



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:51 PM UTC

PDB ID : 9HD5 / pdb\_00009hd5  
Title : Crystal structure of CD73 (ecto-5'-nucleotidase) in complex with the AOPCP derivative PSB19427 in the closed state  
Authors : Strater, N.; Moschuetz, S.; Dobelmann, C.; Schmies, C.C.; Jacobson, K.A.; Muller, C.E.; Junker, A.  
Deposited on : 2024-11-11  
Resolution : 2.91 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.

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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

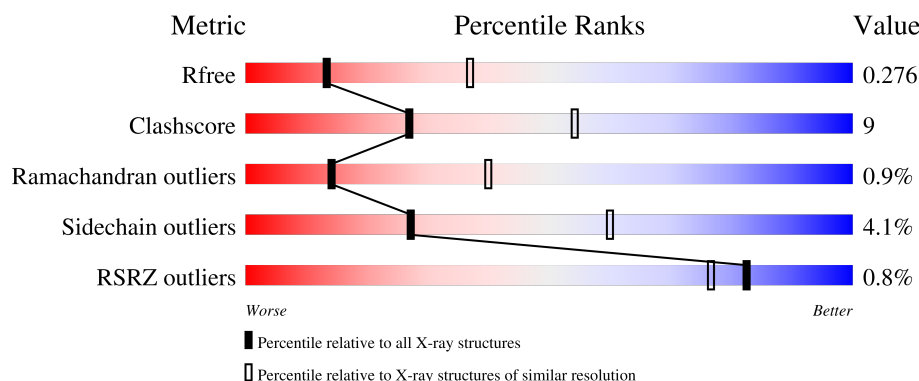
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	542	
1	B	542	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8195 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 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			3987	2535	676	757	19			
1	B	513	Total	C	N	O	S	0	1	0
			3995	2540	679	757	19			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP P21589
A	53	ASP	ASN	conflict	UNP P21589
A	311	ASP	ASN	conflict	UNP P21589
A	333	ASP	ASN	conflict	UNP P21589
A	403	ASP	ASN	conflict	UNP P21589
A	550	GLY	-	expression tag	UNP P21589
A	551	GLY	-	expression tag	UNP P21589
A	552	GLY	-	expression tag	UNP P21589
A	553	GLY	-	expression tag	UNP P21589
A	554	ALA	-	expression tag	UNP P21589
A	555	GLY	-	expression tag	UNP P21589
A	556	GLY	-	expression tag	UNP P21589
A	557	GLY	-	expression tag	UNP P21589
A	558	GLY	-	expression tag	UNP P21589
A	559	GLY	-	expression tag	UNP P21589
A	560	THR	-	expression tag	UNP P21589
A	561	LYS	-	expression tag	UNP P21589
A	562	HIS	-	expression tag	UNP P21589
A	563	HIS	-	expression tag	UNP P21589
A	564	HIS	-	expression tag	UNP P21589
A	565	HIS	-	expression tag	UNP P21589
A	566	HIS	-	expression tag	UNP P21589
A	567	HIS	-	expression tag	UNP P21589
B	26	MET	-	initiating methionine	UNP P21589
B	53	ASP	ASN	conflict	UNP P21589

*Continued on next page...*

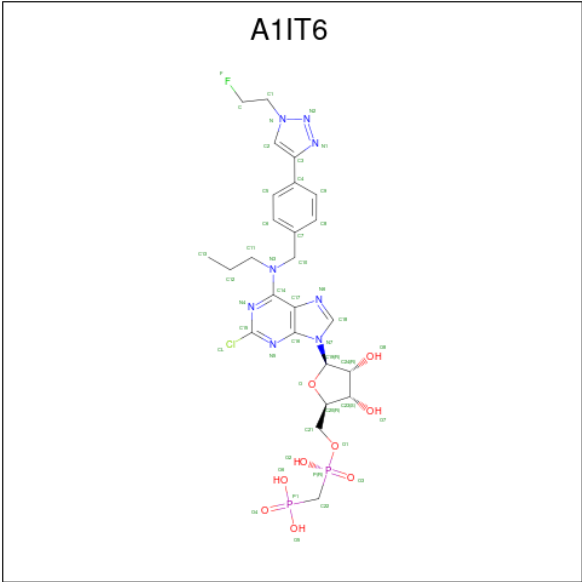
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	311	ASP	ASN	conflict	UNP P21589
B	333	ASP	ASN	conflict	UNP P21589
B	403	ASP	ASN	conflict	UNP P21589
B	550	GLY	-	expression tag	UNP P21589
B	551	GLY	-	expression tag	UNP P21589
B	552	GLY	-	expression tag	UNP P21589
B	553	GLY	-	expression tag	UNP P21589
B	554	ALA	-	expression tag	UNP P21589
B	555	GLY	-	expression tag	UNP P21589
B	556	GLY	-	expression tag	UNP P21589
B	557	GLY	-	expression tag	UNP P21589
B	558	GLY	-	expression tag	UNP P21589
B	559	GLY	-	expression tag	UNP P21589
B	560	THR	-	expression tag	UNP P21589
B	561	LYS	-	expression tag	UNP P21589
B	562	HIS	-	expression tag	UNP P21589
B	563	HIS	-	expression tag	UNP P21589
B	564	HIS	-	expression tag	UNP P21589
B	565	HIS	-	expression tag	UNP P21589
B	566	HIS	-	expression tag	UNP P21589
B	567	HIS	-	expression tag	UNP P21589

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is [(2 {R},3 {S},4 {R},5 {R})-5-[2-chloranyl-6-[[4-[1-(2-fluoranylethyl)-1,2,3-triazol-4-yl]phenyl]methyl-propyl-amino]purin-9-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl]methylphosphonic acid (CCD ID: A1IT6) (formula: C<sub>25</sub>H<sub>32</sub>ClFN<sub>8</sub>O<sub>9</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	P	0	0
			46	25	1	1	8	9	2		
3	B	1	Total	C	Cl	F	N	O	P	0	0
			46	25	1	1	8	9	2		

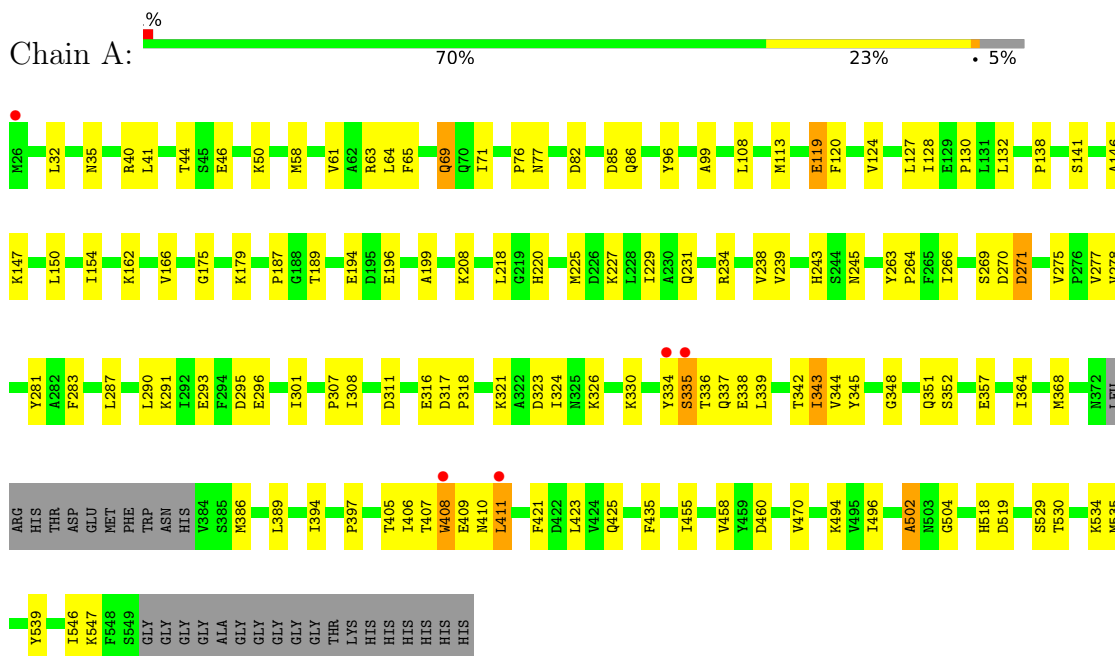
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	50	Total	O	0	0
			50	50		

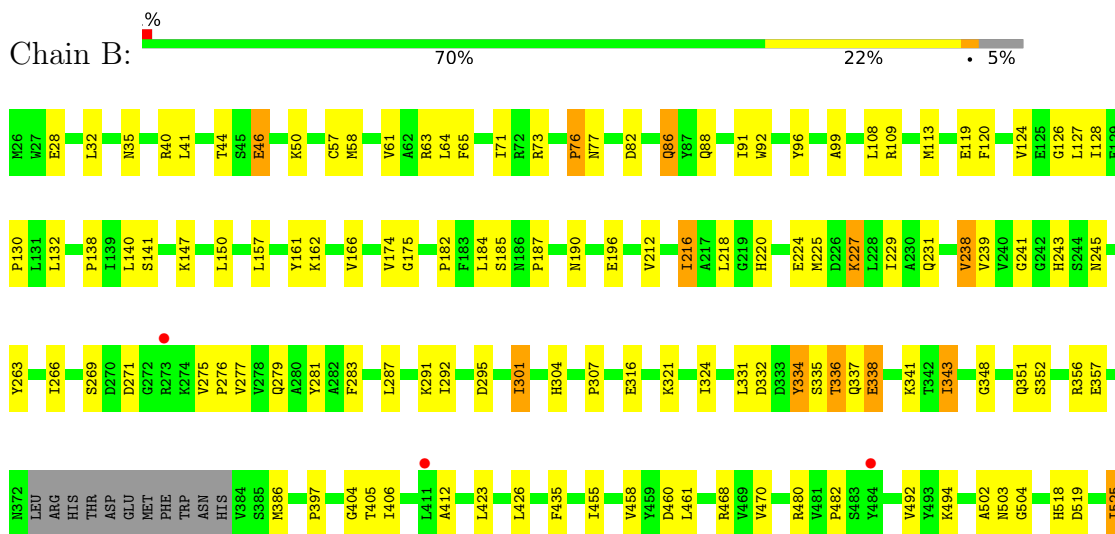
### 3 Residue-property plots

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: 5'-nucleotidase



#### • Molecule 1: 5'-nucleotidase



S529	I530	Y531	I532	Y539	I546	K547	F548	S549	GLY	GLY	GLY	GLY	ALA	GLY	GLY	GLY	GLY	GLY	GLY	THR	LYS	HIS	HIS	HIS	HIS	HIS	HIS
------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.64Å 233.37Å 54.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.91 49.37 – 2.91	Depositor EDS
% Data completeness (in resolution range)	63.9 (49.37-2.91) 63.8 (49.37-2.91)	Depositor EDS
$R_{merge}$	0.95	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.92 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3 (18-SEP-2020)	Depositor
R, $R_{free}$	0.190 , 0.273 0.208 , 0.276	Depositor DCC
$R_{free}$ test set	978 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.5	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 68.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8195	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.7415e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: A1IT6, 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	0.75	0/4067	1.18	16/5505 (0.3%)
1	B	0.74	0/4078	1.17	17/5519 (0.3%)
All	All	0.74	0/8145	1.17	33/11024 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ILE	N-CA-C	-8.57	102.47	110.53
1	A	227	LYS	N-CA-C	7.90	119.89	111.28
1	A	502	ALA	N-CA-C	-6.93	103.81	111.36
1	B	227	LYS	N-CA-C	6.91	118.81	111.28
1	A	271	ASP	CA-CB-CG	6.71	119.31	112.60
1	A	270	ASP	CA-C-N	6.70	130.16	120.38
1	A	270	ASP	C-N-CA	6.70	130.16	120.38
1	B	212	VAL	CA-C-N	6.06	129.52	120.31
1	B	212	VAL	C-N-CA	6.06	129.52	120.31
1	B	271	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	336	THR	CA-C-N	5.84	132.50	121.69
1	B	336	THR	C-N-CA	5.84	132.50	121.69
1	A	229	ILE	N-CA-CB	5.83	118.03	110.57
1	B	229	ILE	N-CA-C	-5.80	105.08	110.53
1	A	86	GLN	CA-C-N	5.75	130.94	121.39
1	A	86	GLN	C-N-CA	5.75	130.94	121.39
1	B	334	TYR	CA-C-N	5.63	132.29	121.54
1	B	334	TYR	C-N-CA	5.63	132.29	121.54
1	B	86	GLN	CA-C-N	5.60	129.21	120.75
1	B	86	GLN	C-N-CA	5.60	129.21	120.75
1	A	435	PHE	CA-CB-CG	-5.57	108.23	113.80
1	B	435	PHE	CA-CB-CG	-5.36	108.44	113.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	VAL	N-CA-C	5.31	113.71	107.77
1	B	301	ILE	N-CA-C	-5.29	106.53	111.45
1	B	126	GLY	CA-C-N	5.29	131.63	121.54
1	B	126	GLY	C-N-CA	5.29	131.63	121.54
1	B	504	GLY	N-CA-C	5.25	122.98	114.90
1	A	308	ILE	N-CA-C	5.22	115.12	108.12
1	A	504	GLY	N-CA-C	-5.15	107.94	115.72
1	A	408	TRP	CA-C-N	5.14	127.43	120.44
1	A	408	TRP	C-N-CA	5.14	127.43	120.44
1	B	266	ILE	N-CA-C	5.05	115.04	107.51
1	A	411	LEU	N-CA-C	-5.02	107.10	113.43

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	3987	0	3978	77	0
1	B	3995	0	3991	74	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	46	0	0	0	0
3	B	46	0	0	0	0
4	A	67	0	0	1	0
4	B	50	0	0	2	0
All	All	8195	0	7969	147	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 9.

All (147) 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:295:ASP:HB3	1:A:301:ILE:HD11	1.19	1.17

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:VAL:HG22	1:A:128:ILE:HD11	1.46	0.96
1:B:502:ALA:HB1	1:B:518:HIS:CD2	2.16	0.81
1:A:502:ALA:HB1	1:A:518:HIS:CD2	2.16	0.80
1:A:124:VAL:HG22	1:A:128:ILE:CD1	2.12	0.80
1:A:41:LEU:HA	1:A:61:VAL:HG13	1.65	0.79
1:B:224:GLU:HA	1:B:227:LYS:NZ	1.99	0.78
1:B:128:ILE:HA	1:B:132:LEU:HB2	1.66	0.76
1:A:336:THR:HG23	1:A:337:GLN:NE2	2.00	0.75
1:B:82:ASP:HB3	1:B:113:MET:HG3	1.69	0.73
1:A:82:ASP:HB3	1:A:113:MET:HG3	1.70	0.73
1:A:234:ARG:HG2	1:A:271:ASP:OD1	1.87	0.73
1:B:338:GLU:HB3	1:B:405:THR:HG23	1.70	0.73
1:B:224:GLU:HA	1:B:227:LYS:HZ3	1.55	0.71
1:A:344:VAL:CG1	1:B:482:PRO:HD3	2.20	0.71
1:A:124:VAL:HG21	1:A:150:LEU:HD11	1.72	0.69
1:B:494:LYS:NZ	4:B:701:HOH:O	2.06	0.69
1:A:389:LEU:HD21	1:A:394:ILE:HD11	1.76	0.68
1:A:344:VAL:HG13	1:B:482:PRO:HD3	1.76	0.68
1:A:96:TYR:HB3	1:A:99:ALA:HB3	1.78	0.66
1:B:40:ARG:HD2	1:B:44:THR:HG21	1.78	0.66
1:B:96:TYR:HB3	1:B:99:ALA:HB3	1.78	0.66
1:B:412:ALA:HA	1:B:525:ILE:HD11	1.78	0.65
1:A:120:PHE:HB3	1:A:187:PRO:HA	1.77	0.65
1:B:458:VAL:HG22	1:B:547:LYS:HB2	1.79	0.64
1:A:458:VAL:HG22	1:A:547:LYS:HB2	1.79	0.64
1:B:65:PHE:HZ	1:B:109[B]:ARG:HH11	1.47	0.63
1:A:40:ARG:HD2	1:A:44:THR:HG21	1.81	0.62
1:B:40:ARG:HG3	1:B:283:PHE:HB3	1.81	0.62
1:A:336:THR:HG23	1:A:337:GLN:CD	2.25	0.61
1:A:502:ALA:HB1	1:A:518:HIS:NE2	2.14	0.61
1:B:502:ALA:HB1	1:B:518:HIS:NE2	2.14	0.60
1:A:40:ARG:HG3	1:A:283:PHE:HB3	1.82	0.60
1:A:323:ASP:HA	1:A:326:LYS:HE2	1.83	0.60
1:B:65:PHE:HZ	1:B:109[B]:ARG:NH1	2.01	0.59
1:B:28:GLU:HG2	1:B:291:LYS:HE2	1.85	0.59
1:A:124:VAL:CG2	1:A:128:ILE:HD11	2.26	0.57
1:B:41:LEU:HA	1:B:61:VAL:HG13	1.85	0.57
1:A:138:PRO:HG3	1:A:162:LYS:HG2	1.86	0.57
1:A:64:LEU:HD11	1:A:287:LEU:HD13	1.87	0.56
1:B:357:GLU:HB2	1:B:546:ILE:HB	1.87	0.56
1:B:196:GLU:HB2	1:B:225:MET:HE3	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD11	1:B:287:LEU:HD13	1.88	0.55
1:A:146:ALA:CB	1:A:154:ILE:HD11	2.37	0.55
1:A:409:GLU:C	1:A:411:LEU:H	2.15	0.55
1:B:216:ILE:HB	1:B:238:VAL:HG13	1.89	0.55
1:B:231:GLN:HA	1:B:269:SER:HA	1.87	0.55
1:B:120:PHE:HB3	1:B:187:PRO:HA	1.89	0.55
1:A:61:VAL:HG23	1:A:324:ILE:HD11	1.90	0.54
1:B:161:TYR:HB3	1:B:174:VAL:HG12	1.90	0.54
1:A:344:VAL:HG11	1:B:482:PRO:HD3	1.90	0.53
1:B:65:PHE:HD1	1:B:108:LEU:HD23	1.72	0.53
1:B:138:PRO:HG3	1:B:162:LYS:HG2	1.89	0.53
1:A:175:GLY:HA2	1:A:218:LEU:O	2.09	0.53
1:B:32:LEU:HD21	1:B:71:ILE:HG21	1.90	0.53
1:A:65:PHE:O	1:A:69:GLN:HB2	2.09	0.52
1:B:76:PRO:HD2	4:B:711:HOH:O	2.09	0.52
1:B:124:VAL:HG21	1:B:150:LEU:HD21	1.91	0.52
1:B:182:PRO:HA	1:B:187:PRO:CG	2.40	0.52
1:A:208:LYS:HD2	4:A:734:HOH:O	2.08	0.52
1:A:32:LEU:HD21	1:A:71:ILE:HG21	1.92	0.52
1:A:61:VAL:CG2	1:A:324:ILE:HD11	2.40	0.52
1:A:502:ALA:CB	1:A:518:HIS:NE2	2.73	0.52
1:A:194:GLU:CD	1:A:199:ALA:HB2	2.34	0.52
1:B:295:ASP:HB3	1:B:301:ILE:HD11	1.90	0.52
1:B:502:ALA:CB	1:B:518:HIS:NE2	2.73	0.51
1:A:460:ASP:HB2	1:A:470:VAL:HG21	1.92	0.51
1:B:175:GLY:HA2	1:B:218:LEU:O	2.10	0.51
1:A:65:PHE:HD1	1:A:108:LEU:HD23	1.75	0.51
1:B:460:ASP:HB2	1:B:470:VAL:HG21	1.93	0.50
1:A:409:GLU:O	1:A:411:LEU:N	2.44	0.50
1:A:196:GLU:HB2	1:A:225:MET:HE3	1.92	0.50
1:A:220:HIS:CD2	1:A:243:HIS:ND1	2.80	0.50
1:A:231:GLN:HA	1:A:269:SER:HA	1.93	0.50
1:B:220:HIS:CD2	1:B:243:HIS:ND1	2.80	0.49
1:B:239:VAL:HB	1:B:277:VAL:HG22	1.93	0.49
1:A:278:VAL:HG11	1:A:290:LEU:HD22	1.95	0.49
1:A:407:THR:OG1	1:A:410:ASN:ND2	2.45	0.49
1:B:321:LYS:HA	1:B:324:ILE:HD12	1.95	0.48
1:A:321:LYS:HA	1:A:324:ILE:HD12	1.95	0.48
1:B:224:GLU:HA	1:B:227:LYS:HZ1	1.75	0.48
1:A:64:LEU:HD23	1:A:108:LEU:HD22	1.96	0.48
1:A:423:LEU:HD11	1:A:494:LYS:HG2	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ASP:O	1:B:336:THR:OG1	2.29	0.48
1:B:64:LEU:HD23	1:B:108:LEU:HD22	1.97	0.47
1:A:239:VAL:HB	1:A:277:VAL:HG22	1.96	0.46
1:A:85:ASP:CG	1:A:220:HIS:CE1	2.94	0.46
1:A:128:ILE:HA	1:A:132:LEU:HB2	1.98	0.46
1:A:263:TYR:CD2	1:A:307:PRO:HD3	2.50	0.46
1:A:535:MET:HA	1:A:535:MET:HE2	1.97	0.46
1:A:364:ILE:O	1:A:368:MET:HG3	2.15	0.46
1:B:263:TYR:CD2	1:B:307:PRO:HD3	2.51	0.46
1:B:147:LYS:O	1:B:190:ASN:HB3	2.15	0.46
1:B:140:LEU:HD21	1:B:162:LYS:HB2	1.97	0.46
1:B:343:ILE:HG13	1:B:539:TYR:HB3	1.97	0.46
1:A:119:GLU:HB3	1:A:127:LEU:HD13	1.97	0.46
1:B:423:LEU:HB3	1:B:519:ASP:HB2	1.97	0.45
1:A:423:LEU:HB3	1:A:519:ASP:HB2	1.97	0.45
1:A:351:GLN:H	1:A:351:GLN:CD	2.25	0.45
1:A:357:GLU:HB2	1:A:546:ILE:HB	1.97	0.45
1:B:351:GLN:H	1:B:351:GLN:CD	2.25	0.45
1:B:77:ASN:HB3	1:B:166:VAL:HG12	1.99	0.44
1:B:91:ILE:HG23	1:B:331:LEU:HD23	1.98	0.44
1:A:63:ARG:HA	1:A:316:GLU:HA	2.00	0.44
1:B:61:VAL:HG23	1:B:324:ILE:HD11	1.99	0.44
1:A:343:ILE:HG13	1:A:539:TYR:HB3	1.99	0.44
1:B:63:ARG:HA	1:B:316:GLU:HA	2.00	0.44
1:B:46:GLU:HG3	1:B:58:MET:HE1	2.00	0.43
1:B:86:GLN:HG2	1:B:113:MET:HE3	1.99	0.43
1:A:77:ASN:HB3	1:A:166:VAL:HG12	2.00	0.43
1:A:534:LYS:HD3	1:A:535:MET:HE3	1.99	0.43
1:A:425:GLN:HG2	1:A:494:LYS:HG3	2.00	0.43
1:B:341:LYS:HA	1:B:404:GLY:O	2.18	0.43
1:A:348:GLY:H	1:A:397:PRO:HB3	1.83	0.43
1:A:334:TYR:O	1:A:335:SER:HB3	2.19	0.43
1:B:291:LYS:HG2	1:B:304:HIS:CE1	2.54	0.43
1:B:245:ASN:HA	1:B:281:TYR:O	2.19	0.43
1:B:335:SER:C	1:B:337:GLN:H	2.27	0.43
1:B:386:MET:HB3	1:B:455:ILE:HD11	2.00	0.43
1:A:323:ASP:HA	1:A:326:LYS:CE	2.46	0.42
1:A:339:LEU:HD11	1:A:408:TRP:CD2	2.54	0.42
1:B:128:ILE:HG23	1:B:157:LEU:CD2	2.49	0.42
1:B:348:GLY:H	1:B:397:PRO:HB3	1.84	0.42
1:A:345:TYR:CD1	1:B:480:ARG:NH1	2.87	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:MET:HE3	1:A:421:PHE:HB3	2.01	0.42
1:A:336:THR:HG23	1:A:337:GLN:HE22	1.78	0.42
1:A:264:PRO:HG2	1:A:266:ILE:HD11	2.02	0.42
1:A:338:GLU:HG3	1:A:405:THR:HG23	2.00	0.42
1:B:406:ILE:HG21	1:B:532:ILE:HD13	2.02	0.42
1:A:342:THR:HB	1:A:406:ILE:HD11	2.02	0.42
1:B:28:GLU:OE2	1:B:291:LYS:NZ	2.48	0.41
1:B:185:SER:O	1:B:187:PRO:HD3	2.20	0.41
1:B:92:TRP:HA	1:B:331:LEU:HD21	2.02	0.41
1:B:224:GLU:CD	1:B:227:LYS:HZ1	2.28	0.41
1:B:461:LEU:HA	1:B:468:ARG:HD2	2.01	0.41
1:A:58:MET:HG2	1:A:311:ASP:HA	2.01	0.41
1:A:386:MET:HB3	1:A:455:ILE:HD11	2.02	0.41
1:A:296:GLU:H	1:A:296:GLU:CD	2.29	0.41
1:A:368:MET:HE2	1:A:496:ILE:HG23	2.01	0.41
1:B:91:ILE:HD11	1:B:334:TYR:CG	2.56	0.41
1:B:224:GLU:CA	1:B:227:LYS:HZ3	2.31	0.41
1:B:241:GLY:O	1:B:279:GLN:HG3	2.21	0.41
1:A:317:ASP:HA	1:A:318:PRO:HD3	1.92	0.41
1:B:275:VAL:HA	1:B:276:PRO:HD3	1.93	0.41
1:A:245:ASN:HA	1:A:281:TYR:O	2.21	0.40
1:A:409:GLU:C	1:A:411:LEU:N	2.75	0.40
1:B:224:GLU:CA	1:B:227:LYS:NZ	2.79	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/542 (94%)	472 (93%)	33 (6%)	4 (1%)	16	43
1	B	510/542 (94%)	474 (93%)	31 (6%)	5 (1%)	12	37

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1019/1084 (94%)	946 (93%)	64 (6%)	9 (1%)	14	40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	SER
1	B	88	GLN
1	B	127	LEU
1	B	141	SER
1	A	141	SER
1	B	130	PRO
1	A	130	PRO
1	B	76	PRO
1	A	76	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	441/460 (96%)	425 (96%)	16 (4%)	31	63
1	B	442/460 (96%)	422 (96%)	20 (4%)	24	56
All	All	883/920 (96%)	847 (96%)	36 (4%)	27	60

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	46	GLU
1	A	50	LYS
1	A	69	GLN
1	A	119	GLU
1	A	147	LYS
1	A	179	LYS
1	A	189	THR
1	A	238	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	291	LYS
1	A	293	GLU
1	A	330	LYS
1	A	343	ILE
1	A	352	SER
1	A	529	SER
1	A	530	THR
1	B	35	ASN
1	B	46	GLU
1	B	50	LYS
1	B	57	CYS
1	B	73	ARG
1	B	119	GLU
1	B	184	LEU
1	B	216	ILE
1	B	238	VAL
1	B	292	ILE
1	B	338	GLU
1	B	343	ILE
1	B	352	SER
1	B	356	ARG
1	B	426	LEU
1	B	492	VAL
1	B	503	ASN
1	B	525	ILE
1	B	529	SER
1	B	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	ASN
1	A	370	ASN
1	A	410	ASN
1	A	425	GLN
1	A	437	HIS
1	A	499	ASN
1	A	523	GLN
1	A	526	ASN
1	B	304	HIS
1	B	370	ASN
1	B	523	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\# Z  > 2$
3	A1IT6	B	603	2	47,50,50	0.59	3 (6%)	66,74,74	0.57	2 (3%)
3	A1IT6	A	603	2	47,50,50	0.60	3 (6%)	66,74,74	0.58	2 (3%)

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
3	A1IT6	B	603	2	-	3/34/50/50	0/5/5/5
3	A1IT6	A	603	2	-	3/34/50/50	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	603	A1IT6	C-C1	2.58	1.58	1.48

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	A1IT6	C-C1	2.42	1.58	1.48
3	B	603	A1IT6	P-O2	-2.09	1.51	1.56
3	B	603	A1IT6	P-O3	2.06	1.56	1.51
3	A	603	A1IT6	P-O3	2.03	1.56	1.51
3	A	603	A1IT6	P-O2	-2.01	1.51	1.56

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	A1IT6	O2-P-C22	2.76	118.14	106.73
3	A	603	A1IT6	O2-P-C22	2.66	117.75	106.73
3	A	603	A1IT6	C15-N4-C14	2.41	117.79	110.98
3	B	603	A1IT6	C15-N4-C14	2.38	117.71	110.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

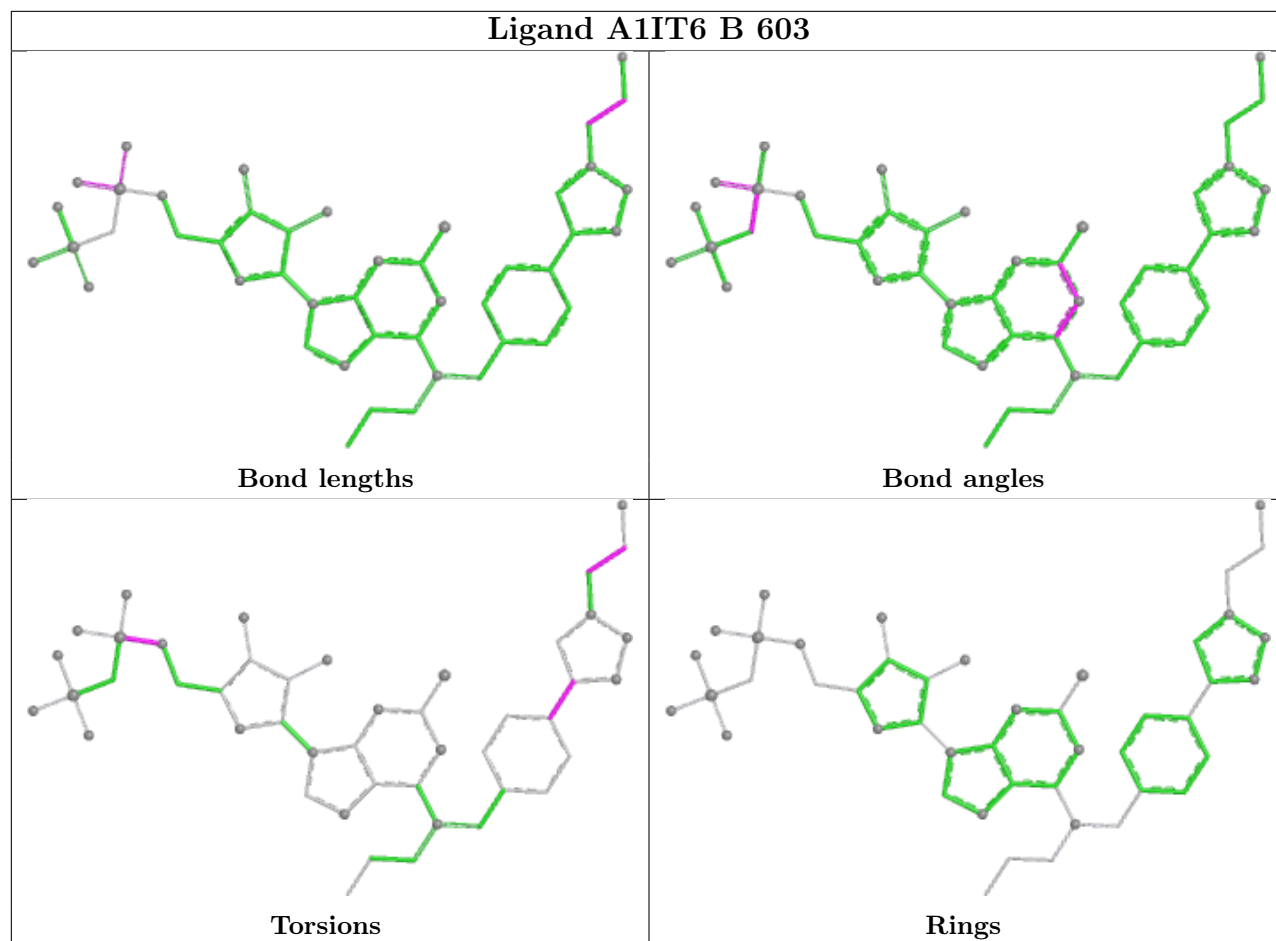
Mol	Chain	Res	Type	Atoms
3	A	603	A1IT6	C21-O1-P-C22
3	A	603	A1IT6	F-C-C1-N
3	B	603	A1IT6	C21-O1-P-C22
3	B	603	A1IT6	F-C-C1-N
3	B	603	A1IT6	C2-C3-C4-C9
3	A	603	A1IT6	P-C22-P1-O4

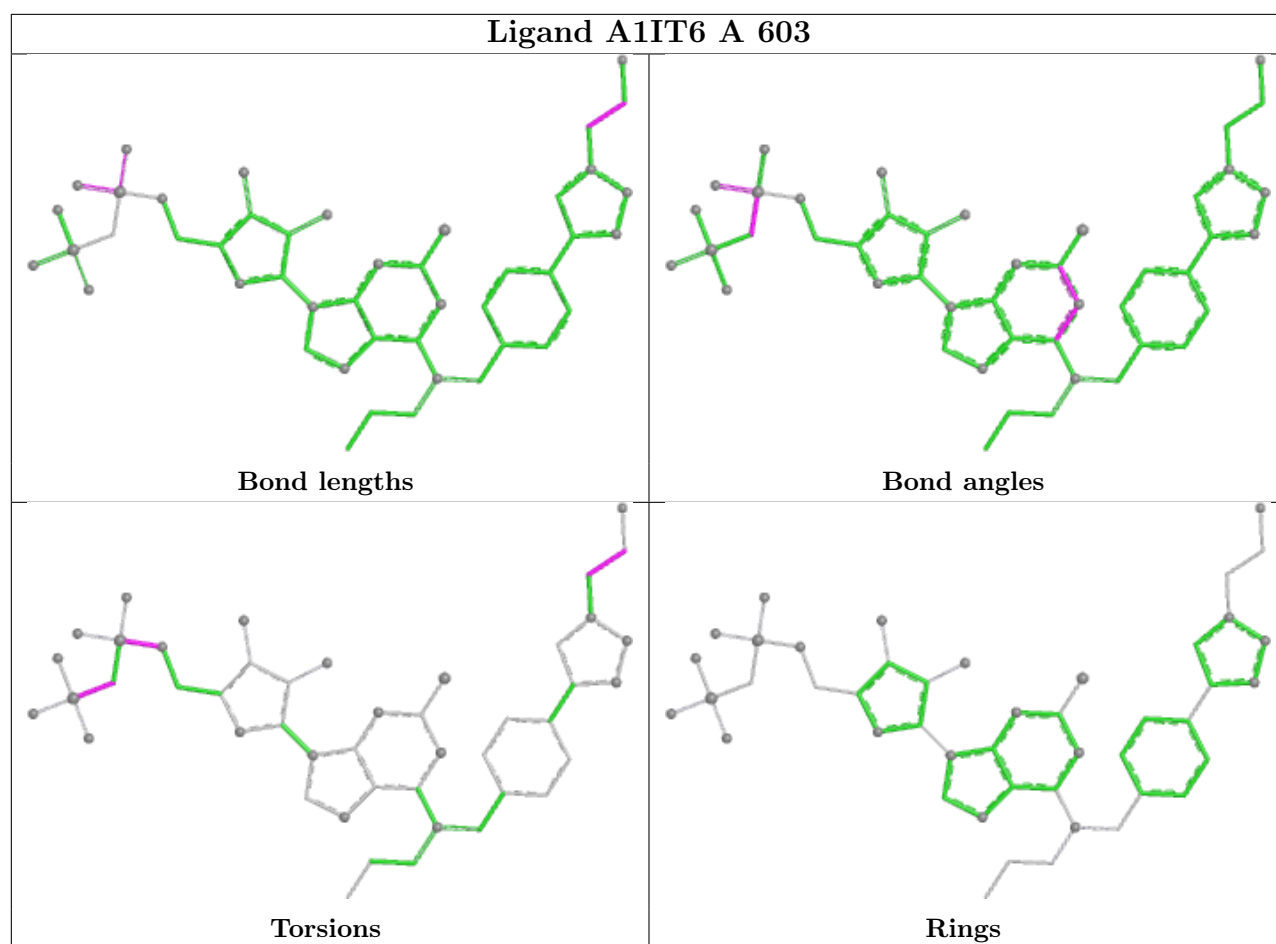
There are no ring outliers.

No monomer is involved in short contacts.

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.

## Ligand A1IT6 B 603





## 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	513/542 (94%)	-0.07	5 (0%)	79 72	23, 54, 78, 99	0
1	B	513/542 (94%)	0.07	3 (0%)	85 81	25, 60, 88, 97	1 (0%)
All	All	1026/1084 (94%)	-0.00	8 (0%)	82 76	23, 57, 86, 99	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	TRP	4.5
1	A	26	MET	2.6
1	A	334	TYR	2.4
1	A	411	LEU	2.4
1	B	484	TYR	2.3
1	B	411	LEU	2.3
1	B	273	ARG	2.2
1	A	335	SER	2.1

### 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 oligosaccharides 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,

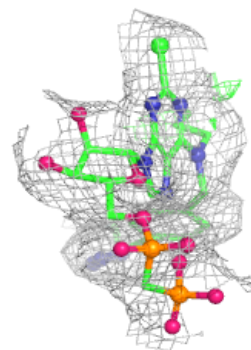
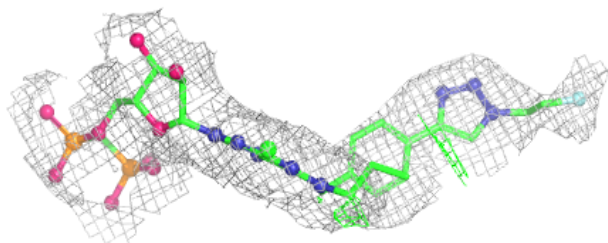
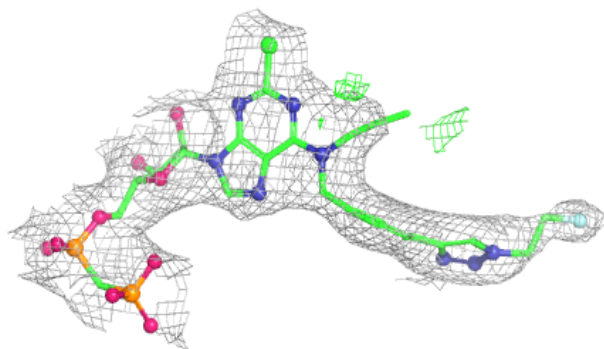
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1IT6	A	603	46/46	0.93	0.09	48,54,65,67	0
3	A1IT6	B	603	46/46	0.93	0.08	52,64,72,72	0
2	ZN	B	601	1/1	0.97	0.04	73,73,73,73	0
2	ZN	B	602	1/1	0.99	0.03	60,60,60,60	0
2	ZN	A	601	1/1	1.00	0.03	62,62,62,62	0
2	ZN	A	602	1/1	1.00	0.03	52,52,52,52	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.

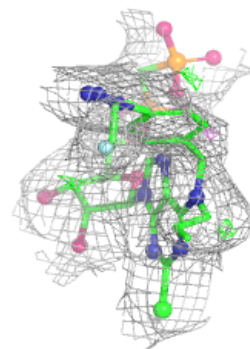
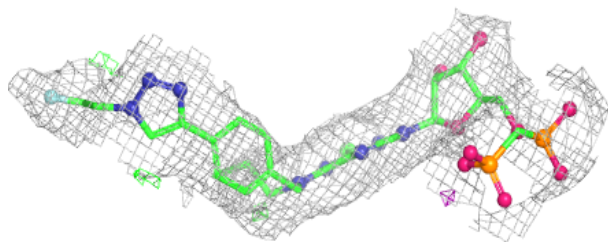
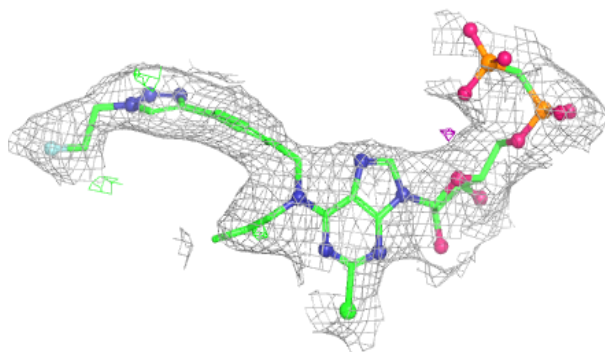
**Electron density around A1IT6 A 603:**

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



**Electron density around A1IT6 B 603:**

$2mF_o-DF_c$  (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.