



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2021 – 03:12 pm BST

PDB ID : 7AH3  
Title : Kinase domain of cSrc in complex with a pyrazolopyrimidine  
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Deposited on : 2020-09-24  
Resolution : 1.95 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 : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

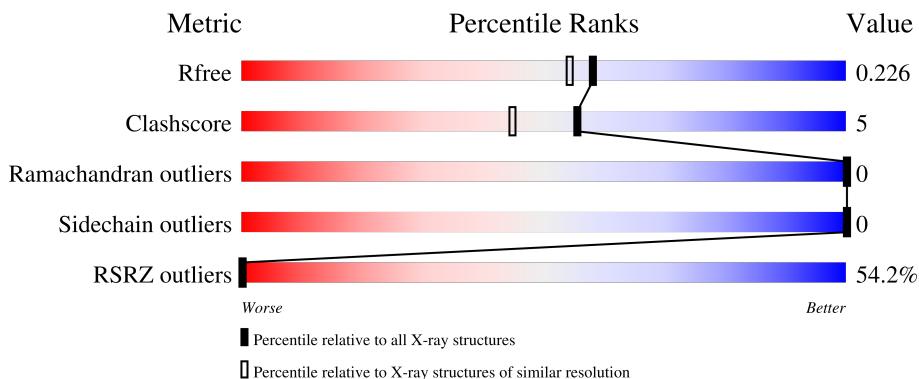
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	286	<p>50% 84% 7% • 7%</p>
1	B	286	<p>49% 77% 11% • 11%</p>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4534 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.

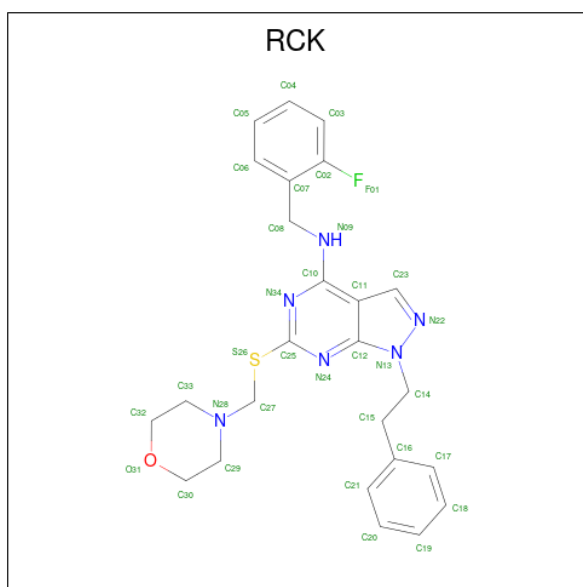
- Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase Src.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	2087	1344	347	379	17	0	4	0
1	B	255	2016	1300	334	367	15	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	GLY	-	expression tag	UNP P00523
A	249	HIS	-	expression tag	UNP P00523
A	250	MET	-	expression tag	UNP P00523
B	248	GLY	-	expression tag	UNP P00523
B	249	HIS	-	expression tag	UNP P00523
B	250	MET	-	expression tag	UNP P00523

- Molecule 2 is {N}-[(2-fluorophenyl)methyl]-6-(morpholin-4-ylmethylsulfanyl)-1-(2-phenylethyl)pyrazolo[3,4-d]pyrimidin-4-amine (three-letter code: RCK) (formula: C<sub>25</sub>H<sub>27</sub>FN<sub>6</sub>OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
2	A	1	34	25	1	6	1	1	0	0
2	B	1	34	25	1	6	1	1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



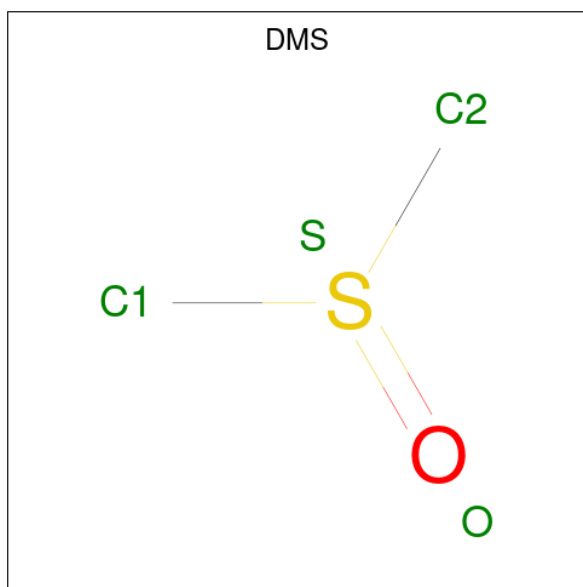
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C O		
3	A	1	4	2 2	0	0
3	A	1	4	2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	172	Total O 172 172	0	0
6	B	159	Total O 159 159	0	0



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	42.26Å 63.42Å 74.93Å 101.72° 90.89° 90.01°	Depositor
Resolution (Å)	43.26 – 1.95 43.26 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.0 (43.26-1.95) 97.0 (43.26-1.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 1.95Å)	Xtrriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.187 , 0.226 0.187 , 0.226	Depositor DCC
$R_{free}$ test set	2693 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.0	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.028 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.83% 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: RCK, DMS, EDO, GOL

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	0.54	1/2150 (0.0%)	0.85	7/2921 (0.2%)
1	B	0.50	1/2069 (0.0%)	1.24	14/2807 (0.5%)
All	All	0.52	2/4219 (0.0%)	1.06	21/5728 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	ARG	CZ-NH2	7.77	1.43	1.33
1	B	332	GLU	CD-OE2	5.71	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	GLU	OE1-CD-OE2	-39.00	76.50	123.30
1	B	332	GLU	CG-CD-OE2	-19.02	80.27	118.30
1	B	332	GLU	CG-CD-OE1	18.73	155.77	118.30
1	A	268	ARG	NE-CZ-NH1	-17.58	111.51	120.30
1	A	268	ARG	NE-CZ-NH2	14.03	127.32	120.30
1	B	438	ARG	NE-CZ-NH1	-10.92	114.84	120.30
1	B	388	ARG	CD-NE-CZ	10.84	138.78	123.60
1	B	331	GLU	C-N-CA	-9.07	99.03	121.70
1	A	318	ARG	CG-CD-NE	9.01	130.72	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	474	GLN	CA-CB-CG	8.61	132.35	113.40
1	B	438	ARG	NE-CZ-NH2	8.28	124.44	120.30
1	B	438	ARG	CD-NE-CZ	8.06	134.88	123.60
1	B	388	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	A	407	LEU	CB-CG-CD2	7.82	124.29	111.00
1	B	291	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	B	291	ARG	CD-NE-CZ	7.10	133.54	123.60
1	A	318	ARG	CB-CG-CD	6.66	128.91	111.60
1	A	318	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	B	451	LEU	CB-CG-CD2	5.77	120.81	111.00
1	A	302	MET	CB-CG-SD	-5.39	96.23	112.40
1	B	501	LYS	CA-CB-CG	5.17	124.77	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	388	ARG	Sidechain

## 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	2087	0	2038	21	0
1	B	2016	0	1962	21	1
2	A	34	0	0	1	0
2	B	34	0	0	2	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
4	A	4	0	6	3	0
5	B	12	0	16	0	0
6	A	172	0	0	2	0
6	B	159	0	0	0	0
All	All	4534	0	4046	42	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 5.

All (42) 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:283:MET:HE3	1:B:291:ARG:HE	1.49	0.77
1:B:283:MET:CE	1:B:291:ARG:HE	2.05	0.69
1:B:378:GLU:HG3	1:B:441:ILE:HG12	1.76	0.67
1:B:476:GLU:OE1	1:B:501:LYS:NZ	2.27	0.66
1:B:386:ASP:CG	1:B:388:ARG:HH11	2.00	0.64
1:B:281:VAL:HG21	2:B:1001:RCK:S26	2.38	0.64
1:B:386:ASP:OD2	1:B:388:ARG:NH1	2.28	0.61
1:A:267:LEU:C	1:A:268:ARG:HD2	2.21	0.60
1:B:295:LYS:HE2	2:B:1001:RCK:F01	1.92	0.59
1:B:329:VAL:HB	1:B:335:TYR:HB2	1.85	0.59
1:A:268:ARG:HD2	1:A:268:ARG:N	2.19	0.58
1:B:266:SER:HB2	1:B:287:ASN:ND2	2.19	0.56
1:A:297:LEU:HD13	1:A:302:MET:HE2	1.88	0.56
1:A:314:MET:HE3	1:A:407:LEU:HD12	1.87	0.56
1:A:318:ARG:HE	1:A:324:GLN:CD	2.09	0.55
1:A:314:MET:CE	1:A:407:LEU:HD12	2.38	0.53
1:A:351:LYS:HZ2	4:A:604:DMS:C2	2.21	0.53
1:B:383:VAL:HG12	1:B:385:ARG:HG3	1.90	0.52
1:B:272:LYS:HE3	1:B:275:GLN:HE21	1.77	0.49
1:B:528:GLN:HE21	1:B:529:PRO:HD2	1.78	0.49
1:A:513:GLN:NE2	6:A:702:HOH:O	2.46	0.48
1:A:351:LYS:HZ2	4:A:604:DMS:H23	1.77	0.48
1:B:262:ILE:HG12	1:B:327:ALA:HB1	1.96	0.48
1:A:318:ARG:NH2	6:A:703:HOH:O	2.47	0.47
1:A:466:MET:HA	1:A:470:GLU:OE2	2.15	0.46
1:B:279:GLY:HA3	1:B:296:THR:O	2.15	0.46
1:A:283:MET:SD	1:A:340:TYR:CZ	3.10	0.45
1:A:338:THR:HG21	2:A:601:RCK:C07	2.47	0.45
1:A:319:HIS:HB3	1:A:322:LEU:HD13	1.98	0.44
1:A:446:TRP:CE3	1:A:499:TRP:HA	2.52	0.44
1:B:283:MET:HE1	1:B:291:ARG:HH11	1.82	0.43
1:A:341:MET:HG3	1:A:393:LEU:HB2	2.00	0.43
1:A:351:LYS:HB3	4:A:604:DMS:H13	2.01	0.43
1:B:466:MET:HB3	1:B:470:GLU:HG3	2.01	0.43
1:B:266:SER:HB2	1:B:287:ASN:HD21	1.84	0.42
1:A:297:LEU:HD13	1:A:302:MET:CE	2.50	0.42
1:A:314:MET:CE	1:A:407:LEU:HB2	2.50	0.42
1:B:470:GLU:O	1:B:474:GLN:HB2	2.20	0.41
1:A:494:LEU:HD11	1:A:512:LEU:HD23	2.02	0.41
1:B:257:LYS:HD2	1:B:261:GLU:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PRO:HA	1:A:520:PHE:CE2	2.55	0.41
1:B:263:PRO:HB2	1:B:265:GLU:OE2	2.21	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:397:ASN:OD1	1:B:438:ARG:NH2[1_455]	2.01	0.19

## 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	265/286 (93%)	260 (98%)	5 (2%)	0	100	100
1	B	250/286 (87%)	242 (97%)	8 (3%)	0	100	100
All	All	515/572 (90%)	502 (98%)	13 (2%)	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	217/245 (89%)	217 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	210/245 (86%)	210 (100%)	0	100	100
All	All	427/490 (87%)	427 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	275	GLN
1	A	391	ASN
1	A	513	GLN
1	B	287	ASN
1	B	528	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](#)

9 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
5	GOL	B	1004	-	5,5,5	0.81	0	5,5,5	1.01	0
3	EDO	B	1002	-	3,3,3	0.52	0	2,2,2	0.29	0
3	EDO	A	602	-	3,3,3	0.46	0	2,2,2	0.35	0
2	RCK	B	1001	-	36,38,38	2.45	9 (25%)	39,51,51	2.10	11 (28%)
4	DMS	A	604	-	3,3,3	0.64	0	3,3,3	0.92	0
2	RCK	A	601	-	36,38,38	2.49	10 (27%)	39,51,51	2.30	10 (25%)
3	EDO	B	1003	-	3,3,3	0.43	0	2,2,2	0.49	0
3	EDO	A	603	-	3,3,3	0.49	0	2,2,2	0.31	0
5	GOL	B	1005	-	5,5,5	1.00	0	5,5,5	0.87	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
5	GOL	B	1004	-	-	0/4/4/4	-
3	EDO	B	1002	-	-	1/1/1/1	-
3	EDO	A	602	-	-	1/1/1/1	-
2	RCK	B	1001	-	-	9/13/23/23	0/5/5/5
2	RCK	A	601	-	-	5/13/23/23	0/5/5/5
3	EDO	B	1003	-	-	0/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
5	GOL	B	1005	-	-	4/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	RCK	C27-N28	-9.51	1.32	1.45
2	B	1001	RCK	C27-N28	-9.26	1.32	1.45
2	A	601	RCK	C10-N09	7.44	1.48	1.34
2	B	1001	RCK	C10-N09	7.28	1.47	1.34
2	A	601	RCK	C07-C02	3.34	1.43	1.38
2	B	1001	RCK	C05-C04	2.95	1.45	1.38
2	B	1001	RCK	C29-N28	-2.92	1.38	1.46
2	B	1001	RCK	C07-C02	2.92	1.43	1.38
2	A	601	RCK	C05-C04	2.89	1.45	1.38
2	A	601	RCK	C29-N28	-2.75	1.39	1.46
2	B	1001	RCK	C27-S26	2.57	1.87	1.81
2	B	1001	RCK	C33-N28	-2.51	1.40	1.46
2	B	1001	RCK	C25-S26	2.51	1.80	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	RCK	C33-N28	-2.47	1.40	1.46
2	A	601	RCK	C14-N13	2.35	1.51	1.47
2	A	601	RCK	C08-C07	2.35	1.58	1.50
2	A	601	RCK	C27-S26	2.32	1.86	1.81
2	A	601	RCK	C25-S26	2.26	1.79	1.75
2	B	1001	RCK	C08-C07	2.07	1.57	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	RCK	C08-N09-C10	-7.49	113.12	123.11
2	B	1001	RCK	C08-N09-C10	-6.44	114.52	123.11
2	A	601	RCK	C32-C33-N28	5.41	118.31	110.10
2	A	601	RCK	C25-N24-C12	5.13	122.39	115.32
2	B	1001	RCK	C25-N24-C12	4.65	121.73	115.32
2	A	601	RCK	C33-N28-C27	-3.94	106.31	111.57
2	A	601	RCK	C23-N22-N13	3.79	108.17	104.23
2	B	1001	RCK	C27-S26-C25	3.77	116.09	100.65
2	B	1001	RCK	C23-N22-N13	3.67	108.05	104.23
2	B	1001	RCK	C32-C33-N28	3.60	115.56	110.10
2	B	1001	RCK	N24-C25-N34	-3.33	120.86	126.98
2	A	601	RCK	N24-C25-N34	-3.02	121.42	126.98
2	B	1001	RCK	C06-C07-C02	2.66	121.27	116.61
2	A	601	RCK	C30-C29-N28	2.59	114.04	110.10
2	A	601	RCK	C33-N28-C29	2.53	114.52	108.83
2	B	1001	RCK	C07-C08-N09	-2.39	105.60	113.38
2	A	601	RCK	C06-C07-C02	2.28	120.60	116.61
2	B	1001	RCK	C23-C11-C12	2.26	107.28	105.20
2	A	601	RCK	O31-C32-C33	2.14	116.51	111.80
2	B	1001	RCK	C29-N28-C27	-2.08	108.79	111.57
2	B	1001	RCK	C21-C16-C17	2.04	121.37	118.17

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	RCK	C15-C14-N13-C12
2	B	1001	RCK	C15-C14-N13-C12
2	B	1001	RCK	N28-C27-S26-C25
5	B	1005	GOL	C1-C2-C3-O3
2	B	1001	RCK	N24-C25-S26-C27
2	B	1001	RCK	N34-C25-S26-C27

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Mol	Chain	Res	Type	Atoms
2	A	601	RCK	C02-C07-C08-N09
5	B	1005	GOL	O2-C2-C3-O3
2	A	601	RCK	C14-C15-C16-C21
2	A	601	RCK	C14-C15-C16-C17
2	B	1001	RCK	N34-C10-N09-C08
2	B	1001	RCK	C14-C15-C16-C21
2	B	1001	RCK	C14-C15-C16-C17
2	B	1001	RCK	C11-C10-N09-C08
5	B	1005	GOL	O1-C1-C2-O2
3	A	602	EDO	O1-C1-C2-O2
2	B	1001	RCK	C15-C14-N13-N22
2	A	601	RCK	C06-C07-C08-N09
5	B	1005	GOL	O1-C1-C2-C3
3	B	1002	EDO	O1-C1-C2-O2

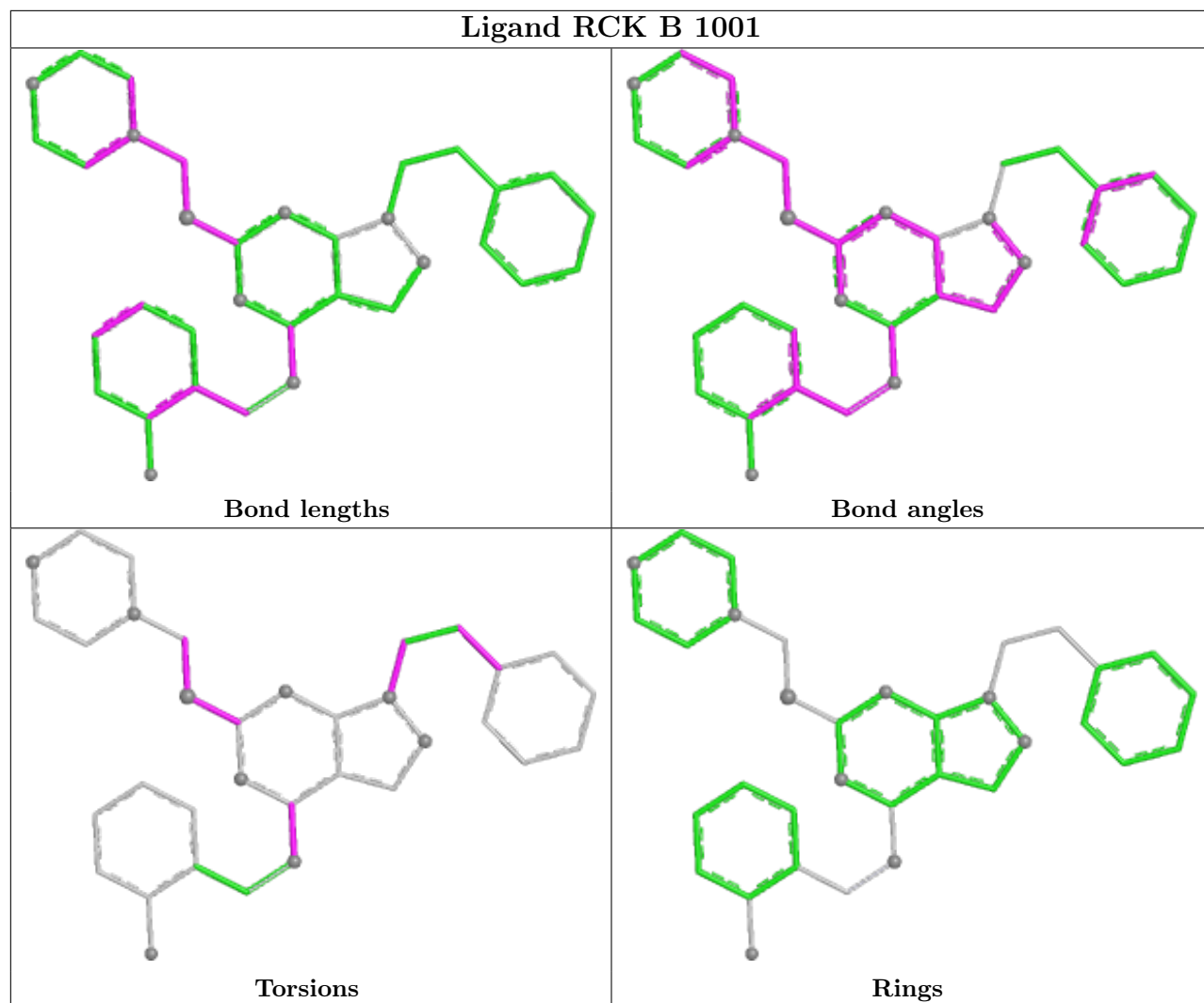
There are no ring outliers.

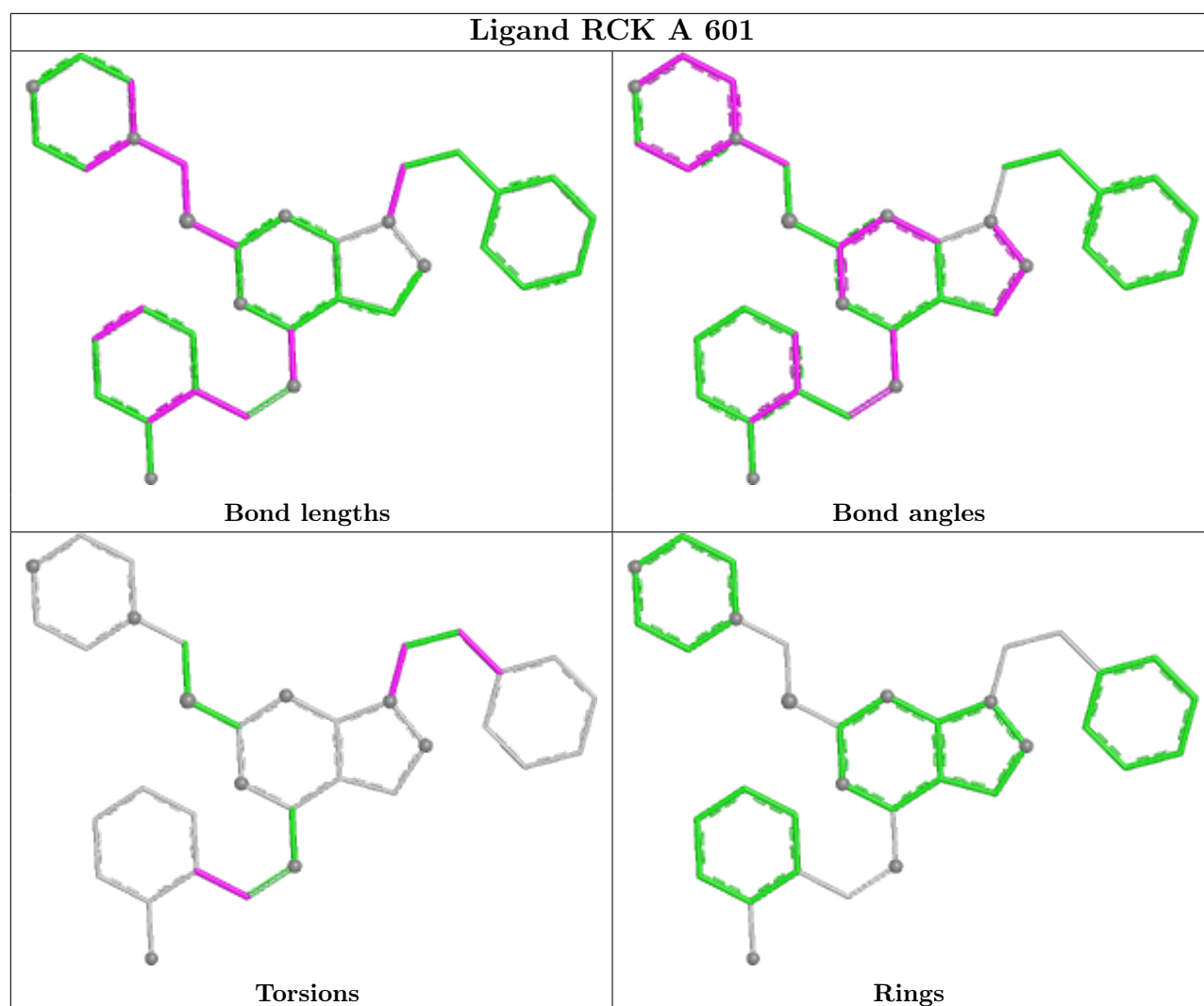
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	RCK	2	0
4	A	604	DMS	3	0
2	A	601	RCK	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	265/286 (92%)	2.46	143 (53%) 0 0	26, 45, 87, 114	0
1	B	255/286 (89%)	2.55	139 (54%) 0 0	27, 45, 98, 141	0
All	All	520/572 (90%)	2.51	282 (54%) 0 0	26, 45, 96, 141	0

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	307	PHE	12.2
1	B	275	GLN	11.1
1	A	411	ILE	10.8
1	A	302	MET	10.4
1	A	410	LEU	10.1
1	A	304	PRO	8.7
1	B	278	PHE	8.7
1	A	303	SER	8.6
1	B	277	CYS	8.6
1	B	406	GLY	8.5
1	B	424	PHE	8.4
1	A	308	LEU	8.0
1	B	333	PRO	7.9
1	B	334	ILE	7.7
1	A	311	ALA	7.4
1	A	313	VAL	7.4
1	B	279	GLY	7.3
1	A	260	TRP	7.2
1	A	306	ALA	6.9
1	A	305	GLU	6.5
1	B	297	LEU	6.4
1	B	271	VAL	6.3
1	B	298	LYS	6.3
1	B	270	GLU	6.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	289	THR	6.2
1	B	311	ALA	6.1
1	B	313	VAL	6.1
1	B	308	LEU	5.9
1	A	312	GLN	5.8
1	A	289	THR	5.8
1	B	276	GLY	5.7
1	A	258	ASP	5.7
1	B	435	LEU	5.6
1	B	331	GLU	5.5
1	B	269	LEU	5.4
1	A	318	ARG	5.3
1	A	404	ASP	5.3
1	B	263	PRO	5.2
1	B	299	PRO	5.2
1	B	335	TYR	5.2
1	A	257	LYS	5.2
1	A	271	VAL	5.2
1	A	278	PHE	5.1
1	A	333	PRO	5.1
1	A	297	LEU	5.1
1	B	404	ASP	5.0
1	B	329	VAL	5.0
1	A	259	ALA	4.9
1	A	403	ALA	4.9
1	A	300	GLY	4.7
1	A	307	PHE	4.7
1	B	332	GLU	4.6
1	A	298	LYS	4.5
1	B	282	TRP	4.5
1	B	296	THR	4.5
1	B	264	ARG	4.4
1	A	310	GLU	4.4
1	A	471	VAL	4.4
1	B	471	VAL	4.4
1	A	435	LEU	4.4
1	A	408	ALA	4.4
1	B	274	GLY	4.3
1	B	405	PHE	4.2
1	A	290	THR	4.2
1	A	331	GLU	4.2
1	B	256	ALA	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	276	GLY	4.1
1	A	425	PRO	4.1
1	A	334	ILE	4.1
1	A	299	PRO	4.0
1	B	290	THR	4.0
1	A	309	GLN	4.0
1	B	285	THR	4.0
1	B	472	LEU	3.9
1	B	262	ILE	3.9
1	B	267	LEU	3.8
1	B	309	GLN	3.8
1	A	301	THR	3.8
1	A	337	VAL	3.8
1	B	377	VAL	3.8
1	B	328	VAL	3.7
1	B	287	ASN	3.7
1	A	277	CYS	3.7
1	B	310	GLU	3.6
1	A	407	LEU	3.6
1	A	491	LEU	3.6
1	B	286	TRP	3.6
1	A	469	ARG	3.6
1	A	330	SER	3.6
1	B	467	VAL	3.6
1	B	280	GLU	3.5
1	A	473	ASP	3.5
1	B	323	VAL	3.5
1	A	262	ILE	3.4
1	A	472	LEU	3.4
1	A	275	GLN	3.4
1	B	284	GLY	3.4
1	A	494	LEU	3.4
1	A	516	LEU	3.4
1	B	358	LEU	3.4
1	A	382	TYR	3.4
1	B	265	GLU	3.4
1	B	330	SER	3.4
1	B	425	PRO	3.4
1	A	370	ILE	3.4
1	A	502	ASP	3.3
1	B	498	CYS	3.3
1	B	531	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	312	GLN	3.3
1	A	477	ARG	3.2
1	B	291	ARG	3.2
1	B	483	CYS	3.2
1	B	349	PHE	3.2
1	A	438	ARG	3.2
1	A	328	VAL	3.2
1	B	399	VAL	3.2
1	A	268	ARG	3.1
1	B	346	LEU	3.1
1	B	449	GLY	3.1
1	B	367	ALA	3.1
1	B	343	LYS	3.1
1	A	428	TRP	3.0
1	A	358	LEU	3.0
1	B	350	LEU	3.0
1	A	498	CYS	3.0
1	A	364	VAL	3.0
1	A	434	ALA	3.0
1	B	261	GLU	3.0
1	B	281	VAL	3.0
1	A	286	TRP	3.0
1	B	441	ILE	3.0
1	A	296	THR	3.0
1	B	266	SER	3.0
1	A	336	ILE	3.0
1	A	390	ALA	3.0
1	B	462	PRO	3.0
1	A	317	LEU	2.9
1	A	360	LEU	2.9
1	A	509	PHE	2.9
1	A	436	TYR	2.9
1	B	428	TRP	2.9
1	A	399[A]	VAL	2.9
1	A	267	LEU	2.9
1	A	446	TRP	2.9
1	A	350	LEU	2.9
1	B	528	GLN	2.8
1	A	294	ILE	2.8
1	A	392	ILE	2.8
1	A	462	PRO	2.8
1	A	409	ARG	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	463	TYR	2.8
1	B	317	LEU	2.8
1	A	484	PRO	2.8
1	B	294	ILE	2.8
1	B	450	ILE	2.8
1	A	439	PHE	2.8
1	B	283	MET	2.8
1	A	315	LYS	2.7
1	A	451	LEU	2.7
1	A	323	VAL	2.7
1	A	377	VAL	2.7
1	B	394	VAL	2.7
1	B	456	THR	2.7
1	B	436	TYR	2.7
1	B	475	VAL	2.7
1	A	394	VAL	2.7
1	A	283	MET	2.7
1	A	533	LEU	2.7
1	B	455	LEU	2.7
1	A	329	VAL	2.7
1	B	527	TYR	2.7
1	A	452	LEU	2.7
1	A	398	LEU	2.6
1	B	398	LEU	2.6
1	A	371	ALA	2.6
1	A	426	ILE	2.6
1	A	405	PHE	2.6
1	B	382	TYR	2.6
1	B	453	THR	2.6
1	B	407	LEU	2.6
1	B	368	ALA	2.6
1	A	496	CYS	2.6
1	B	336	ILE	2.6
1	B	461	VAL	2.6
1	B	451	LEU	2.6
1	B	426	ILE	2.6
1	B	337	VAL	2.6
1	A	520	PHE	2.5
1	A	512	LEU	2.5
1	A	499	TRP	2.5
1	A	441	ILE	2.5
1	A	381	ASN	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	502	ASP	2.5
1	A	285	THR	2.5
1	B	499	TRP	2.5
1	A	445	VAL	2.5
1	B	512	LEU	2.5
1	A	266	SER	2.5
1	A	263	PRO	2.5
1	B	388	ARG	2.5
1	A	346	LEU	2.5
1	A	287	ASN	2.5
1	B	392	ILE	2.4
1	A	456	THR	2.4
1	B	347	LEU	2.4
1	B	360	LEU	2.4
1	B	515	PHE	2.4
1	A	389	ALA	2.4
1	B	389	ALA	2.4
1	B	447	SER	2.4
1	B	268	ARG	2.4
1	B	452	LEU	2.4
1	B	533	LEU	2.4
1	A	340	TYR	2.4
1	A	453	THR	2.4
1	A	467	VAL	2.4
1	A	475	VAL	2.4
1	A	367	ALA	2.4
1	A	368	ALA	2.4
1	B	318	ARG	2.4
1	B	292	VAL	2.4
1	A	455	LEU	2.3
1	B	363	LEU	2.3
1	B	457	THR	2.3
1	A	493[A]	ASP	2.3
1	A	519	TYR	2.3
1	B	529	PRO	2.3
1	A	487	CYS	2.3
1	A	481	MET	2.3
1	B	314	MET	2.3
1	B	403	ALA	2.3
1	B	434	ALA	2.3
1	B	516	LEU	2.3
1	A	463	TYR	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	495	MET	2.3
1	A	325	LEU	2.3
1	B	438	ARG	2.3
1	A	261	GLU	2.3
1	B	393	LEU	2.3
1	B	473	ASP	2.3
1	B	370	ILE	2.2
1	A	387	LEU	2.2
1	A	448	PHE	2.2
1	A	508	THR	2.2
1	B	445	VAL	2.2
1	A	526	GLN	2.2
1	A	511	TYR	2.2
1	B	400	CYS	2.2
1	B	525	PRO	2.2
1	B	508	THR	2.2
1	B	520	PHE	2.2
1	A	314	MET	2.2
1	B	504	GLU	2.2
1	B	429	THR	2.2
1	B	352	GLY	2.2
1	B	474	GLN	2.2
1	B	371	ALA	2.2
1	B	257	LYS	2.2
1	A	366	MET	2.1
1	A	374	MET	2.1
1	A	490	SER	2.1
1	B	351	LYS	2.1
1	A	363	LEU	2.1
1	B	390	ALA	2.1
1	B	260	TRP	2.1
1	A	348	ASP	2.1
1	A	402	VAL	2.1
1	A	380	MET	2.1
1	A	465	GLY	2.1
1	A	450	ILE	2.1
1	B	322	LEU	2.1
1	B	387	LEU	2.1
1	B	494	LEU	2.1
1	B	505	GLU	2.1
1	A	274	GLY	2.1
1	B	501	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	515	PHE	2.1
1	B	446	TRP	2.1
1	A	322	LEU	2.1
1	A	514	ALA	2.0
1	A	345	SER	2.0
1	A	429	THR	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](#)

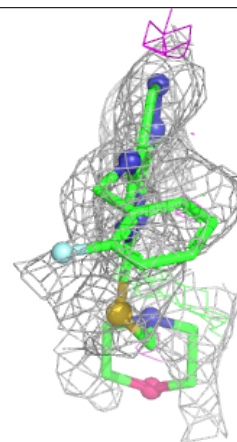
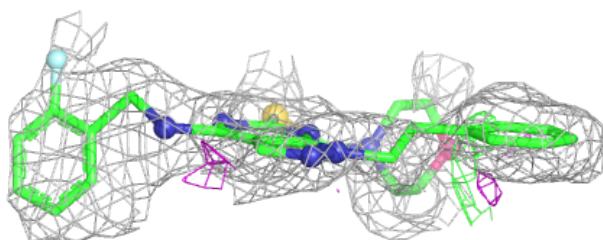
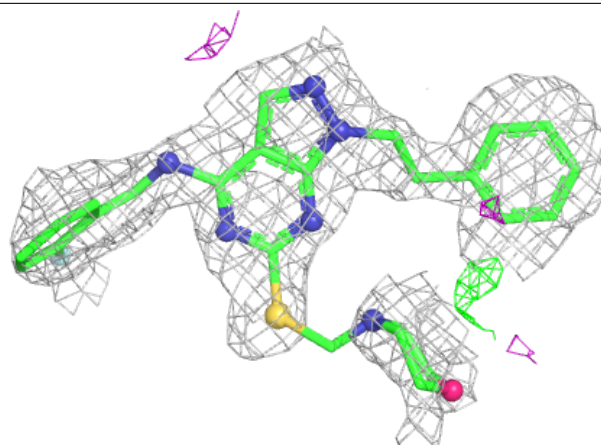
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	EDO	B	1002	4/4	0.33	0.23	66,70,71,72	0
2	RCK	B	1001	34/34	0.39	0.36	50,65,84,87	0
4	DMS	A	604	4/4	0.48	0.32	73,78,83,84	4
3	EDO	B	1003	4/4	0.49	0.33	52,57,67,70	0
3	EDO	A	603	4/4	0.52	0.27	60,60,60,66	0
5	GOL	B	1005	6/6	0.54	0.23	59,66,70,72	0
2	RCK	A	601	34/34	0.63	0.28	36,50,68,73	34
3	EDO	A	602	4/4	0.65	0.24	73,74,78,80	0
5	GOL	B	1004	6/6	0.82	0.24	37,43,46,46	6

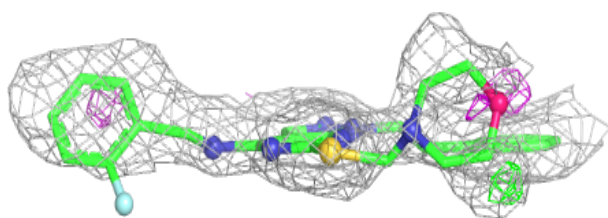
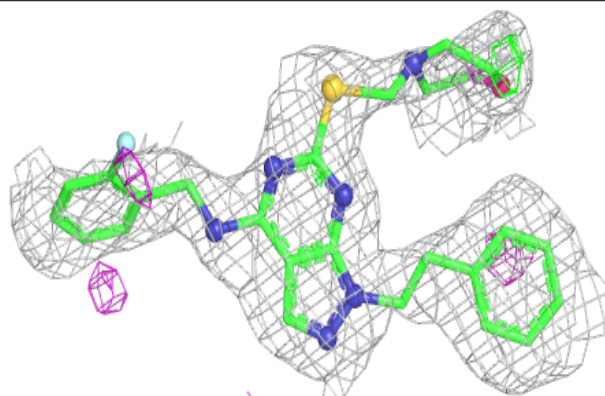
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around RCK B 1001:**

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

**Electron density around RCK A 601:**

$2mF_o-DF_c$  (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.