

# wwPDB X-ray Structure Validation Summary Report (i)

#### Aug 20, 2023 - 03:53 AM EDT

PDB ID	:	2G1T
Title	:	A Src-like Inactive Conformation in the Abl Tyrosine Kinase Domain
Authors	:	Levinson, N.M.; Kuchment, O.
Deposited on		
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

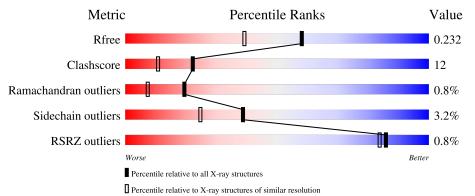
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.35
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

The reported resolution of this entry is 1.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 >=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 <=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	А	287	.% • 78%	15% • 6%
1	В	287	71%	22% • 5%
1	С	287	71%	24% •••
1	D	287	.% 	15% ••••
2	Е	13	62%	38%



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Mol	Chain	Length	Quality of chain							
2	F	13	62%		8%	8%	23%			
2	G	13	46%	%		46%				
2	Н	13	54%	8%		38%				



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10249 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	٨	971	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	A	271	2210	1424	359	410	17	0	0	0
1	В	273	Total	С	Ν	0	S	0	0	0
	D	213	2225	1433	362	413	17	0	0	
1	С	276	Total	С	Ν	0	S	0	0	0
	C	270	2249	1446	364	422	17	0	0	U
1	П	277	Total	С	Ν	0	S	0	0	0
		277	2253	1449	368	418	18	0	0	0

• Molecule 1 is a protein called Proto-oncogene tyrosine-protein kinase ABL1.

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	226	GLY	-	cloning artifact	UNP P00519
А	227	HIS	-	cloning artifact	UNP P00519
А	228	MET	-	cloning artifact	UNP P00519
В	226	GLY	-	cloning artifact	UNP P00519
В	227	HIS	-	cloning artifact	UNP P00519
В	228	MET	-	cloning artifact	UNP P00519
С	226	GLY	-	cloning artifact	UNP P00519
С	227	HIS	-	cloning artifact	UNP P00519
С	228	MET	-	cloning artifact	UNP P00519
D	226	GLY	-	cloning artifact	UNP P00519
D	227	HIS	-	cloning artifact	UNP P00519
D	228	MET	_	cloning artifact	UNP P00519

• Molecule 2 is a protein called ATP-Peptide Conjugate.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	Е	8	Total         C         N         O           66         44         8         14	0	0	0
2	F	10	Total         C         N         O           76         50         10         16	0	0	0



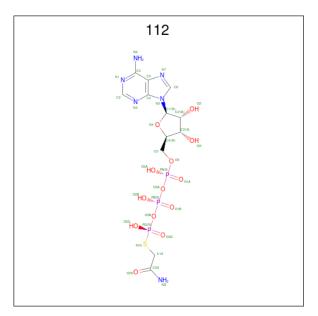
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	G	7	Total C N O 57 39 7 11	0	0	0
2	Н	8	Total         C         N         O           70         46         8         16	0	0	0

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mg 1 1	0	0
3	В	1	Total Mg 1 1	0	0
3	С	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

• Molecule 4 is THIOPHOSPHORIC ACID O-((ADENOSYL-PHOSPHO)PHOSPHO)-S-AC ETAMIDYL-DIESTER (three-letter code: 112) (formula:  $C_{12}H_{19}N_6O_{13}P_3S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	Е	1	Total	-		-			0	0
			35			13				
4	F	1	Total	-		-			0	0
			35		-	13	-			
4	G	1	Total					$\mathbf{S}$	0	0
	, u	Ĩ	35	12	6	13	3	1		9



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	Н	1	Total 35	C 12	N 6	0	Р 3	S 1	0	0

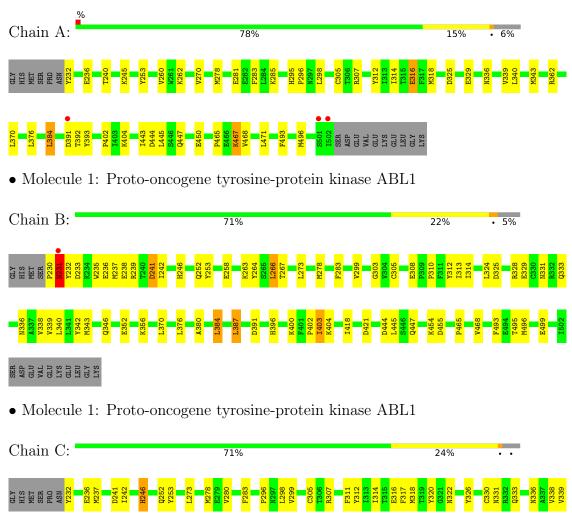
• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	244	Total O 244 244	0	0
5	В	197	Total O 197 197	0	0
5	С	172	Total O 172 172	0	0
5	D	209	Total O 209 209	0	0
5	Е	19	Total O 19 19	0	0
5	F	29	TotalO2929	0	0
5	G	15	Total O 15 15	0	0
5	Н	14	Total         O           14         14	0	0

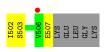


# 3 Residue-property plots (i)

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: Proto-oncogene tyrosine-protein kinase ABL1



• Molecule 1: Proto-oncogene tyrosine-protein kinase ABL1



Chain D:	79%		15% ••••	
C226 H227 N228 S229 P230 N231 N231 N237 D241 1242	R286 R262 V260 V260 V260 V260 R266 R266 R266 R266 R266 R306 R307 R312 V312	1314 1314 1336 1336 1337 1338 1338 1338 1338 1338 1338 1338	H361 R362 L370 L370 R385 R385 R385 R385 R385 R385 R385 R385	H396 A397 G398
• Molecule 2: A7	P-Peptide Conjugate	SER ASP ASP ASP ASP CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU		
Chain E:	62%		38%	
ALA GLU GLU HI2 HI2 LYS LYS				
• Molecule 2: AT	P-Peptide Conjugate			
Chain E				
Chain F:	62%	8% 8%	23%	
ALA GLU E104 E107 G108 E109 K113 LYS				
• Molecule 2: AT	P-Peptide Conjugate			
Chain G:	46% 8%	46	5%	
ALA GLU GLU E105 F107 E111 ALA LYS LYS				
• Molecule 2: AT	P-Peptide Conjugate			
Chain H:	54%	8%	38%	



# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	62.59Å 78.44Å 141.61Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.11° 90.00°	
Resolution (Å)	$50.00 - 1.80 \ 48.92 - 1.83$	Depositor EDS
% Data completeness	92.6 (50.00-1.80)	Depositor
(in resolution range)	96.9 (48.92-1.83)	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.90 (at 1.83 \text{\AA})$	Xtriage
Refinement program	CNS 1.1	Depositor
P. P.	0.219 , $0.244$	Depositor
$R, R_{free}$	0.205 , $0.232$	DCC
$R_{free}$ test set	11279  reflections  (9.59%)	wwPDB-VP
Wilson B-factor $(Å^2)$	21.8	Xtriage
Anisotropy	0.824	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, $30.2$	EDS
L-test for twinning <sup>2</sup>	$< L >=0.45, < L^2>=0.27$	Xtriage
Estimated twinning fraction	0.084 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10249	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 12.08% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: MG,  $112\,$ 

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	Bo	ond angles
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.33	0/2267	0.62	1/3068~(0.0%)
1	В	0.32	0/2283	0.60	1/3090~(0.0%)
1	С	0.31	0/2306	0.58	1/3121~(0.0%)
1	D	0.35	0/2312	0.61	2/3129~(0.1%)
2	Е	0.50	0/67	0.55	0/88
2	F	0.48	0/77	0.57	0/102
2	G	0.49	0/58	0.65	0/76
2	Н	0.48	0/71	0.50	0/93
All	All	0.33	0/9441	0.60	5/12767~(0.0%)

There are no bond length outliers.

All $(5)$	bond	angle	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	402	PRO	N-CA-C	-6.78	94.47	112.10
1	В	402	PRO	N-CA-C	-6.65	94.81	112.10
1	D	402	PRO	N-CA-C	-5.67	97.36	112.10
1	С	402	PRO	N-CA-C	-5.32	98.28	112.10
1	D	229	SER	N-CA-C	5.31	125.33	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.



0	$\cap$	1	Π		
4	G	T	1	L	

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2210	0	2163	34	0
1	В	2225	0	2177	61	0
1	С	2249	0	2193	71	0
1	D	2253	0	2200	50	0
2	Е	66	0	54	0	0
2	F	76	0	58	3	0
2	G	57	0	45	1	0
2	Н	70	0	55	1	0
3	А	1	0	0	0	0
3	В	1	0	0	0	0
3	С	1	0	0	0	0
3	D	1	0	0	0	0
4	Ε	35	0	14	0	0
4	F	35	0	14	0	0
4	G	35	0	14	0	0
4	Н	35	0	15	1	0
5	А	244	0	0	4	0
5	В	197	0	0	1	0
5	С	172	0	0	1	0
5	D	209	0	0	3	0
5	Е	19	0	0	0	0
5	F	29	0	0	0	0
5	G	15	0	0	0	0
5	Н	14	0	0	1	0
All	All	10249	0	9002	215	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 12.

The worst 5 of 215 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:D:307:ARG:HH11	1:D:307:ARG:HB2	1.08	1.15
1:D:473:ARG:HH11	1:D:473:ARG:HB3	1.33	0.94
1:C:278:MET:HE1	1:C:283:PHE:HD1	1.34	0.91
1:D:307:ARG:HH11	1:D:307:ARG:CB	1.87	0.86
1:D:484:PRO:HG2	1:D:489:ILE:HD11	1.58	0.86

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	А	269/287~(94%)	260~(97%)	9~(3%)	0	100 100
1	В	271/287~(94%)	261 (96%)	8 (3%)	2(1%)	22 10
1	С	274/287~(96%)	265~(97%)	6(2%)	3 (1%)	14 4
1	D	275/287~(96%)	262~(95%)	9~(3%)	4(2%)	10 2
2	Ε	6/13~(46%)	6 (100%)	0	0	100 100
2	F	8/13~(62%)	8 (100%)	0	0	100 100
2	G	5/13~(38%)	5~(100%)	0	0	100 100
2	Н	6/13~(46%)	6 (100%)	0	0	100 100
All	All	1114/1200~(93%)	1073 (96%)	32 (3%)	9~(1%)	19 7

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	С	397	ALA
1	D	229	SER
1	В	231	ASN
1	D	228	MET
1	D	230	PRO

#### 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	А	237/251~(94%)	230~(97%)	7 (3%)	41 27



Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	В	239/251~(95%)	231~(97%)	8~(3%)	38	23
1	$\mathbf{C}$	242/251~(96%)	237~(98%)	5(2%)	53	42
1	D	242/251~(96%)	232~(96%)	10 (4%)	30	16
2	Ε	6/10~(60%)	6 (100%)	0	100	100
2	F	6/10~(60%)	5 (83%)	1 (17%)	2	0
2	G	5/10~(50%)	5(100%)	0	100	100
2	Н	7/10~(70%)	7~(100%)	0	100	100
All	All	984/1044~(94%)	953~(97%)	31 (3%)	39	25

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5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	391	ASP
1	D	450	GLU
1	С	373	GLU
1	D	473	ARG
1	D	370	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	С	447	GLN
1	D	375	HIS
1	D	491	GLN
1	D	447	GLN
1	В	375	HIS

#### 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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	Turne	Chain	hain Res	Res Link	Bond lengths			Bond angles		
	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z >2
4	112	G	1301	3,2	27,37,37	3.72	7 (25%)	$27,\!57,\!57$	1.66	9 (33%)
4	112	Е	1101	3,2	27,37,37	<mark>3.79</mark>	8 (29%)	$27,\!57,\!57$	1.66	9 (33%)
4	112	F	1201	3,2	27,37,37	<mark>3.69</mark>	7 (25%)	$27,\!57,\!57$	1.57	9 (33%)
4	112	Н	1401	3,2	27,37,37	3.55	8 (29%)	$27,\!57,\!57$	1.72	8 (29%)

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	112	G	1301	3,2	-	0/19/44/44	0/3/3/3
4	112	Е	1101	3,2	-	0/19/44/44	0/3/3/3
4	112	F	1201	3,2	-	0/19/44/44	0/3/3/3
4	112	Н	1401	3,2	-	0/19/44/44	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}(\operatorname{\AA})$
4	Е	1101	112	C1S-S1G	-16.58	1.64	1.84
4	F	1201	112	C1S-S1G	-16.33	1.65	1.84
4	G	1301	112	C1S-S1G	-16.23	1.65	1.84
4	Н	1401	112	C1S-S1G	-15.12	1.66	1.84
4	Е	1101	112	C4-N3	5.73	1.43	1.35

The worst 5 of 35 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
4	Н	1401	112	C4-C5-N7	3.83	113.39	109.40
4	G	1301	112	C4-C5-N7	3.64	113.19	109.40
4	Е	1101	112	C4-C5-N7	3.61	113.16	109.40
4	F	1201	112	C4-C5-N7	3.40	112.94	109.40
4	Н	1401	112	PA-O3A-PB	3.10	143.47	132.83

There are no chirality outliers.

There are no torsion outliers.

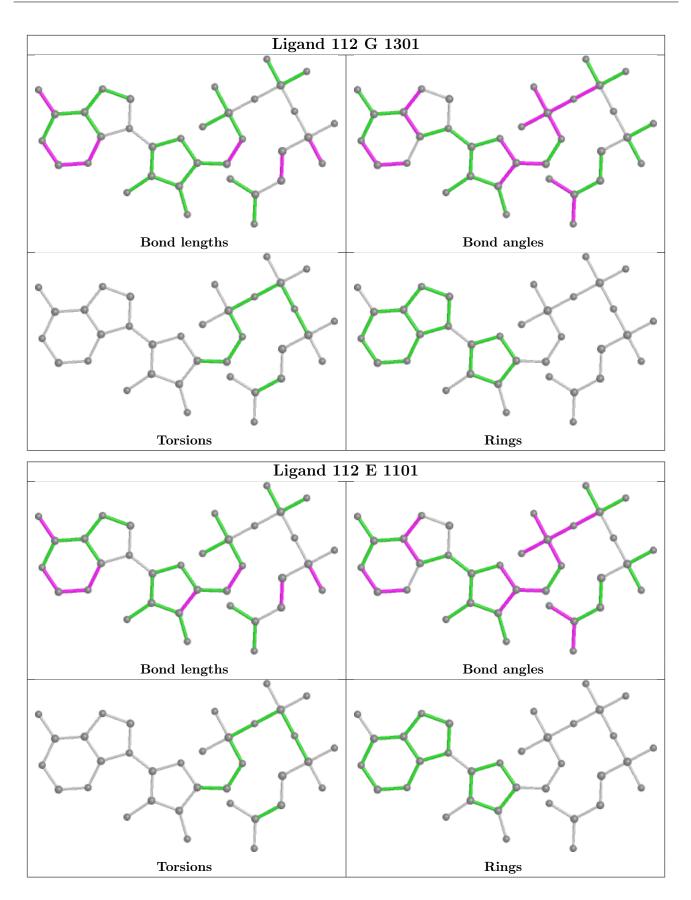
There are no ring outliers.

1 monomer is involved in 1 short contact:

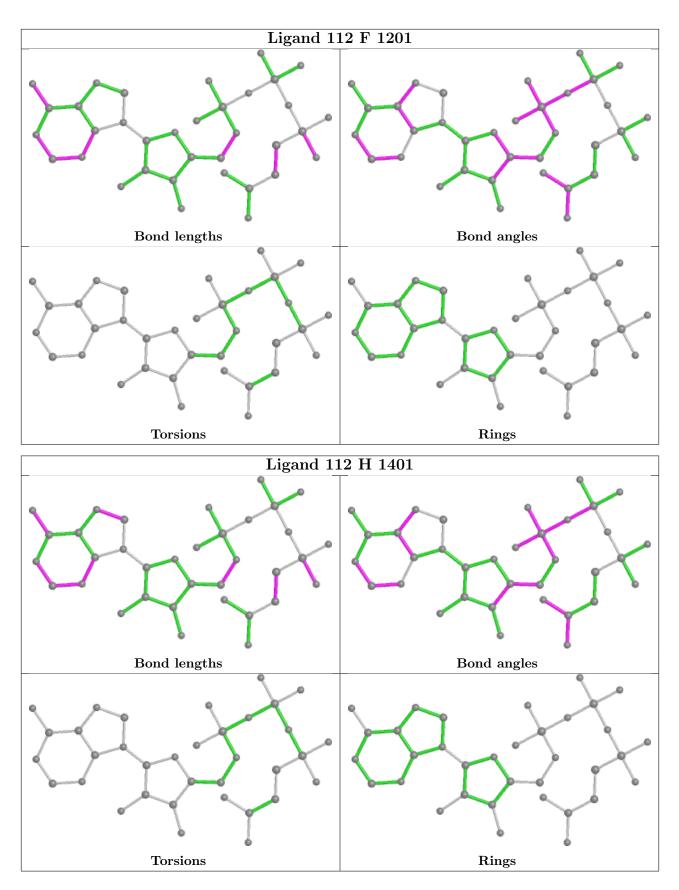
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Н	1401	112	1	0

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 then 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,  $95^{th}$  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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	271/287~(94%)	-0.30	3 (1%) 80 78	13, 23, 43, 66	0
1	В	273/287~(95%)	-0.22	1 (0%) 92 90	13, 27, 45, 70	0
1	С	276/287~(96%)	-0.16	1 (0%) 92 90	18, 28, 49, 66	0
1	D	277/287~(96%)	-0.24	4 (1%) 75 72	15, 24, 45, 70	0
2	Е	8/13~(61%)	0.14	0 100 100	22, 28, 37, 39	0
2	F	10/13~(76%)	-0.06	0 100 100	23, 33, 44, 44	0
2	G	7/13~(53%)	0.12	0 100 100	28, 30, 45, 45	0
2	Н	8/13~(61%)	0.46	0 100 100	23, 44, 48, 51	0
All	All	1130/1200~(94%)	-0.22	9 (0%) 86 84	13, 26, 46, 70	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	501	SER	4.6
1	D	229	SER	4.3
1	В	231	ASN	3.5
1	С	506	VAL	3.4
1	А	391	ASP	3.2

# 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.

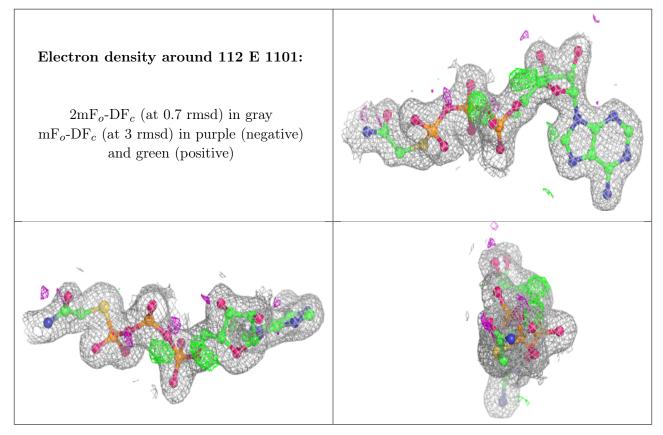


## 6.4 Ligands (i)

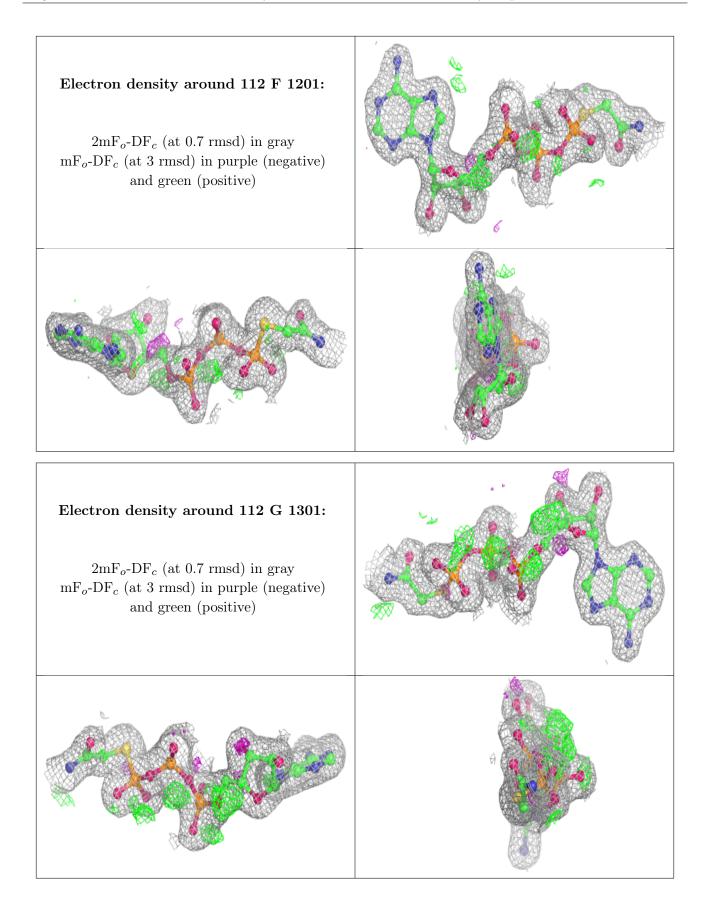
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	112	Е	1101	35/35	0.97	0.10	$15,\!21,\!28,\!30$	0
4	112	F	1201	35/35	0.97	0.10	20,24,27,30	0
4	112	G	1301	35/35	0.97	0.10	18,24,28,29	0
4	112	Н	1401	35/35	0.97	0.10	15,19,26,27	0
3	MG	D	1801	1/1	0.98	0.09	20,20,20,20	0
3	MG	С	1701	1/1	0.99	0.13	20,20,20,20	0
3	MG	А	1501	1/1	0.99	0.06	17,17,17,17	0
3	MG	В	1601	1/1	0.99	0.08	21,21,21,21	0

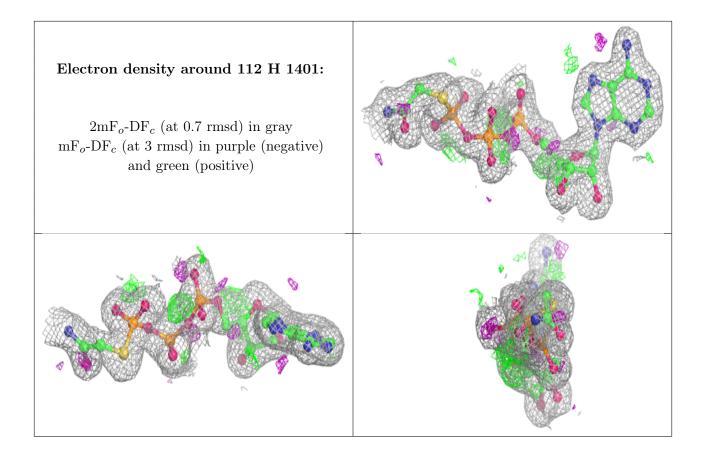
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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











## 6.5 Other polymers (i)

There are no such residues in this entry.

