:2:GLY:HA3	1:D:138:GLY:O	2.15	0.47
1:C:224:THR:HG22	1:C:225:THR:N	2.30	0.47
1:D:268:LEU:O	1:D:272:LEU:HG	2.15	0.47
1:A:57:LEU:O	1:A:61:LYS:HG2	2.15	0.46
1:D:21:THR:HA	1:D:25:THR:O	2.15	0.46
1:B:62:SER:HB2	1:B:64:HIS:NE2	2.30	0.46
1:A:76:ARG:NH1	3:A:503:HOH:O	2.34	0.46
1:C:12:LYS:HE2	1:C:155:ASP:O	2.16	0.46
1:D:198[B]:THR:HG22	1:D:238:ASN:OD1	2.16	0.46
1:C:115:LEU:HD11	1:C:122:PRO:HB3	1.97	0.45
1:C:210:ALA:HB2	1:C:296:VAL:HG13	1.98	0.45
1:C:9:PRO:HG2	1:D:122:PRO:HB2	1.98	0.45
1:A:18:VAL:HG12	1:A:70:ALA:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:SER:N	1:D:166:GLU:OE2	2.41	0.45
1:C:86:VAL:HG23	1:C:179:GLY:CA	2.44	0.45
1:D:283:GLY:N	3:D:503:HOH:O	2.32	0.45
1:B:117:CYS:O	1:B:144:SER:HA	2.17	0.45
1:B:39:PRO:HB3	1:B:164:HIS:CD2	2.52	0.45
1:A:210:ALA:HB2	1:A:296:VAL:HG13	1.99	0.45
1:C:1:SER:HB2	1:D:166:GLU:OE2	2.18	0.44
1:A:288[B]:GLU:OE2	1:A:290:GLU:N	2.46	0.44
1:A:123:SER:O	1:B:298:ARG:NH1	2.48	0.44
1:C:226:THR:OG1	1:C:229:ASP:HB2	2.18	0.44
1:B:224:THR:HG22	1:B:225:THR:H	1.83	0.44
1:D:114:VAL:HG11	1:D:140:PHE:CZ	2.52	0.44
1:B:86:VAL:HG23	1:B:179:GLY:HA2	1.99	0.44
1:D:132:PRO:HG2	1:D:198[A]:THR:HG23	2.00	0.43
1:D:247:VAL:HG22	1:D:261:VAL:HG11	2.00	0.43
1:A:218:TRP:CE3	1:A:279:ARG:CZ	3.00	0.43
1:B:43:ILE:HD11	1:B:54:TYR:HD1	1.84	0.43
1:A:165:MET:HE2	1:A:167:LEU:HD21	1.99	0.43
1:D:95:ASN:HB3	1:D:98:THR:OG1	2.18	0.43
1:D:230:PHE:HA	1:D:269:LYS:CE	2.48	0.43
1:A:113:SER:O	1:A:149:GLY:HA2	2.18	0.43
1:A:225:THR:O	1:A:262:LEU:HD13	2.19	0.43
1:A:206:ALA:O	1:A:296:VAL:HG21	2.18	0.43
1:B:95:ASN:HB3	1:B:98:THR:OG1	2.19	0.43
1:C:188:ARG:CZ	1:C:190:THR:HG21	2.48	0.43
1:A:251:GLY:O	1:A:254:SER:HB3	2.19	0.43
1:D:114:VAL:O	1:D:125:VAL:HA	2.19	0.43
1:B:33:ASP:O	1:B:94:ALA:HA	2.19	0.42
1:D:68:VAL:HB	1:D:75:LEU:HB2	2.02	0.42
1:A:164:HIS:HB2	1:A:174:GLY:HA2	2.02	0.42
1:D:140:PHE:HB3	1:D:144:SER:OG	2.19	0.42
1:A:49[B]:MET:HG3	1:A:189:GLN:HB2	2.01	0.42
1:D:67:LEU:CD1	1:D:74:GLN:HG3	2.49	0.42
1:A:40:ARG:O	1:A:43:ILE:HG12	2.19	0.42
1:B:237:TYR:OH	1:B:273:GLN:HG2	2.20	0.42
1:D:224:THR:HG22	1:D:225:THR:H	1.85	0.41
1:B:84:ASN:HB2	1:B:179:GLY:HA3	2.02	0.41
1:D:53:ASN:OD1	1:D:55:GLU:HG2	2.20	0.41
1:D:53:ASN:OD1	1:D:56:ASP:HB2	2.20	0.41
1:B:102:LYS:N	1:B:157:VAL:O	2.46	0.41
1:D:244:GLN:OE1	3:D:501:HOH:O	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:ALA:HB1	1:D:216:ASP:CB	2.50	0.41
1:D:230:PHE:HA	1:D:269:LYS:HE2	2.01	0.41
1:C:251:GLY:O	1:C:254:SER:HB3	2.21	0.41
1:D:116:ALA:O	1:D:123:SER:HB3	2.20	0.41
1:D:117:CYS:SG	1:D:122:PRO:HA	2.61	0.41
1:B:132:PRO:HD2	1:B:197:ASP:OD1	2.21	0.41
1:C:138:GLY:O	1:D:2:GLY:HA3	2.20	0.41
1:C:236:LYS:NZ	3:C:505:HOH:O	2.43	0.41
1:C:286[B]:LEU:C	1:C:286[B]:LEU:HD12	2.41	0.41
1:B:165:MET:HB3	2:B:401:KKO:CL19	2.57	0.40
1:D:113:SER:O	1:D:149:GLY:HA2	2.21	0.40
1:C:163:HIS:NE2	2:C:401:KKO:N27	2.70	0.40
1:D:19:GLN:OE1	1:D:26:THR:HG21	2.21	0.40

All (4) 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:65:ASN:ND2	1:B:273:GLN:O[1_556]	2.00	0.20
1:C:1:SER:OG	1:D:255:ALA:O[1_655]	2.04	0.16
1:A:65:ASN:HD21	1:B:273:GLN:O[1_556]	1.48	0.12
1:C:65:ASN:ND2	1:D:273:GLN:O[1_454]	2.12	0.08

## 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	311/306 (102%)	297 (96%)	14 (4%)	0	100 100
1	B	302/306 (99%)	289 (96%)	12 (4%)	1 (0%)	41 50
1	C	312/306 (102%)	297 (95%)	13 (4%)	2 (1%)	25 30
1	D	304/306 (99%)	292 (96%)	11 (4%)	1 (0%)	41 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1229/1224 (100%)	1175 (96%)	50 (4%)	4 (0%)	41   50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	154[A]	TYR
1	C	154[B]	TYR
1	B	154	TYR
1	D	5	LYS

### 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	270/263 (103%)	269 (100%)	1 (0%)	91   96
1	B	263/263 (100%)	262 (100%)	1 (0%)	91   96
1	C	271/263 (103%)	268 (99%)	3 (1%)	73   85
1	D	265/263 (101%)	263 (99%)	2 (1%)	81   90
All	All	1069/1052 (102%)	1062 (99%)	7 (1%)	84   92

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	B	104	VAL
1	C	27	LEU
1	C	53	ASN
1	C	153	ASP
1	D	27	LEU
1	D	107	GLN

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 [\(i\)](#)

4 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	KKO	B	401	-	36,36,36	0.45	0	42,50,50	0.80	4 (9%)
2	KKO	A	401	-	36,36,36	0.46	0	42,50,50	0.77	3 (7%)
2	KKO	C	401	-	36,36,36	0.49	0	42,50,50	0.81	3 (7%)
2	KKO	D	401	-	36,36,36	0.41	0	42,50,50	0.79	3 (7%)

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	KKO	B	401	-	-	2/21/36/36	0/4/4/4
2	KKO	A	401	-	-	2/21/36/36	0/4/4/4
2	KKO	C	401	-	-	2/21/36/36	0/4/4/4
2	KKO	D	401	-	-	2/21/36/36	0/4/4/4

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	KKO	C11-N12-C24	2.65	129.68	122.44
2	B	401	KKO	C11-N12-C24	2.62	129.61	122.44
2	D	401	KKO	C11-N12-C24	2.60	129.54	122.44
2	A	401	KKO	C11-N12-C24	2.55	129.41	122.44
2	D	401	KKO	C14-N15-C10	2.42	116.64	110.58
2	A	401	KKO	C14-N15-C10	2.37	116.52	110.58
2	B	401	KKO	C14-N15-C10	2.36	116.50	110.58
2	C	401	KKO	C14-N15-C10	2.33	116.42	110.58
2	B	401	KKO	C13-N12-C11	-2.18	108.69	113.06
2	C	401	KKO	C5-C4-N3	-2.12	108.11	112.71
2	A	401	KKO	C13-N12-C11	-2.12	108.82	113.06
2	D	401	KKO	C13-N12-C11	-2.08	108.90	113.06
2	B	401	KKO	C5-C4-N3	-2.01	108.36	112.71

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	KKO	C17-C16-N15-C14
2	A	401	KKO	C22-C16-N15-C14
2	C	401	KKO	C17-C16-N15-C14
2	D	401	KKO	C17-C16-N15-C14
2	D	401	KKO	C22-C16-N15-C14
2	B	401	KKO	C17-C16-N15-C14
2	B	401	KKO	C22-C16-N15-C14
2	C	401	KKO	C22-C16-N15-C14

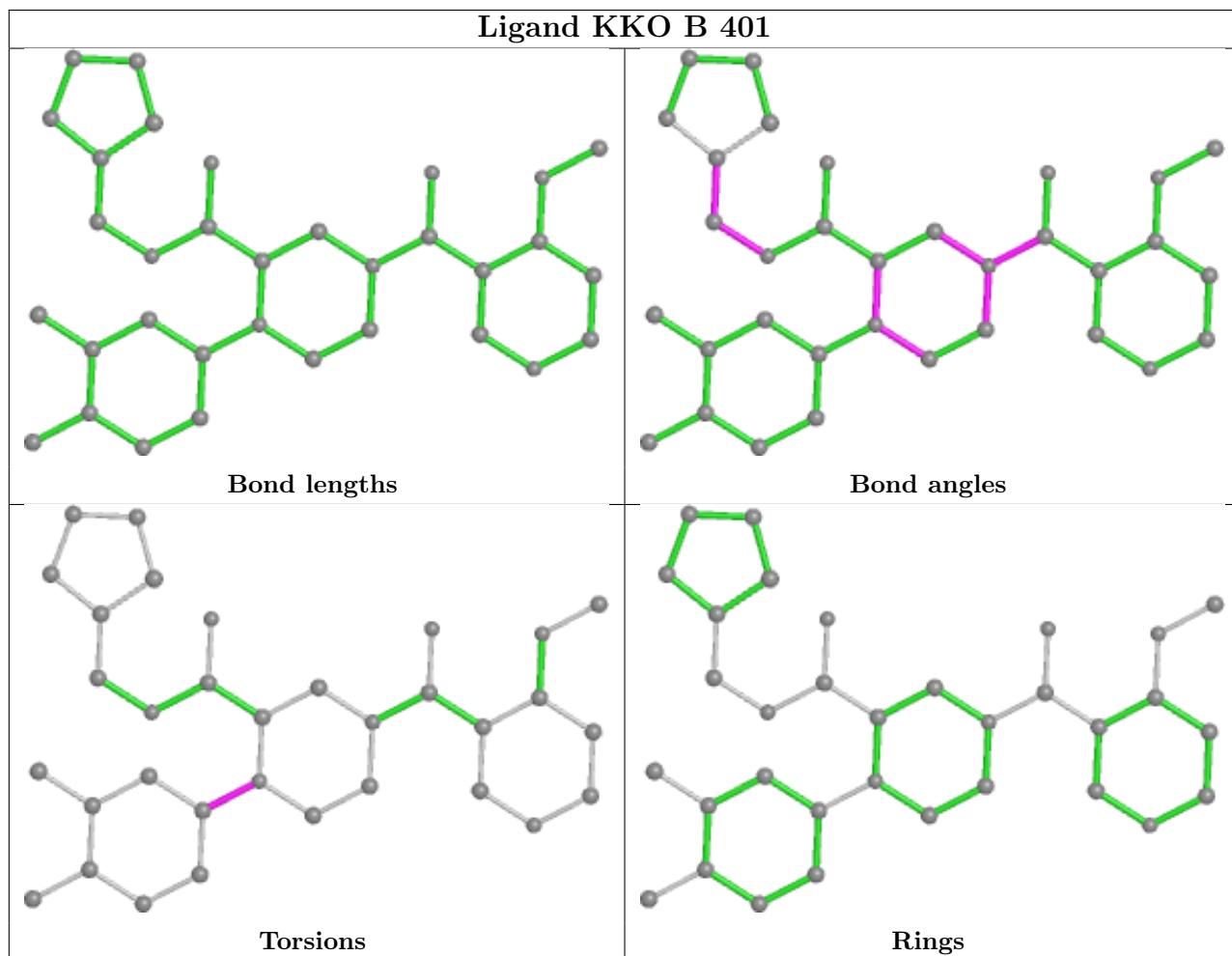
There are no ring outliers.

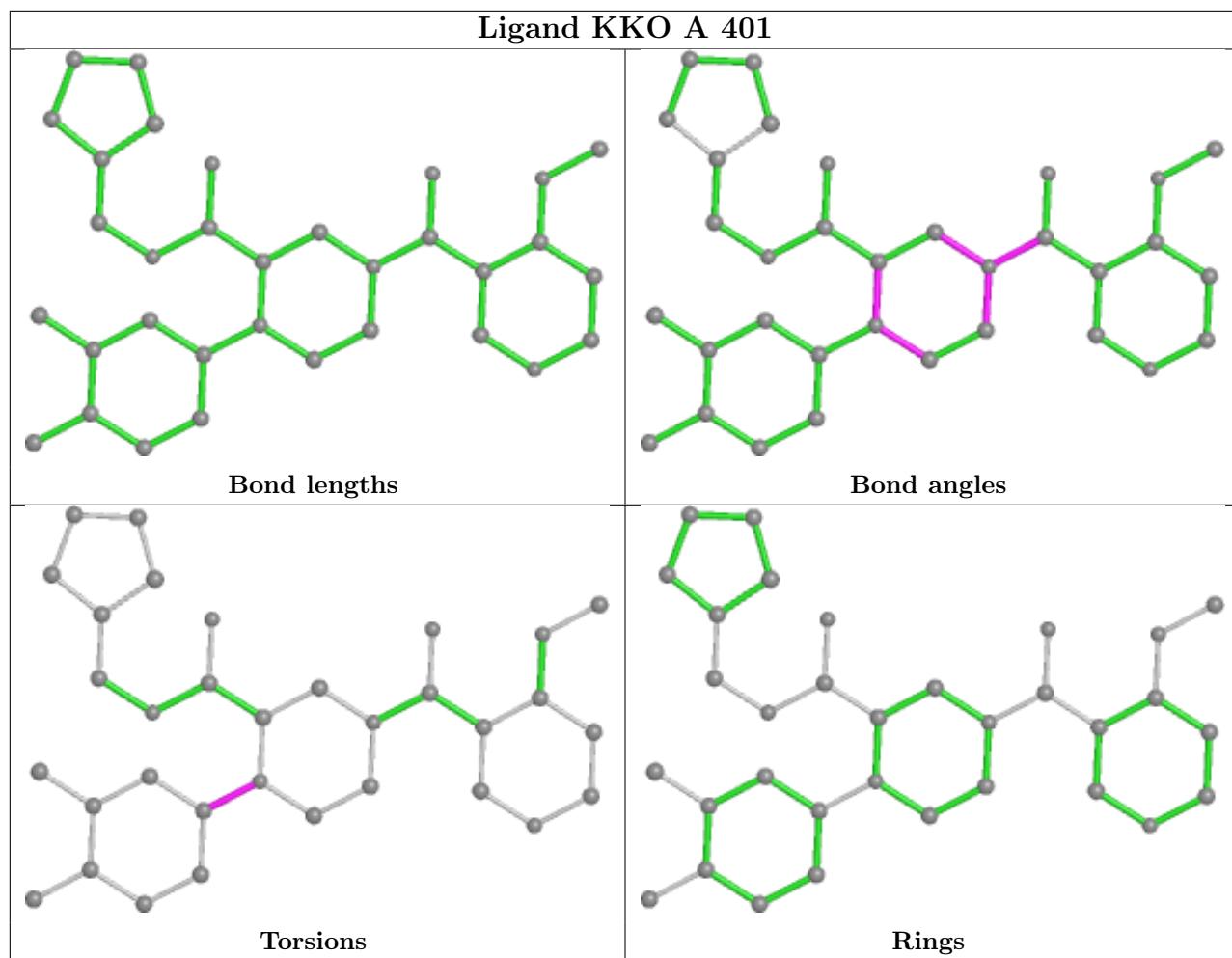
2 monomers are involved in 2 short contacts:

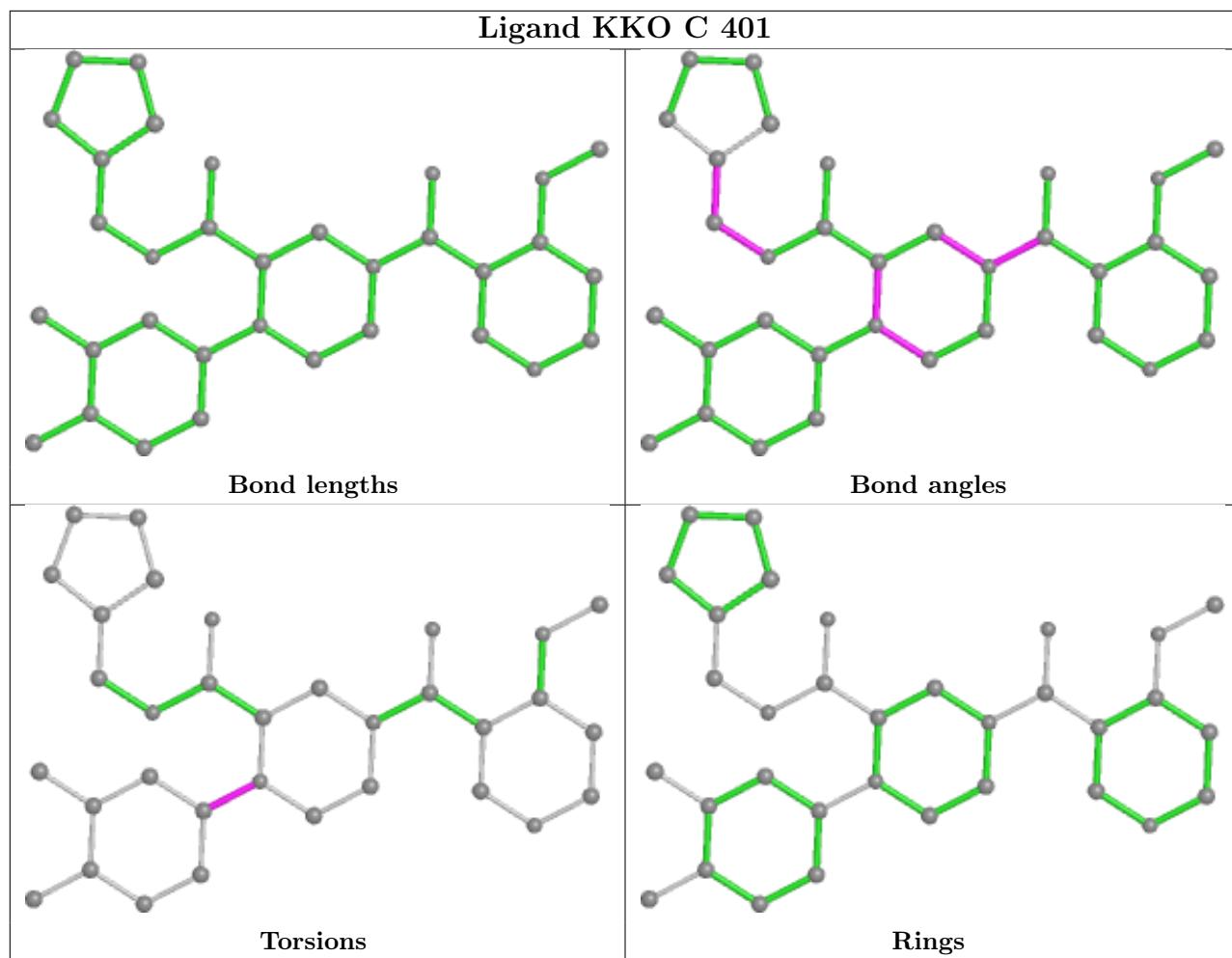
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	KKO	1	0
2	C	401	KKO	1	0

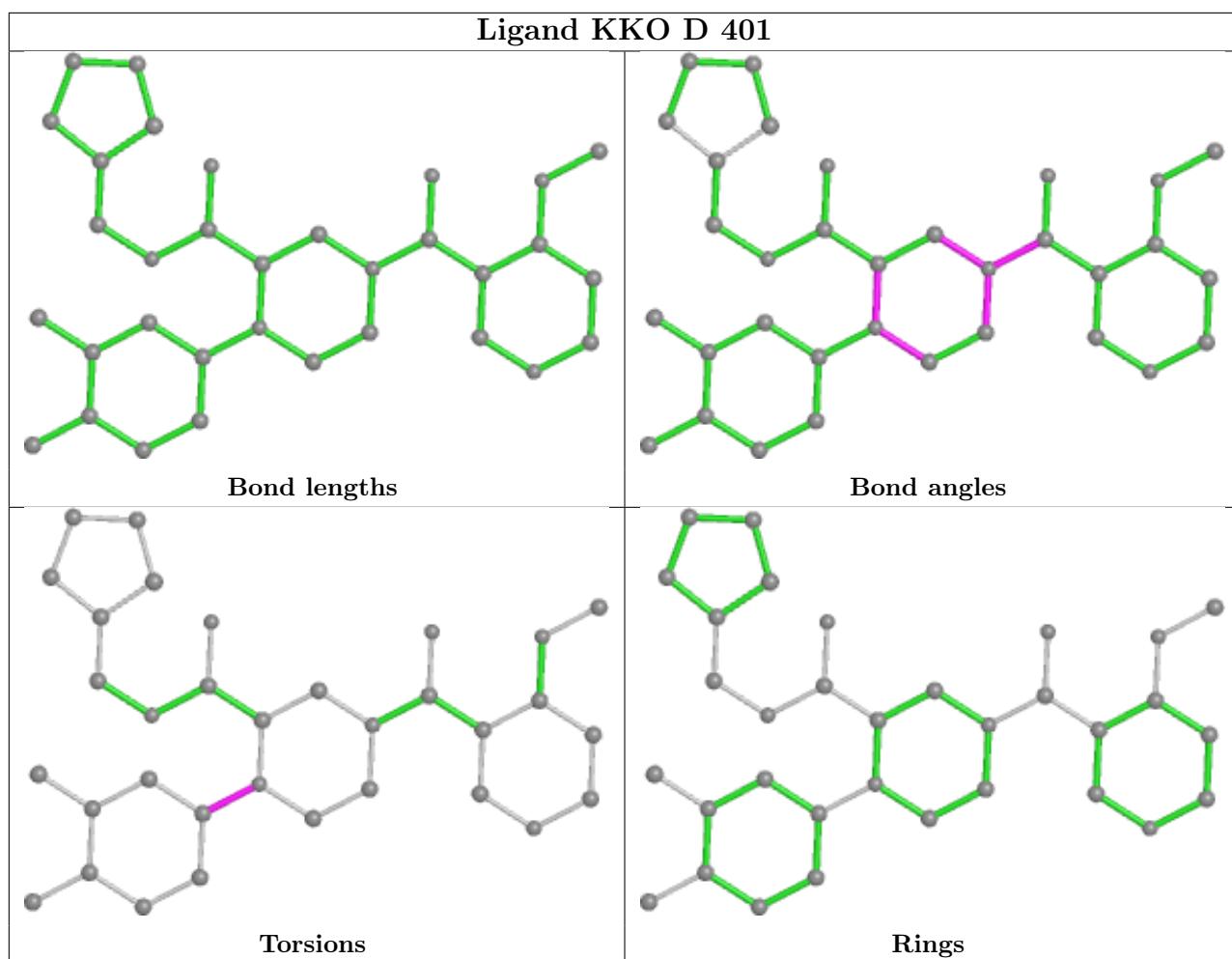
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	301/306 (98%)	2.96	216 (71%) 0   0	26, 32, 44, 58	0
1	B	295/306 (96%)	3.39	224 (75%) 0   0	29, 36, 60, 72	0
1	C	301/306 (98%)	3.22	225 (74%) 0   0	28, 34, 43, 53	0
1	D	293/306 (95%)	3.28	228 (77%) 0   0	29, 37, 52, 63	0
All	All	1190/1224 (97%)	3.21	893 (75%) 0   0	26, 35, 50, 72	0

All (893) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	LEU	14.3
1	B	301	SER	12.4
1	D	35	VAL	10.8
1	D	72	ASN	10.5
1	C	29	GLY	10.1
1	A	220	LEU	9.7
1	B	6	MET	9.5
1	D	43	ILE	9.2
1	B	250	LEU	9.1
1	B	86	VAL	9.1
1	B	139	SER	9.0
1	D	122	PRO	8.9
1	B	249	ILE	8.8
1	C	66	PHE	8.7
1	B	59	ILE	8.7
1	C	161	TYR	8.6
1	B	237	TYR	8.5
1	B	80	HIS	8.5
1	C	282	LEU	8.5
1	B	106	ILE	8.3
1	D	224	THR	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	291	PHE	8.3
1	D	189	GLN	7.9
1	D	22	CYS	7.9
1	C	56	ASP	7.8
1	B	22	CYS	7.7
1	D	240	GLU	7.7
1	D	301	SER	7.7
1	C	44	CYS	7.6
1	B	1	SER	7.6
1	C	42	VAL	7.6
1	A	296	VAL	7.5
1	A	194	ALA	7.5
1	C	154[A]	TYR	7.4
1	D	36	VAL	7.3
1	C	235	MET	7.3
1	C	140	PHE	7.3
1	A	125	VAL	7.1
1	D	57	LEU	7.1
1	C	22	CYS	7.1
1	D	87[A]	LEU	6.9
1	B	159	PHE	6.8
1	D	44	CYS	6.8
1	B	295	ASP	6.7
1	A	193	ALA	6.7
1	A	152	ILE	6.7
1	B	38	CYS	6.6
1	A	89	LEU	6.6
1	A	104[A]	VAL	6.6
1	A	177	LEU	6.6
1	C	30	LEU	6.6
1	C	109	GLY	6.6
1	A	58	LEU	6.6
1	C	13	VAL	6.5
1	C	222	ARG	6.5
1	B	167	LEU	6.5
1	A	60	ARG	6.5
1	B	71	GLY	6.4
1	D	66	PHE	6.4
1	C	185	PHE	6.4
1	D	223	PHE	6.4
1	C	150	PHE	6.4
1	D	190	THR	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	1	SER	6.3
1	B	78	ILE	6.3
1	B	54	TYR	6.2
1	B	182	TYR	6.2
1	D	3	PHE	6.2
1	A	154	TYR	6.2
1	B	26	THR	6.2
1	B	181	PHE	6.1
1	D	32	LEU	6.1
1	D	177	LEU	6.1
1	D	230	PHE	6.1
1	D	62	SER	5.9
1	A	190	THR	5.9
1	C	163	HIS	5.9
1	D	64	HIS	5.9
1	A	162	MET	5.9
1	D	125	VAL	5.9
1	B	44	CYS	5.9
1	D	60	ARG	5.8
1	D	174	GLY	5.8
1	B	154	TYR	5.8
1	C	166	GLU	5.8
1	A	136	ILE	5.8
1	B	189	GLN	5.8
1	B	283	GLY	5.8
1	B	20	VAL	5.8
1	C	170	GLY	5.7
1	C	135	THR	5.7
1	A	271[A]	LEU	5.7
1	D	205	LEU	5.7
1	B	255	ALA	5.7
1	C	54	TYR	5.7
1	C	57	LEU	5.7
1	C	81	SER	5.7
1	C	232	LEU	5.6
1	C	52	PRO	5.6
1	C	71	GLY	5.6
1	D	37	TYR	5.5
1	C	275	GLY	5.5
1	D	186	VAL	5.5
1	D	213	ILE	5.5
1	D	259	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	173	ALA	5.5
1	D	102	LYS	5.5
1	A	181	PHE	5.4
1	C	20	VAL	5.4
1	A	3	PHE	5.4
1	A	49[A]	MET	5.4
1	C	300	CYS	5.4
1	D	117	CYS	5.4
1	C	269	LYS	5.4
1	B	148	VAL	5.3
1	C	287[A]	LEU	5.3
1	A	293	PRO	5.3
1	C	31	TRP	5.3
1	C	118	TYR	5.3
1	B	65	ASN	5.3
1	D	63	ASN	5.3
1	C	212	VAL	5.3
1	B	228	ASN	5.3
1	D	29	GLY	5.3
1	B	216	ASP	5.3
1	C	132	PRO	5.3
1	A	23	GLY	5.3
1	B	72	ASN	5.3
1	C	89	LEU	5.3
1	C	286[A]	LEU	5.3
1	C	49	MET	5.2
1	C	224	THR	5.2
1	B	277[A]	ASN	5.2
1	C	3	PHE	5.2
1	D	58	LEU	5.2
1	A	157	VAL	5.2
1	A	122	PRO	5.2
1	B	281	ILE	5.2
1	B	217	ARG	5.2
1	A	65	ASN	5.2
1	B	52	PRO	5.2
1	D	165	MET	5.1
1	A	10	SER	5.1
1	B	224	THR	5.1
1	B	269	LYS	5.1
1	D	134	PHE	5.1
1	B	152	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	69	GLN	5.1
1	B	118	TYR	5.1
1	B	296	VAL	5.1
1	C	233	VAL	5.1
1	D	33	ASP	5.1
1	D	298	ARG	5.1
1	D	154	TYR	5.1
1	C	16	CYS	5.1
1	A	59	ILE	5.1
1	B	242	LEU	5.0
1	C	301	SER	5.0
1	B	84	ASN	5.0
1	B	60	ARG	5.0
1	B	185	PHE	5.0
1	D	231	ASN	5.0
1	C	78	ILE	5.0
1	B	115	LEU	5.0
1	B	89	LEU	5.0
1	C	179	GLY	4.9
1	D	1	SER	4.9
1	B	160	CYS	4.9
1	C	294	PHE	4.9
1	D	25	THR	4.9
1	B	235	MET	4.9
1	A	153	ASP	4.9
1	B	2	GLY	4.9
1	C	251	GLY	4.9
1	A	202	VAL	4.9
1	A	297	VAL	4.9
1	B	18	VAL	4.9
1	A	273	GLN	4.9
1	D	188	ARG	4.9
1	A	55	GLU	4.9
1	B	192	GLN	4.8
1	B	291	PHE	4.8
1	A	18	VAL	4.8
1	C	32	LEU	4.8
1	B	134	PHE	4.8
1	D	296	VAL	4.8
1	B	32	LEU	4.8
1	B	25	THR	4.8
1	B	61	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	101	TYR	4.7
1	A	171	VAL	4.7
1	A	118	TYR	4.7
1	C	73	VAL	4.7
1	C	143	GLY	4.7
1	D	13	VAL	4.7
1	A	75	LEU	4.7
1	A	142	ASN	4.7
1	C	299	GLN	4.7
1	D	101	TYR	4.7
1	B	157	VAL	4.7
1	B	187	ASP	4.6
1	C	155	ASP	4.6
1	D	27	LEU	4.6
1	D	237	TYR	4.6
1	C	77	VAL	4.6
1	A	155	ASP	4.6
1	C	297	VAL	4.6
1	B	112	PHE	4.6
1	B	77	VAL	4.6
1	B	104	VAL	4.6
1	B	268	LEU	4.6
1	C	110[A]	GLN	4.5
1	A	46	SER	4.5
1	D	253	LEU	4.5
1	D	124	GLY	4.5
1	B	62	SER	4.5
1	C	58	LEU	4.5
1	B	13	VAL	4.5
1	C	15	GLY	4.5
1	D	81	SER	4.5
1	B	180	ASN	4.5
1	A	174	GLY	4.5
1	C	2	GLY	4.5
1	D	182	TYR	4.5
1	B	103	PHE	4.4
1	D	93	THR	4.4
1	B	164	HIS	4.4
1	B	129	ALA	4.4
1	B	271[A]	LEU	4.4
1	C	165	MET	4.4
1	A	241	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	158	SER	4.4
1	C	129	ALA	4.4
1	C	114	VAL	4.4
1	D	86	VAL	4.4
1	C	291	PHE	4.4
1	B	222	ARG	4.4
1	D	160	CYS	4.4
1	C	146	GLY	4.4
1	C	169	THR	4.4
1	D	266	ALA	4.4
1	A	235	MET	4.3
1	A	87[A]	LEU	4.3
1	A	117	CYS	4.3
1	C	60	ARG	4.3
1	C	128	CYS	4.3
1	D	88	LYS	4.3
1	C	62	SER	4.3
1	D	225	THR	4.3
1	B	19	GLN	4.3
1	D	123	SER	4.3
1	B	55	GLU	4.3
1	C	37	TYR	4.3
1	D	126[A]	TYR	4.3
1	A	224	THR	4.3
1	C	198	THR	4.3
1	B	126[A]	TYR	4.3
1	D	103	PHE	4.3
1	A	253	LEU	4.3
1	C	227	LEU	4.3
1	C	257	THR	4.3
1	B	293	PRO	4.2
1	A	230	PHE	4.2
1	B	223	PHE	4.2
1	B	153	ASP	4.2
1	A	184	PRO	4.2
1	D	128	CYS	4.2
1	A	286	LEU	4.2
1	D	115	LEU	4.2
1	D	198[A]	THR	4.2
1	D	17	MET	4.2
1	B	70	ALA	4.2
1	C	189	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	53	ASN	4.2
1	A	11	GLY	4.2
1	A	156	CYS	4.2
1	B	241	PRO	4.1
1	A	294	PHE	4.1
1	D	299	GLN	4.1
1	D	28	ASN	4.1
1	D	118	TYR	4.1
1	C	249	ILE	4.1
1	B	31	TRP	4.1
1	C	223	PHE	4.1
1	D	247	VAL	4.1
1	C	250	LEU	4.1
1	A	61	LYS	4.1
1	D	42	VAL	4.1
1	D	261	VAL	4.1
1	C	190	THR	4.1
1	B	218	TRP	4.1
1	A	233	VAL	4.1
1	B	233	VAL	4.1
1	B	162	MET	4.1
1	A	50	LEU	4.1
1	D	250	LEU	4.1
1	D	140	PHE	4.1
1	D	26	THR	4.0
1	A	30	LEU	4.0
1	B	262	LEU	4.0
1	B	39	PRO	4.0
1	C	258	GLY	4.0
1	A	27	LEU	4.0
1	D	287[A]	LEU	4.0
1	C	107	GLN	4.0
1	A	44	CYS	4.0
1	B	85	CYS	4.0
1	C	39	PRO	4.0
1	D	218	TRP	4.0
1	A	72	ASN	4.0
1	B	150	PHE	4.0
1	C	126[A]	TYR	4.0
1	D	191	ALA	4.0
1	B	3	PHE	4.0
1	B	146	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	94	ALA	4.0
1	A	147	SER	4.0
1	C	147	SER	4.0
1	C	239	TYR	3.9
1	B	125	VAL	3.9
1	C	230	PHE	3.9
1	D	200	ILE	3.9
1	B	23	GLY	3.9
1	D	179	GLY	3.9
1	A	209	TYR	3.9
1	C	27	LEU	3.9
1	A	215	GLY	3.9
1	D	212	VAL	3.9
1	B	221	ASN	3.9
1	A	167	LEU	3.9
1	A	43	ILE	3.9
1	D	294	PHE	3.9
1	A	106	ILE	3.9
1	B	75	LEU	3.9
1	B	239	TYR	3.8
1	D	15	GLY	3.8
1	A	219	PHE	3.8
1	B	207	TRP	3.8
1	D	38	CYS	3.8
1	D	80	HIS	3.8
1	D	255	ALA	3.8
1	A	57	LEU	3.8
1	C	271[A]	LEU	3.8
1	C	192	GLN	3.8
1	A	9	PRO	3.8
1	B	51	ASN	3.8
1	D	206	ALA	3.8
1	D	279	ARG	3.8
1	C	272	LEU	3.8
1	A	237	TYR	3.8
1	C	256	GLN	3.8
1	A	47	GLU	3.8
1	C	88	LYS	3.8
1	C	175	THR	3.8
1	C	38	CYS	3.8
1	A	239	TYR	3.8
1	A	93	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	169	THR	3.7
1	B	298	ARG	3.7
1	C	69	GLN	3.7
1	A	99	PRO	3.7
1	B	98	THR	3.7
1	D	24	THR	3.7
1	D	204	VAL	3.7
1	D	271[A]	LEU	3.7
1	D	34	ASP	3.7
1	B	270	GLU	3.7
1	A	85	CYS	3.7
1	C	191	ALA	3.7
1	B	198	THR	3.7
1	C	280	THR	3.7
1	A	300	CYS	3.7
1	A	229	ASP	3.7
1	C	270	GLU	3.7
1	D	235	MET	3.7
1	A	67	LEU	3.7
1	A	121	SER	3.7
1	C	281	ILE	3.7
1	D	227	LEU	3.7
1	D	256	GLN	3.7
1	A	48	ASP	3.7
1	D	129	ALA	3.7
1	B	275	GLY	3.7
1	D	67	LEU	3.6
1	B	24	THR	3.6
1	B	169	THR	3.6
1	B	280	THR	3.6
1	C	168	PRO	3.6
1	A	182	TYR	3.6
1	B	82	MET	3.6
1	A	188	ARG	3.6
1	C	72	ASN	3.6
1	B	130	MET	3.6
1	C	98	THR	3.6
1	D	180	ASN	3.6
1	D	136	ILE	3.6
1	C	167	LEU	3.6
1	A	25	THR	3.6
1	A	38	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	116	ALA	3.6
1	A	130	MET	3.6
1	B	243	THR	3.6
1	B	230	PHE	3.6
1	D	242	LEU	3.6
1	A	37	TYR	3.6
1	A	259	ILE	3.5
1	D	91	VAL	3.5
1	A	161	TYR	3.5
1	B	161	TYR	3.5
1	A	223	PHE	3.5
1	B	138	GLY	3.5
1	C	55	GLU	3.5
1	B	276	MET	3.5
1	D	30	LEU	3.5
1	D	92	ASP	3.5
1	B	163	HIS	3.5
1	D	291	PHE	3.5
1	B	286	LEU	3.5
1	C	43	ILE	3.5
1	C	177	LEU	3.5
1	B	21	THR	3.5
1	B	246	HIS	3.5
1	D	109	GLY	3.5
1	D	14	GLU	3.5
1	B	136	ILE	3.4
1	C	106	ILE	3.4
1	A	20	VAL	3.4
1	B	7	ALA	3.4
1	C	92	ASP	3.4
1	A	141	LEU	3.4
1	C	35	VAL	3.4
1	C	121	SER	3.4
1	C	173	ALA	3.4
1	A	53	ASN	3.4
1	D	184	PRO	3.4
1	A	285	ALA	3.4
1	C	157	VAL	3.4
1	C	296	VAL	3.4
1	C	51	ASN	3.4
1	A	185	PHE	3.4
1	A	266	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	89	LEU	3.4
1	B	212	VAL	3.4
1	D	207	TRP	3.4
1	D	297	VAL	3.4
1	A	82	MET	3.4
1	B	259	ILE	3.4
1	D	20	VAL	3.4
1	A	94	ALA	3.4
1	B	193	ALA	3.4
1	D	222	ARG	3.4
1	D	100	LYS	3.4
1	B	122	PRO	3.3
1	D	96	PRO	3.3
1	B	121	SER	3.3
1	A	280	THR	3.3
1	C	4	ARG	3.3
1	D	161	TYR	3.3
1	D	137	LYS	3.3
1	D	274	ASN	3.3
1	A	211	ALA	3.3
1	B	94	ALA	3.3
1	B	30	LEU	3.3
1	B	200	ILE	3.3
1	A	64	HIS	3.3
1	C	127	GLN	3.3
1	B	285	ALA	3.3
1	D	178	GLU	3.3
1	D	193	ALA	3.3
1	B	56	ASP	3.3
1	B	87[A]	LEU	3.3
1	D	23	GLY	3.3
1	A	164	HIS	3.3
1	C	221	ASN	3.3
1	C	253	LEU	3.3
1	D	220	LEU	3.3
1	C	260	ALA	3.3
1	A	103	PHE	3.3
1	B	43	ILE	3.3
1	C	19	GLN	3.3
1	D	249	ILE	3.3
1	C	202	VAL	3.3
1	A	5	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	61	LYS	3.3
1	B	238	ASN	3.3
1	A	256	GLN	3.2
1	D	120	GLY	3.2
1	B	264	MET	3.2
1	D	121	SER	3.2
1	B	261	VAL	3.2
1	A	225	THR	3.2
1	B	194	ALA	3.2
1	C	46	SER	3.2
1	C	205	LEU	3.2
1	C	174	GLY	3.2
1	C	245	ASP	3.2
1	A	254	SER	3.2
1	C	242	LEU	3.2
1	D	82	MET	3.2
1	A	31	TRP	3.2
1	D	54	TYR	3.2
1	B	186	VAL	3.2
1	B	297	VAL	3.2
1	C	125	VAL	3.2
1	C	164	HIS	3.2
1	A	52	PRO	3.2
1	A	252	PRO	3.2
1	A	214	ASN	3.2
1	B	76	ARG	3.2
1	C	26	THR	3.2
1	A	267	SER	3.2
1	C	266	ALA	3.2
1	D	168	PRO	3.2
1	C	75	LEU	3.2
1	C	68	VAL	3.2
1	D	73	VAL	3.2
1	D	270[A]	GLU	3.1
1	B	10	SER	3.1
1	D	239	TYR	3.1
1	A	295	ASP	3.1
1	C	33	ASP	3.1
1	A	262	LEU	3.1
1	D	106	ILE	3.1
1	A	140	PHE	3.1
1	A	263	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	258	GLY	3.1
1	D	183	GLY	3.1
1	D	208	LEU	3.1
1	C	25	THR	3.1
1	C	244	GLN	3.1
1	A	83	GLN	3.1
1	B	171	VAL	3.1
1	D	59	ILE	3.1
1	B	79	GLY	3.1
1	C	70	ALA	3.1
1	A	35	VAL	3.1
1	B	68	VAL	3.1
1	C	36	VAL	3.1
1	A	45	THR	3.1
1	B	225	THR	3.1
1	B	140	PHE	3.1
1	D	289[A]	ASP	3.0
1	C	90	LYS	3.0
1	C	274	ASN	3.0
1	A	272	LEU	3.0
1	C	141	LEU	3.0
1	C	276	MET	3.0
1	D	155	ASP	3.0
1	A	204	VAL	3.0
1	B	175	THR	3.0
1	C	67	LEU	3.0
1	C	197	ASP	3.0
1	A	301	SER	3.0
1	B	145	CYS	3.0
1	A	108	PRO	3.0
1	C	243	THR	3.0
1	C	82	MET	3.0
1	A	173	ALA	3.0
1	B	173	ALA	3.0
1	D	8	PHE	3.0
1	C	86	VAL	3.0
1	B	69	GLN	3.0
1	A	238	ASN	3.0
1	C	298	ARG	3.0
1	A	90	LYS	3.0
1	C	8	PHE	3.0
1	A	186	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	275	GLY	3.0
1	B	179	GLY	3.0
1	C	217	ARG	3.0
1	B	267	SER	3.0
1	C	211	ALA	3.0
1	B	215	GLY	3.0
1	A	261	VAL	3.0
1	D	257	THR	3.0
1	B	165	MET	2.9
1	C	85	CYS	2.9
1	D	2	GLY	2.9
1	C	259	ILE	2.9
1	B	108	PRO	2.9
1	A	73	VAL	2.9
1	B	37	TYR	2.9
1	B	128	CYS	2.9
1	C	288[A]	GLU	2.9
1	A	76	ARG	2.9
1	B	195	GLY	2.9
1	C	6	MET	2.9
1	C	76	ARG	2.9
1	C	278[A]	GLY	2.9
1	C	151	ASN	2.9
1	C	182	TYR	2.9
1	C	59	ILE	2.9
1	B	117	CYS	2.9
1	A	218	TRP	2.9
1	D	110[A]	GLN	2.9
1	A	216	ASP	2.9
1	C	252	PRO	2.9
1	D	108	PRO	2.9
1	A	134	PHE	2.9
1	D	71	GLY	2.9
1	C	228	ASN	2.9
1	B	236	LYS	2.9
1	C	295	ASP	2.9
1	C	213	ILE	2.8
1	A	98	THR	2.8
1	D	214	ASN	2.8
1	A	42	VAL	2.8
1	D	114	VAL	2.8
1	B	57	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	211	ALA	2.8
1	B	260	ALA	2.8
1	A	109	GLY	2.8
1	C	133	ASN	2.8
1	C	225	THR	2.8
1	D	111[A]	THR	2.8
1	D	284	SER	2.8
1	A	217	ARG	2.8
1	D	70	ALA	2.8
1	D	6	MET	2.8
1	D	162	MET	2.8
1	A	74	GLN	2.8
1	A	54	TYR	2.8
1	C	207	TRP	2.8
1	C	41	HIS	2.8
1	B	9	PRO	2.8
1	A	298	ARG	2.8
1	D	130	MET	2.8
1	A	200	ILE	2.8
1	B	266	ALA	2.8
1	C	65	ASN	2.8
1	A	197	ASP	2.8
1	C	23	GLY	2.8
1	D	275	GLY	2.8
1	C	93	THR	2.8
1	C	199[A]	THR	2.8
1	C	117	CYS	2.8
1	A	163	HIS	2.8
1	B	64	HIS	2.8
1	D	84	ASN	2.8
1	B	5	LYS	2.8
1	C	236	LYS	2.8
1	A	36	VAL	2.7
1	A	247	VAL	2.7
1	A	278[A]	GLY	2.7
1	D	202	VAL	2.7
1	D	268	LEU	2.7
1	A	243	THR	2.7
1	D	288[A]	GLU	2.7
1	B	245	ASP	2.7
1	B	254	SER	2.7
1	D	68	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	219	PHE	2.7
1	B	199[A]	THR	2.7
1	C	102	LYS	2.7
1	C	83	GLN	2.7
1	B	114	VAL	2.7
1	B	282	LEU	2.7
1	C	279	ARG	2.7
1	B	166	GLU	2.7
1	C	209	TYR	2.7
1	D	150	PHE	2.7
1	A	208	LEU	2.7
1	B	93	THR	2.7
1	D	245	ASP	2.7
1	C	47	GLU	2.7
1	C	290	GLU	2.7
1	D	132	PRO	2.7
1	D	210	ALA	2.7
1	C	48	ASP	2.7
1	D	203	ASN	2.7
1	B	67	LEU	2.7
1	D	167	LEU	2.7
1	A	222	ARG	2.6
1	B	133	ASN	2.6
1	D	7	ALA	2.6
1	A	115	LEU	2.6
1	C	1	SER	2.6
1	D	267	SER	2.6
1	A	203	ASN	2.6
1	A	7	ALA	2.6
1	B	190	THR	2.6
1	D	135	THR	2.6
1	D	156	CYS	2.6
1	A	232	LEU	2.6
1	B	272	LEU	2.6
1	C	219	PHE	2.6
1	C	237	TYR	2.6
1	C	268	LEU	2.6
1	D	119	ASN	2.6
1	D	157	VAL	2.6
1	C	206	ALA	2.6
1	C	210	ALA	2.6
1	B	213	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	238	ASN	2.6
1	A	282	LEU	2.6
1	B	220	LEU	2.6
1	D	112	PHE	2.6
1	A	244	GLN	2.6
1	B	248	ASP	2.6
1	D	263	ASP	2.6
1	D	78	ILE	2.6
1	A	288[A]	GLU	2.6
1	C	5	LYS	2.6
1	B	99	PRO	2.6
1	A	159	PHE	2.6
1	A	2	GLY	2.6
1	C	119	ASN	2.6
1	D	142	ASN	2.6
1	A	135	THR	2.5
1	B	168	PRO	2.5
1	C	115	LEU	2.5
1	D	265	CYS	2.5
1	C	18	VAL	2.5
1	C	229	ASP	2.5
1	A	195	GLY	2.5
1	B	142	ASN	2.5
1	B	292	THR	2.5
1	A	39	PRO	2.5
1	A	250	LEU	2.5
1	D	18	VAL	2.5
1	A	95	ASN	2.5
1	D	209	TYR	2.5
1	D	243	THR	2.5
1	D	41	HIS	2.5
1	D	280	THR	2.5
1	A	32	LEU	2.5
1	A	8	PHE	2.5
1	B	147	SER	2.5
1	A	175	THR	2.5
1	B	257	THR	2.5
1	C	214	ASN	2.5
1	D	170	GLY	2.5
1	D	286[A]	LEU	2.5
1	C	112	PHE	2.5
1	C	263	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	172	HIS	2.5
1	C	122	PRO	2.4
1	D	217	ARG	2.4
1	A	290	GLU	2.4
1	A	114	VAL	2.4
1	B	191	ALA	2.4
1	B	210	ALA	2.4
1	C	181	PHE	2.4
1	A	192	GLN	2.4
1	A	56	ASP	2.4
1	B	188	ARG	2.4
1	A	137	LYS	2.4
1	B	174	GLY	2.4
1	D	159	PHE	2.4
1	D	31	TRP	2.4
1	B	83	GLN	2.4
1	D	273	GLN	2.4
1	A	22	CYS	2.4
1	A	260	ALA	2.4
1	D	194	ALA	2.4
1	B	137	LYS	2.4
1	A	236	LYS	2.4
1	D	149	GLY	2.4
1	A	21	THR	2.4
1	B	201	THR	2.4
1	C	156	CYS	2.4
1	D	233	VAL	2.4
1	A	19	GLN	2.4
1	B	263	ASP	2.4
1	D	146	GLY	2.4
1	D	229	ASP	2.4
1	B	177	LEU	2.4
1	C	50	LEU	2.4
1	B	252	PRO	2.4
1	C	108	PRO	2.4
1	D	277[A]	ASN	2.4
1	A	80	HIS	2.3
1	B	124	GLY	2.3
1	C	262	LEU	2.3
1	A	150	PHE	2.3
1	B	8	PHE	2.3
1	C	139	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	197	ASP	2.3
1	B	278[A]	GLY	2.3
1	D	138	GLY	2.3
1	D	166	GLU	2.3
1	A	107	GLN	2.3
1	B	287[A]	LEU	2.3
1	C	201	THR	2.3
1	D	201	THR	2.3
1	B	288[A]	GLU	2.3
1	B	74	GLN	2.3
1	A	40	ARG	2.3
1	C	218	TRP	2.3
1	B	91	VAL	2.3
1	A	274	ASN	2.3
1	B	53	ASN	2.3
1	C	153	ASP	2.3
1	A	287[A]	LEU	2.3
1	D	75	LEU	2.3
1	D	69	GLN	2.3
1	D	74	GLN	2.3
1	B	42	VAL	2.3
1	D	181	PHE	2.3
1	C	176	ASP	2.3
1	C	100	LYS	2.3
1	A	81	SER	2.3
1	D	211	ALA	2.3
1	A	29	GLY	2.3
1	B	66	PHE	2.3
1	A	299	GLN	2.3
1	D	281	ILE	2.3
1	B	120	GLY	2.2
1	C	188	ARG	2.2
1	A	246	HIS	2.2
1	B	97	LYS	2.2
1	D	97	LYS	2.2
1	C	247	VAL	2.2
1	C	261	VAL	2.2
1	D	131	ARG	2.2
1	B	17	MET	2.2
1	D	163	HIS	2.2
1	B	12	LYS	2.2
1	A	24	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	213	ILE	2.2
1	A	41	HIS	2.2
1	C	216	ASP	2.2
1	B	209	TYR	2.2
1	C	99	PRO	2.2
1	A	88	LYS	2.2
1	B	73	VAL	2.2
1	C	91	VAL	2.2
1	A	284	SER	2.2
1	C	215	GLY	2.2
1	A	187	ASP	2.2
1	A	231	ASN	2.2
1	A	126[A]	TYR	2.2
1	A	91	VAL	2.2
1	C	53	ASN	2.2
1	C	160	CYS	2.2
1	A	70	ALA	2.2
1	A	257	THR	2.2
1	D	192	GLN	2.2
1	C	220	LEU	2.2
1	C	162	MET	2.2
1	B	119	ASN	2.2
1	C	84	ASN	2.2
1	C	21	THR	2.2
1	D	169	THR	2.2
1	B	16	CYS	2.2
1	A	166	GLU	2.2
1	C	240	GLU	2.2
1	A	6	MET	2.2
1	B	29	GLY	2.2
1	D	269	LYS	2.1
1	B	36	VAL	2.1
1	A	92	ASP	2.1
1	A	102	LYS	2.1
1	B	155	ASP	2.1
1	A	127	GLN	2.1
1	B	63	ASN	2.1
1	D	10	SER	2.1
1	D	65	ASN	2.1
1	D	282	LEU	2.1
1	D	196	THR	2.1
1	A	66	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	131	ARG	2.1
1	D	144	SER	2.1
1	D	246	HIS	2.1
1	A	210	ALA	2.1
1	C	204	VAL	2.1
1	C	9	PRO	2.1
1	D	141	LEU	2.1
1	B	256	GLN	2.1
1	D	145	CYS	2.1
1	A	62	SER	2.1
1	A	269	LYS	2.1
1	D	254	SER	2.1
1	B	27	LEU	2.1
1	C	264	MET	2.1
1	A	100	LYS	2.1
1	B	111[A]	THR	2.1
1	B	35	VAL	2.1
1	D	76	ARG	2.0
1	A	12	LYS	2.0
1	C	137	LYS	2.0
1	A	170	GLY	2.0
1	A	168	PRO	2.0
1	D	293	PRO	2.0
1	D	185	PHE	2.0
1	A	228	ASN	2.0
1	A	124	GLY	2.0
1	B	123	SER	2.0
1	C	7	ALA	2.0
1	D	148	VAL	2.0
1	A	71	GLY	2.0
1	D	226	THR	2.0
1	D	260	ALA	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 [\(i\)](#)

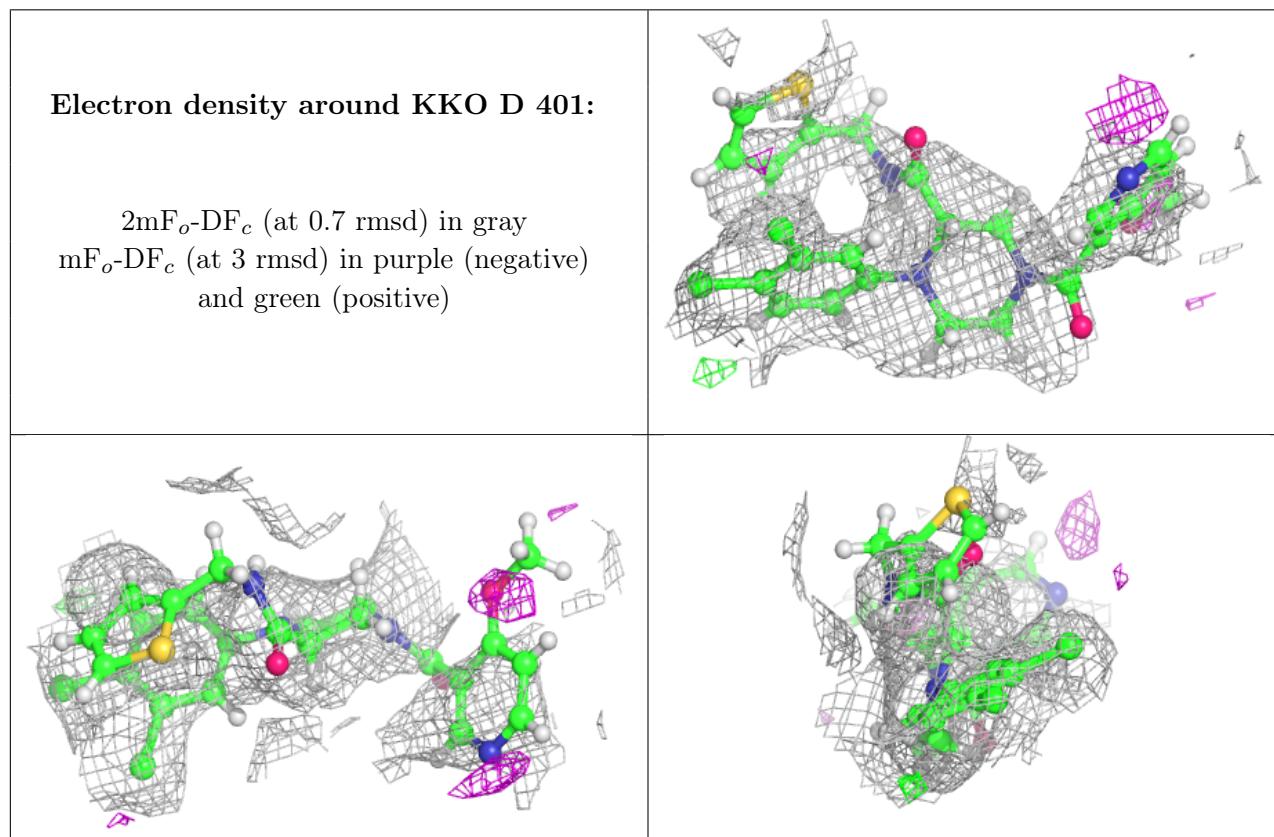
There are no monosaccharides in this entry.

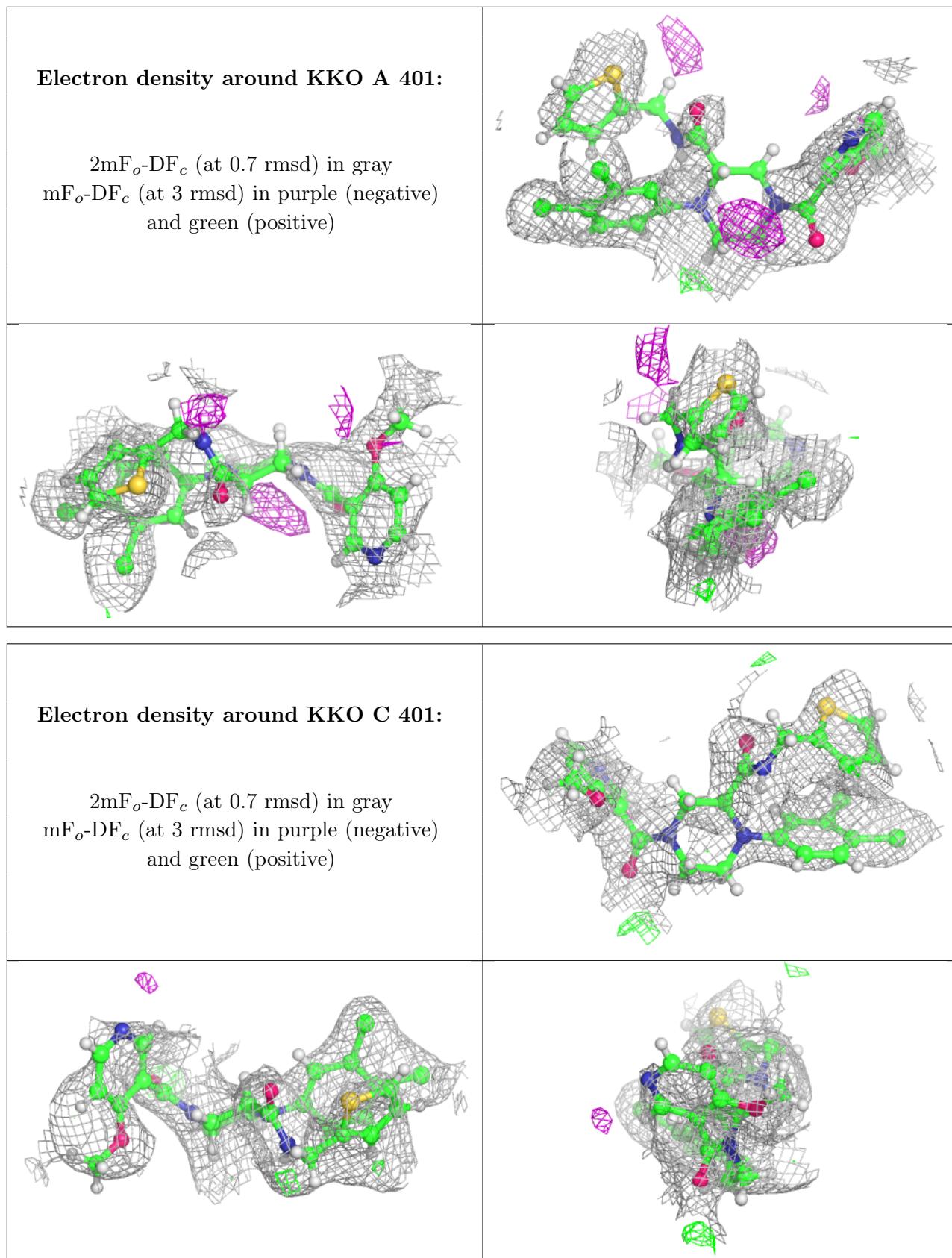
## 6.4 Ligands [\(i\)](#)

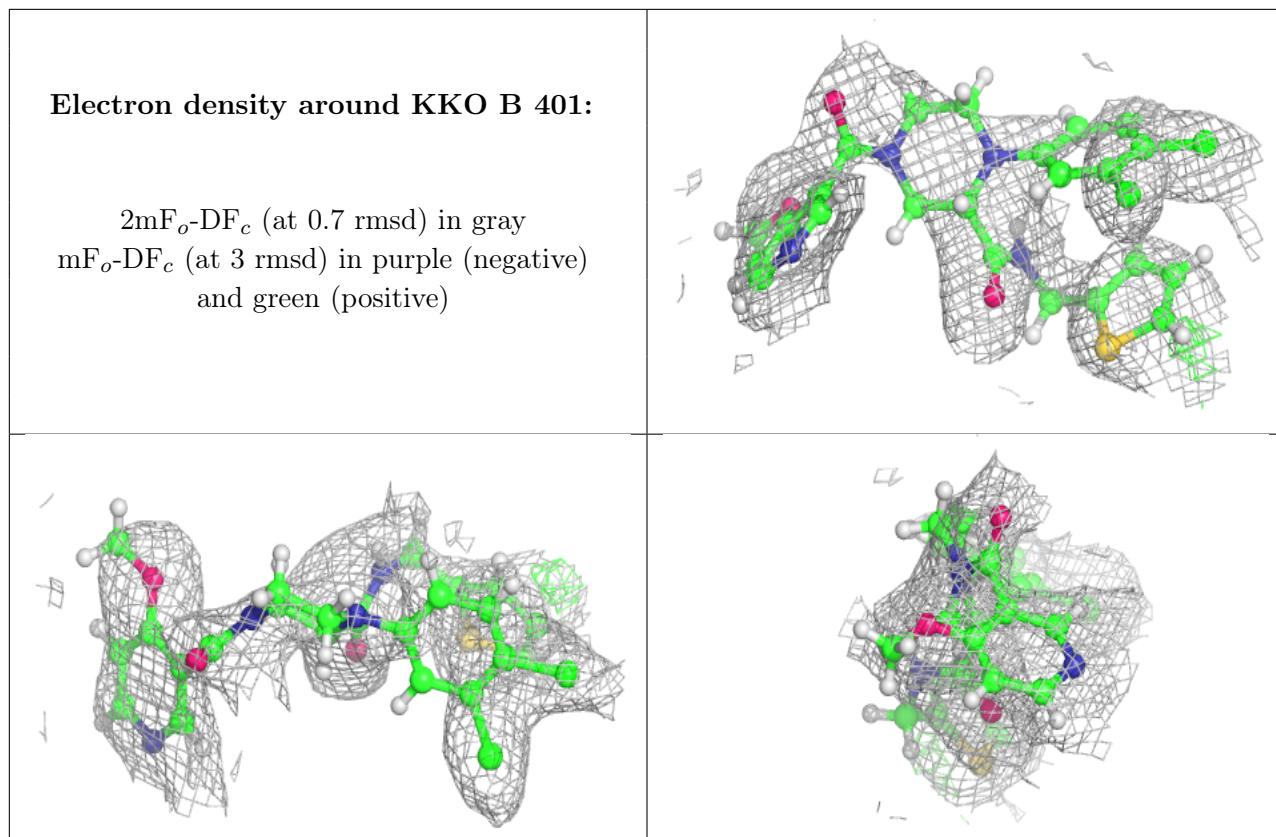
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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	KKO	D	401	33/33	0.55	0.40	39,46,61,68	0
2	KKO	A	401	33/33	0.61	0.39	31,34,41,43	0
2	KKO	C	401	33/33	0.68	0.28	34,41,49,52	0
2	KKO	B	401	33/33	0.73	0.30	32,38,46,53	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.







## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.