



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 05:24 pm BST

PDB ID : 1G8H  
Title : ATP SULFURYLASE FROM S. CEREVISIAE: THE TERNARY PRODUCT  
COMPLEX WITH APS AND PPI  
Authors : Ullrich, T.C.; Blaesle, M.; Huber, R.  
Deposited on : 2000-11-17  
Resolution : 2.80 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 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 : 2.11  
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) : 2.11

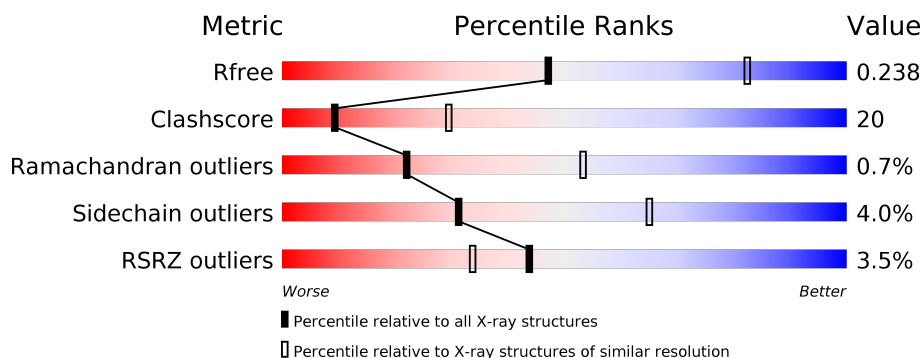
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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	511	<div> <div>4%</div> <div>66%</div> <div>31%</div> <div>.</div> </div>
1	B	511	<div> <div>3%</div> <div>65%</div> <div>32%</div> <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
5	MG	B	539	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 8917 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 SULFATE ADENYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4077	2598	707	767	5			
1	B	510	Total	C	N	O	S	0	0	0
			4077	2598	707	767	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	ARG	LYS	CONFLICT	UNP P08536
A	457	ASP	ASN	CONFLICT	UNP P08536
B	131	ARG	LYS	CONFLICT	UNP P08536
B	457	ASP	ASN	CONFLICT	UNP P08536

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Cd	0	0
			5	5		
2	A	6	Total	Cd	0	0
			6	6		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Ca	0	0
			3	3		
3	A	3	Total	Ca	0	0
			3	3		

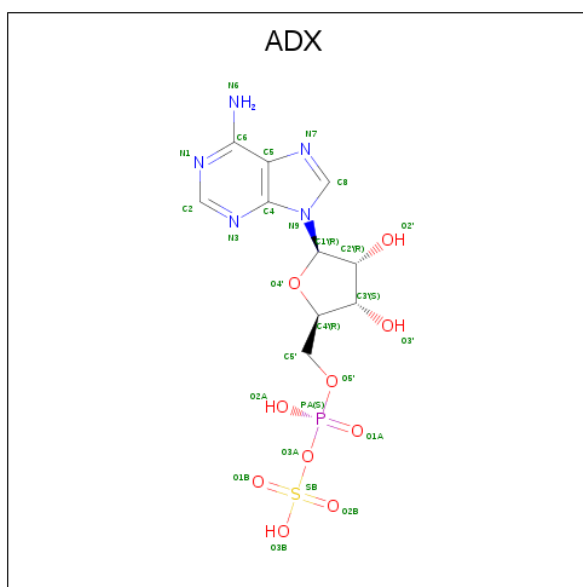
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	6	Total	Na	0	0
			6	6		
4	A	6	Total	Na	0	0
			6	6		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

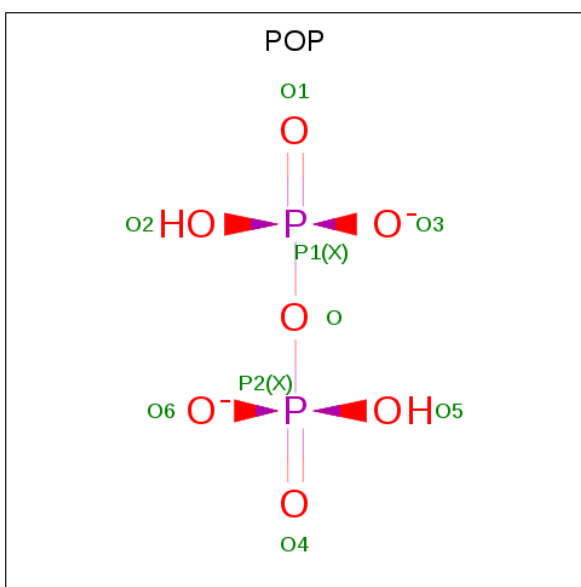
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is ADENOSINE-5'-PHOSPHOSULFATE (three-letter code: ADX) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>10</sub>PS).



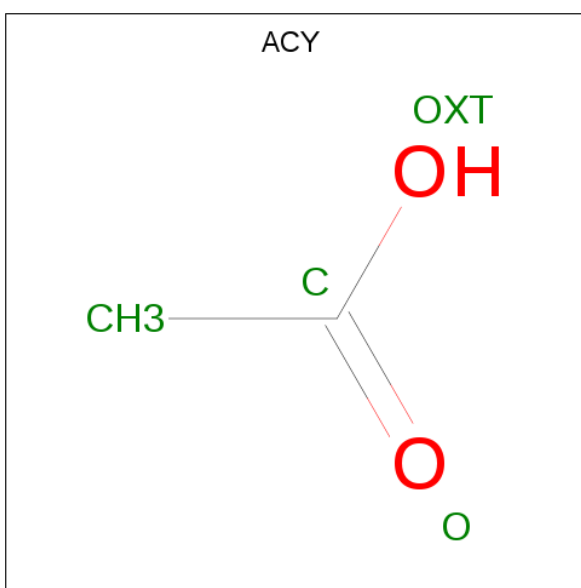
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		
6	B	1	Total	C	N	O	P	S	0	0
			27	10	5	10	1	1		

- Molecule 7 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			9	7	2		
7	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 8 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

*Continued on next page...*

*Continued from previous page...*

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

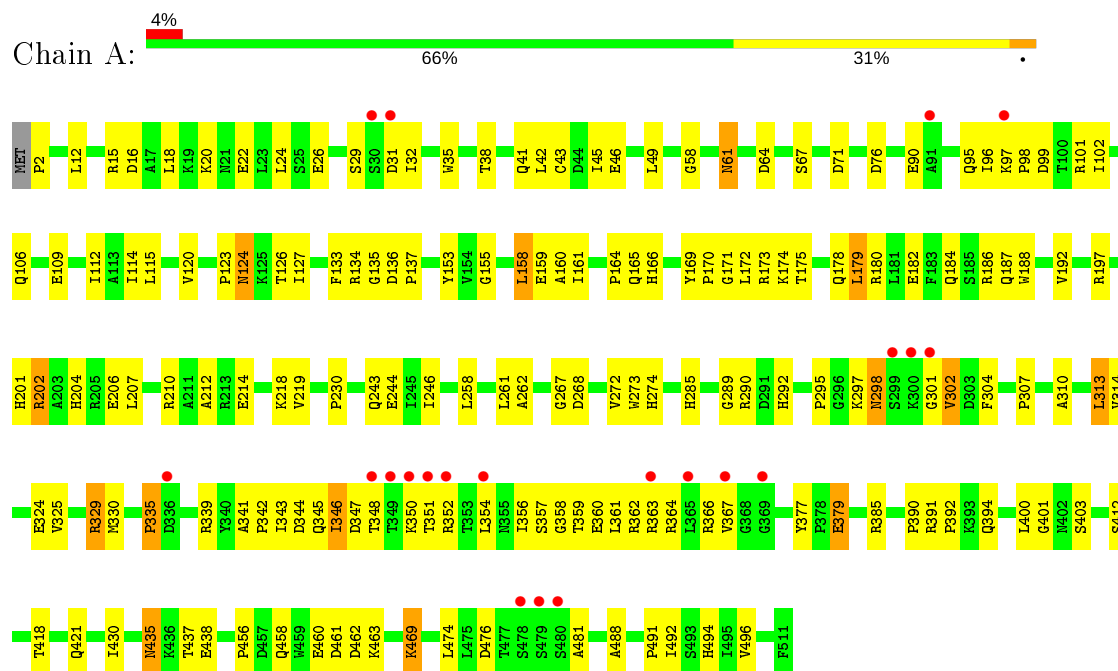
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	301	Total O 301 301	0	0
9	B	299	Total O 299 299	0	0

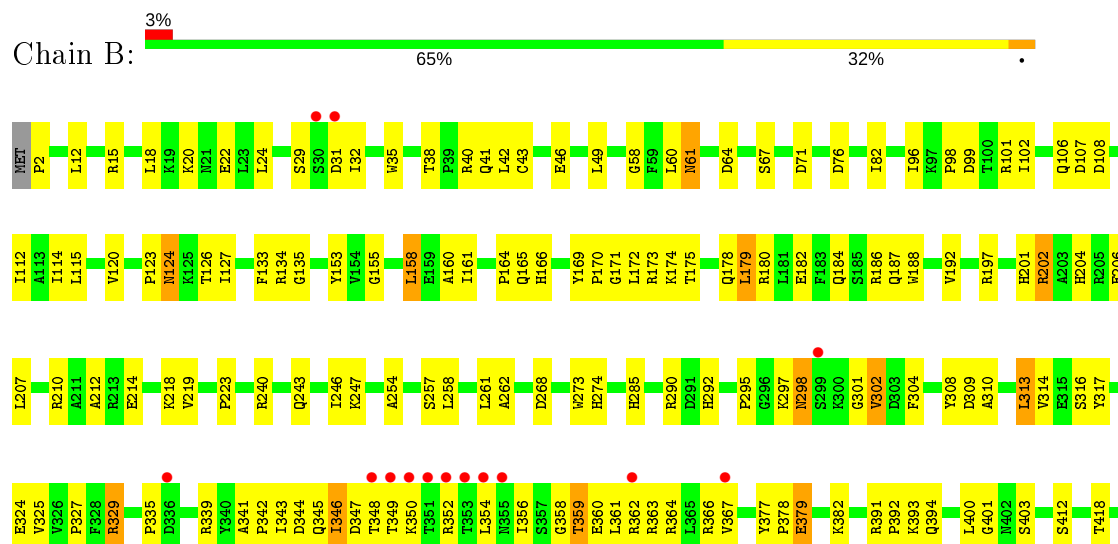
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

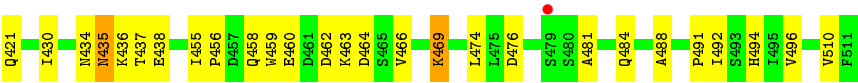
#### • Molecule 1: SULFATE ADENYLYLTRANSFERASE



#### • Molecule 1: SULFATE ADENYLYLTRANSFERASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	186.01Å 186.01Å 223.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.87 – 2.80 24.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (24.87-2.80) 95.4 (24.87-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.80Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.194 , 0.245 0.186 , 0.238	Depositor DCC
$R_{free}$ test set	1801 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 62.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.018 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.012 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.46% 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: MG, NA, CA, ADX, CD, POP, ACY

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	0.37	0/4173	0.62	1/5670 (0.0%)
1	B	0.38	0/4173	0.62	1/5670 (0.0%)
All	All	0.37	0/8346	0.62	2/11340 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	GLY	N-CA-C	5.42	126.65	113.10
1	A	135	GLY	N-CA-C	5.20	126.10	113.10

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4077	0	4033	159	0
1	B	4077	0	4033	165	0
2	A	6	0	0	0	1
2	B	5	0	0	0	1
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	6	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	27	0	13	5	0
6	B	27	0	13	0	0
7	A	9	0	0	1	0
7	B	9	0	0	0	0
8	A	32	0	24	2	0
8	B	28	0	21	2	0
9	A	301	0	0	14	0
9	B	299	0	0	14	0
All	All	8917	0	8137	326	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 20.

All (326) 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:329:ARG:HD2	1:A:329:ARG:H	1.06	1.08
1:B:329:ARG:H	1:B:329:ARG:HD2	1.06	1.06
1:A:106:GLN:HE22	1:A:165:GLN:H	1.12	0.98
1:A:58:GLY:HA2	1:A:158:LEU:HD22	1.48	0.95
1:B:106:GLN:HE22	1:B:165:GLN:H	1.09	0.94
1:A:362:ARG:NH1	1:A:362:ARG:HB2	1.86	0.91
1:B:362:ARG:NH1	1:B:362:ARG:HB2	1.86	0.90
1:B:469:LYS:N	1:B:469:LYS:HE2	1.86	0.90
1:B:329:ARG:N	1:B:329:ARG:HD2	1.87	0.90
1:B:469:LYS:H	1:B:469:LYS:HE2	1.35	0.89
1:A:329:ARG:HD2	1:A:329:ARG:N	1.87	0.89
1:B:58:GLY:HA2	1:B:158:LEU:HD22	1.55	0.88
1:A:469:LYS:N	1:A:469:LYS:HE2	1.94	0.83
1:A:61:ASN:ND2	1:A:64:ASP:H	1.77	0.83
1:B:329:ARG:CD	1:B:329:ARG:H	1.92	0.81
1:A:469:LYS:H	1:A:469:LYS:HE2	1.45	0.80
1:B:412:SER:HB3	1:B:430:ILE:HD12	1.64	0.79
1:A:175:THR:H	1:A:178:GLN:HE21	1.27	0.78
1:A:348:THR:HG21	1:A:350:LYS:HZ2	1.48	0.78
1:B:61:ASN:ND2	1:B:64:ASP:H	1.82	0.78
1:A:412:SER:HB3	1:A:430:ILE:HD12	1.68	0.76
1:B:210:ARG:O	1:B:214:GLU:HG2	1.85	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:THR:H	1:B:178:GLN:HE21	1.31	0.74
1:A:61:ASN:HD21	1:A:64:ASP:H	1.35	0.74
1:A:314:VAL:CG1	1:A:325:VAL:HG21	2.18	0.73
1:B:35:TRP:HE1	1:B:41:GLN:HE22	1.36	0.73
1:A:295:PRO:HG2	1:A:304:PHE:CD1	2.24	0.73
1:B:49:LEU:HD22	1:B:160:ALA:HB2	1.71	0.72
1:A:210:ARG:O	1:A:214:GLU:HG2	1.89	0.72
1:A:96:ILE:HG21	1:A:102:ILE:HD11	1.70	0.71
1:A:49:LEU:HD22	1:A:160:ALA:HB2	1.72	0.71
1:B:314:VAL:CG1	1:B:325:VAL:HG21	2.20	0.71
1:A:35:TRP:HE1	1:A:41:GLN:HE22	1.38	0.71
1:B:295:PRO:HG2	1:B:304:PHE:CD1	2.27	0.70
1:B:290:ARG:HD2	9:B:1001:HOH:O	1.92	0.70
1:A:61:ASN:C	1:A:61:ASN:HD22	1.93	0.69
1:B:469:LYS:H	1:B:469:LYS:CE	2.02	0.69
1:B:96:ILE:HG21	1:B:102:ILE:HD11	1.73	0.69
1:A:201:HIS:H	1:A:204:HIS:HD2	1.38	0.69
1:B:98:PRO:O	1:B:99:ASP:HB2	1.91	0.69
1:A:98:PRO:O	1:A:99:ASP:HB2	1.93	0.69
1:A:175:THR:H	1:A:178:GLN:NE2	1.90	0.69
1:B:201:HIS:H	1:B:204:HIS:HD2	1.41	0.68
1:B:314:VAL:HG11	1:B:325:VAL:HG21	1.76	0.67
1:A:362:ARG:CZ	1:A:362:ARG:HB2	2.23	0.67
1:A:366:ARG:HH21	1:A:366:ARG:HG2	1.58	0.67
1:A:352:ARG:HB3	1:A:352:ARG:NH2	2.10	0.67
1:B:61:ASN:HD22	1:B:61:ASN:C	1.97	0.67
1:B:362:ARG:HB2	1:B:362:ARG:CZ	2.22	0.67
1:A:329:ARG:CD	1:A:329:ARG:H	1.92	0.67
1:A:352:ARG:HA	9:A:649:HOH:O	1.95	0.66
1:B:166:HIS:HD2	9:B:646:HOH:O	1.78	0.66
1:A:298:ASN:C	1:A:298:ASN:HD22	1.98	0.66
1:B:366:ARG:HH21	1:B:366:ARG:HG2	1.60	0.66
1:B:61:ASN:HD21	1:B:64:ASP:H	1.44	0.66
1:A:67:SER:O	1:A:71:ASP:HB2	1.95	0.66
1:A:58:GLY:HA2	1:A:158:LEU:CD2	2.23	0.66
1:B:175:THR:H	1:B:178:GLN:NE2	1.93	0.65
1:B:247:LYS:HE3	9:B:1031:HOH:O	1.97	0.65
1:A:124:ASN:HD21	1:A:126:THR:HB	1.62	0.65
1:B:67:SER:O	1:B:71:ASP:HB2	1.96	0.65
1:B:352:ARG:NH2	1:B:352:ARG:HB3	2.11	0.65
1:A:314:VAL:HG11	1:A:325:VAL:HG21	1.79	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:HIS:H	1:B:204:HIS:CD2	2.15	0.64
1:A:243:GLN:O	1:A:246:ILE:HG22	1.98	0.64
1:A:469:LYS:CE	1:A:469:LYS:H	2.09	0.63
1:B:348:THR:HG21	1:B:350:LYS:HZ2	1.64	0.63
1:B:243:GLN:O	1:B:246:ILE:HG22	1.99	0.62
1:A:201:HIS:H	1:A:204:HIS:CD2	2.17	0.62
1:B:363:ARG:O	1:B:367:VAL:HG13	2.00	0.62
1:B:298:ASN:C	1:B:298:ASN:HD22	2.03	0.62
1:A:166:HIS:HD2	9:A:705:HOH:O	1.83	0.61
1:A:169:TYR:N	1:A:170:PRO:HD3	2.15	0.61
1:B:435:ASN:HD21	1:B:460:GLU:HB2	1.66	0.61
1:A:363:ARG:O	1:A:367:VAL:HG13	2.01	0.61
1:A:351:THR:HG21	9:A:1192:HOH:O	2.00	0.60
1:A:335:PRO:HG3	1:A:354:LEU:HD12	1.83	0.60
1:B:298:ASN:HD21	1:B:302:VAL:HG13	1.65	0.60
1:B:124:ASN:HD21	1:B:126:THR:HB	1.66	0.60
1:B:180:ARG:O	1:B:184:GLN:HG3	2.02	0.60
1:B:362:ARG:HH11	1:B:362:ARG:CB	2.15	0.60
1:A:2:PRO:HD2	9:A:1105:HOH:O	2.01	0.60
1:A:20:LYS:HB3	8:A:550:ACY:H2	1.84	0.59
1:A:364:ARG:HA	1:A:367:VAL:HG22	1.84	0.59
1:B:115:LEU:HD23	1:B:158:LEU:HD13	1.85	0.59
1:B:188:TRP:CE2	1:B:218:LYS:HG3	2.37	0.59
1:A:352:ARG:HH21	1:A:352:ARG:CB	2.15	0.59
1:B:335:PRO:HD2	1:B:352:ARG:O	2.01	0.59
1:B:364:ARG:HA	1:B:367:VAL:HG22	1.84	0.59
1:B:382:LYS:HD3	9:B:770:HOH:O	2.02	0.59
1:B:172:LEU:N	1:B:172:LEU:HD12	2.17	0.59
1:B:362:ARG:NH1	1:B:362:ARG:CB	2.63	0.59
1:B:240:ARG:HD2	9:B:878:HOH:O	2.03	0.59
1:A:362:ARG:HH11	1:A:362:ARG:CB	2.16	0.58
1:A:46:GLU:HB2	1:A:164:PRO:HD2	1.84	0.58
1:A:362:ARG:NH1	1:A:362:ARG:CB	2.64	0.58
1:A:385:ARG:HA	9:A:760:HOH:O	2.02	0.58
1:A:435:ASN:HD21	1:A:460:GLU:HB2	1.69	0.58
1:B:46:GLU:HB2	1:B:164:PRO:HD2	1.85	0.58
1:A:180:ARG:O	1:A:184:GLN:HG3	2.04	0.58
1:A:362:ARG:HH11	1:A:362:ARG:HB2	1.64	0.58
1:B:169:TYR:N	1:B:170:PRO:HD3	2.19	0.57
1:B:352:ARG:CB	1:B:352:ARG:HH21	2.16	0.57
1:A:348:THR:C	1:A:350:LYS:H	2.08	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ARG:NH1	1:B:114:ILE:HG21	2.20	0.57
1:B:335:PRO:HG3	1:B:354:LEU:HD12	1.87	0.57
1:A:356:ILE:HG23	1:A:360:GLU:HG3	1.86	0.56
1:A:363:ARG:O	1:A:367:VAL:HG22	2.05	0.56
1:A:329:ARG:HD3	1:A:342:PRO:HB3	1.87	0.56
1:A:438:GLU:HG2	9:A:1100:HOH:O	2.03	0.56
1:B:298:ASN:ND2	1:B:302:VAL:HG13	2.19	0.56
1:B:348:THR:C	1:B:350:LYS:H	2.08	0.56
1:B:348:THR:HG21	1:B:350:LYS:NZ	2.20	0.56
1:A:335:PRO:HD2	1:A:352:ARG:O	2.05	0.56
1:B:329:ARG:HG2	1:B:344:ASP:HB3	1.88	0.56
1:B:207:LEU:HD23	1:B:207:LEU:C	2.27	0.56
1:A:115:LEU:HD23	1:A:158:LEU:HD13	1.88	0.55
1:A:172:LEU:HD12	1:A:172:LEU:N	2.20	0.55
1:B:58:GLY:HA2	1:B:158:LEU:CD2	2.33	0.55
1:A:202:ARG:HH21	1:A:202:ARG:HG3	1.71	0.55
1:A:357:SER:HB2	9:A:755:HOH:O	2.06	0.55
1:A:298:ASN:HD21	1:A:302:VAL:HG13	1.71	0.55
1:B:20:LYS:HB3	8:B:560:ACY:H2	1.89	0.55
1:B:274:HIS:ND1	1:B:292:HIS:HE1	2.05	0.54
1:A:366:ARG:HG3	1:A:394:GLN:HE22	1.71	0.54
1:B:356:ILE:HG23	1:B:360:GLU:HG3	1.89	0.54
1:A:38:THR:H	1:A:41:GLN:NE2	2.05	0.53
1:B:178:GLN:O	1:B:182:GLU:HG2	2.07	0.53
1:A:329:ARG:HG2	1:A:344:ASP:HB3	1.89	0.53
1:B:329:ARG:HD3	1:B:342:PRO:HB3	1.91	0.53
1:A:346:ILE:HG13	1:A:347:ASP:N	2.24	0.53
1:B:352:ARG:HB3	1:B:352:ARG:HH21	1.71	0.53
1:B:38:THR:H	1:B:41:GLN:NE2	2.06	0.53
1:A:437:THR:HG22	1:A:463:LYS:HD3	1.91	0.53
1:A:298:ASN:ND2	1:A:302:VAL:HG13	2.24	0.53
1:A:352:ARG:HH21	1:A:352:ARG:HB3	1.71	0.53
1:A:289:GLY:HA3	6:A:635:ADX:N3	2.24	0.53
1:A:462:ASP:OD1	1:A:463:LYS:HG3	2.09	0.52
1:A:274:HIS:ND1	1:A:292:HIS:HE1	2.07	0.52
1:B:362:ARG:HB2	1:B:362:ARG:HH11	1.65	0.52
1:A:343:ILE:HD12	1:A:346:ILE:HD11	1.90	0.52
1:A:400:LEU:HG	1:A:456:PRO:HA	1.92	0.52
1:A:22:GLU:OE2	1:A:22:GLU:N	2.36	0.52
1:B:61:ASN:HA	1:B:155:GLY:HA3	1.91	0.52
1:A:61:ASN:HA	1:A:155:GLY:HA3	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ASP:HB3	9:B:704:HOH:O	2.11	0.51
1:B:363:ARG:O	1:B:367:VAL:HG22	2.10	0.51
1:A:207:LEU:HD23	1:A:207:LEU:C	2.30	0.51
1:B:343:ILE:HD12	1:B:346:ILE:HD11	1.92	0.51
1:B:437:THR:HG22	1:B:463:LYS:HD3	1.92	0.50
1:A:391:ARG:N	1:A:392:PRO:HD2	2.26	0.50
1:B:366:ARG:HG3	1:B:394:GLN:HE22	1.77	0.50
1:A:348:THR:HG21	1:A:350:LYS:NZ	2.22	0.50
1:A:101:ARG:NH1	1:A:114:ILE:HG21	2.25	0.50
1:B:106:GLN:NE2	1:B:165:GLN:H	1.94	0.50
1:A:173:ARG:HG2	1:A:173:ARG:HH21	1.77	0.50
6:A:635:ADX:N7	7:A:637:POP:O6	2.45	0.49
1:A:298:ASN:C	1:A:298:ASN:ND2	2.65	0.49
1:B:346:ILE:HG13	1:B:347:ASP:N	2.27	0.49
1:B:510:VAL:HA	9:B:841:HOH:O	2.11	0.49
1:B:469:LYS:CD	1:B:469:LYS:H	2.25	0.49
1:A:285:HIS:HA	1:A:324:GLU:O	2.12	0.49
1:B:123:PRO:HG3	1:B:153:TYR:CE1	2.47	0.49
1:A:12:LEU:HD22	1:A:15:ARG:CZ	2.43	0.49
1:A:346:ILE:HG13	1:A:347:ASP:H	1.78	0.49
1:A:358:GLY:N	9:A:755:HOH:O	2.39	0.49
1:A:469:LYS:CD	1:A:469:LYS:H	2.25	0.49
1:A:347:ASP:CG	1:A:348:THR:H	2.15	0.49
1:B:124:ASN:HD22	1:B:127:ILE:H	1.60	0.49
1:A:178:GLN:O	1:A:182:GLU:HG2	2.12	0.48
1:B:133:PHE:O	1:B:134:ARG:HB2	2.13	0.48
1:B:171:GLY:O	1:B:174:LYS:HE2	2.13	0.48
1:B:401:GLY:HA3	1:B:476:ASP:OD1	2.12	0.48
1:A:345:GLN:O	1:A:346:ILE:HG23	2.12	0.48
1:A:401:GLY:HA3	1:A:476:ASP:OD1	2.13	0.48
1:A:29:SER:O	1:A:32:ILE:HG22	2.14	0.48
1:A:346:ILE:CG1	1:A:347:ASP:H	2.26	0.48
1:A:292:HIS:CD2	6:A:635:ADX:O3'	2.67	0.48
1:B:179:LEU:O	1:B:182:GLU:HB2	2.13	0.48
1:B:462:ASP:OD1	1:B:463:LYS:HG3	2.13	0.48
1:B:2:PRO:HD2	9:B:658:HOH:O	2.13	0.48
1:B:391:ARG:N	1:B:392:PRO:HD2	2.28	0.48
1:B:435:ASN:HD21	1:B:460:GLU:CB	2.27	0.48
1:A:124:ASN:HD22	1:A:124:ASN:C	2.17	0.48
1:B:12:LEU:HD22	1:B:15:ARG:CZ	2.43	0.48
1:B:438:GLU:HG2	9:B:949:HOH:O	2.13	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLU:N	1:B:22:GLU:OE2	2.30	0.47
1:A:461:ASP:HB3	9:A:851:HOH:O	2.13	0.47
1:B:124:ASN:HD22	1:B:124:ASN:C	2.17	0.47
1:A:188:TRP:CE2	1:A:218:LYS:HG3	2.48	0.47
1:B:202:ARG:HG3	1:B:202:ARG:HH21	1.79	0.47
1:B:476:ASP:HB3	1:B:481:ALA:HB2	1.97	0.47
1:A:43:CYS:CB	1:A:262:ALA:HB2	2.45	0.47
1:A:173:ARG:NH2	1:A:173:ARG:HG2	2.30	0.47
1:A:347:ASP:CG	1:A:348:THR:N	2.68	0.47
1:B:223:PRO:HD2	1:B:257:SER:O	2.14	0.47
1:A:435:ASN:HD21	1:A:460:GLU:CB	2.28	0.47
1:B:298:ASN:HD21	1:B:302:VAL:CG1	2.28	0.47
1:B:43:CYS:CB	1:B:262:ALA:HB2	2.45	0.47
1:B:285:HIS:HA	1:B:324:GLU:O	2.14	0.47
1:A:202:ARG:HG2	1:A:377:TYR:CE1	2.50	0.47
1:B:297:LYS:HD3	1:B:301:GLY:O	2.14	0.47
1:B:466:VAL:O	1:B:466:VAL:HG12	2.15	0.47
1:A:297:LYS:HD3	1:A:301:GLY:O	2.15	0.46
1:B:347:ASP:CG	1:B:348:THR:H	2.18	0.46
1:B:35:TRP:HE1	1:B:41:GLN:NE2	2.09	0.46
1:A:492:ILE:O	1:A:496:VAL:HG23	2.15	0.46
1:B:400:LEU:HG	1:B:456:PRO:HA	1.97	0.46
1:B:348:THR:HB	1:B:350:LYS:HZ3	1.81	0.46
1:B:290:ARG:HG3	1:B:308:TYR:CZ	2.51	0.46
1:B:29:SER:O	1:B:32:ILE:HG22	2.16	0.46
1:B:346:ILE:CG1	1:B:347:ASP:H	2.29	0.46
1:B:335:PRO:HG3	1:B:354:LEU:CD1	2.46	0.46
1:A:124:ASN:ND2	1:A:127:ILE:H	2.14	0.46
1:A:335:PRO:HG3	1:A:354:LEU:CD1	2.45	0.46
1:A:339:ARG:HH22	1:A:341:ALA:HB2	1.80	0.46
1:A:35:TRP:HE1	1:A:41:GLN:NE2	2.10	0.46
1:B:106:GLN:HE21	1:B:112:ILE:HD11	1.81	0.46
1:A:133:PHE:O	1:A:134:ARG:HB2	2.15	0.46
1:A:230:PRO:HD2	9:A:873:HOH:O	2.16	0.46
1:A:172:LEU:HB3	1:A:258:LEU:HG	1.98	0.46
1:B:173:ARG:HG2	1:B:173:ARG:HH21	1.81	0.46
1:A:358:GLY:O	1:A:361:LEU:HB3	2.15	0.46
1:A:363:ARG:HH21	1:A:363:ARG:HG2	1.80	0.45
1:B:172:LEU:HB3	1:B:258:LEU:HG	1.99	0.45
1:B:123:PRO:HG3	1:B:153:TYR:CZ	2.51	0.45
1:A:356:ILE:HG23	1:A:360:GLU:CG	2.47	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLN:HB3	9:A:756:HOH:O	2.15	0.45
1:B:96:ILE:HG13	1:B:120:VAL:HG21	1.99	0.45
1:B:124:ASN:ND2	1:B:127:ILE:H	2.15	0.45
1:B:347:ASP:CG	1:B:348:THR:N	2.70	0.45
1:A:329:ARG:HD3	1:A:344:ASP:OD1	2.17	0.45
1:B:358:GLY:O	1:B:361:LEU:HB3	2.16	0.45
1:A:352:ARG:CB	1:A:352:ARG:NH2	2.77	0.45
1:A:458:GLN:HB3	9:A:1190:HOH:O	2.17	0.45
1:B:491:PRO:HG2	1:B:494:HIS:CG	2.52	0.45
1:A:42:LEU:HD11	1:A:106:GLN:HG3	2.00	0.44
1:B:418:THR:O	1:B:421:GLN:HG2	2.17	0.44
1:A:261:LEU:HG	1:A:262:ALA:N	2.32	0.44
1:B:492:ILE:O	1:B:496:VAL:HG23	2.18	0.44
1:A:97:LYS:HD2	9:A:1217:HOH:O	2.16	0.44
1:B:268:ASP:HA	1:B:310:ALA:HA	2.00	0.44
1:A:366:ARG:HH21	1:A:366:ARG:CG	2.28	0.44
1:B:434:ASN:O	1:B:436:LYS:HG3	2.17	0.44
1:A:171:GLY:O	1:A:174:LYS:HE2	2.17	0.44
1:B:298:ASN:C	1:B:298:ASN:ND2	2.69	0.44
1:A:494:HIS:HD1	8:A:552:ACY:C	2.30	0.44
1:B:172:LEU:N	1:B:172:LEU:CD1	2.81	0.44
1:B:261:LEU:HG	1:B:262:ALA:N	2.33	0.44
1:B:202:ARG:HG2	1:B:377:TYR:CE1	2.52	0.44
1:A:403:SER:O	1:A:488:ALA:HB1	2.18	0.44
1:B:346:ILE:HG13	1:B:347:ASP:H	1.82	0.44
6:A:635:ADX:H5"	6:A:635:ADX:SB	2.58	0.44
1:B:313:LEU:HD22	1:B:317:TYR:CE1	2.53	0.44
1:B:403:SER:O	1:B:488:ALA:HB1	2.18	0.44
1:A:298:ASN:HD21	1:A:302:VAL:CG1	2.31	0.44
1:B:366:ARG:CG	1:B:366:ARG:HH21	2.29	0.44
1:A:435:ASN:ND2	1:A:460:GLU:HG2	2.33	0.43
1:A:476:ASP:HB3	1:A:481:ALA:HB2	2.00	0.43
1:A:491:PRO:HG2	1:A:494:HIS:CG	2.53	0.43
1:B:356:ILE:HG23	1:B:360:GLU:CG	2.48	0.43
1:B:459:TRP:NE1	1:B:464:ASP:HA	2.33	0.43
1:A:385:ARG:HH21	1:A:385:ARG:HG2	1.82	0.43
1:B:112:ILE:O	1:B:161:ILE:HB	2.19	0.43
1:B:186:ARG:NH1	8:B:564:ACY:O	2.52	0.43
1:A:418:THR:O	1:A:421:GLN:CG	2.67	0.43
1:B:325:VAL:O	1:B:327:PRO:HD3	2.18	0.43
1:A:192:VAL:HA	1:A:285:HIS:HB2	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ARG:NH2	1:B:173:ARG:HG2	2.33	0.43
1:B:61:ASN:ND2	1:B:61:ASN:C	2.69	0.43
1:B:316:SER:HB3	9:B:1131:HOH:O	2.18	0.43
1:B:339:ARG:HH22	1:B:341:ALA:HB2	1.84	0.43
1:B:42:LEU:HD11	1:B:106:GLN:HG3	2.01	0.43
1:A:123:PRO:HG3	1:A:153:TYR:CE1	2.54	0.43
1:B:219:VAL:O	1:B:254:ALA:HA	2.19	0.43
1:A:172:LEU:CD1	1:A:172:LEU:N	2.82	0.42
1:B:60:LEU:HA	9:B:905:HOH:O	2.18	0.42
1:A:169:TYR:N	1:A:170:PRO:CD	2.83	0.42
1:B:348:THR:CB	1:B:350:LYS:HZ3	2.32	0.42
1:B:359:THR:HG23	1:B:362:ARG:HH21	1.85	0.42
1:B:393:LYS:HA	9:B:999:HOH:O	2.19	0.42
1:A:42:LEU:O	1:A:45:ILE:HG22	2.20	0.42
1:B:107:ASP:O	1:B:108:ASP:C	2.58	0.42
1:B:366:ARG:HD3	9:B:1029:HOH:O	2.20	0.42
1:A:136:ASP:HA	1:A:137:PRO:HD2	1.89	0.42
1:A:268:ASP:HA	1:A:310:ALA:HA	2.02	0.42
1:A:290:ARG:NH2	1:A:307:PRO:HB3	2.34	0.42
1:A:390:PRO:HB2	1:A:392:PRO:HD2	2.02	0.42
1:B:192:VAL:HA	1:B:285:HIS:HB2	2.01	0.42
1:B:455:ILE:HA	1:B:456:PRO:HD2	1.86	0.42
1:A:112:ILE:O	1:A:161:ILE:HB	2.20	0.41
1:A:16:ASP:OD1	1:A:159:GLU:HA	2.19	0.41
1:A:330:MET:HB3	1:A:343:ILE:HG21	2.02	0.41
1:B:166:HIS:CD2	9:B:711:HOH:O	2.73	0.41
1:A:186:ARG:O	1:A:187:GLN:HB2	2.19	0.41
1:B:313:LEU:HA	1:B:313:LEU:HD23	1.89	0.41
1:A:212:ALA:HB2	1:A:219:VAL:CG2	2.51	0.41
1:A:272:VAL:HG21	1:A:313:LEU:HD13	2.02	0.41
1:B:378:PRO:HG2	1:B:379:GLU:HG3	2.02	0.41
1:B:458:GLN:HE21	1:B:458:GLN:HB3	1.58	0.41
1:B:184:GLN:C	1:B:186:ARG:N	2.73	0.41
1:B:212:ALA:HB2	1:B:219:VAL:CG2	2.50	0.41
1:B:345:GLN:O	1:B:346:ILE:HG23	2.21	0.41
1:A:261:LEU:HD11	1:A:273:TRP:CH2	2.56	0.41
1:A:96:ILE:HG13	1:A:120:VAL:HG21	2.02	0.41
1:A:123:PRO:HG3	1:A:153:TYR:CZ	2.56	0.41
1:A:46:GLU:OE2	1:A:166:HIS:HE1	2.04	0.41
1:A:292:HIS:HD2	6:A:635:ADX:O3'	2.03	0.41
1:B:186:ARG:O	1:B:187:GLN:HB2	2.20	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:HG3	1:B:262:ALA:HB1	2.03	0.41
1:B:347:ASP:C	1:B:349:THR:N	2.74	0.41
1:B:76:ASP:OD2	1:B:76:ASP:C	2.60	0.41
1:A:295:PRO:HG2	1:A:304:PHE:CG	2.56	0.41
1:A:90:GLU:HG3	9:A:747:HOH:O	2.21	0.41
1:B:188:TRP:CD2	1:B:218:LYS:HG3	2.56	0.41
1:A:179:LEU:O	1:A:182:GLU:HB2	2.21	0.40
1:A:76:ASP:C	1:A:76:ASP:OD2	2.59	0.40
1:B:46:GLU:OE2	1:B:166:HIS:HE1	2.04	0.40
1:A:124:ASN:ND2	1:A:127:ILE:HG13	2.36	0.40
1:A:26:GLU:OE1	1:A:101:ARG:NE	2.39	0.40
1:B:82:ILE:HG13	1:B:273:TRP:CE3	2.56	0.40
1:A:366:ARG:HG2	1:A:366:ARG:NH2	2.32	0.40
1:B:476:ASP:O	1:B:484:GLN:HA	2.21	0.40
1:B:348:THR:O	1:B:349:THR:HB	2.22	0.40
1:A:244:GLU:HG3	1:A:379:GLU:OE2	2.22	0.40
1:B:391:ARG:HA	1:B:391:ARG:HD3	1.86	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)
2:A:515:CD:CD	2:B:533:CD:CD[2_765]	1.19	1.01

## 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	508/511 (99%)	475 (94%)	28 (6%)	5 (1%)	15	44
1	B	508/511 (99%)	470 (92%)	36 (7%)	2 (0%)	34	66
All	All	1016/1022 (99%)	945 (93%)	64 (6%)	7 (1%)	22	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	346	ILE
1	B	346	ILE
1	A	109	GLU
1	A	359	THR
1	B	359	THR
1	A	267	GLY
1	A	335	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	445/446 (100%)	427 (96%)	18 (4%)	31	65
1	B	445/446 (100%)	427 (96%)	18 (4%)	31	65
All	All	890/892 (100%)	854 (96%)	36 (4%)	31	65

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

Mol	Chain	Res	Type
1	A	18	LEU
1	A	24	LEU
1	A	31	ASP
1	A	61	ASN
1	A	124	ASN
1	A	158	LEU
1	A	179	LEU
1	A	197	ARG
1	A	202	ARG
1	A	206	GLU
1	A	298	ASN
1	A	302	VAL
1	A	313	LEU
1	A	329	ARG
1	A	379	GLU
1	A	435	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	469	LYS
1	A	474	LEU
1	B	18	LEU
1	B	24	LEU
1	B	31	ASP
1	B	61	ASN
1	B	124	ASN
1	B	158	LEU
1	B	179	LEU
1	B	197	ARG
1	B	202	ARG
1	B	206	GLU
1	B	298	ASN
1	B	302	VAL
1	B	313	LEU
1	B	329	ARG
1	B	379	GLU
1	B	435	ASN
1	B	469	LYS
1	B	474	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	21	ASN
1	A	41	GLN
1	A	61	ASN
1	A	63	ASN
1	A	94	ASN
1	A	95	GLN
1	A	106	GLN
1	A	118	GLN
1	A	124	ASN
1	A	147	ASN
1	A	166	HIS
1	A	178	GLN
1	A	184	GLN
1	A	198	ASN
1	A	204	HIS
1	A	243	GLN
1	A	292	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	298	ASN
1	A	434	ASN
1	A	435	ASN
1	A	471	ASN
1	A	484	GLN
1	A	506	ASN
1	B	10	GLN
1	B	21	ASN
1	B	41	GLN
1	B	61	ASN
1	B	94	ASN
1	B	106	GLN
1	B	118	GLN
1	B	124	ASN
1	B	147	ASN
1	B	166	HIS
1	B	178	GLN
1	B	184	GLN
1	B	198	ASN
1	B	204	HIS
1	B	243	GLN
1	B	292	HIS
1	B	298	ASN
1	B	434	ASN
1	B	435	ASN
1	B	471	ASN
1	B	484	GLN
1	B	506	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 50 ligands modelled in this entry, 31 are monoatomic - leaving 19 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
8	ACY	A	553	-	1,3,3	5.62	1 (100%)	0,3,3	0.00	-
8	ACY	A	554	2	1,3,3	5.54	1 (100%)	0,3,3	0.00	-
8	ACY	B	561	2	1,3,3	5.78	1 (100%)	0,3,3	0.00	-
8	ACY	A	550	2	1,3,3	5.18	1 (100%)	0,3,3	0.00	-
8	ACY	B	560	2	1,3,3	4.70	1 (100%)	0,3,3	0.00	-
6	ADX	A	635	-	25,29,29	1.42	4 (16%)	26,45,45	1.55	2 (7%)
8	ACY	B	564	2	1,3,3	6.27	1 (100%)	0,3,3	0.00	-
8	ACY	B	563	-	1,3,3	5.70	1 (100%)	0,3,3	0.00	-
8	ACY	A	556	2	1,3,3	4.36	1 (100%)	0,3,3	0.00	-
6	ADX	B	636	-	25,29,29	1.46	5 (20%)	26,45,45	1.53	2 (7%)
8	ACY	A	567	2	1,3,3	5.58	1 (100%)	0,3,3	0.00	-
8	ACY	A	555	2	1,3,3	5.71	1 (100%)	0,3,3	0.00	-
7	POP	A	637	-	6,8,8	1.46	0	13,13,13	1.35	2 (15%)
8	ACY	B	565	2	1,3,3	5.27	1 (100%)	0,3,3	0.00	-
8	ACY	B	562	-	1,3,3	5.55	1 (100%)	0,3,3	0.00	-
8	ACY	A	551	2	1,3,3	5.62	1 (100%)	0,3,3	0.00	-
7	POP	B	638	-	6,8,8	1.42	0	13,13,13	1.37	3 (23%)
8	ACY	B	566	2	1,3,3	5.68	1 (100%)	0,3,3	0.00	-
8	ACY	A	552	-	1,3,3	5.72	1 (100%)	0,3,3	0.00	-

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
6	ADX	B	636	-	-	2/6/32/32	0/3/3/3

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	POP	B	638	-	-	5/6/6/6	-
7	POP	A	637	-	-	2/6/6/6	-
6	ADX	A	635	-	-	2/6/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	564	ACY	CH3-C	6.27	1.56	1.48
8	B	561	ACY	CH3-C	5.78	1.56	1.48
8	A	552	ACY	CH3-C	5.72	1.56	1.48
8	A	555	ACY	CH3-C	5.71	1.56	1.48
8	B	563	ACY	CH3-C	5.70	1.56	1.48
8	B	566	ACY	CH3-C	5.68	1.56	1.48
8	A	551	ACY	CH3-C	5.62	1.55	1.48
8	A	553	ACY	CH3-C	5.62	1.55	1.48
8	A	567	ACY	CH3-C	5.58	1.55	1.48
8	B	562	ACY	CH3-C	5.55	1.55	1.48
8	A	554	ACY	CH3-C	5.54	1.55	1.48
8	B	565	ACY	CH3-C	5.27	1.55	1.48
8	A	550	ACY	CH3-C	5.18	1.55	1.48
8	B	560	ACY	CH3-C	4.70	1.54	1.48
6	B	636	ADX	O2B-SB	4.40	1.64	1.45
8	A	556	ACY	CH3-C	4.36	1.54	1.48
6	A	635	ADX	O2B-SB	3.99	1.62	1.45
6	A	635	ADX	O4'-C1'	2.87	1.45	1.41
6	B	636	ADX	O4'-C1'	2.64	1.44	1.41
6	A	635	ADX	C5-N7	-2.52	1.30	1.39
6	B	636	ADX	PA-O3A	-2.28	1.57	1.59
6	B	636	ADX	C5-N7	-2.17	1.31	1.39
6	A	635	ADX	PA-O3A	-2.09	1.57	1.59
6	B	636	ADX	C2-N3	2.01	1.35	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	636	ADX	N3-C2-N1	-6.32	118.80	128.68
6	A	635	ADX	N3-C2-N1	-6.32	118.81	128.68
7	A	637	POP	O5-P2-O4	-2.70	100.13	110.68
6	B	636	ADX	C4-C5-N7	-2.64	106.65	109.40
6	A	635	ADX	C4-C5-N7	-2.54	106.76	109.40
7	B	638	POP	O5-P2-O4	-2.47	101.00	110.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	638	POP	O6-P2-O4	2.46	120.31	110.68
7	A	637	POP	O6-P2-O4	2.36	119.92	110.68
7	B	638	POP	O6-P2-O	2.14	111.80	104.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	637	POP	P2-O-P1-O2
7	A	637	POP	P2-O-P1-O3
7	B	638	POP	P2-O-P1-O3
7	B	638	POP	P1-O-P2-O6
6	B	636	ADX	O4'-C4'-C5'-O5'
6	B	636	ADX	C3'-C4'-C5'-O5'
6	A	635	ADX	O4'-C4'-C5'-O5'
6	A	635	ADX	C3'-C4'-C5'-O5'
7	B	638	POP	P1-O-P2-O4
7	B	638	POP	P2-O-P1-O2
7	B	638	POP	P1-O-P2-O5

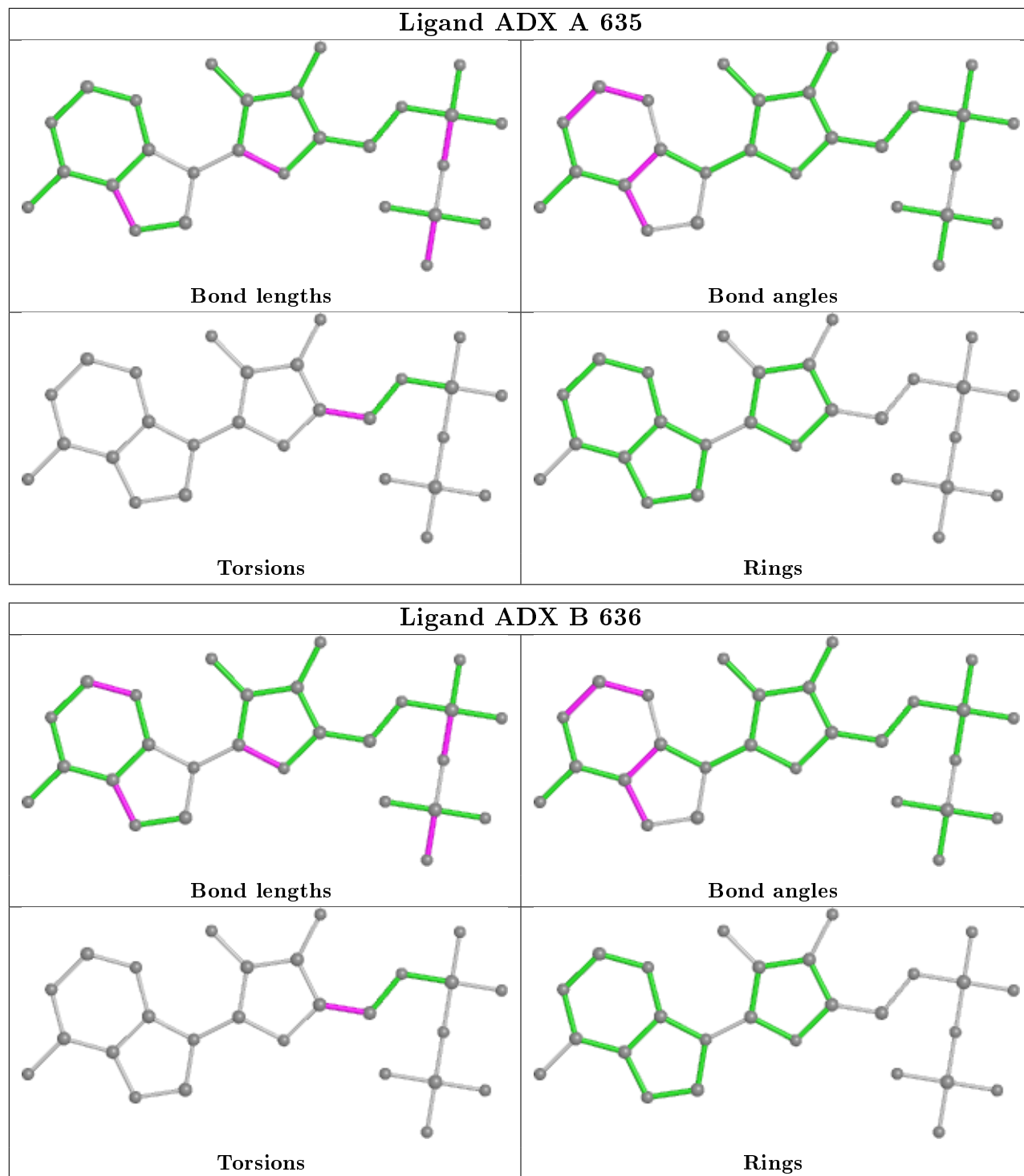
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	550	ACY	1	0
8	B	560	ACY	1	0
6	A	635	ADX	5	0
8	B	564	ACY	1	0
7	A	637	POP	1	0
8	A	552	ACY	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 ⓘ

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	510/511 (99%)	-0.16	21 (4%)	37 27	15, 31, 72, 90	0
1	B	510/511 (99%)	-0.22	15 (2%)	51 41	14, 31, 72, 90	0
All	All	1020/1022 (99%)	-0.19	36 (3%)	44 34	14, 31, 72, 90	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	369	GLY	4.6
1	A	349	THR	3.9
1	A	348	THR	3.8
1	A	350	LYS	3.2
1	B	350	LYS	3.2
1	B	354	LEU	3.1
1	A	30	SER	3.1
1	B	349	THR	3.0
1	B	348	THR	3.0
1	A	367	VAL	2.9
1	A	299	SER	2.7
1	B	351	THR	2.7
1	A	336	ASP	2.7
1	B	30	SER	2.6
1	B	367	VAL	2.6
1	A	352	ARG	2.6
1	A	354	LEU	2.5
1	A	301	GLY	2.5
1	B	352	ARG	2.4
1	A	300	LYS	2.4
1	B	31	ASP	2.4
1	B	479	SER	2.4
1	A	31	ASP	2.4
1	A	351	THR	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	97	LYS	2.4
1	A	480	SER	2.3
1	A	363	ARG	2.3
1	A	91	ALA	2.3
1	A	478	SER	2.2
1	B	299	SER	2.2
1	A	365	LEU	2.2
1	B	355	ASN	2.2
1	A	479	SER	2.1
1	B	353	THR	2.1
1	B	362	ARG	2.0
1	B	336	ASP	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	B	539	1/1	0.58	0.41	70,70,70,70	0
3	CA	B	537	1/1	0.80	0.12	73,73,73,73	0
8	ACY	B	562	4/4	0.85	0.23	63,64,65,65	0
4	NA	A	527	1/1	0.87	0.07	35,35,35,35	0
2	CD	A	513	1/1	0.88	0.07	127,127,127,127	0
8	ACY	A	552	4/4	0.89	0.17	53,54,55,55	0
4	NA	B	544	1/1	0.89	0.11	29,29,29,29	0
3	CA	A	519	1/1	0.90	0.06	63,63,63,63	0
4	NA	A	523	1/1	0.91	0.10	35,35,35,35	0
3	CA	A	520	1/1	0.92	0.05	45,45,45,45	0
4	NA	B	543	1/1	0.92	0.11	34,34,34,34	0

*Continued on next page...*

*Continued from previous page...*

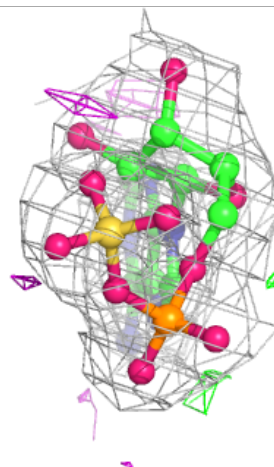
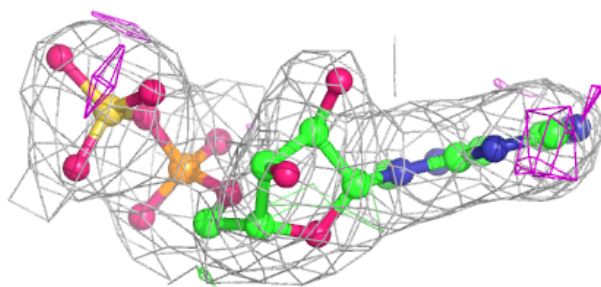
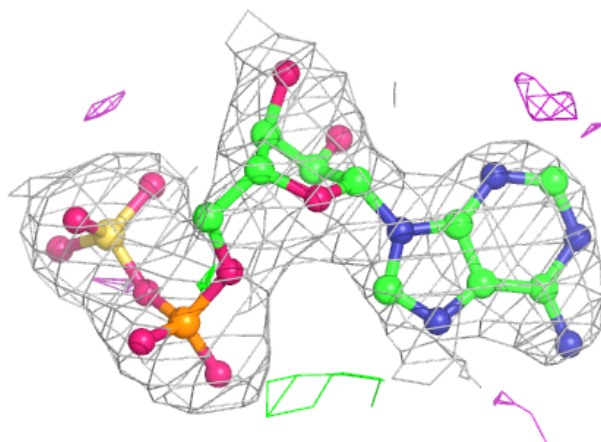
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	POP	B	638	9/9	0.92	0.19	92,93,93,93	0
8	ACY	B	563	4/4	0.92	0.19	31,33,33,34	0
4	NA	B	542	1/1	0.93	0.12	56,56,56,56	0
4	NA	A	518	1/1	0.93	0.11	42,42,42,42	0
8	ACY	A	553	4/4	0.94	0.19	34,36,36,36	0
4	NA	B	536	1/1	0.94	0.08	42,42,42,42	0
7	POP	A	637	9/9	0.94	0.15	47,50,51,51	0
4	NA	B	541	1/1	0.95	0.06	20,20,20,20	0
2	CD	B	531	1/1	0.95	0.05	113,113,113,113	0
8	ACY	A	551	4/4	0.95	0.22	35,36,37,38	0
4	NA	B	540	1/1	0.96	0.06	30,30,30,30	0
4	NA	A	525	1/1	0.96	0.10	6,6,6,6	0
4	NA	A	522	1/1	0.96	0.06	19,19,19,19	0
8	ACY	A	555	4/4	0.97	0.36	46,47,48,49	0
6	ADX	A	635	27/27	0.97	0.15	21,33,40,40	0
5	MG	A	521	1/1	0.97	0.10	22,22,22,22	0
6	ADX	B	636	27/27	0.97	0.16	24,29,43,45	0
8	ACY	B	564	4/4	0.97	0.23	22,22,25,26	0
8	ACY	A	554	4/4	0.97	0.14	19,21,22,23	0
4	NA	A	526	1/1	0.97	0.05	20,20,20,20	0
8	ACY	B	561	4/4	0.98	0.21	29,32,32,33	0
8	ACY	B	565	4/4	0.98	0.45	73,74,74,74	0
3	CA	B	535	1/1	0.98	0.12	38,38,38,38	0
8	ACY	B	566	4/4	0.98	0.22	22,24,25,25	0
8	ACY	B	560	4/4	0.99	0.27	29,30,30,31	0
8	ACY	A	556	4/4	0.99	0.23	28,30,31,31	0
8	ACY	A	550	4/4	0.99	0.26	22,25,25,27	0
2	CD	A	514	1/1	0.99	0.06	36,36,36,36	0
3	CA	B	538	1/1	0.99	0.09	26,26,26,26	0
3	CA	A	517	1/1	0.99	0.04	31,31,31,31	0
8	ACY	A	567	4/4	0.99	0.14	21,24,25,27	0
2	CD	B	532	1/1	0.99	0.05	40,40,40,40	0
2	CD	A	516	1/1	1.00	0.02	43,43,43,43	0
2	CD	B	534	1/1	1.00	0.03	35,35,35,35	0
2	CD	B	533	1/1	1.00	0.05	47,47,47,47	0
2	CD	A	512	1/1	1.00	0.04	32,32,32,32	0
2	CD	A	524	1/1	1.00	0.04	56,56,56,56	0
2	CD	B	530	1/1	1.00	0.04	38,38,38,38	0
2	CD	A	515	1/1	1.00	0.07	78,78,78,78	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 ADX A 635:**

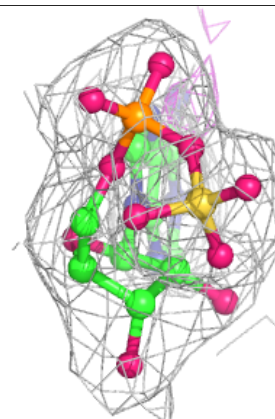
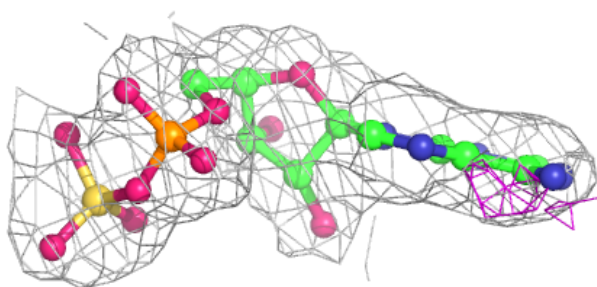
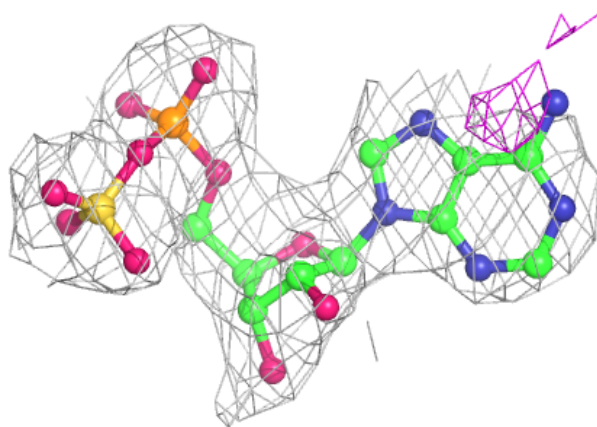
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ADX B 636:**

$2mF_o-DF_c$  (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.