



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 02:02 PM EDT

PDB ID : 6NR0  
Title : SIRT2(56-356) with covalent intermediate between mechanism-based inhibitor  
Glucose-TM-1beta and 1'-SH ADP-ribose  
Authors : Price, I.R.; Hong, J.  
Deposited on : 2019-01-22  
Resolution : 2.45 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 : 2.23.2  
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) : 2.23.2

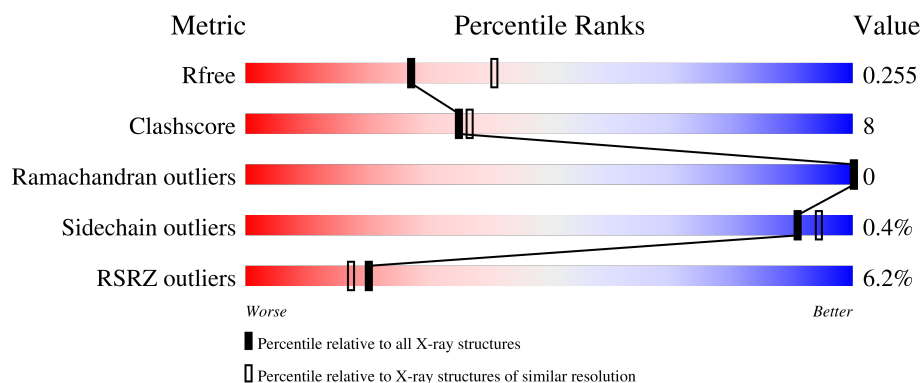
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	319	 4% 77% 13% 9%
1	B	319	 7% 70% 21% 9%

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
6	SO4	B	406	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9501 atoms, of which 4535 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.

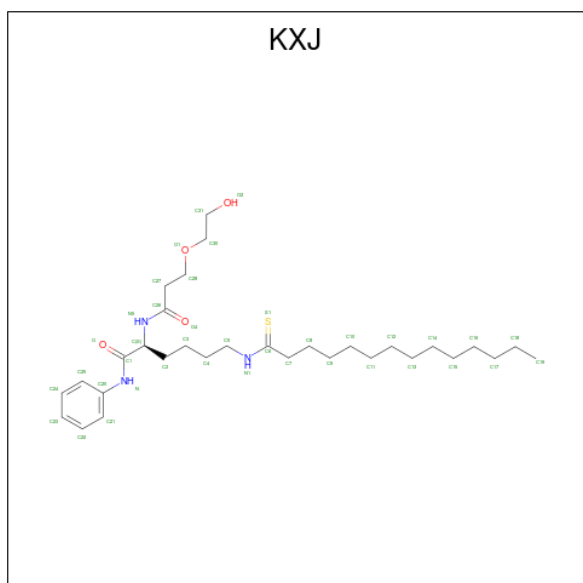
- Molecule 1 is a protein called NAD-dependent protein deacetylase sirtuin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	H	N	O	S	0	2	0
			4526	1481	2214	385	429	17			
1	B	291	Total	C	H	N	O	S	0	6	0
			4594	1497	2255	390	435	17			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

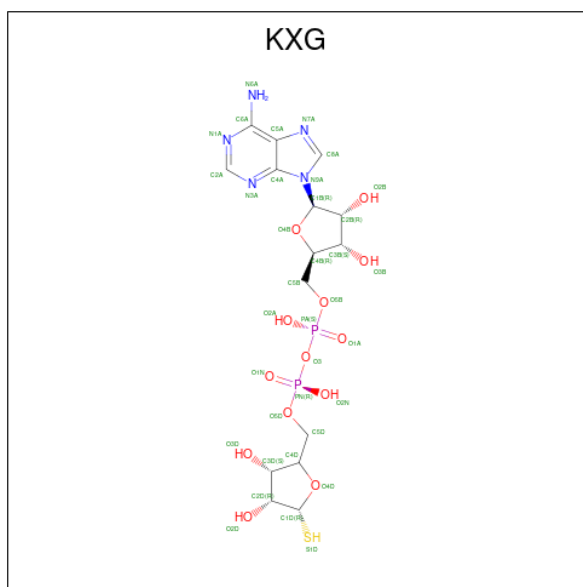
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is N 2 -[3-(2-hydroxyethoxy)propanoyl]-N-phenyl-N 6 -tetradecanethioyl-L-lys inamide (three-letter code: KXJ) (formula: C<sub>31</sub>H<sub>53</sub>N<sub>3</sub>O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 34	C 29	N 3	O 2	0	0
3	B	1	Total 35	C 28	N 3	O 4	0	0

- Molecule 4 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(3 {S},4 {R},5 {R})-3,4-bis(oxidanyl)-5-sulfanyl-oxolan-2-yl]methyl hydrogen phosphate (three-letter code: KXG) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>5</sub>O<sub>13</sub>P<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total 56	C 15	H 20	N 5	O 13	P 2	S 1	0	0
4	B	1	Total 56	C 15	H 20	N 5	O 13	P 2	S 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

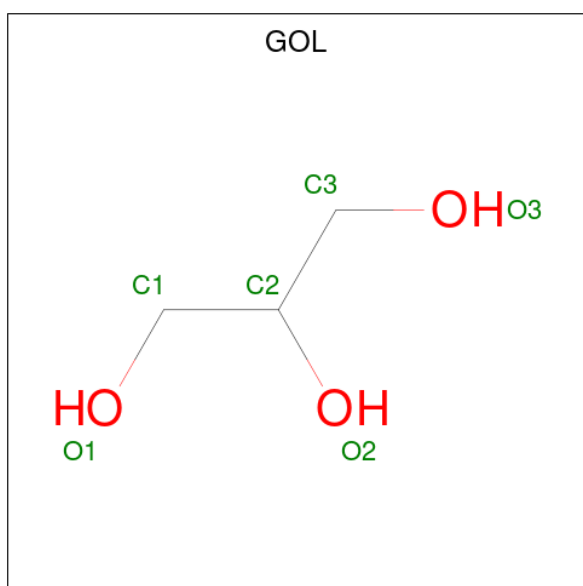
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Na 2 2	0	0
5	B	2	Total Na 2 2	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			12	3	6	3		
7	B	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	H	O	0	0
			12	3	6	3		
7	B	1	Total	C	H	O	0	0
			12	3	6	3		

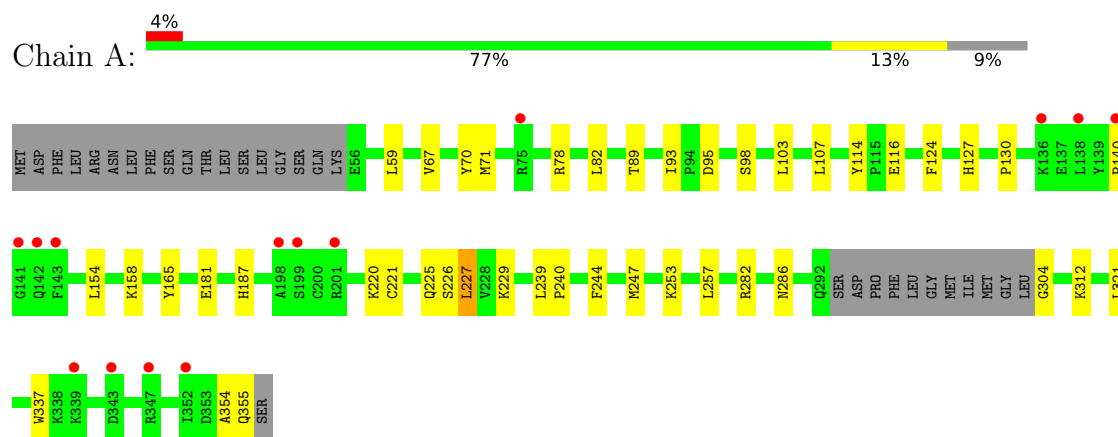
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	69	Total	O	0	0
			69	69		
8	B	65	Total	O	0	0
			65	65		

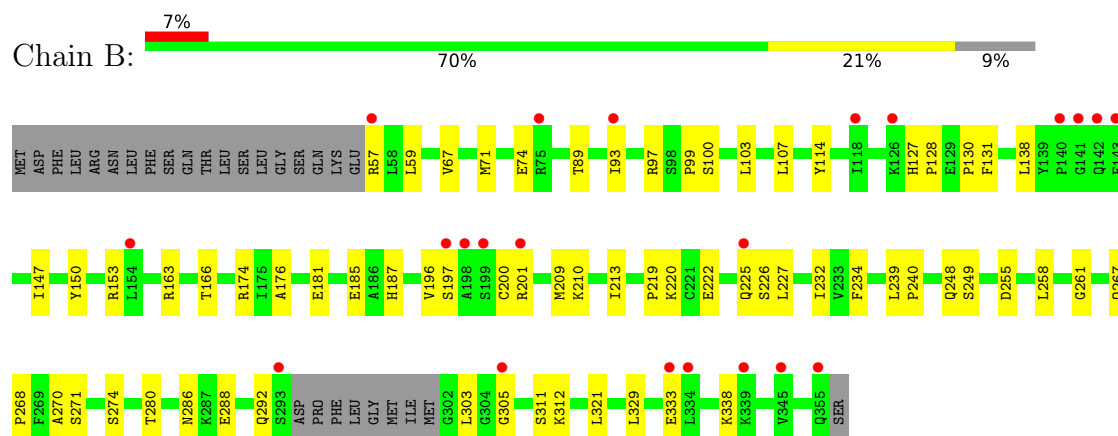
### 3 Residue-property plots [i](#)

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: NAD-dependent protein deacetylase sirtuin-2



- Molecule 1: NAD-dependent protein deacetylase sirtuin-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.31Å 76.84Å 114.46Å 90.00° 95.87° 90.00°	Depositor
Resolution (Å)	63.69 – 2.45 63.69 – 2.45	Depositor EDS
% Data completeness (in resolution range)	91.8 (63.69-2.45) 91.5 (63.69-2.45)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.220 , 0.256 0.220 , 0.255	Depositor DCC
$R_{free}$ test set	2013 reflections (7.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.9	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for $-1/2^*h+1/2^*k+1/2^*l, 1/2^*h-1/2^*k+1/2^*l, h+k$ 0.025 for $-1/2^*h-1/2^*k+1/2^*l, -1/2^*h-1/2^*k-1/2^*l, h-k$	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% 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: KXG, NA, GOL, KXJ, SO4, ZN

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	0.42	0/2373	0.63	1/3202 (0.0%)
1	B	0.45	1/2413 (0.0%)	0.64	2/3254 (0.1%)
All	All	0.44	1/4786 (0.0%)	0.64	3/6456 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	138	LEU	CG-CD2	5.33	1.71	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LEU	CD1-CG-CD2	-5.74	93.28	110.50
1	B	138	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	A	227	LEU	CB-CG-CD1	-5.03	102.45	111.00

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	2312	2214	2279	28	0
1	B	2339	2255	2297	54	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	34	0	0	1	0
3	B	35	0	0	1	0
4	A	36	20	0	2	0
4	B	36	20	0	3	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	6	6	8	0	0
7	B	18	20	24	0	0
8	A	69	0	0	1	0
8	B	65	0	0	3	0
All	All	4966	4535	4608	78	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 8.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:HIS:ND1	4:A:403:KXG:O3D	2.08	0.85
1:B:267:GLN:OE1	1:B:270:ALA:HB3	1.95	0.66
1:B:103:LEU:O	1:B:107:LEU:HG	1.98	0.64
1:B:267:GLN:HB3	1:B:268:PRO:HA	1.80	0.63
1:B:128:PRO:HG3	1:B:227:LEU:HD21	1.80	0.63
1:B:97:ARG:HG2	8:B:524:HOH:O	1.99	0.63
1:B:127:HIS:O	1:B:130:PRO:HD2	1.99	0.62
1:A:286:ASN:O	1:A:321:LEU:HA	1.99	0.61
1:A:67:VAL:O	1:A:71:MET:HG3	2.00	0.60
1:B:333:GLU:HB2	1:B:338:LYS:HD2	1.86	0.57
1:B:286:ASN:O	1:B:321:LEU:HA	2.05	0.57
1:B:267:GLN:HE22	1:B:271:SER:H	1.51	0.57
1:B:232:ILE:HD11	1:B:234:PHE:CZ	2.41	0.55
1:B:153:ARG:HD3	1:B:176:ALA:O	2.07	0.55
1:A:304:GLY:N	8:A:509:HOH:O	2.39	0.55
1:B:220:LYS:HA	1:B:226:SER:O	2.06	0.55
1:B:222:GLU:O	1:B:225:GLN:NE2	2.37	0.54
1:A:312:LYS:HB2	1:B:114:TYR:CZ	2.44	0.53
1:B:147:ILE:H	1:B:147:ILE:HD12	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:SER:HB3	1:B:305:GLY:HA3	1.92	0.51
1:B:292[A]:GLN:O	1:B:303:LEU:HD23	2.10	0.51
1:B:97:ARG:HD2	4:B:403:KXG:O2A	2.11	0.50
1:B:292[B]:GLN:O	1:B:303:LEU:HD23	2.10	0.50
1:B:220:LYS:HE3	1:B:225:GLN:O	2.12	0.49
1:B:239:LEU:HB3	1:B:240:PRO:HD2	1.94	0.49
1:B:163:ARG:NH1	1:B:181[A]:GLU:O	2.45	0.48
1:B:89:THR:HA	1:B:93:ILE:O	2.14	0.48
1:A:312:LYS:HG3	1:B:114:TYR:CE1	2.49	0.48
1:B:219:PRO:O	1:B:227:LEU:HD12	2.14	0.48
1:B:67:VAL:O	1:B:71:MET:HG3	2.14	0.48
1:B:197:SER:O	1:B:201:ARG:HG3	2.14	0.48
1:A:59:LEU:HD23	1:A:70:TYR:HB2	1.96	0.47
1:A:127:HIS:O	1:A:130:PRO:HD2	2.14	0.47
1:A:257:LEU:HB2	1:A:282:ARG:HG2	1.97	0.47
1:B:274:SER:HB3	1:B:305:GLY:CA	2.45	0.46
1:B:288:GLU:OE2	4:B:403:KXG:O3B	2.33	0.46
1:A:154:LEU:O	1:A:158:LYS:HG2	2.15	0.46
1:B:163:ARG:NH1	1:B:181[B]:GLU:O	2.49	0.46
1:B:209:MET:HG3	1:B:213:ILE:HD12	1.96	0.46
1:B:249:SER:OG	8:B:502:HOH:O	2.20	0.46
1:A:116:GLU:OE1	1:B:311:SER:HA	2.16	0.46
1:A:95:ASP:OD2	1:A:98:SER:HB2	2.15	0.46
1:B:227:LEU:HD12	1:B:227:LEU:HA	1.71	0.46
1:B:220:LYS:HD2	1:B:226:SER:O	2.16	0.45
1:B:261:GLY:HA2	1:B:286:ASN:OD1	2.17	0.45
1:A:181:GLU:OE1	1:A:181:GLU:HA	2.17	0.45
1:A:220:LYS:HA	1:A:226:SER:O	2.17	0.45
1:B:197:SER:HB3	1:B:200:CYS:HB3	1.99	0.45
1:B:255:ASP:C	1:B:280:THR:HG23	2.38	0.44
1:A:78:ARG:HH11	1:A:253:LYS:HB2	1.82	0.44
1:A:114:TYR:CZ	1:B:312:LYS:HB2	2.52	0.44
1:A:221:CYS:O	1:A:225:GLN:HA	2.17	0.44
1:B:267:GLN:HE22	1:B:271:SER:N	2.15	0.44
1:A:187:HIS:CE1	4:A:403:KXG:O3D	2.70	0.44
1:B:174:ARG:HD2	1:B:185:GLU:OE2	2.18	0.44
1:A:103:LEU:O	1:A:107:LEU:HG	2.17	0.43
1:B:196:VAL:HG13	1:B:227:LEU:O	2.18	0.43
1:A:154:LEU:HD13	1:A:337:TRP:HB3	2.00	0.43
1:A:78:ARG:NH1	1:A:253:LYS:HB2	2.34	0.43
1:B:153:ARG:NH1	1:B:176:ALA:O	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:LEU:HD23	1:B:329:LEU:HA	1.94	0.42
1:B:99:PRO:O	1:B:100:SER:HB3	2.19	0.42
1:A:82:LEU:CD2	1:A:165:TYR:HB2	2.49	0.42
1:A:140:PRO:HD3	3:A:402:KXJ:C18	2.49	0.41
1:A:239:LEU:HB3	1:A:240:PRO:HD2	2.01	0.41
1:A:354:ALA:O	1:A:355:GLN:HB3	2.19	0.41
1:B:181[A]:GLU:HA	1:B:181[A]:GLU:OE1	2.20	0.41
1:A:124:PHE:CZ	1:A:229:LYS:HB3	2.55	0.41
1:B:166:THR:HG22	1:B:185:GLU:HA	2.02	0.41
1:A:89:THR:HA	1:A:93:ILE:O	2.20	0.41
1:B:150:TYR:O	1:B:153:ARG:HB3	2.21	0.41
1:A:244:PHE:HA	1:A:247:MET:HE2	2.02	0.41
1:B:187:HIS:ND1	4:B:403:KXG:O3D	2.53	0.41
1:B:209:MET:HE2	1:B:209:MET:HB2	1.89	0.41
1:B:248:GLN:OE1	8:B:503:HOH:O	2.21	0.41
1:B:57:ARG:HG3	1:B:59:LEU:O	2.21	0.40
1:B:131:PHE:HE2	3:B:402:KXJ:C12	2.34	0.40
1:B:232:ILE:HD11	1:B:234:PHE:CE2	2.56	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:B:74:GLU:OE2	1:B:210:LYS:HZ2[4_545]	1.56	0.04

## 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	287/319 (90%)	278 (97%)	9 (3%)	0	100	100
1	B	292/319 (92%)	281 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	579/638 (91%)	559 (96%)	20 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	254/279 (91%)	253 (100%)	1 (0%)	91	94
1	B	259/279 (93%)	258 (100%)	1 (0%)	91	94
All	All	513/558 (92%)	511 (100%)	2 (0%)	91	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	LEU
1	B	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	GLN
1	B	167	GLN
1	B	355	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](#)

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 for Mogul analysis.

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
7	GOL	B	409	-	5,5,5	1.08	0	5,5,5	1.22	1 (20%)
7	GOL	B	408	-	5,5,5	0.84	0	5,5,5	1.15	0
7	GOL	A	407	-	5,5,5	1.12	1 (20%)	5,5,5	1.34	1 (20%)
6	SO4	B	406	-	4,4,4	0.14	0	6,6,6	0.06	0
7	GOL	B	407	-	5,5,5	0.84	0	5,5,5	1.01	0
4	KXG	A	403	3	32,39,39	2.38	10 (31%)	36,60,60	2.13	9 (25%)
6	SO4	A	406	-	4,4,4	0.14	0	6,6,6	0.06	0
4	KXG	B	403	3,5	32,39,39	1.73	4 (12%)	36,60,60	1.93	7 (19%)
3	KXJ	A	402	4	34,34,39	1.98	5 (14%)	38,38,44	1.84	8 (21%)
3	KXJ	B	402	4	35,35,39	2.19	7 (20%)	38,39,44	1.61	7 (18%)

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
7	GOL	B	409	-	-	0/4/4/4	-
7	GOL	B	408	-	-	1/4/4/4	-
7	GOL	A	407	-	-	2/4/4/4	-
7	GOL	B	407	-	-	2/4/4/4	-
4	KXG	A	403	3	-	5/18/54/54	0/4/4/4
4	KXG	B	403	3,5	-	7/18/54/54	0/4/4/4
3	KXJ	A	402	4	-	15/33/33/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KXJ	B	402	4	-	18/34/34/39	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	KXJ	C26-N5	7.18	1.49	1.34
3	B	402	KXJ	C1-N	6.98	1.51	1.35
3	B	402	KXJ	C26-N5	6.43	1.47	1.34
3	A	402	KXJ	C1-N	5.80	1.48	1.35
4	A	403	KXG	PA-O1A	-5.10	1.32	1.50
4	A	403	KXG	PN-O2N	-4.98	1.32	1.55
4	A	403	KXG	PN-O1N	-4.97	1.33	1.50
4	A	403	KXG	PA-O2A	-4.74	1.33	1.55
4	B	403	KXG	C4A-N3A	-4.72	1.29	1.35
3	B	402	KXJ	C20-N	4.56	1.50	1.41
3	B	402	KXJ	C6-N1	-4.55	1.31	1.46
4	A	403	KXG	C4A-N3A	-4.06	1.30	1.35
4	A	403	KXG	C3D-C2D	-3.84	1.42	1.53
4	B	403	KXG	O4B-C1B	3.70	1.46	1.41
3	A	402	KXJ	C9-C8	-3.68	1.30	1.51
4	B	403	KXG	C5A-N7A	3.65	1.53	1.39
4	A	403	KXG	C5A-N7A	3.48	1.52	1.39
3	B	402	KXJ	C9-C8	-3.33	1.32	1.51
3	A	402	KXJ	C20-N	3.22	1.48	1.41
4	B	403	KXG	C6A-N6A	3.17	1.45	1.34
3	A	402	KXJ	C6-N1	-3.10	1.36	1.46
3	B	402	KXJ	O4-C26	-2.45	1.18	1.23
4	A	403	KXG	C6A-N6A	2.43	1.42	1.34
4	A	403	KXG	O5D-C5D	-2.40	1.35	1.44
3	B	402	KXJ	O-C1	-2.09	1.19	1.23
7	A	407	GOL	O2-C2	-2.04	1.37	1.43
4	A	403	KXG	C2A-N1A	-2.01	1.30	1.33

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	403	KXG	C4A-C5A-N7A	-7.34	101.75	109.40
3	A	402	KXJ	C27-C26-N5	6.72	124.42	115.77
4	A	403	KXG	C1D-C2D-C3D	6.54	111.59	102.26
4	A	403	KXG	C4A-C5A-N7A	-6.39	102.74	109.40
4	B	403	KXG	N3A-C2A-N1A	-4.78	121.20	128.68
3	B	402	KXJ	O-C1-C	-4.60	110.76	120.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	KXJ	C2-C-C1	-4.56	99.54	110.20
3	B	402	KXJ	C7-C6-N1	-3.81	101.85	112.14
4	A	403	KXG	O4B-C1B-C2B	-3.72	101.49	106.93
3	B	402	KXJ	C27-C26-N5	3.63	122.13	115.83
3	A	402	KXJ	O4-C26-N5	-3.56	116.94	122.95
4	B	403	KXG	O4B-C1B-C2B	-3.54	101.76	106.93
3	B	402	KXJ	C1-C-N5	-3.52	101.57	111.16
4	A	403	KXG	N3A-C2A-N1A	-3.37	123.42	128.68
3	B	402	KXJ	O-C1-N	2.99	130.36	123.93
3	A	402	KXJ	O-C1-N	2.97	130.31	123.93
4	A	403	KXG	O3D-C3D-C4D	2.93	119.53	111.05
7	A	407	GOL	C3-C2-C1	-2.70	101.22	111.70
4	B	403	KXG	PN-O3-PA	-2.55	124.08	132.83
4	A	403	KXG	O2A-PA-O1A	-2.54	99.69	112.24
3	A	402	KXJ	C-N5-C26	2.42	127.86	121.65
4	A	403	KXG	C1B-N9A-C4A	-2.38	122.47	126.64
7	B	409	GOL	C3-C2-C1	-2.35	102.55	111.70
4	B	403	KXG	O2N-PN-O1N	-2.28	100.96	112.24
4	B	403	KXG	O3D-C3D-C4D	2.28	117.64	111.05
3	A	402	KXJ	C8-C7-C6	-2.26	102.86	113.56
3	B	402	KXJ	O4-C26-N5	-2.26	119.14	122.95
4	B	403	KXG	O2A-PA-O1A	-2.25	101.11	112.24
3	A	402	KXJ	C9-C8-C7	2.19	125.54	114.42
4	A	403	KXG	O3B-C3B-C4B	2.13	117.20	111.05
3	A	402	KXJ	C-C1-N	-2.11	108.80	115.10
4	A	403	KXG	O2N-PN-O1N	-2.10	101.88	112.24
3	B	402	KXJ	C4-C3-C2	2.05	120.88	113.62

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	KXJ	C1-C-C2-C3
4	B	403	KXG	C5D-O5D-PN-O1N
4	B	403	KXG	C5D-O5D-PN-O2N
4	B	403	KXG	C5D-O5D-PN-O3
7	B	407	GOL	C1-C2-C3-O3
3	A	402	KXJ	C27-C26-N5-C
3	B	402	KXJ	C27-C26-N5-C
3	A	402	KXJ	N5-C-C2-C3
3	B	402	KXJ	N5-C-C2-C3
3	A	402	KXJ	O4-C26-N5-C

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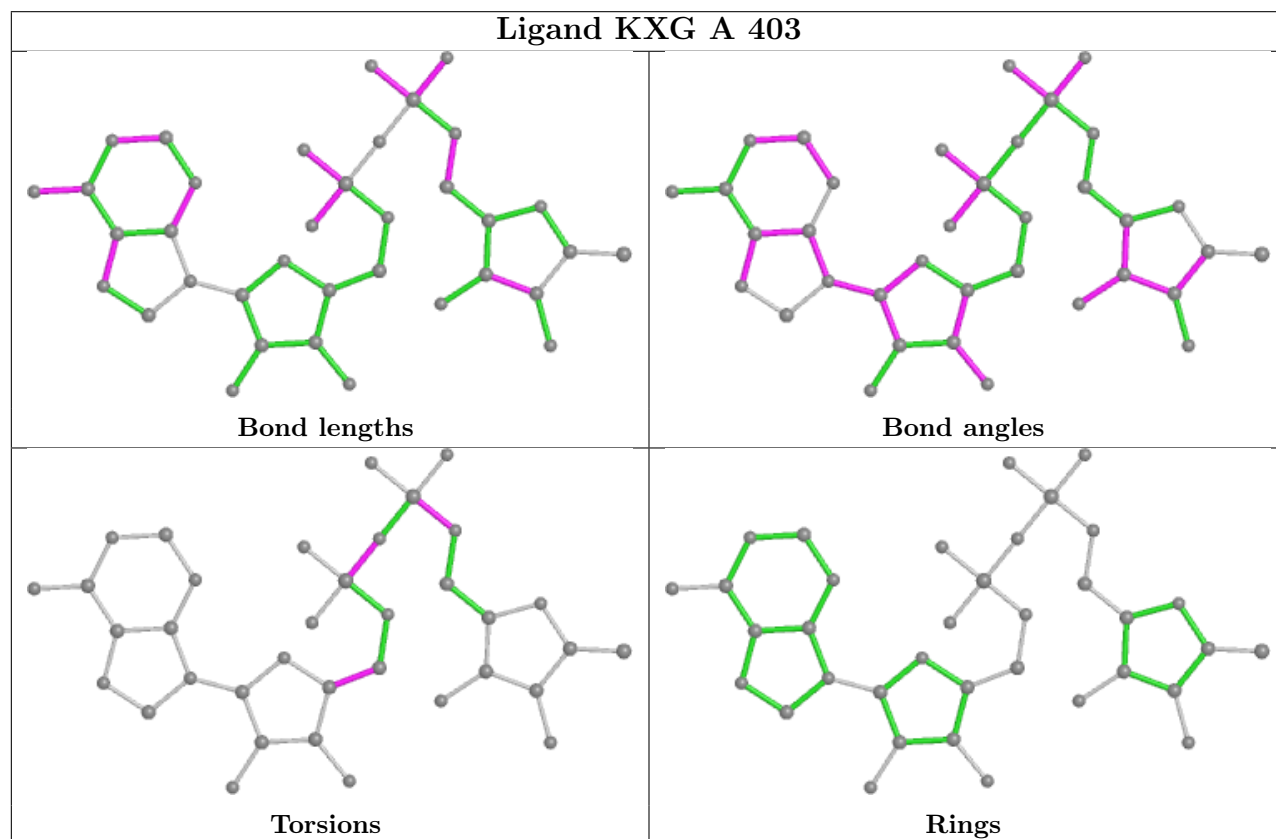
Mol	Chain	Res	Type	Atoms
3	B	402	KXJ	O4-C26-N5-C
4	B	403	KXG	O4D-C4D-C5D-O5D
3	B	402	KXJ	C1-C-C2-C3
3	A	402	KXJ	N1-C6-C7-C8
3	B	402	KXJ	C3-C4-C5-N1
3	A	402	KXJ	C3-C4-C5-N1
3	B	402	KXJ	N1-C6-C7-C8
3	B	402	KXJ	C4-C5-N1-C6
4	B	403	KXG	C3D-C4D-C5D-O5D
3	B	402	KXJ	C-C2-C3-C4
3	B	402	KXJ	O1-C30-C31-O2
3	A	402	KXJ	C21-C20-N-C1
3	A	402	KXJ	C10-C11-C12-C13
3	B	402	KXJ	C10-C11-C12-C13
7	B	407	GOL	O2-C2-C3-O3
3	A	402	KXJ	C2-C3-C4-C5
3	B	402	KXJ	C6-C7-C8-C9
3	A	402	KXJ	C9-C10-C11-C12
3	A	402	KXJ	C25-C20-N-C1
3	A	402	KXJ	C4-C5-N1-C6
3	B	402	KXJ	C13-C14-C15-C16
3	B	402	KXJ	C9-C10-C11-C12
7	A	407	GOL	O1-C1-C2-O2
3	A	402	KXJ	C6-C7-C8-C9
4	B	403	KXG	C4D-C5D-O5D-PN
4	A	403	KXG	PN-O3-PA-O5B
3	B	402	KXJ	C11-C10-C9-C8
3	A	402	KXJ	C16-C17-C18-C19
4	A	403	KXG	C5D-O5D-PN-O3
4	A	403	KXG	C5D-O5D-PN-O1N
4	A	403	KXG	C5D-O5D-PN-O2N
3	A	402	KXJ	C12-C13-C14-C15
3	B	402	KXJ	C7-C6-N1-C5
3	B	402	KXJ	C12-C13-C14-C15
3	B	402	KXJ	C31-C30-O1-C28
7	B	408	GOL	C1-C2-C3-O3
4	A	403	KXG	O4B-C4B-C5B-O5B
4	B	403	KXG	O4B-C4B-C5B-O5B
3	B	402	KXJ	C11-C12-C13-C14
7	A	407	GOL	O1-C1-C2-C3

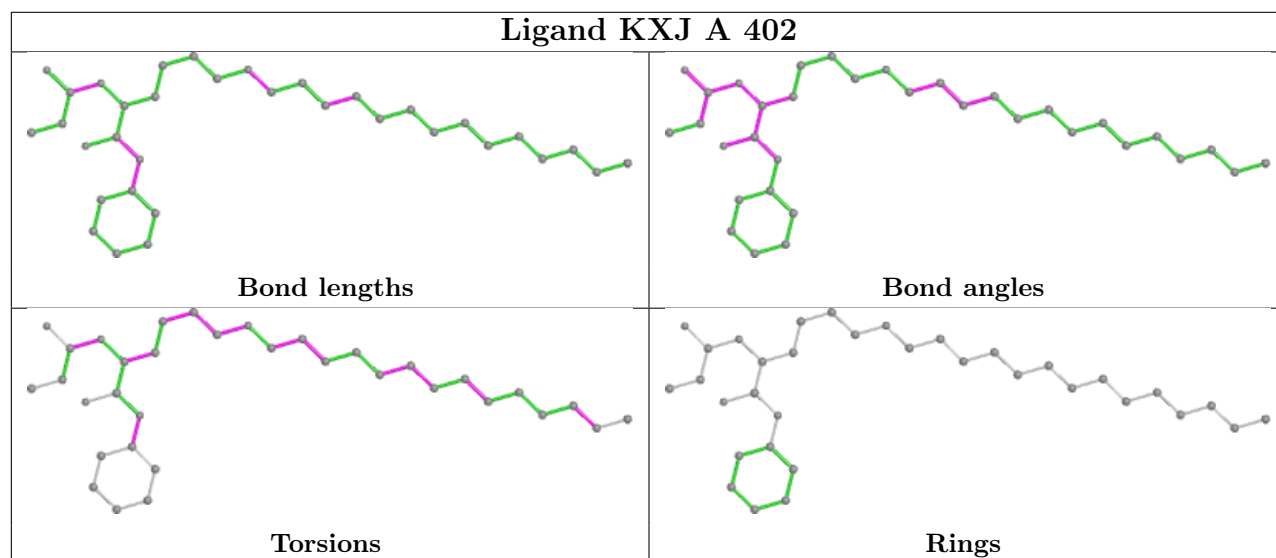
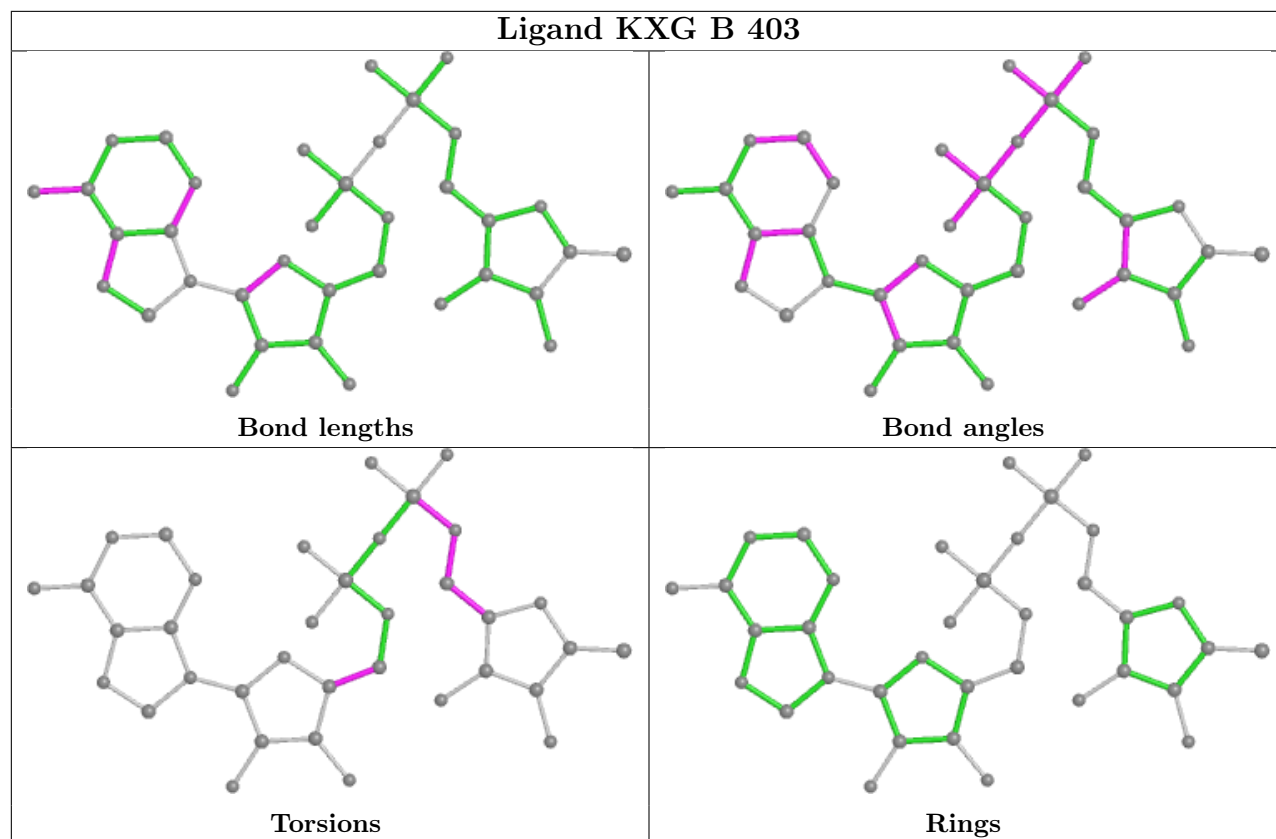
There are no ring outliers.

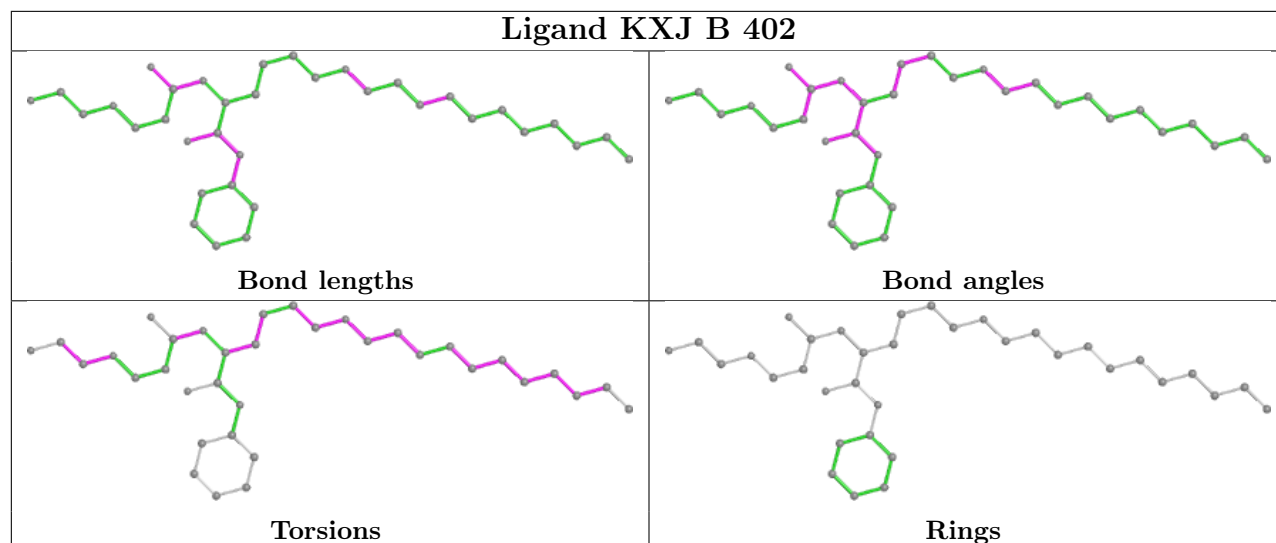
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	KXG	2	0
4	B	403	KXG	3	0
3	A	402	KXJ	1	0
3	B	402	KXJ	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	289/319 (90%)	0.44	14 (4%) 30 28	25, 42, 67, 96	0
1	B	291/319 (91%)	0.60	22 (7%) 13 10	26, 46, 77, 99	0
All	All	580/638 (90%)	0.52	36 (6%) 20 17	25, 44, 74, 99	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	GLY	7.3
1	B	199	SER	6.5
1	A	198	ALA	5.8
1	B	225	GLN	5.1
1	B	339	LYS	4.5
1	B	305	GLY	4.1
1	B	141	GLY	3.8
1	B	201	ARG	3.7
1	B	143	PHE	3.7
1	B	198	ALA	3.7
1	B	140	PRO	3.6
1	A	199	SER	3.5
1	B	142	GLN	3.3
1	A	142	GLN	3.1
1	A	143	PHE	3.0
1	B	355	GLN	2.9
1	B	333	GLU	2.6
1	B	154	LEU	2.5
1	A	343	ASP	2.5
1	B	334	LEU	2.4
1	B	118	ILE	2.4
1	B	57	ARG	2.4
1	B	197	SER	2.4
1	B	75	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	75	ARG	2.3
1	A	347	ARG	2.2
1	B	126	LYS	2.2
1	A	352	ILE	2.2
1	B	93	ILE	2.2
1	B	345	VAL	2.2
1	A	138	LEU	2.2
1	A	201	ARG	2.1
1	A	140	PRO	2.1
1	B	293[A]	SER	2.1
1	A	136	LYS	2.1
1	A	339	LYS	2.1

## 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.

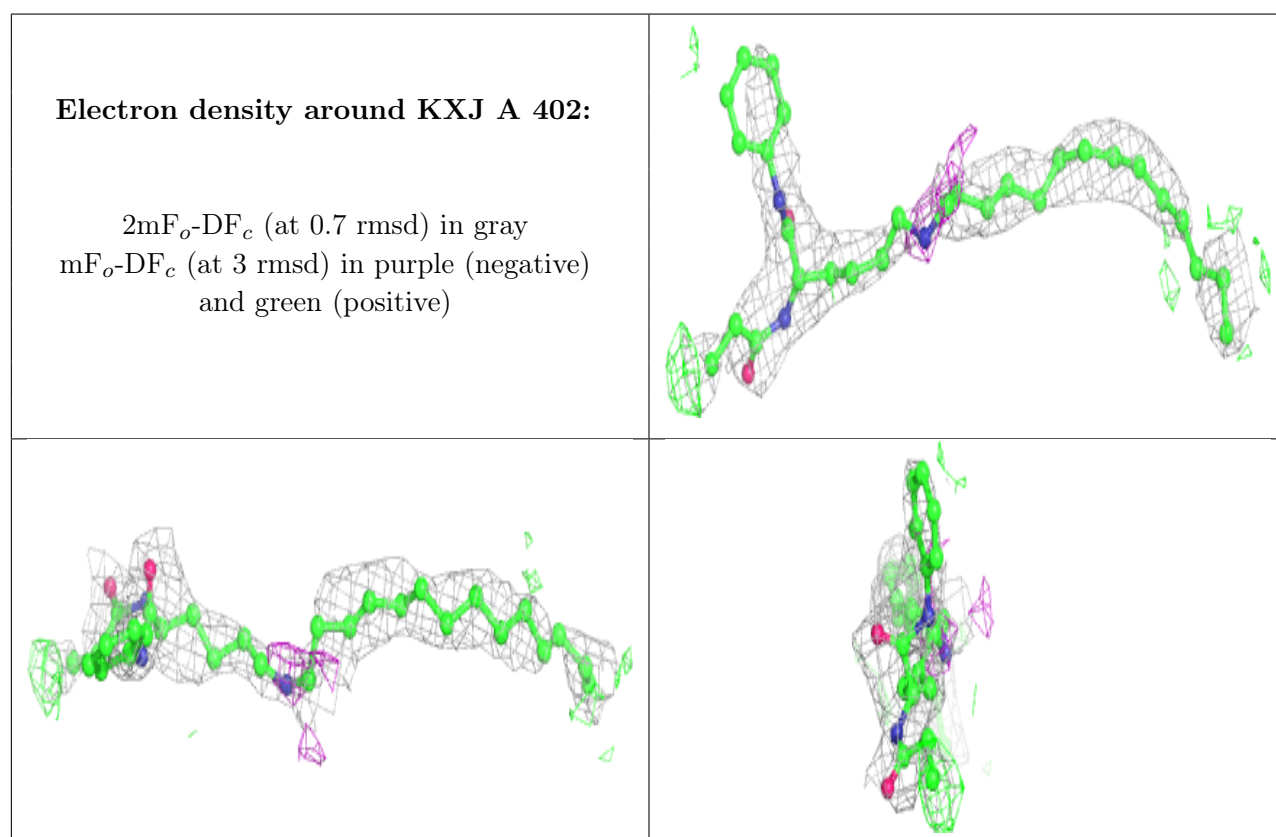
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	GOL	B	408	6/6	0.54	0.29	46,77,101,101	0
7	GOL	B	407	6/6	0.72	0.19	52,65,84,101	0
6	SO4	B	406	5/5	0.73	0.52	62,70,91,107	0
3	KXJ	A	402	34/39	0.77	0.30	31,59,74,77	0
5	NA	B	404	1/1	0.81	0.23	49,49,49,49	0
5	NA	B	405	1/1	0.83	0.10	43,43,43,43	0
3	KXJ	B	402	35/39	0.83	0.30	45,59,71,81	0
7	GOL	B	409	6/6	0.83	0.31	55,74,81,89	0
2	ZN	B	401	1/1	0.85	0.10	87,87,87,87	0
5	NA	A	405	1/1	0.86	0.20	43,43,43,43	0
7	GOL	A	407	6/6	0.90	0.21	43,72,99,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	401	1/1	0.92	0.11	63,63,63,63	0
6	SO4	A	406	5/5	0.93	0.21	72,74,87,92	0
4	KXG	A	403	36/36	0.93	0.17	31,48,65,79	0
4	KXG	B	403	36/36	0.94	0.19	30,46,65,80	0
5	NA	A	404	1/1	0.95	0.11	41,41,41,41	0

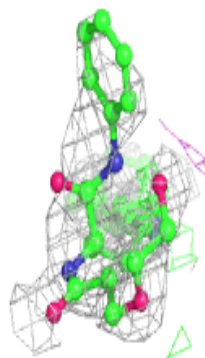
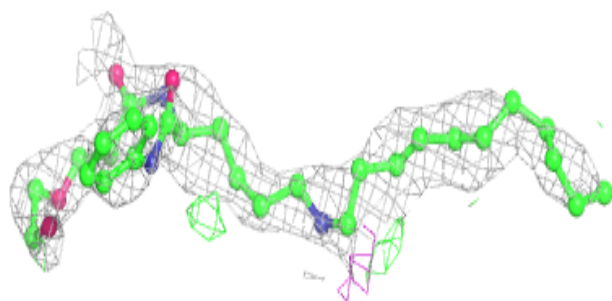
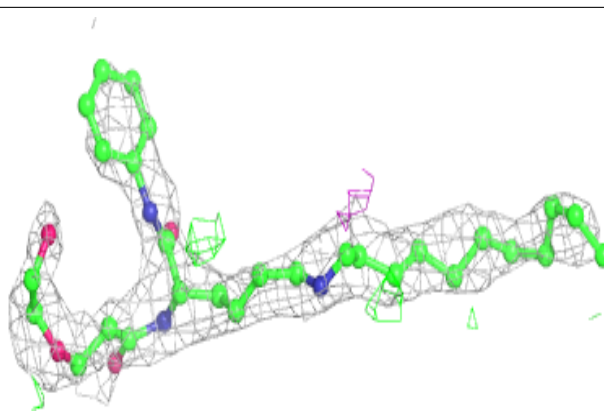
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



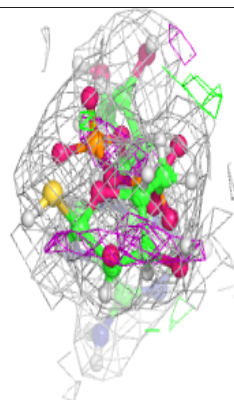
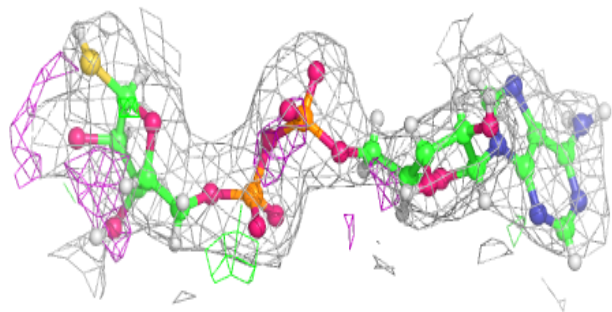
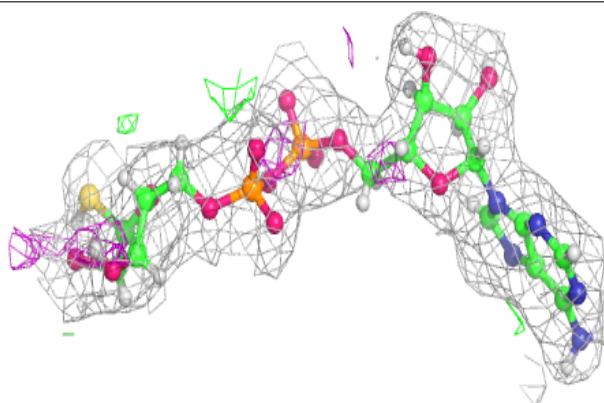


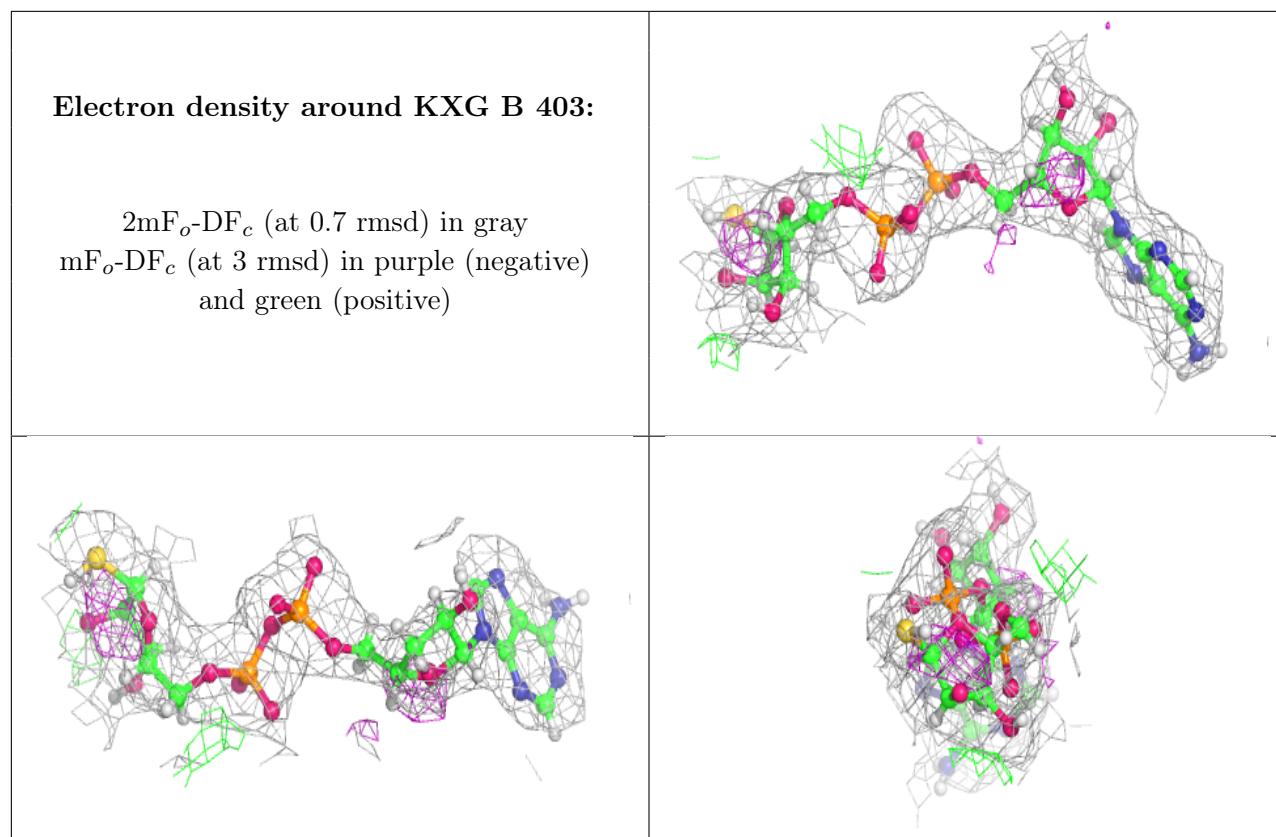
**Electron density around KXJ B 402:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around KXG A 403:**

$2mF_o-DF_c$  (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.