



# Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2021 – 04:09 PM EDT

PDB ID : 4DKU  
Title : Crystal structure of clade A/E 93TH057 HIV-1 gp120 core in complex with NBD-09027  
Authors : Kwon, Y.D.; Debnath, A.K.; Kwong, P.D.  
Deposited on : 2012-02-04  
Resolution : 2.49 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.

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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	:	2.18
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)	:	2.18

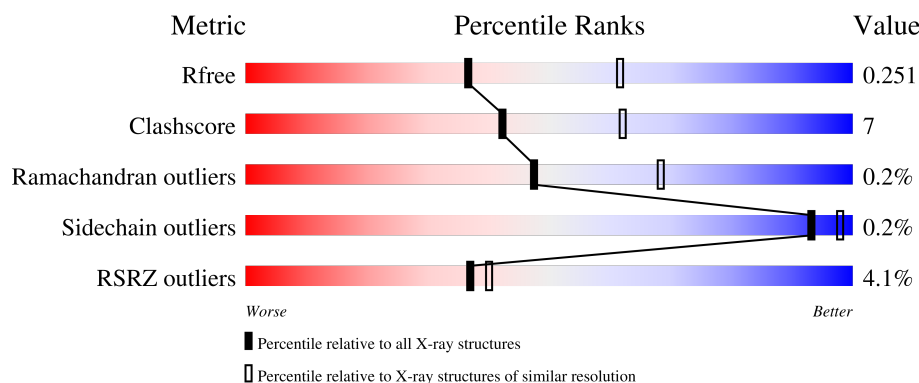
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.49 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	353	
1	B	353	

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
4	0KU	B	511	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5807 atoms, of which 46 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.

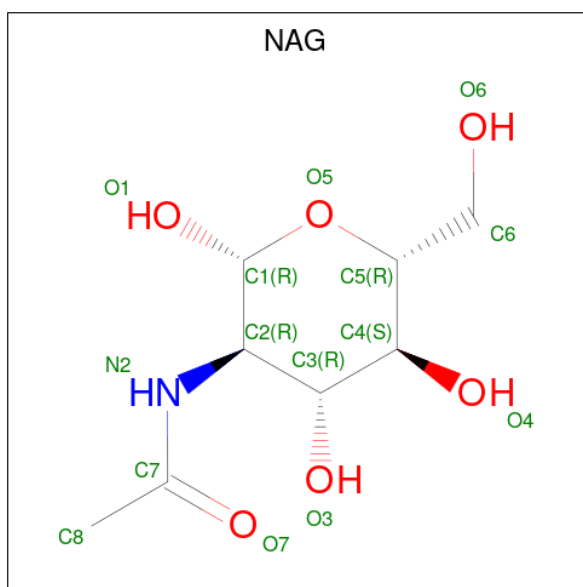
- Molecule 1 is a protein called HIV-1 gp120 core.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			
1	B	339	Total	C	N	O	S	0	0	0
			2654	1666	460	507	21			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	GLY	-	linker	UNP Q0ED31
A	198	GLY	-	linker	UNP Q0ED31
A	318	GLY	-	linker	UNP Q0ED31
A	319	GLY	-	linker	UNP Q0ED31
A	320	SER	-	linker	UNP Q0ED31
A	321	GLY	-	linker	UNP Q0ED31
A	322	SER	-	linker	UNP Q0ED31
A	323	GLY	-	linker	UNP Q0ED31
A	375	SER	HIS	engineered mutation	UNP Q0ED31
B	124	GLY	-	linker	UNP Q0ED31
B	198	GLY	-	linker	UNP Q0ED31
B	318	GLY	-	linker	UNP Q0ED31
B	319	GLY	-	linker	UNP Q0ED31
B	320	SER	-	linker	UNP Q0ED31
B	321	GLY	-	linker	UNP Q0ED31
B	322	SER	-	linker	UNP Q0ED31
B	323	GLY	-	linker	UNP Q0ED31
B	375	SER	HIS	engineered mutation	UNP Q0ED31

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



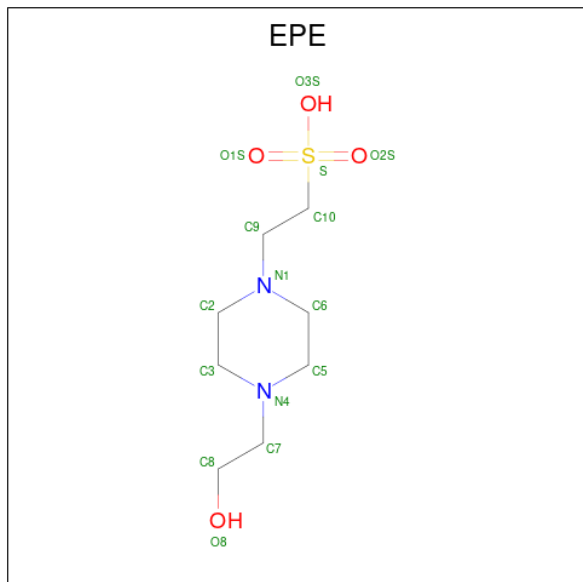
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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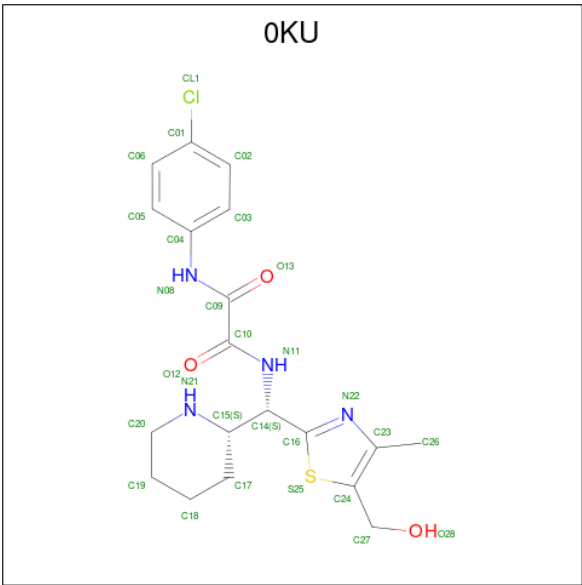
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is N-(4-chlorophenyl)-N'-{(S)-[5-(hydroxymethyl)-4-methyl-1,3-thiazol-2-yl]}[(2S)-piperidin-2-yl]methyl}ethanediamide (three-letter code: 0KU) (formula: C<sub>19</sub>H<sub>23</sub>ClN<sub>4</sub>O<sub>3</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	Cl	H	N	O	S	0	0
			51	19	1	23	4	3	1		
4	B	1	Total	C	Cl	H	N	O	S	0	0
			51	19	1	23	4	3	1		

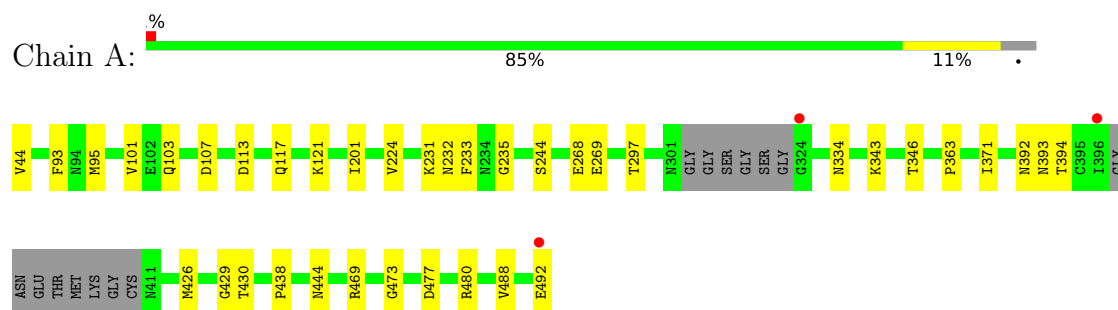
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	71	Total	O	0	0
			71	71		
5	B	30	Total	O	0	0
			30	30		

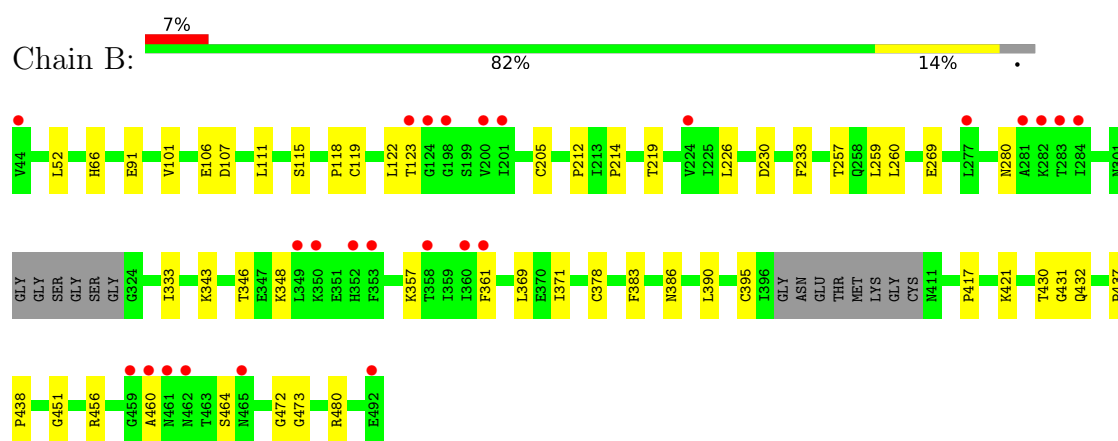
### 3 Residue-property plots

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: HIV-1 gp120 core



#### • Molecule 1: HIV-1 gp120 core





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.23Å 68.44Å 93.97Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	28.50 – 2.49 46.96 – 2.49	Depositor EDS
% Data completeness (in resolution range)	92.4 (28.50-2.49) 88.1 (46.96-2.49)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.46 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, $R_{free}$	0.200 , 0.249 0.204 , 0.251	Depositor DCC
$R_{free}$ test set	1283 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5807	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, EPE, OKU

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	0.23	0/2709	0.42	0/3678
1	B	0.23	0/2709	0.42	0/3678
All	All	0.23	0/5418	0.42	0/7356

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

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	2654	0	2589	29	0
1	B	2654	0	2590	45	0
2	A	140	0	130	3	0
2	B	126	0	116	0	0
3	A	15	0	17	3	0
3	B	15	0	17	2	0
4	A	28	23	23	7	0
4	B	28	23	23	14	0
5	A	71	0	0	5	0
5	B	30	0	0	6	0
All	All	5761	46	5505	77	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 7.

All (77) 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:395:CYS:SG	5:B:623:HOH:O	2.18	0.97
1:B:371:ILE:CD1	4:B:511:0KU:H14	2.05	0.87
1:B:371:ILE:HD11	4:B:511:0KU:C18	2.11	0.80
1:B:106:GLU:OE1	5:B:620:HOH:O	1.98	0.80
1:A:488:VAL:O	5:A:665:HOH:O	2.01	0.76
1:B:371:ILE:HD11	4:B:511:0KU:C19	2.16	0.76
1:A:473:GLY:HA3	4:A:512:0KU:H9	1.69	0.74
1:A:438:PRO:O	5:A:611:HOH:O	2.06	0.74
1:B:371:ILE:HD11	4:B:511:0KU:H14	1.70	0.72
1:A:269:GLU:OE2	5:A:666:HOH:O	2.10	0.69
1:A:477:ASP:OD1	1:A:480:ARG:NH1	2.25	0.69
1:B:472:GLY:O	5:B:622:HOH:O	2.10	0.68
1:B:473:GLY:HA3	4:B:511:0KU:H9	1.75	0.68
1:A:371:ILE:HD11	4:A:512:0KU:H10	1.77	0.66
1:B:371:ILE:HD11	4:B:511:0KU:H10	1.78	0.66
1:A:480:ARG:NH2	5:A:618:HOH:O	2.28	0.65
1:B:122:LEU:HB2	1:B:432:GLN:HB3	1.77	0.65
1:B:371:ILE:HD11	4:B:511:0KU:C17	2.28	0.64
1:B:269:GLU:OE1	1:B:348:LYS:NZ	2.32	0.63
1:A:121:LYS:HB2	1:A:201:ILE:HB	1.83	0.61
1:B:473:GLY:CA	4:B:511:0KU:H9	2.31	0.60
1:B:123:THR:HG21	1:B:430:THR:HB	1.83	0.59
1:B:333:ILE:HD12	1:B:390:LEU:HD21	1.83	0.59
1:B:115:SER:O	5:B:624:HOH:O	2.17	0.58
1:A:113:ASP:O	1:A:117:GLN:NE2	2.28	0.58
1:A:473:GLY:CA	4:A:512:0KU:H9	2.33	0.58
1:A:473:GLY:HA3	4:A:512:0KU:C17	2.33	0.57
1:A:224:VAL:HG11	1:A:244:SER:HB2	1.87	0.57
1:A:480:ARG:NE	5:A:605:HOH:O	2.11	0.53
1:B:101:VAL:HG21	1:B:480:ARG:HG2	1.90	0.52
1:B:280:ASN:OD1	1:B:456:ARG:NH2	2.43	0.52
1:B:386:ASN:HB3	1:B:417:PRO:HG2	1.92	0.52
1:A:107:ASP:OD2	3:A:511:EPE:H72	2.10	0.52
1:A:392:ASN:O	1:A:394:THR:N	2.37	0.51
2:A:508:NAG:H62	1:B:214:PRO:HG2	1.91	0.51
1:B:346:THR:HG22	1:B:361:PHE:HE1	1.75	0.51
1:B:66:HIS:CD2	1:B:111:LEU:HD21	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:CYS:SG	1:B:205:CYS:N	2.84	0.50
1:B:230:ASP:HB2	1:B:233:PHE:HB2	1.93	0.49
1:B:371:ILE:CD1	4:B:511:0KU:C18	2.86	0.48
1:B:378:CYS:HB3	1:B:383:PHE:CE1	2.49	0.48
1:A:363:PRO:O	1:A:469:ARG:NH1	2.45	0.48
1:A:93:PHE:HB2	1:A:233:PHE:HZ	1.79	0.48
1:B:371:ILE:CD1	4:B:511:0KU:H11	2.45	0.47
1:B:371:ILE:HD11	4:B:511:0KU:H11	1.96	0.47
4:A:512:0KU:H21	4:A:512:0KU:O28	2.15	0.47
1:A:426:MET:SD	1:A:430:THR:OG1	2.73	0.47
1:A:44:VAL:HG13	1:A:492:GLU:HB2	1.96	0.46
1:A:429:GLY:HA2	4:A:512:0KU:H20	1.97	0.46
1:B:260:LEU:HD12	1:B:451:GLY:HA3	1.97	0.46
1:B:371:ILE:CD1	4:B:511:0KU:C19	2.78	0.45
4:B:511:0KU:H21	4:B:511:0KU:O28	2.15	0.45
1:B:257:THR:O	1:B:259:LEU:N	2.48	0.45
1:B:357:LYS:HB3	1:B:464:SER:O	2.17	0.45
1:B:395:CYS:CB	5:B:623:HOH:O	2.57	0.45
1:A:429:GLY:CA	4:A:512:0KU:H20	2.47	0.45
1:A:297:THR:HG22	1:A:444:ASN:HB2	1.99	0.44
1:B:107:ASP:OD2	3:B:510:EPE:H72	2.17	0.44
1:B:473:GLY:HA3	4:B:511:0KU:C17	2.43	0.44
1:A:101:VAL:HG21	1:A:480:ARG:HG2	2.00	0.44
1:B:52:LEU:O	3:B:510:EPE:H81	2.18	0.44
1:B:219:THR:OG1	5:B:621:HOH:O	2.21	0.43
1:A:232:ASN:OD1	1:A:268:GLU:HB3	2.19	0.43
1:A:95:MET:SD	1:A:235:GLY:HA3	2.60	0.42
1:B:91:GLU:HG3	1:B:226:LEU:HD13	1.99	0.42
1:A:343:LYS:O	1:A:346:THR:OG1	2.31	0.42
1:B:123:THR:HB	1:B:431:GLY:HA3	2.01	0.42
1:B:357:LYS:NZ	1:B:460:ALA:O	2.52	0.42
1:B:66:HIS:CD2	1:B:212:PRO:HA	2.54	0.42
1:A:103:GLN:HB3	3:A:511:EPE:O8	2.20	0.42
1:B:437:PRO:HA	1:B:438:PRO:HD3	1.91	0.42
1:B:343:LYS:O	1:B:346:THR:OG1	2.28	0.41
2:A:510:NAG:H83	2:A:510:NAG:H2	1.94	0.41
1:A:107:ASP:OD1	3:A:511:EPE:H31	2.19	0.41
1:B:369:LEU:HD12	1:B:421:LYS:HE3	2.01	0.41
1:B:118:PRO:C	1:B:205:CYS:HB3	2.42	0.40
1:A:334:ASN:HA	2:A:507:NAG:H82	2.03	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	A	333/353 (94%)	316 (95%)	16 (5%)	1 (0%)	41	61
1	B	333/353 (94%)	316 (95%)	17 (5%)	0	100	100
All	All	666/706 (94%)	632 (95%)	33 (5%)	1 (0%)	47	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	393	ASN

### 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	303/311 (97%)	302 (100%)	1 (0%)	92	97
1	B	303/311 (97%)	303 (100%)	0	100	100
All	All	606/622 (97%)	605 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	LYS

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	432	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](#)

23 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	NAG	B	502	1	14,14,15	0.57	0	17,19,21	1.09	1 (5%)
2	NAG	B	504	1	14,14,15	0.48	0	17,19,21	0.86	0
2	NAG	A	504	1	14,14,15	0.55	0	17,19,21	0.69	0
2	NAG	B	503	1	14,14,15	0.52	0	17,19,21	0.92	1 (5%)
2	NAG	A	509	1	14,14,15	0.54	0	17,19,21	0.67	0
2	NAG	A	501	1	14,14,15	0.58	0	17,19,21	0.67	0
2	NAG	A	505	1	14,14,15	0.49	0	17,19,21	0.84	1 (5%)
2	NAG	B	508	1	14,14,15	0.48	0	17,19,21	0.81	0
2	NAG	B	506	1	14,14,15	0.50	0	17,19,21	0.95	0
2	NAG	A	508	1	14,14,15	0.61	0	17,19,21	0.93	1 (5%)
3	EPE	A	511	-	15,15,15	2.43	4 (26%)	18,20,20	3.82	5 (27%)
4	OKU	B	511	-	27,30,30	2.18	9 (33%)	28,41,41	1.93	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	506	1	14,14,15	0.45	0	17,19,21	1.28	3 (17%)
2	NAG	B	507	1	14,14,15	0.58	0	17,19,21	0.82	0
2	NAG	B	505	1	14,14,15	0.58	0	17,19,21	0.76	0
2	NAG	A	507	1	14,14,15	0.54	0	17,19,21	0.75	0
2	NAG	A	502	1	14,14,15	0.51	0	17,19,21	0.70	0
3	EPE	B	510	-	15,15,15	2.46	4 (26%)	18,20,20	3.88	5 (27%)
2	NAG	B	501	1	14,14,15	0.50	0	17,19,21	0.78	0
2	NAG	A	503	1	14,14,15	0.52	0	17,19,21	0.86	1 (5%)
4	OKU	A	512	-	27,30,30	2.18	9 (33%)	28,41,41	1.93	4 (14%)
2	NAG	B	509	1	14,14,15	0.49	0	17,19,21	0.78	0
2	NAG	A	510	1	14,14,15	0.48	0	17,19,21	0.68	0

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	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	504	1	-	0/6/23/26	0/1/1/1
2	NAG	A	504	1	-	0/6/23/26	0/1/1/1
2	NAG	B	503	1	-	0/6/23/26	0/1/1/1
2	NAG	A	509	1	-	0/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1	-	2/6/23/26	0/1/1/1
2	NAG	B	508	1	-	2/6/23/26	0/1/1/1
2	NAG	B	506	1	-	2/6/23/26	0/1/1/1
2	NAG	A	508	1	-	4/6/23/26	0/1/1/1
3	EPE	A	511	-	-	2/9/19/19	0/1/1/1
4	OKU	B	511	-	-	4/16/30/30	0/3/3/3
2	NAG	A	506	1	-	0/6/23/26	0/1/1/1
2	NAG	B	507	1	-	2/6/23/26	0/1/1/1
2	NAG	B	505	1	-	2/6/23/26	0/1/1/1
2	NAG	A	507	1	-	2/6/23/26	0/1/1/1
2	NAG	A	502	1	-	2/6/23/26	0/1/1/1
3	EPE	B	510	-	-	3/9/19/19	0/1/1/1
2	NAG	B	501	1	-	1/6/23/26	0/1/1/1
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1
4	OKU	A	512	-	-	4/16/30/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	509	1	-	2/6/23/26	0/1/1/1
2	NAG	A	510	1	-	2/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	510	EPE	O2S-S	5.08	1.60	1.45
3	A	511	EPE	O2S-S	5.02	1.59	1.45
3	B	510	EPE	O1S-S	4.94	1.59	1.45
3	A	511	EPE	O1S-S	4.94	1.59	1.45
4	B	511	OKU	C10-N11	4.90	1.44	1.34
4	A	512	OKU	C10-N11	4.85	1.43	1.34
4	A	512	OKU	C17-C15	-4.59	1.45	1.53
4	B	511	OKU	C17-C15	-4.57	1.45	1.53
3	B	510	EPE	O3S-S	4.27	1.62	1.47
4	A	512	OKU	C15-N21	-4.24	1.41	1.47
3	A	511	EPE	O3S-S	4.22	1.62	1.47
4	B	511	OKU	C15-N21	-4.17	1.41	1.47
3	B	510	EPE	O8-C8	-3.95	1.21	1.42
3	A	511	EPE	O8-C8	-3.88	1.22	1.42
4	A	512	OKU	O13-C09	-3.17	1.17	1.23
4	B	511	OKU	O13-C09	-3.15	1.17	1.23
4	B	511	OKU	O12-C10	-2.76	1.18	1.23
4	B	511	OKU	C09-N08	2.74	1.41	1.35
4	A	512	OKU	C09-N08	2.72	1.41	1.35
4	A	512	OKU	O12-C10	-2.72	1.18	1.23
4	A	512	OKU	C14-N11	-2.62	1.41	1.46
4	B	511	OKU	C14-N11	-2.55	1.41	1.46
4	A	512	OKU	C01-CL1	-2.44	1.69	1.74
4	B	511	OKU	C01-CL1	-2.44	1.69	1.74
4	B	511	OKU	C10-C09	-2.38	1.49	1.53
4	A	512	OKU	C10-C09	-2.33	1.49	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	510	EPE	O1S-S-C10	11.07	120.25	106.92
3	A	511	EPE	O1S-S-C10	10.86	119.99	106.92
3	B	510	EPE	O2S-S-C10	8.64	117.32	106.92
3	A	511	EPE	O2S-S-C10	8.49	117.14	106.92
3	B	510	EPE	O3S-S-O2S	-5.29	98.34	111.27
3	A	511	EPE	O3S-S-O1S	-5.06	98.91	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	510	EPE	O3S-S-O1S	-4.87	99.37	111.27
3	A	511	EPE	O3S-S-O2S	-4.80	99.56	111.27
4	A	512	0KU	C10-C09-N08	4.68	119.71	112.31
4	B	511	0KU	C10-C09-N08	4.68	119.70	112.31
4	B	511	0KU	C17-C15-C14	4.51	117.40	112.61
4	A	512	0KU	C17-C15-C14	4.48	117.37	112.61
4	B	511	0KU	C17-C15-N21	-4.46	105.34	111.90
4	A	512	0KU	C17-C15-N21	-4.46	105.35	111.90
2	A	508	NAG	C1-O5-C5	2.90	116.13	112.19
3	A	511	EPE	O8-C8-C7	2.83	122.91	111.19
3	B	510	EPE	O8-C8-C7	2.81	122.85	111.19
4	A	512	0KU	C09-C10-N11	2.76	120.35	113.73
4	B	511	0KU	C09-C10-N11	2.74	120.30	113.73
2	A	506	NAG	C1-O5-C5	2.61	115.73	112.19
2	A	506	NAG	O5-C1-C2	-2.33	107.60	111.29
2	B	502	NAG	O5-C1-C2	2.29	114.90	111.29
2	A	503	NAG	O5-C5-C6	2.27	110.77	107.20
2	A	505	NAG	O5-C5-C6	2.23	110.70	107.20
2	B	503	NAG	O5-C5-C6	2.05	110.42	107.20
2	A	506	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	NAG	C8-C7-N2-C2
2	A	502	NAG	O7-C7-N2-C2
2	A	508	NAG	C8-C7-N2-C2
2	A	508	NAG	O7-C7-N2-C2
2	A	510	NAG	C8-C7-N2-C2
2	A	510	NAG	O7-C7-N2-C2
3	A	511	EPE	C10-C9-N1-C6
3	B	510	EPE	C10-C9-N1-C6
4	A	512	0KU	N11-C14-C15-C17
4	A	512	0KU	N11-C14-C15-N21
4	A	512	0KU	C16-C14-C15-C17
4	A	512	0KU	C16-C14-C15-N21
4	B	511	0KU	N11-C14-C15-C17
4	B	511	0KU	N11-C14-C15-N21
4	B	511	0KU	C16-C14-C15-C17
4	B	511	0KU	C16-C14-C15-N21
2	B	505	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	505	NAG	C4-C5-C6-O6
2	B	507	NAG	C8-C7-N2-C2
2	B	509	NAG	C8-C7-N2-C2
2	B	509	NAG	O7-C7-N2-C2
2	A	505	NAG	C8-C7-N2-C2
2	A	507	NAG	C8-C7-N2-C2
2	B	506	NAG	C8-C7-N2-C2
2	B	507	NAG	O7-C7-N2-C2
2	A	507	NAG	O7-C7-N2-C2
2	B	506	NAG	O7-C7-N2-C2
2	A	505	NAG	O7-C7-N2-C2
2	B	508	NAG	C8-C7-N2-C2
2	B	501	NAG	O5-C5-C6-O6
3	B	510	EPE	C10-C9-N1-C2
2	B	508	NAG	O7-C7-N2-C2
2	A	508	NAG	C1-C2-N2-C7
3	B	510	EPE	C9-C10-S-O1S
3	A	511	EPE	C10-C9-N1-C2
2	A	508	NAG	C3-C2-N2-C7

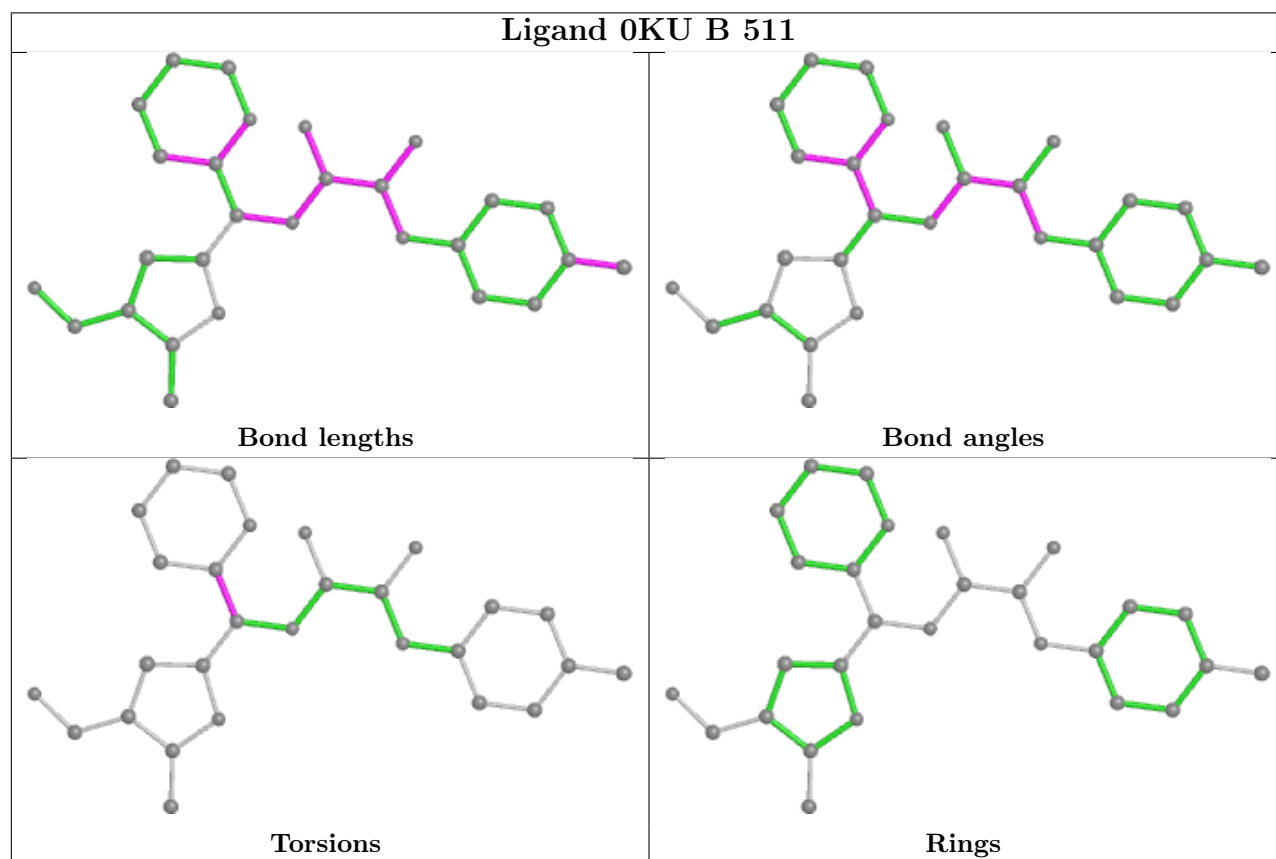
There are no ring outliers.

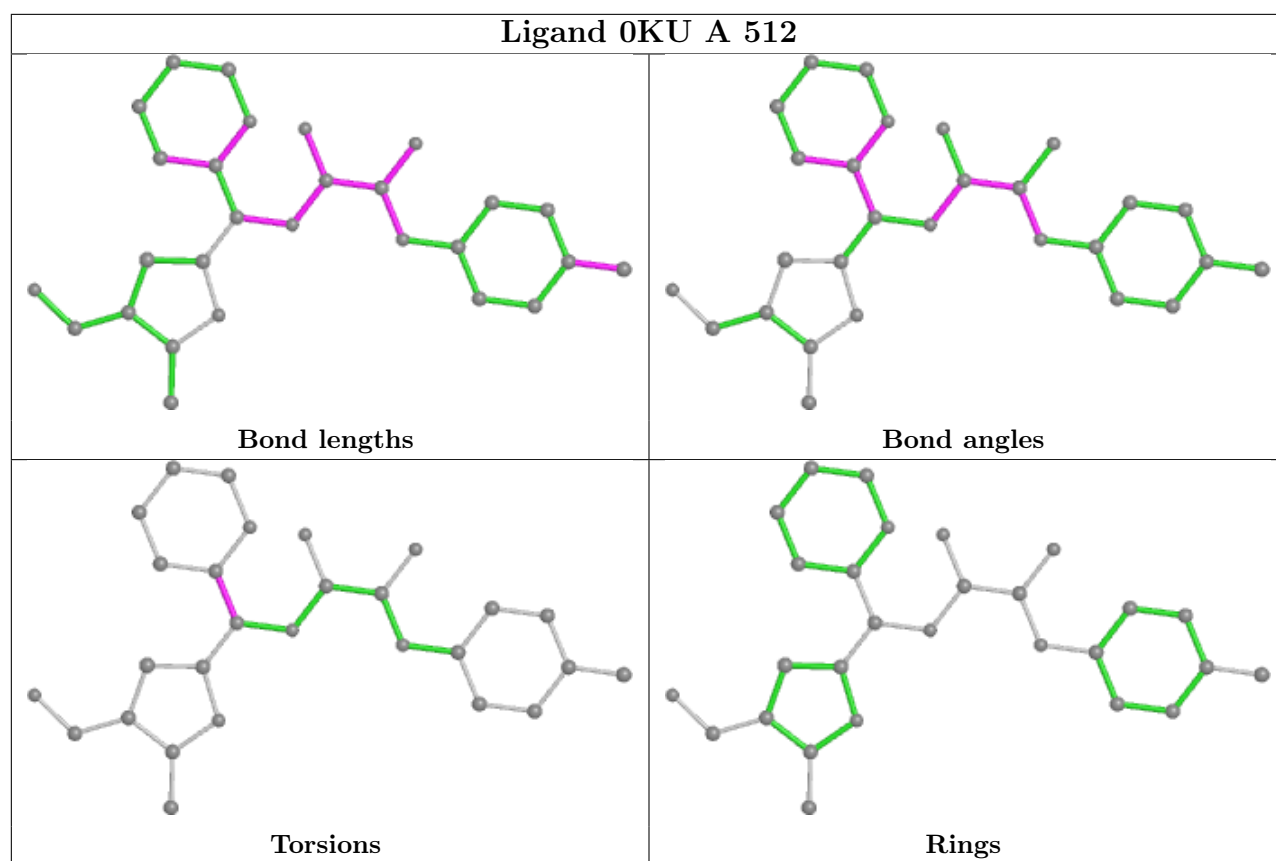
7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	508	NAG	1	0
3	A	511	EPE	3	0
4	B	511	0KU	14	0
2	A	507	NAG	1	0
3	B	510	EPE	2	0
4	A	512	0KU	7	0
2	A	510	NAG	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	339/353 (96%)	-0.19	3 (0%) 84 86	30, 50, 87, 106	0
1	B	339/353 (96%)	0.34	25 (7%) 14 15	38, 68, 115, 158	0
All	All	678/706 (96%)	0.08	28 (4%) 37 40	30, 58, 104, 158	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	462	ASN	6.7
1	B	124	GLY	5.1
1	B	353	PHE	4.3
1	B	200	VAL	3.7
1	B	358	THR	3.6
1	B	492	GLU	3.4
1	B	44	VAL	3.4
1	A	396	ILE	3.2
1	B	283	THR	3.1
1	B	460	ALA	3.0
1	B	459	GLY	2.9
1	B	277	LEU	2.8
1	A	492	GLU	2.8
1	B	201	ILE	2.8
1	B	198	GLY	2.8
1	B	224	VAL	2.8
1	B	461	ASN	2.7
1	B	123	THR	2.6
1	B	350	LYS	2.5
1	B	361	PHE	2.5
1	B	281	ALA	2.4
1	B	352	HIS	2.3
1	B	465	ASN	2.2
1	B	360	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	282	LYS	2.1
1	A	324	GLY	2.1
1	B	284	ILE	2.1
1	B	349	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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
4	OKU	B	511	28/28	0.62	0.59	67,87,109,157	0
2	NAG	B	502	14/15	0.69	0.30	102,124,134,138	0
2	NAG	B	509	14/15	0.76	0.29	101,121,135,138	0
2	NAG	A	502	14/15	0.76	0.38	110,136,151,157	0
2	NAG	A	507	14/15	0.77	0.25	94,118,123,126	0
2	NAG	B	504	14/15	0.78	0.31	82,99,114,124	0
2	NAG	B	507	14/15	0.79	0.32	91,121,130,132	0
2	NAG	B	501	14/15	0.81	0.31	85,115,147,161	0
2	NAG	B	505	14/15	0.83	0.14	50,87,97,105	0
4	OKU	A	512	28/28	0.84	0.25	50,83,112,160	0
2	NAG	A	506	14/15	0.87	0.23	65,77,95,103	0
2	NAG	B	506	14/15	0.89	0.16	52,72,92,94	0
2	NAG	A	510	14/15	0.92	0.19	64,79,87,87	0
2	NAG	A	508	14/15	0.92	0.20	41,54,89,95	0
2	NAG	A	505	14/15	0.93	0.13	55,62,83,87	0
2	NAG	B	508	14/15	0.94	0.12	73,93,97,99	0
2	NAG	A	504	14/15	0.94	0.12	61,66,73,77	0
2	NAG	A	509	14/15	0.94	0.14	53,77,94,98	0
2	NAG	A	501	14/15	0.94	0.14	52,71,85,87	0

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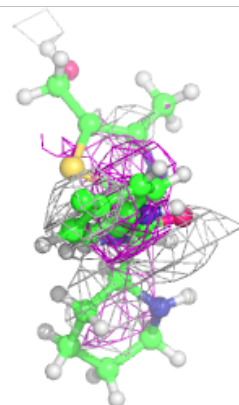
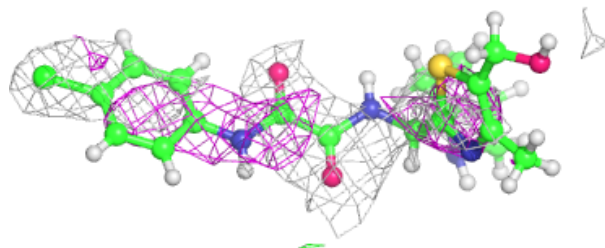
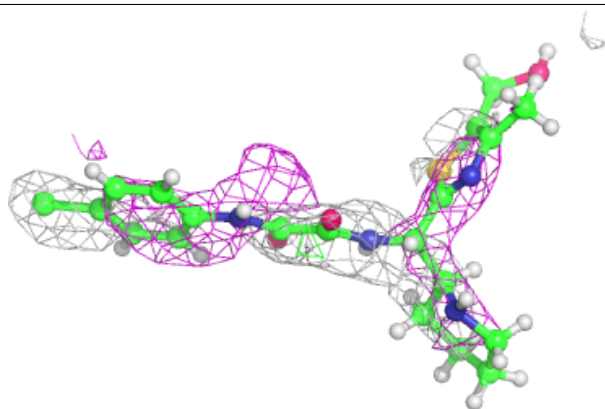
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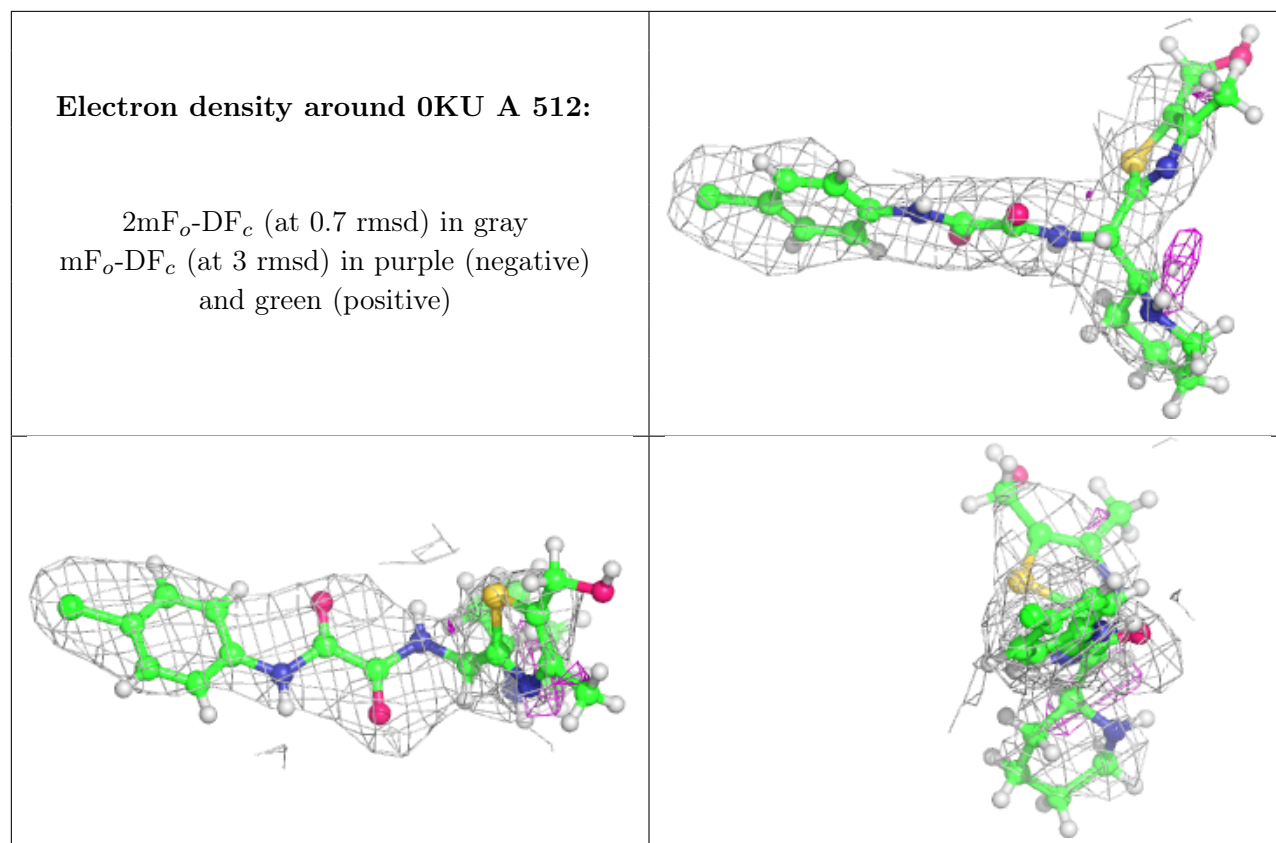
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	B	503	14/15	0.95	0.16	24,41,47,48	0
2	NAG	A	503	14/15	0.96	0.12	35,42,52,53	0
3	EPE	A	511	15/15	0.97	0.16	29,43,47,50	0
3	EPE	B	510	15/15	0.97	0.18	40,54,75,102	0

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 0KU B 511:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.