



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 04:01 AM EDT

PDB ID : 2QZO  
Title : Crystal Structure of the Estrogen Receptor Alpha Ligand Binding Domain  
Complexed with WAY-169916  
Authors : Bruning, J.B.; Gil, G.; Nowak, J.; Katzenellenbogen, J.; Nettles, K.W.  
Deposited on : 2007-08-16  
Resolution : 1.72 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

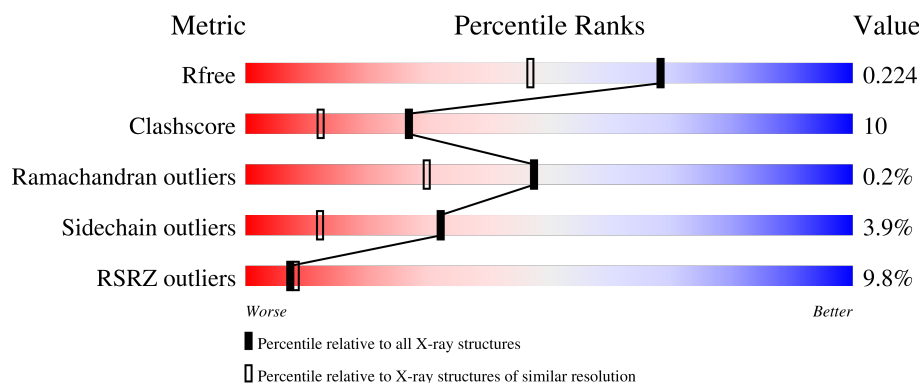
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	258	<div> <div>12%</div> <div> <div></div> <div>72%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>
2	B	258	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>•</div> <div>8%</div> </div> </div>
3	C	13	<div> <div>23%</div> <div> <div></div> <div>54%</div> <div>8%</div> <div>8%</div> <div>31%</div> </div> </div>
3	D	13	<div> <div></div> <div> <div>46%</div> <div>23%</div> <div>31%</div> </div> </div>

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	CME	B	381	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4364 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	0	7	0
			1823	1168	313	323	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	SER	-	expression tag	UNP P03372
A	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 2 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	10	0
			1920	1237	319	341	23			

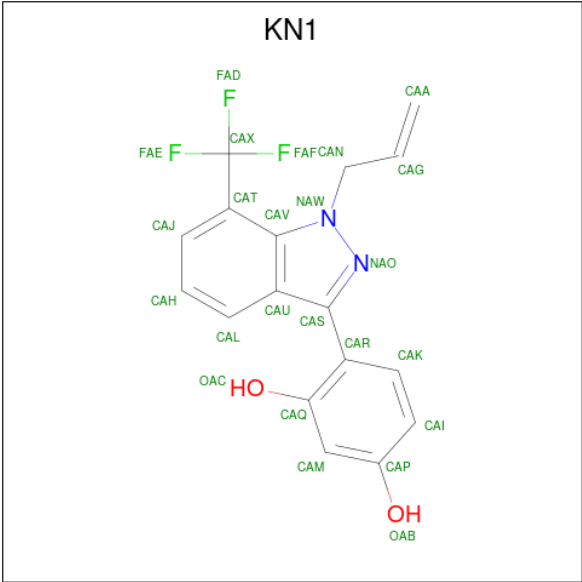
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	SER	-	expression tag	UNP P03372
B	537	SER	TYR	engineered mutation	UNP P03372

- Molecule 3 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			72	47	15	10			
3	D	9	Total	C	N	O	0	0	0
			79	51	16	12			

- Molecule 4 is 4-[1-allyl-7-(trifluoromethyl)-1H-indazol-3-yl]benzene-1,3-diol (three-letter code: KN1) (formula: C<sub>17</sub>H<sub>13</sub>F<sub>3</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			24	17	3	2	2		
4	B	1	Total	C	F	N	O	0	0
			24	17	3	2	2		

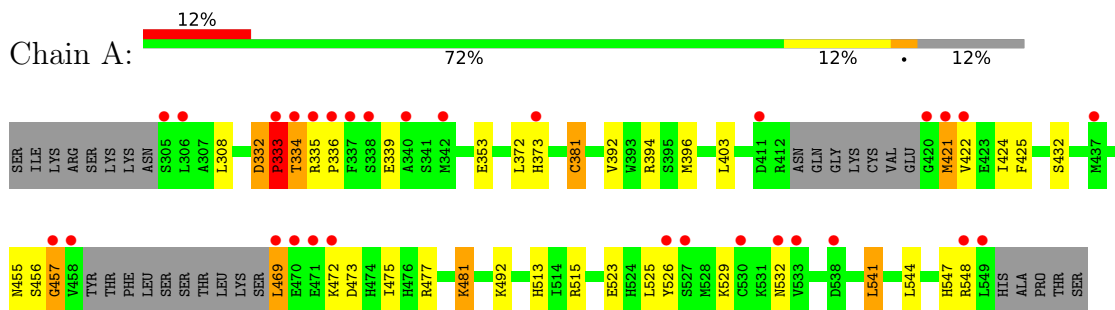
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	178	Total	O	0	0
			178	178		
5	B	236	Total	O	0	0
			236	236		
5	C	1	Total	O	0	0
			1	1		
5	D	7	Total	O	0	0
			7	7		

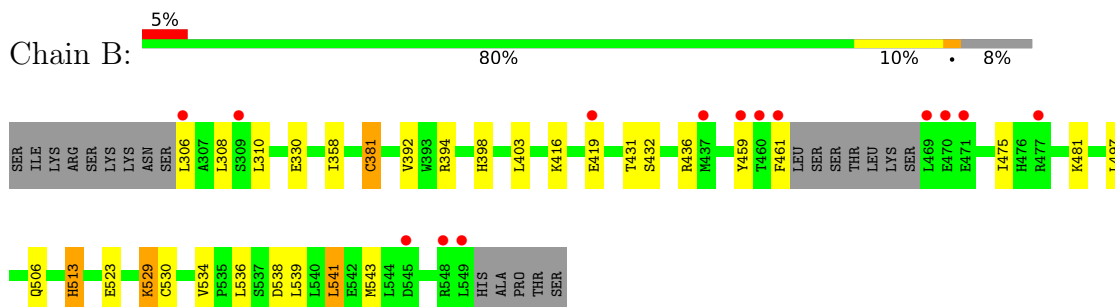
### 3 Residue-property plots

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.

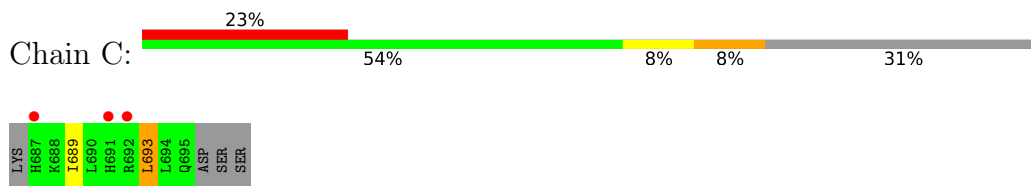
- Molecule 1: Estrogen receptor



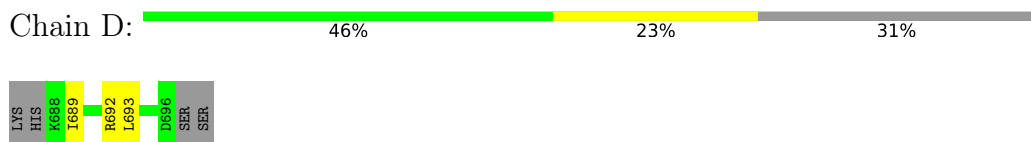
- Molecule 2: Estrogen receptor



- Molecule 3: Nuclear receptor coactivator 2



- Molecule 3: Nuclear receptor coactivator 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.81Å 82.03Å 58.52Å 90.00° 109.04° 90.00°	Depositor
Resolution (Å)	9.91 – 1.72 9.84 – 1.72	Depositor EDS
% Data completeness (in resolution range)	91.6 (9.91-1.72) 91.6 (9.84-1.72)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.85 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.178 , 0.221 0.182 , 0.224	Depositor DCC
$R_{free}$ test set	2446 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 70.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: KN1, CME

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	0.57	0/1866	0.70	0/2521
2	B	0.66	0/1963	0.70	1/2652 (0.0%)
3	C	0.44	0/72	0.64	0/96
3	D	0.55	0/79	0.72	0/104
All	All	0.61	0/3980	0.70	1/5373 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	436	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	ASP	Peptide
1	A	333	PRO	Peptide
1	A	334	THR	Peptide
1	A	339	GLU	Peptide
1	A	456	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	457	GLY	Peptide

## 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	1823	0	1858	51	0
2	B	1920	0	1981	33	0
3	C	72	0	75	3	0
3	D	79	0	88	2	0
4	A	24	0	11	5	0
4	B	24	0	12	0	0
5	A	178	0	0	10	0
5	B	236	0	0	6	0
5	C	1	0	0	0	0
5	D	7	0	0	0	0
All	All	4364	0	4025	81	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 10.

All (81) 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)
2:B:381:CME:OH	2:B:381:CME:HB2	1.26	1.29
1:A:513[B]:HIS:NE2	2:B:459:TYR:CE2	2.14	1.15
1:A:334:THR:HG23	1:A:335:ARG:CA	1.78	1.13
2:B:381:CME:OH	2:B:381:CME:CB	1.99	1.10
1:A:513[B]:HIS:NE2	2:B:459:TYR:HE2	1.50	1.09
1:A:334:THR:CG2	1:A:335:ARG:HA	1.82	1.09
1:A:335:ARG:H	1:A:336:PRO:HD2	1.34	0.93
1:A:335:ARG:N	1:A:336:PRO:HD2	1.83	0.92
2:B:381:CME:SD	5:B:674:HOH:O	2.26	0.91
1:A:513[B]:HIS:CE1	2:B:459:TYR:CD2	2.59	0.90
1:A:547:HIS:HD2	5:A:708:HOH:O	1.61	0.83
1:A:513[B]:HIS:CD2	2:B:459:TYR:CE2	2.67	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:CME:HB2	2:B:381:CME:HH	1.49	0.78
1:A:513[B]:HIS:CE1	2:B:459:TYR:CE2	2.72	0.77
1:A:335:ARG:N	1:A:336:PRO:CD	2.45	0.77
1:A:513[B]:HIS:CE1	2:B:459:TYR:HD2	2.04	0.72
1:A:334:THR:HG23	1:A:335:ARG:HA	0.86	0.71
1:A:332:ASP:O	1:A:334:THR:O	2.10	0.69
1:A:425:PHE:CE1	4:A:1:KN1:HAA2	2.28	0.69
1:A:332:ASP:O	1:A:336:PRO:HD2	1.95	0.66
1:A:547:HIS:HE1	5:A:724:HOH:O	1.78	0.65
2:B:381:CME:CB	2:B:381:CME:HH	1.96	0.63
1:A:457:GLY:HA3	1:A:515:ARG:HH12	1.65	0.62
1:A:421:MET:HE2	1:A:424:ILE:HD12	1.81	0.62
1:A:457:GLY:HA3	1:A:515:ARG:NH1	2.16	0.60
1:A:455:ASN:O	2:B:513:HIS:HE1	1.85	0.59
2:B:392:VAL:HG13	2:B:432:SER:HA	1.84	0.59
2:B:392:VAL:HG13	2:B:432:SER:CA	2.33	0.58
1:A:526:TYR:HA	1:A:544:LEU:HD21	1.86	0.57
1:A:422:VAL:HG23	5:A:719:HOH:O	2.06	0.56
2:B:523:GLU:HG3	5:B:616:HOH:O	2.06	0.55
1:A:335:ARG:H	1:A:336:PRO:CD	2.11	0.55
1:A:547:HIS:CD2	5:A:708:HOH:O	2.44	0.54
3:C:689:ILE:O	3:C:693:LEU:HD22	2.07	0.54
1:A:396:MET:CE	5:A:685:HOH:O	2.56	0.53
1:A:394:ARG:HG3	5:A:726:HOH:O	2.09	0.53
1:A:403:LEU:HG	5:A:722:HOH:O	2.08	0.53
1:A:421:MET:CE	1:A:424:ILE:HD12	2.38	0.53
2:B:538:ASP:HB3	3:D:689:ILE:HD11	1.91	0.53
2:B:419:GLU:HG3	5:B:683:HOH:O	2.08	0.52
2:B:358:ILE:HD13	3:D:693:LEU:HB3	1.91	0.52
2:B:310:LEU:O	2:B:481[B]:LYS:HE3	2.10	0.52
3:C:689:ILE:HG22	3:C:693:LEU:CD2	2.40	0.51
1:A:394:ARG:CG	5:A:726:HOH:O	2.59	0.51
1:A:396:MET:HE2	5:A:685:HOH:O	2.11	0.51
2:B:529:LYS:HG3	2:B:536:LEU:HD22	1.93	0.50
1:A:473:ASP:OD2	1:A:477:ARG:NH1	2.45	0.49
2:B:330:GLU:HB2	5:B:784:HOH:O	2.11	0.49
2:B:381:CME:OH	2:B:381:CME:SG	2.53	0.49
1:A:525:LEU:HD23	1:A:544:LEU:HD13	1.94	0.49
1:A:469:LEU:HB2	1:A:472:LYS:HB2	1.93	0.49
1:A:425:PHE:CD1	4:A:1:KN1:HAA2	2.49	0.48
1:A:523[A]:GLU:OE1	1:A:548:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:LEU:HG	2:B:308:LEU:H	1.78	0.47
2:B:536:LEU:CB	2:B:541:LEU:HD13	2.45	0.47
2:B:536:LEU:HB3	2:B:541:LEU:HD13	1.97	0.47
1:A:333:PRO:N	1:A:334:THR:C	2.69	0.46
1:A:392:VAL:HG13	1:A:432[B]:SER:CA	2.46	0.46
1:A:392:VAL:HG13	1:A:432[A]:SER:CA	2.46	0.46
1:A:381:CME:HZ2	1:A:547:HIS:CD2	2.51	0.46
1:A:308:LEU:HA	1:A:481:LYS:HD2	1.98	0.45
1:A:332:ASP:O	1:A:336:PRO:CD	2.65	0.45
2:B:392:VAL:HG11	2:B:431:THR:HG22	1.99	0.45
4:A:1:KN1:FAD	4:A:1:KN1:HAN1	2.07	0.45
2:B:461:PHE:HE2	2:B:475:ILE:CD1	2.30	0.45
1:A:353:GLU:OE1	4:A:1:KN1:OAB	2.35	0.44
2:B:394:ARG:HB3	2:B:403[B]:LEU:HD23	1.98	0.44
1:A:333:PRO:CD	1:A:335:ARG:H	2.31	0.44
1:A:392:VAL:HG13	1:A:432[B]:SER:HA	1.99	0.43
1:A:392:VAL:HG13	1:A:432[A]:SER:HA	1.99	0.43
1:A:333:PRO:CD	1:A:335:ARG:N	2.82	0.43
2:B:506:GLN:NE2	5:B:777:HOH:O	2.47	0.42
1:A:455:ASN:O	2:B:513:HIS:CE1	2.69	0.42
2:B:539:LEU:O	2:B:543:MET:HG2	2.19	0.42
4:A:1:KN1:HAL	4:A:1:KN1:HAK	2.02	0.41
3:C:689:ILE:HG22	3:C:693:LEU:HD23	2.01	0.41
1:A:373:HIS:CD2	1:A:373:HIS:C	2.94	0.41
1:A:475:ILE:HD12	5:A:604:HOH:O	2.20	0.41
2:B:398:HIS:HE1	5:B:648:HOH:O	2.02	0.41
1:A:541:LEU:HD12	1:A:541:LEU:HA	1.92	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	228/258 (88%)	224 (98%)	3 (1%)	1 (0%)	34	18
2	B	241/258 (93%)	238 (99%)	3 (1%)	0	100	100
3	C	7/13 (54%)	7 (100%)	0	0	100	100
3	D	7/13 (54%)	7 (100%)	0	0	100	100
All	All	483/542 (89%)	476 (99%)	6 (1%)	1 (0%)	47	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	333	PRO

### 5.3.2 Protein sidechains ⓘ

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	201/232 (87%)	193 (96%)	8 (4%)	31	12
2	B	215/231 (93%)	208 (97%)	7 (3%)	38	17
3	C	7/13 (54%)	6 (86%)	1 (14%)	3	0
3	D	9/13 (69%)	8 (89%)	1 (11%)	6	1
All	All	432/489 (88%)	415 (96%)	17 (4%)	32	12

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	372	LEU
1	A	421	MET
1	A	469	LEU
1	A	481	LYS
1	A	492	LYS
1	A	529	LYS
1	A	532	ASN
1	A	541	LEU
2	B	416	LYS
2	B	497	LEU

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Mol	Chain	Res	Type
2	B	513	HIS
2	B	529	LYS
2	B	534[A]	VAL
2	B	534[B]	VAL
2	B	541	LEU
3	C	693	LEU
3	D	692	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	HIS
1	A	474	HIS
2	B	398	HIS
2	B	513	HIS
3	C	691	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CME	A	381	1	8,9,10	0.93	0	5,9,11	2.09	2 (40%)
2	CME	B	381	2	8,9,10	1.00	0	5,9,11	1.81	1 (20%)
2	CME	B	530	2	8,9,10	0.90	0	5,9,11	1.21	1 (20%)

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
1	CME	A	381	1	-	1/5/8/10	-
2	CME	B	381	2	-	3/5/8/10	-
2	CME	B	530	2	-	0/5/8/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	CME	CE-SD-SG	4.06	122.15	103.45
2	B	381	CME	CB-SG-SD	3.21	112.13	103.82
1	A	381	CME	CZ-CE-SD	-2.25	105.55	113.37
2	B	530	CME	CE-SD-SG	2.16	113.42	103.45

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	381	CME	CZ-CE-SD-SG
2	B	381	CME	CE-SD-SG-CB
2	B	381	CME	SD-CE-CZ-OH
1	A	381	CME	CZ-CE-SD-SG

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	381	CME	1	0
2	B	381	CME	6	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	KN1	A	1	-	23,26,26	3.45	4 (17%)	29,39,39	3.79	11 (37%)
4	KN1	B	1	-	23,26,26	3.33	6 (26%)	29,39,39	2.09	10 (34%)

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
4	KN1	A	1	-	-	5/9/13/13	0/3/3/3
4	KN1	B	1	-	-	1/9/13/13	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	KN1	NAO-NAW	-12.92	1.23	1.37
4	B	1	KN1	NAO-NAW	-11.60	1.24	1.37
4	A	1	KN1	CAR-CAS	-7.97	1.39	1.49
4	B	1	KN1	CAR-CAS	-7.74	1.39	1.49
4	B	1	KN1	CAN-CAG	-4.83	1.40	1.49
4	A	1	KN1	CAN-CAG	-4.66	1.40	1.49
4	B	1	KN1	CAX-CAT	3.11	1.54	1.50
4	B	1	KN1	CAJ-CAT	2.63	1.40	1.37
4	A	1	KN1	CAS-NAO	-2.62	1.33	1.35
4	B	1	KN1	CAS-NAO	-2.01	1.33	1.35

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	KN1	FAF-CAX-CAT	11.96	124.73	112.32
4	A	1	KN1	CAX-CAT-CAV	9.89	125.78	119.46
4	A	1	KN1	FAD-CAX-CAT	-7.61	104.43	112.32
4	B	1	KN1	FAE-CAX-CAT	-5.47	106.64	112.32
4	B	1	KN1	CAX-CAT-CAV	5.25	122.82	119.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	KN1	CAQ-CAR-CAS	-4.67	116.67	121.28
4	A	1	KN1	FAE-CAX-CAT	-4.61	107.53	112.32
4	A	1	KN1	FAD-CAX-FAF	-3.89	91.46	105.72
4	A	1	KN1	CAJ-CAT-CAX	-3.77	114.90	119.87
4	A	1	KN1	FAF-CAX-FAE	3.72	119.35	105.72
4	B	1	KN1	CAK-CAR-CAS	3.24	124.16	120.14
4	B	1	KN1	FAF-CAX-CAT	3.22	115.66	112.32
4	B	1	KN1	CAQ-CAM-CAP	3.19	122.58	119.70
4	A	1	KN1	CAK-CAR-CAS	3.03	123.91	120.14
4	A	1	KN1	CAR-CAS-NAO	2.61	125.26	120.78
4	B	1	KN1	CAI-CAP-CAM	-2.60	117.33	120.17
4	B	1	KN1	CAR-CAS-NAO	2.47	125.02	120.78
4	A	1	KN1	CAL-CAU-CAV	2.44	121.29	116.73
4	B	1	KN1	CAQ-CAR-CAS	-2.40	118.91	121.28
4	B	1	KN1	CAL-CAU-CAV	2.25	120.93	116.73
4	B	1	KN1	FAD-CAX-CAT	-2.04	110.21	112.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	KN1	CAV-CAT-CAX-FAF
4	A	1	KN1	CAK-CAR-CAS-NAO
4	B	1	KN1	CAK-CAR-CAS-NAO
4	A	1	KN1	CAV-CAT-CAX-FAD
4	A	1	KN1	CAJ-CAT-CAX-FAF
4	A	1	KN1	CAJ-CAT-CAX-FAD

There are no ring outliers.

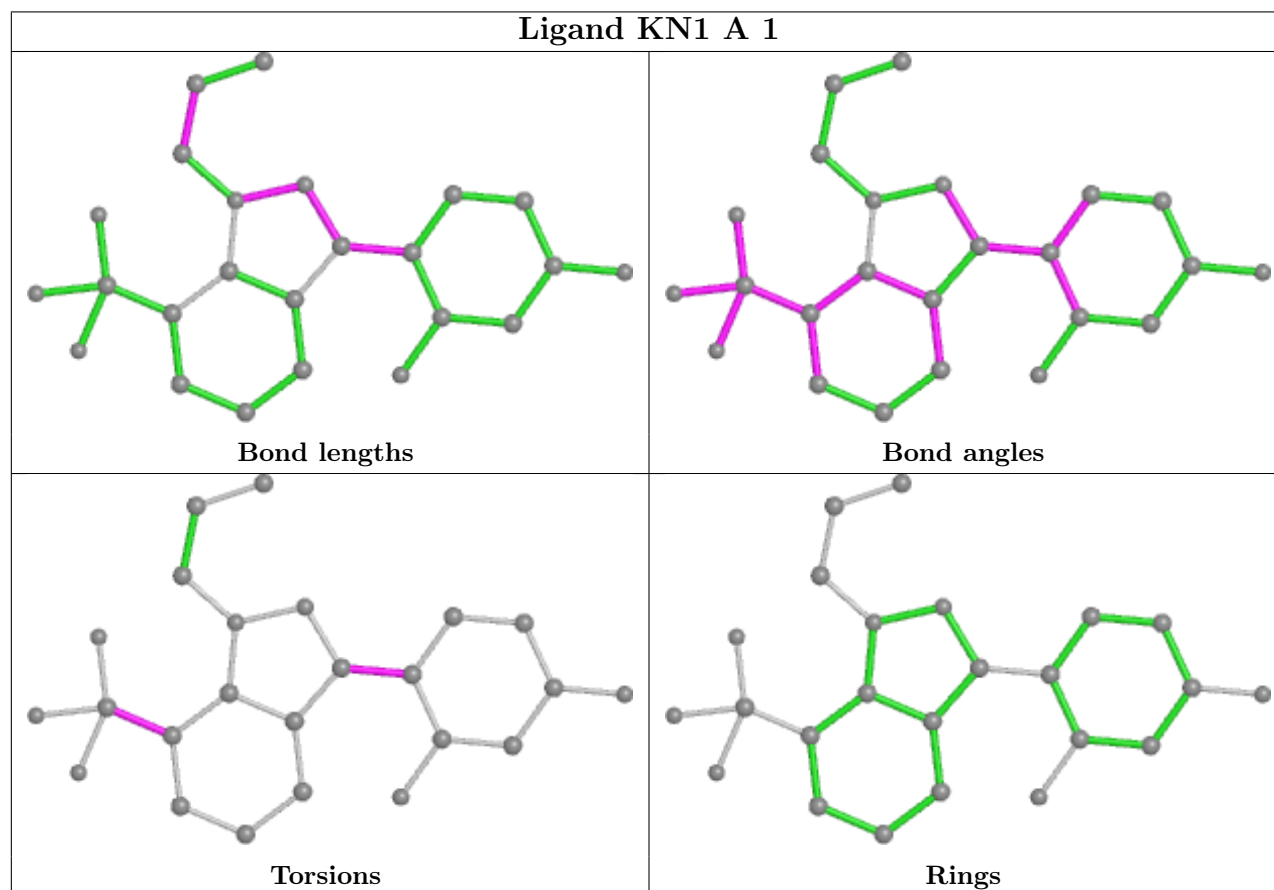
1 monomer is involved in 5 short contacts:

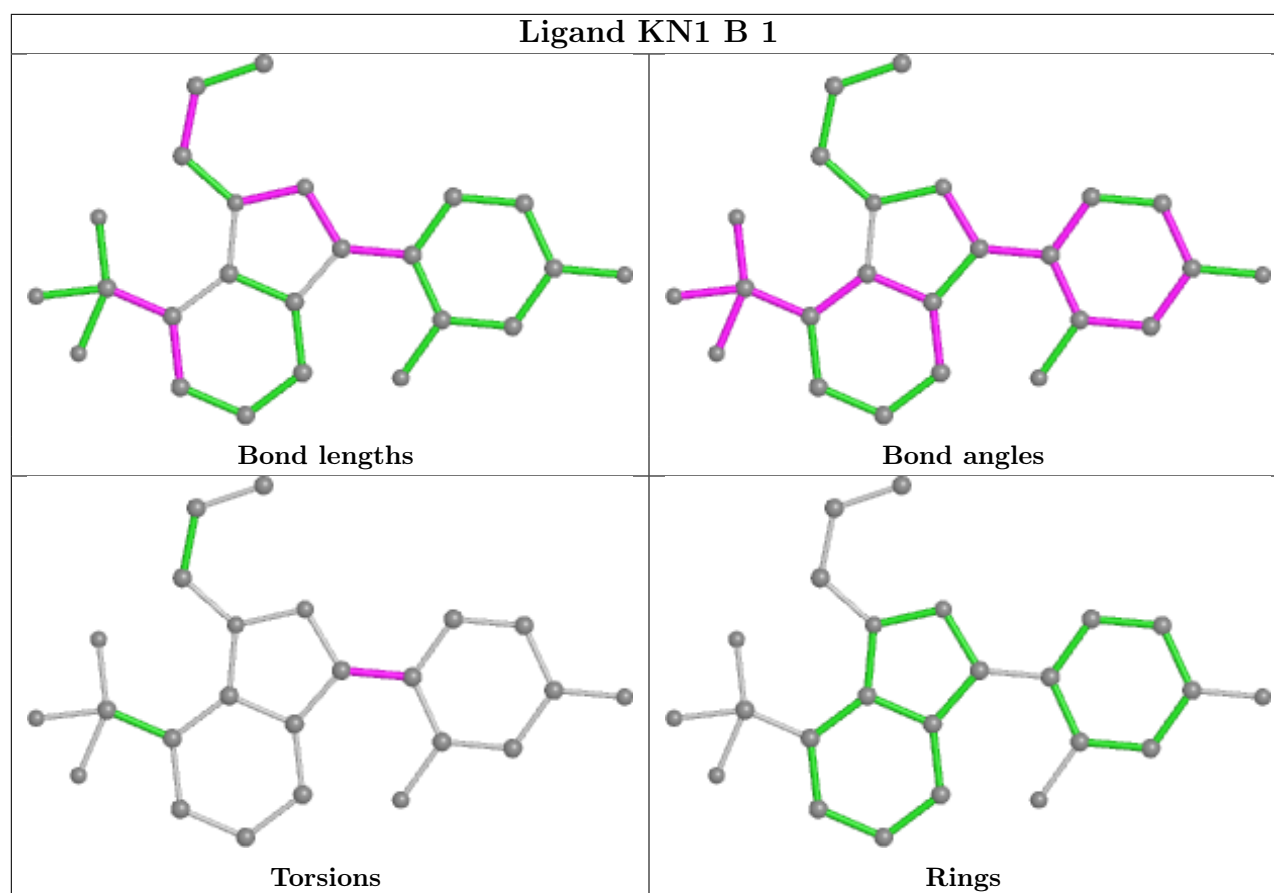
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	KN1	5	0

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	227/258 (87%)	0.45	30 (13%) <b>3</b> <b>3</b>	12, 22, 41, 47	4 (1%)
2	B	235/258 (91%)	-0.10	14 (5%) <b>21</b> <b>24</b>	12, 18, 36, 51	3 (1%)
3	C	9/13 (69%)	1.39	3 (33%) <b>0</b> <b>0</b>	18, 22, 25, 25	0
3	D	9/13 (69%)	0.25	0 <b>100</b> <b>100</b>	22, 23, 29, 30	0
All	All	480/542 (88%)	0.19	47 (9%) <b>7</b> <b>8</b>	12, 19, 40, 51	7 (1%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	THR	11.5
1	A	549	LEU	10.7
1	A	469	LEU	8.0
2	B	306	LEU	6.1
1	A	458	VAL	5.4
1	A	457	GLY	5.2
2	B	549	LEU	5.2
1	A	340	ALA	4.7
1	A	337	PHE	4.7
1	A	526	TYR	4.6
1	A	336	PRO	4.3
2	B	461	PHE	4.3
2	B	548	ARG	4.2
2	B	469	LEU	4.2
1	A	306	LEU	4.2
1	A	533	VAL	4.0
3	C	687	HIS	3.7
1	A	548	ARG	3.6
1	A	305	SER	3.6
2	B	309	SER	3.6
1	A	338	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	B	471	GLU	3.5
1	A	420	GLY	3.5
1	A	333	PRO	3.4
1	A	470	GLU	3.4
2	B	460	THR	3.3
1	A	472	LYS	3.1
2	B	459	TYR	3.1
1	A	532	ASN	3.1
2	B	470	GLU	3.0
1	A	471	GLU	2.9
3	C	691	HIS	2.8
1	A	373	HIS	2.6
2	B	419	GLU	2.6
2	B	437	MET	2.5
1	A	437	MET	2.5
3	C	692	ARG	2.4
2	B	545	ASP	2.4
1	A	538	ASP	2.4
1	A	342	MET	2.3
1	A	421	MET	2.3
1	A	335	ARG	2.1
1	A	527	SER	2.1
1	A	411	ASP	2.1
1	A	422	VAL	2.1
2	B	477	ARG	2.1
1	A	530	CYS	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	CME	B	381	10/11	0.83	0.15	12,15,30,37	3
1	CME	A	381	10/11	0.90	0.13	17,18,38,42	0
2	CME	B	530	10/11	0.90	0.12	12,15,36,40	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

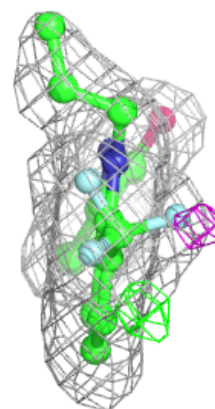
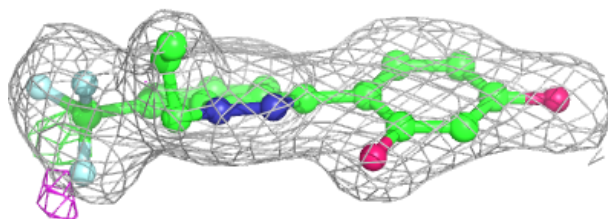
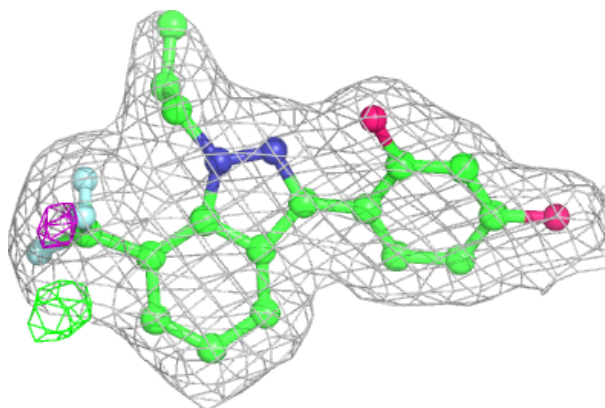
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

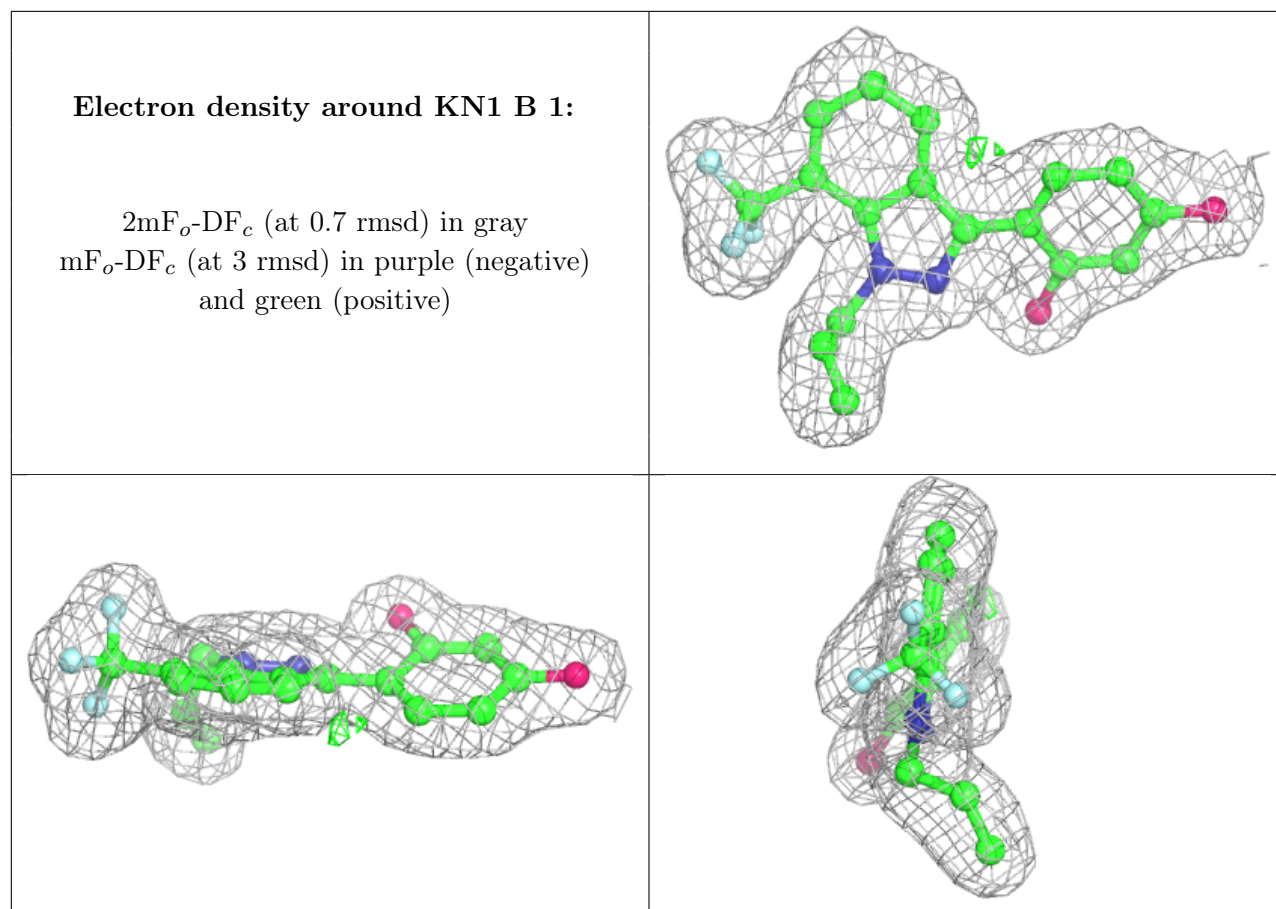
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	KN1	A	1	24/24	0.94	0.07	30,39,46,49	0
4	KN1	B	1	24/24	0.97	0.05	20,25,31,32	0

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 KN1 A 1:**

$2mF_o-DF_c$  (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.