



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2021 – 03:15 PM EDT

PDB ID : 3HZI  
Title : Structure of mdt protein  
Authors : Schumacher, M.A.  
Deposited on : 2009-06-23  
Resolution : 2.98 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

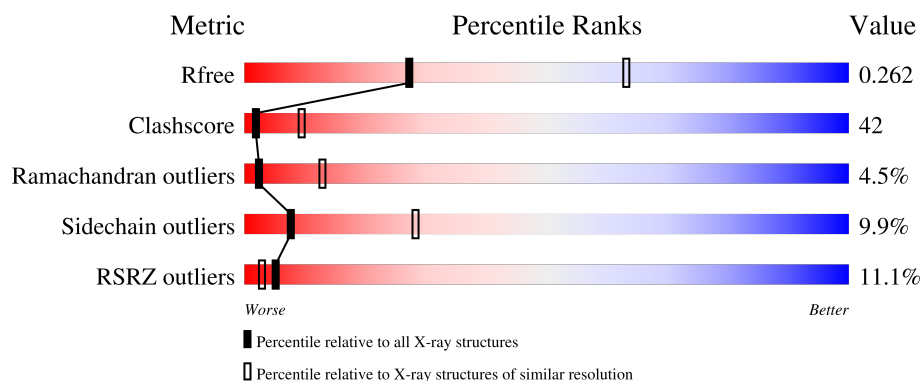
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


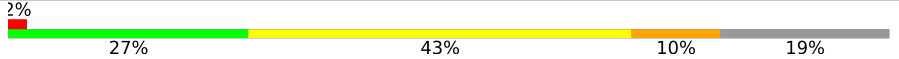

The reported resolution of this entry is 2.98 Å.

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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	440	
2	B	88	
3	T	21	

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	SO4	A	833	-	-	X	-
5	SO4	A	834	-	-	X	-
5	SO4	A	836	-	-	X	-
5	SO4	A	878	-	-	X	-
5	SO4	B	640	-	-	X	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4420 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 Protein hipA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	Se	0	0	0
			3347	2146	585	603	10	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	309	GLN	ASP	engineered mutation	UNP P23874

- Molecule 2 is a protein called HTH-type transcriptional regulator hipB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total	C	N	O	S	0	0	0
			564	358	95	108	3			

- Molecule 3 is a DNA chain called 5'-D(\*DAP\*DCP\*DTP\*DAP\*DTP\*DCP\*DCP\*DCP\*DCP\*DTP\*DTP\*DAP\*DAP\*DGP\*DGP\*DGP\*DGP\*DAP\*DTP\*DAP\*DG)-3'.

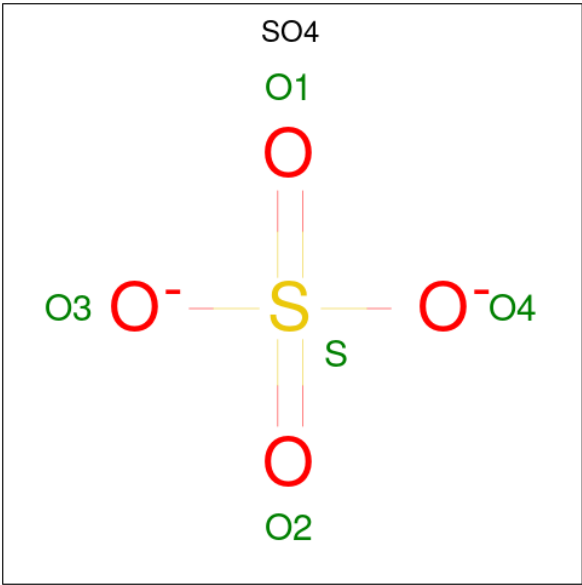
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	21	Total	C	N	O	P	0	0	0
			428	205	80	123	20			

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

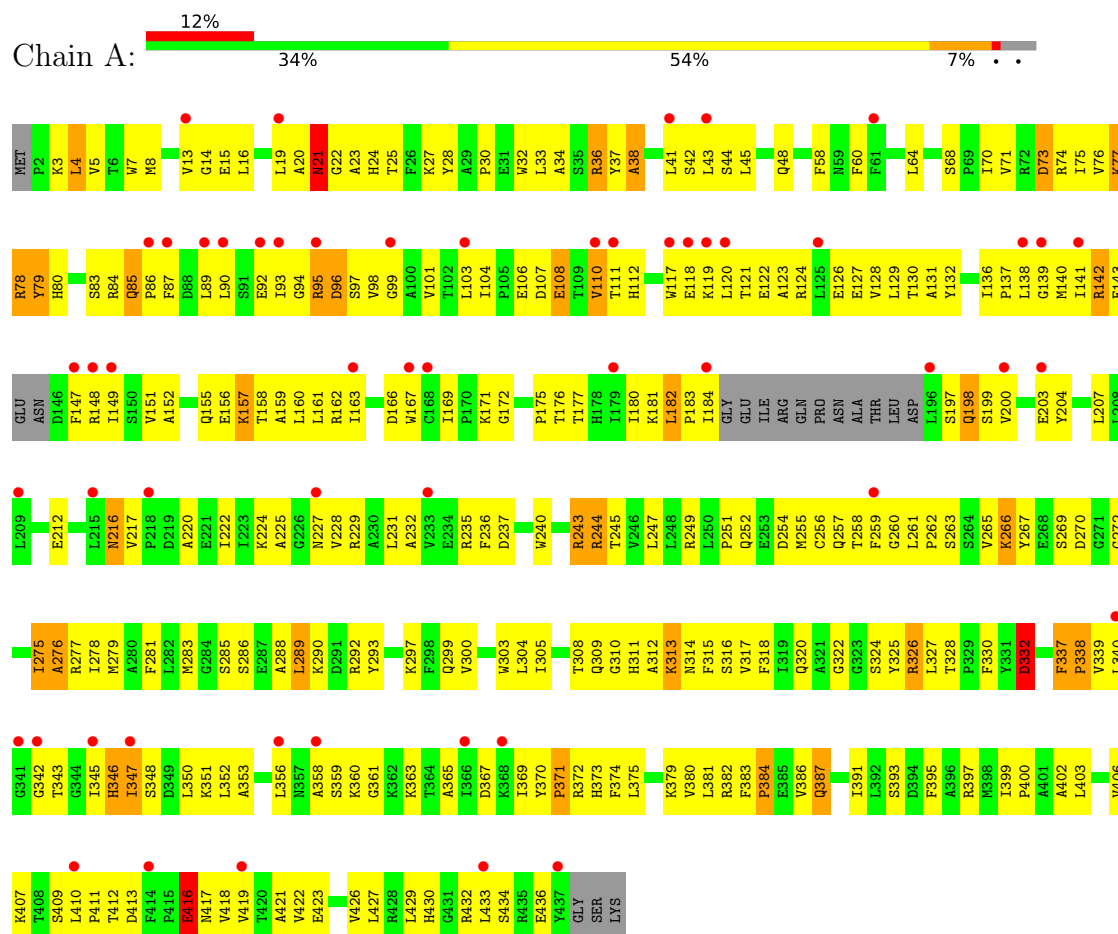
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	T	1	Total	O	0	0
			1	1		

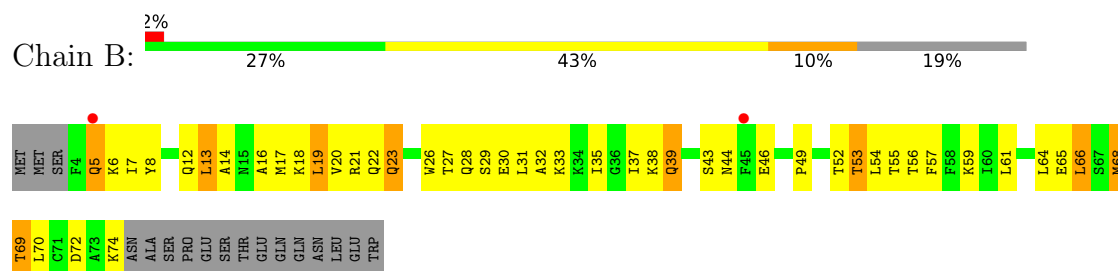
### 3 Residue-property plots [i](#)

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: Protein hipA



#### • Molecule 2: HTH-type transcriptional regulator hipB



- Molecule 3: 5'-D(\*DAP\*DCP\*DTP\*DAP\*DTP\*DCP\*DCP\*DCP\*DCP\*DTP\*DTP\*DAP\*DA  
P\*DGP\*DGP\*DGP\*DGP\*DAP\*DTP\*DAP\*DG)-3'

Chain T: 29% 62% 10%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.25Å 167.25Å 62.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.26 – 2.98 118.26 – 2.97	Depositor EDS
% Data completeness (in resolution range)	99.3 (118.26-2.98) 99.3 (118.26-2.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.96Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.265 , 0.283 0.242 , 0.262	Depositor DCC
$R_{free}$ test set	2435 reflections (13.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	81.5	Xtriage
Anisotropy	0.557	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 89.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, SO4

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	0.67	0/3418	0.79	4/4625 (0.1%)
2	B	0.76	0/572	0.79	0/771
3	T	0.80	0/480	0.82	0/739
All	All	0.70	0/4470	0.79	4/6135 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	T	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	416	GLU	OE1-CD-OE2	-6.97	114.94	123.30
1	A	416	GLU	N-CA-C	6.86	129.51	111.00
1	A	326	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	96	ASP	CB-CG-OD2	5.09	122.88	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	T	713	DG	Sidechain
3	T	715	DG	Sidechain

## 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	3347	0	3399	297	0
2	B	564	0	577	46	0
3	T	428	0	238	29	0
4	A	31	0	12	2	0
5	A	40	0	0	12	0
5	B	5	0	0	4	0
6	A	4	0	0	0	0
6	T	1	0	0	0	0
All	All	4420	0	4226	363	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 42.

All (363) 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:78:ARG:H	1:A:78:ARG:HD3	1.15	1.05
2:B:23:GLN:HE21	2:B:23:GLN:HA	1.18	1.04
1:A:243:ARG:HB2	1:A:245:THR:HG23	1.49	0.95
1:A:33:LEU:HD21	2:B:19:LEU:HD21	1.48	0.93
3:T:703:DT:H2''	3:T:704:DC:H5'	1.51	0.92
1:A:340:LEU:HD22	1:A:346:HIS:HA	1.54	0.90
2:B:29:SER:O	2:B:33:LYS:HG3	1.77	0.84
1:A:399:ILE:HB	1:A:400:PRO:HD3	1.59	0.84
1:A:416:GLU:OE1	1:A:417:ASN:N	2.11	0.83
2:B:6:LYS:HZ1	2:B:74:LYS:HG3	1.42	0.82
2:B:7:ILE:HG23	2:B:12:GLN:HB3	1.62	0.82
2:B:6:LYS:NZ	2:B:74:LYS:HG3	1.96	0.81
1:A:78:ARG:HD3	1:A:78:ARG:N	1.96	0.80
1:A:436:GLU:OE2	5:A:834:SO4:O3	2.00	0.80
1:A:347:ILE:HD12	1:A:350:LEU:HD12	1.62	0.80
1:A:64:LEU:HD22	1:A:97:SER:OG	1.84	0.77
2:B:39:GLN:HE22	3:T:702:DA:H62	1.30	0.77
1:A:161:LEU:HD11	1:A:163:ILE:HD11	1.64	0.77
1:A:370:TYR:CD2	1:A:432:ARG:HD3	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:O	2:B:57:PHE:HB3	1.83	0.77
1:A:382:ARG:NH1	3:T:713:DG:H5''	1.99	0.77
2:B:27:THR:OG1	2:B:30:GLU:HG3	1.85	0.77
2:B:38:LYS:HG2	5:B:640:SO4:O1	1.84	0.76
1:A:399:ILE:HG13	1:A:430:HIS:HD2	1.51	0.75
2:B:38:LYS:HG2	5:B:640:SO4:S	2.26	0.75
2:B:23:GLN:HA	2:B:23:GLN:NE2	1.99	0.74
1:A:340:LEU:HD23	1:A:345:ILE:HG22	1.69	0.74
2:B:16:ALA:O	2:B:20:VAL:HG23	1.88	0.74
1:A:41:LEU:HD11	1:A:101:VAL:HG12	1.69	0.73
2:B:39:GLN:HE22	3:T:702:DA:N6	1.85	0.73
1:A:308:THR:HG22	1:A:351:LYS:O	1.88	0.72
1:A:363:LYS:NZ	5:A:833:SO4:S	2.63	0.72
1:A:429:LEU:HD23	1:A:432:ARG:NH1	2.04	0.72
3:T:714:DG:H5'	3:T:714:DG:H8	1.55	0.72
1:A:175:PRO:HG3	1:A:249:ARG:CZ	2.21	0.71
1:A:200:VAL:HG13	1:A:231:LEU:HB2	1.72	0.70
1:A:255:MET:HE3	1:A:278:ILE:HG23	1.74	0.70
1:A:68:SER:HB3	1:A:71:VAL:HG23	1.73	0.70
1:A:275:ILE:HD11	1:A:299:GLN:HG3	1.73	0.70
1:A:175:PRO:HB3	1:A:249:ARG:HE	1.56	0.70
1:A:58:PHE:CE1	1:A:86:PRO:HG2	2.27	0.69
1:A:138:LEU:HD12	1:A:140:MSE:HE2	1.73	0.69
1:A:19:LEU:HD12	1:A:23:ALA:HB3	1.75	0.69
1:A:99:GLY:HA2	1:A:252:GLN:HG2	1.75	0.69
1:A:4:LEU:HD12	1:A:87:PHE:CE1	2.29	0.68
1:A:107:ASP:O	1:A:108:GLU:HB2	1.94	0.68
1:A:343:THR:OG1	1:A:345:ILE:HD13	1.94	0.68
1:A:243:ARG:HB2	1:A:245:THR:CG2	2.24	0.68
1:A:235:ARG:HB3	1:A:237:ASP:OD1	1.94	0.68
1:A:131:ALA:HB3	1:A:139:GLY:HA2	1.75	0.67
1:A:225:ALA:O	1:A:228:VAL:HG12	1.94	0.67
1:A:300:VAL:HG22	1:A:374:PHE:CE2	2.29	0.67
1:A:4:LEU:HB2	1:A:87:PHE:HE1	1.59	0.66
1:A:16:LEU:HD12	1:A:25:THR:O	1.95	0.66
1:A:345:ILE:HD12	1:A:345:ILE:H	1.59	0.66
1:A:73:ASP:OD1	1:A:84:ARG:HD3	1.96	0.66
1:A:78:ARG:H	1:A:78:ARG:CD	1.99	0.66
3:T:703:DT:C2'	3:T:704:DC:H5'	2.25	0.66
1:A:256:CYS:SG	1:A:313:LYS:HG3	2.36	0.66
1:A:78:ARG:NH2	1:A:140:MSE:HE3	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:SER:O	1:A:45:LEU:HD23	1.95	0.65
1:A:402:ALA:O	1:A:406:VAL:HG23	1.95	0.65
2:B:8:TYR:H	2:B:12:GLN:NE2	1.94	0.65
1:A:155:GLN:CG	1:A:184:ILE:HD13	2.27	0.65
1:A:281:PHE:HE2	1:A:317:VAL:HG11	1.62	0.65
1:A:79:TYR:HE2	1:A:148:ARG:HE	1.44	0.64
1:A:384:PRO:HB2	1:A:387:GLN:HB2	1.80	0.64
1:A:275:ILE:CD1	1:A:299:GLN:HG3	2.28	0.64
1:A:83:SER:OG	1:A:85:GLN:HB2	1.96	0.64
3:T:714:DG:H2''	3:T:715:DG:C5'	2.28	0.64
1:A:293:TYR:CE1	1:A:387:GLN:HG2	2.34	0.63
1:A:42:SER:HB2	1:A:60:PHE:CE1	2.33	0.63
1:A:265:VAL:O	1:A:272:GLY:HA3	1.99	0.63
1:A:155:GLN:HG3	1:A:184:ILE:HD13	1.80	0.62
1:A:98:VAL:HG12	1:A:99:GLY:N	2.14	0.62
1:A:372:ARG:NH2	5:A:833:SO4:O4	2.33	0.62
2:B:68:MET:HG2	2:B:69:THR:N	2.10	0.62
2:B:64:LEU:O	2:B:66:LEU:HD13	2.00	0.62
1:A:122:GLU:H	1:A:122:GLU:CD	2.02	0.62
1:A:255:MET:CE	1:A:278:ILE:HG23	2.29	0.61
1:A:429:LEU:HD23	1:A:432:ARG:HH12	1.65	0.61
1:A:395:PHE:O	1:A:399:ILE:HG12	2.01	0.61
2:B:26:TRP:HA	2:B:30:GLU:OE1	2.01	0.61
1:A:58:PHE:CZ	1:A:86:PRO:HG2	2.36	0.60
1:A:316:SER:O	1:A:328:THR:HG23	2.01	0.60
3:T:705:DC:H2''	3:T:706:DC:O5'	2.00	0.60
1:A:147:PHE:CE2	1:A:169:ILE:HG23	2.36	0.60
1:A:380:VAL:HG23	1:A:381:LEU:HG	1.84	0.60
1:A:360:LYS:HD3	1:A:363:LYS:HZ1	1.67	0.60
1:A:417:ASN:O	1:A:421:ALA:N	2.26	0.60
1:A:95:ARG:HH12	1:A:172:GLY:C	2.05	0.59
1:A:346:HIS:O	1:A:348:SER:N	2.36	0.59
1:A:175:PRO:HA	1:A:249:ARG:HH21	1.66	0.59
1:A:41:LEU:HD11	1:A:101:VAL:CG1	2.32	0.59
2:B:18:LYS:NZ	2:B:46:GLU:OE1	2.36	0.58
1:A:27:LYS:NZ	5:A:878:SO4:O4	2.20	0.58
1:A:42:SER:HB2	1:A:60:PHE:CD1	2.38	0.58
1:A:158:THR:O	1:A:180:ILE:HB	2.03	0.58
1:A:155:GLN:CG	1:A:184:ILE:CD1	2.81	0.58
1:A:155:GLN:HG2	1:A:184:ILE:CD1	2.33	0.58
1:A:120:LEU:HD12	1:A:167:TRP:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ARG:HH11	3:T:713:DG:H5''	1.68	0.58
1:A:326:ARG:NH2	5:A:836:SO4:O1	2.37	0.58
1:A:71:VAL:O	1:A:75:ILE:HG12	2.04	0.58
1:A:130:THR:HA	1:A:132:TYR:CE2	2.38	0.58
1:A:142:ARG:CG	1:A:142:ARG:O	2.52	0.58
3:T:714:DG:H5'	3:T:714:DG:C8	2.38	0.58
1:A:90:LEU:O	1:A:94:GLY:HA3	2.03	0.58
1:A:110:VAL:HG11	1:A:112:HIS:CE1	2.38	0.58
1:A:365:ALA:O	1:A:369:ILE:HG13	2.04	0.58
2:B:7:ILE:HG23	2:B:12:GLN:CB	2.31	0.58
1:A:77:LYS:HB3	1:A:78:ARG:HD3	1.86	0.57
1:A:312:ALA:O	1:A:314:ASN:N	2.37	0.57
2:B:19:LEU:HD22	2:B:23:GLN:HG2	1.86	0.57
3:T:714:DG:H2''	3:T:715:DG:O5'	2.05	0.57
1:A:33:LEU:O	1:A:33:LEU:HD23	2.05	0.57
1:A:117:TRP:HA	1:A:171:LYS:HG2	1.86	0.57
1:A:265:VAL:O	1:A:272:GLY:CA	2.53	0.57
2:B:23:GLN:HE21	2:B:23:GLN:CA	2.01	0.57
1:A:345:ILE:H	1:A:345:ILE:CD1	2.17	0.57
1:A:347:ILE:CD1	1:A:350:LEU:HD12	2.35	0.56
1:A:141:ILE:HD13	1:A:143:GLU:HB3	1.87	0.56
1:A:254:ASP:OD2	1:A:256:CYS:HB2	2.05	0.56
1:A:175:PRO:HG3	1:A:249:ARG:NE	2.19	0.56
1:A:120:LEU:HD22	1:A:124:ARG:HB3	1.88	0.56
1:A:399:ILE:CG1	1:A:430:HIS:HD2	2.16	0.56
1:A:345:ILE:HD12	1:A:345:ILE:N	2.21	0.56
1:A:358:ALA:CB	1:A:363:LYS:HG2	2.36	0.56
1:A:279:MET:HE3	1:A:292:ARG:NH1	2.21	0.56
1:A:142:ARG:O	1:A:142:ARG:HG2	2.05	0.56
1:A:79:TYR:HB3	1:A:92:GLU:OE1	2.06	0.55
1:A:131:ALA:CB	1:A:139:GLY:HA2	2.37	0.54
1:A:243:ARG:HD2	1:A:243:ARG:N	2.22	0.54
1:A:370:TYR:HB2	1:A:372:ARG:NH1	2.22	0.54
3:T:705:DC:H1'	3:T:706:DC:H5'	1.89	0.54
3:T:718:DA:H1'	3:T:719:DG:H5''	1.89	0.54
1:A:347:ILE:HG13	1:A:367:ASP:HB2	1.90	0.54
2:B:55:THR:CG2	2:B:59:LYS:HE3	2.37	0.54
1:A:76:VAL:HG12	1:A:76:VAL:O	2.07	0.54
1:A:159:ALA:O	1:A:160:LEU:HD23	2.08	0.53
1:A:240:TRP:CZ3	1:A:247:LEU:HB2	2.43	0.53
1:A:410:LEU:HD13	1:A:419:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:HG22	1:A:374:PHE:CD2	2.43	0.53
1:A:79:TYR:HE2	1:A:148:ARG:NE	2.05	0.53
1:A:110:VAL:O	1:A:112:HIS:N	2.41	0.53
1:A:375:LEU:O	1:A:379:LYS:HB2	2.08	0.53
1:A:24:HIS:CE1	1:A:85:GLN:HE22	2.26	0.53
1:A:216:ASN:O	1:A:330:PHE:N	2.40	0.53
3:T:713:DG:H2''	3:T:714:DG:OP2	2.09	0.53
1:A:326:ARG:NH2	5:A:836:SO4:S	2.82	0.53
1:A:97:SER:OG	1:A:98:VAL:N	2.40	0.52
2:B:21:ARG:HG3	2:B:26:TRP:HB2	1.91	0.52
1:A:162:ARG:HH21	1:A:162:ARG:HG3	1.73	0.52
1:A:266:LYS:HD2	1:A:267:TYR:CE1	2.45	0.52
1:A:182:LEU:N	1:A:182:LEU:HD22	2.24	0.52
1:A:98:VAL:HG12	1:A:99:GLY:H	1.75	0.52
1:A:78:ARG:NH1	1:A:140:MSE:O	2.42	0.52
1:A:207:LEU:HD13	1:A:220:ALA:HB2	1.92	0.52
1:A:3:LYS:HD2	1:A:106:GLU:OE2	2.10	0.52
1:A:155:GLN:HG2	1:A:184:ILE:HD13	1.92	0.52
1:A:162:ARG:HG3	1:A:162:ARG:NH2	2.26	0.51
1:A:318:PHE:O	1:A:325:TYR:HA	2.10	0.51
2:B:7:ILE:HG13	2:B:12:GLN:HG2	1.92	0.51
1:A:118:GLU:HB2	1:A:171:LYS:HE3	1.92	0.51
1:A:276:ALA:O	1:A:277:ARG:C	2.47	0.51
2:B:7:ILE:HG23	2:B:12:GLN:CG	2.41	0.51
1:A:71:VAL:O	1:A:74:ARG:HB2	2.10	0.51
1:A:78:ARG:NH1	1:A:136:ILE:HG23	2.26	0.51
1:A:279:MET:CE	1:A:292:ARG:NH1	2.74	0.51
1:A:77:LYS:HD3	1:A:78:ARG:HD2	1.92	0.51
1:A:147:PHE:HE2	1:A:169:ILE:HG23	1.75	0.51
1:A:337:PHE:C	1:A:339:VAL:H	2.13	0.51
1:A:93:ILE:O	1:A:93:ILE:HD12	2.10	0.51
1:A:76:VAL:HG22	1:A:89:LEU:HD21	1.93	0.51
1:A:311:HIS:O	1:A:312:ALA:C	2.50	0.51
1:A:343:THR:CB	1:A:345:ILE:HD13	2.41	0.51
1:A:363:LYS:HG3	1:A:373:HIS:CE1	2.45	0.51
1:A:78:ARG:HH22	1:A:140:MSE:HB2	1.76	0.50
2:B:7:ILE:N	2:B:7:ILE:HD12	2.26	0.50
2:B:35:ILE:HD12	2:B:59:LYS:HB3	1.91	0.50
3:T:718:DA:H2''	3:T:719:DG:H5'	1.92	0.50
1:A:152:ALA:O	4:A:500:ATP:H5'1	2.11	0.50
1:A:279:MET:HE1	1:A:292:ARG:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:702:DA:H2''	3:T:703:DT:C5'	2.41	0.50
1:A:403:LEU:HD22	1:A:423:GLU:HG3	1.94	0.50
1:A:203:GLU:OE2	1:A:231:LEU:HD21	2.12	0.50
1:A:304:LEU:O	1:A:426:VAL:HG22	2.12	0.50
1:A:337:PHE:HB2	1:A:338:PRO:HD3	1.92	0.50
2:B:38:LYS:CG	5:B:640:SO4:O1	2.57	0.49
1:A:96:ASP:HB3	1:A:149:ILE:CD1	2.42	0.49
1:A:95:ARG:HH11	1:A:95:ARG:HB3	1.76	0.49
1:A:121:THR:H	1:A:124:ARG:HB2	1.77	0.49
1:A:372:ARG:HD3	5:A:834:SO4:O1	2.12	0.49
1:A:13:VAL:HG13	1:A:32:TRP:NE1	2.28	0.49
1:A:177:THR:O	1:A:235:ARG:HG3	2.12	0.49
1:A:255:MET:HG3	1:A:315:PHE:HB2	1.95	0.49
1:A:131:ALA:HB1	1:A:136:ILE:HB	1.95	0.49
1:A:120:LEU:HG	1:A:169:ILE:HG12	1.94	0.49
1:A:340:LEU:HD22	1:A:346:HIS:CA	2.35	0.49
1:A:372:ARG:CG	5:A:834:SO4:O1	2.60	0.49
2:B:39:GLN:NE2	3:T:702:DA:H62	2.04	0.49
1:A:42:SER:C	1:A:44:SER:N	2.66	0.49
2:B:53:THR:HG22	2:B:56:THR:H	1.77	0.49
2:B:55:THR:HG22	2:B:59:LYS:HE3	1.95	0.49
1:A:128:VAL:HG13	1:A:139:GLY:O	2.13	0.49
1:A:183:PRO:HD3	1:A:229:ARG:O	2.13	0.49
2:B:32:ALA:HB1	2:B:37:ILE:O	2.14	0.48
2:B:53:THR:HG22	2:B:55:THR:N	2.28	0.48
3:T:713:DG:H2''	3:T:714:DG:H5'	1.94	0.48
1:A:96:ASP:HB3	1:A:149:ILE:HD12	1.95	0.48
1:A:237:ASP:HB3	1:A:252:GLN:OE1	2.14	0.48
1:A:4:LEU:HB2	1:A:87:PHE:CE1	2.44	0.48
1:A:279:MET:HE1	1:A:292:ARG:CG	2.44	0.48
1:A:32:TRP:C	1:A:34:ALA:H	2.17	0.48
1:A:36:ARG:NH1	1:A:36:ARG:HG3	2.28	0.48
1:A:119:LYS:HD2	1:A:166:ASP:CG	2.35	0.48
1:A:380:VAL:HG23	1:A:381:LEU:N	2.28	0.48
1:A:79:TYR:CD1	1:A:79:TYR:N	2.82	0.48
1:A:289:LEU:HD13	1:A:289:LEU:HA	1.47	0.48
1:A:161:LEU:HD12	1:A:162:ARG:H	1.79	0.47
1:A:411:PRO:C	1:A:413:ASP:H	2.17	0.47
1:A:20:ALA:C	1:A:22:GLY:H	2.17	0.47
1:A:36:ARG:HG3	1:A:36:ARG:HH11	1.78	0.47
1:A:44:SER:HB3	1:A:258:THR:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:SER:O	1:A:270:ASP:OD2	2.33	0.47
1:A:337:PHE:O	1:A:339:VAL:N	2.48	0.47
3:T:714:DG:H2''	3:T:715:DG:H5'	1.96	0.47
1:A:14:GLY:O	1:A:15:GLU:HB3	2.14	0.47
1:A:225:ALA:HB3	1:A:228:VAL:HG13	1.96	0.47
1:A:337:PHE:C	1:A:339:VAL:N	2.68	0.47
1:A:382:ARG:HH12	3:T:713:DG:H5''	1.79	0.47
1:A:406:VAL:O	1:A:409:SER:HB2	2.14	0.47
3:T:704:DC:H2''	3:T:705:DC:C6	2.49	0.47
1:A:120:LEU:CG	1:A:169:ILE:HG12	2.44	0.47
1:A:183:PRO:O	1:A:184:ILE:C	2.53	0.47
1:A:259:PHE:HB3	1:A:277:ARG:NH1	2.30	0.47
1:A:30:PRO:HG3	5:A:878:SO4:O3	2.15	0.46
1:A:399:ILE:HB	1:A:430:HIS:CD2	2.51	0.46
3:T:702:DA:H2''	3:T:703:DT:H5''	1.96	0.46
1:A:98:VAL:HG11	4:A:500:ATP:H1'	1.96	0.46
1:A:175:PRO:CA	1:A:249:ARG:HH21	2.27	0.46
1:A:360:LYS:HD3	1:A:363:LYS:NZ	2.30	0.46
1:A:399:ILE:HG13	1:A:430:HIS:CD2	2.41	0.46
1:A:399:ILE:HB	1:A:400:PRO:CD	2.40	0.46
1:A:132:TYR:CB	1:A:156:GLU:HG2	2.46	0.46
1:A:204:TYR:CB	1:A:222:ILE:HD11	2.46	0.46
1:A:316:SER:C	1:A:328:THR:HG23	2.36	0.46
2:B:7:ILE:HA	2:B:12:GLN:CD	2.36	0.46
3:T:716:DA:H2''	3:T:717:DT:OP2	2.15	0.46
1:A:120:LEU:HD21	1:A:169:ILE:HG12	1.98	0.46
1:A:5:VAL:HB	1:A:7:TRP:HE1	1.81	0.46
1:A:359:SER:C	1:A:361:GLY:H	2.20	0.46
1:A:120:LEU:HD21	1:A:169:ILE:CG1	2.45	0.46
1:A:128:VAL:HG13	1:A:139:GLY:HA3	1.98	0.46
1:A:281:PHE:CE2	1:A:317:VAL:HG11	2.47	0.46
1:A:293:TYR:CD1	1:A:387:GLN:HG2	2.51	0.46
1:A:78:ARG:HH21	1:A:140:MSE:HE3	1.79	0.45
1:A:3:LYS:HD2	1:A:106:GLU:CD	2.37	0.45
1:A:141:ILE:HD12	1:A:141:ILE:O	2.16	0.45
1:A:180:ILE:N	1:A:180:ILE:HD12	2.31	0.45
1:A:244:ARG:HH11	1:A:244:ARG:HG2	1.82	0.45
1:A:363:LYS:NZ	5:A:833:SO4:O3	2.48	0.45
1:A:181:LYS:C	1:A:182:LEU:HD13	2.36	0.45
1:A:411:PRO:HB2	1:A:413:ASP:OD1	2.16	0.45
2:B:52:THR:O	2:B:53:THR:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LEU:O	1:A:132:TYR:HE2	1.98	0.45
1:A:259:PHE:CD2	1:A:277:ARG:NH1	2.85	0.45
1:A:358:ALA:HB2	1:A:363:LYS:HG2	1.98	0.45
1:A:21:ASN:C	1:A:21:ASN:ND2	2.70	0.45
1:A:236:PHE:C	1:A:236:PHE:CD2	2.89	0.45
1:A:266:LYS:HG3	1:A:267:TYR:CD1	2.51	0.45
2:B:69:THR:OG1	2:B:70:LEU:N	2.49	0.45
3:T:715:DG:H1'	3:T:716:DA:H5'	2.00	0.45
1:A:8:MET:HE1	1:A:251:PRO:HB3	1.98	0.44
1:A:71:VAL:HG12	1:A:75:ILE:HD11	1.99	0.44
1:A:147:PHE:CD2	1:A:169:ILE:HG23	2.52	0.44
1:A:151:VAL:HB	1:A:157:LYS:HD3	1.99	0.44
1:A:403:LEU:O	1:A:406:VAL:HB	2.17	0.44
1:A:320:GLN:HB2	1:A:324:SER:HB2	1.98	0.44
1:A:37:TYR:O	1:A:38:ALA:C	2.56	0.44
1:A:156:GLU:OE1	1:A:156:GLU:HA	2.18	0.44
1:A:155:GLN:HG3	1:A:184:ILE:CD1	2.46	0.44
1:A:110:VAL:CG1	1:A:112:HIS:CE1	3.01	0.44
1:A:75:ILE:C	1:A:77:LYS:H	2.21	0.44
1:A:434:SER:C	1:A:436:GLU:H	2.20	0.43
1:A:372:ARG:HB3	5:A:834:SO4:O1	2.18	0.43
1:A:103:LEU:O	1:A:104:ILE:HD13	2.18	0.43
1:A:309:GLN:O	1:A:311:HIS:N	2.46	0.43
2:B:28:GLN:HE22	2:B:43:SER:HA	1.83	0.43
3:T:701:DT:H2''	3:T:702:DA:C8	2.54	0.43
1:A:98:VAL:CG1	1:A:99:GLY:N	2.81	0.43
1:A:48:GLN:HA	2:B:22:GLN:HE22	1.82	0.43
1:A:263:SER:OG	1:A:266:LYS:NZ	2.52	0.43
1:A:43:LEU:HA	1:A:43:LEU:HD23	1.82	0.43
1:A:68:SER:HB3	1:A:71:VAL:CG2	2.47	0.43
1:A:290:LYS:O	1:A:293:TYR:HB3	2.19	0.43
1:A:300:VAL:O	1:A:303:TRP:HB3	2.19	0.43
1:A:123:ALA:O	1:A:126:GLU:N	2.52	0.43
1:A:197:SER:HB2	1:A:198:GLN:OE1	2.19	0.43
1:A:383:PHE:O	1:A:384:PRO:C	2.57	0.42
1:A:117:TRP:O	1:A:117:TRP:CD1	2.73	0.42
1:A:124:ARG:O	1:A:127:GLU:HB2	2.19	0.42
1:A:147:PHE:CE2	1:A:169:ILE:HD12	2.54	0.42
1:A:266:LYS:HB2	1:A:311:HIS:HB2	2.00	0.42
1:A:285:SER:HB3	1:A:288:ALA:HA	2.00	0.42
1:A:407:LYS:C	1:A:409:SER:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:715:DG:H2''	3:T:716:DA:O5'	2.18	0.42
2:B:39:GLN:N	5:B:640:SO4:O3	2.51	0.42
1:A:7:TRP:N	1:A:7:TRP:CD1	2.87	0.42
1:A:83:SER:OG	1:A:84:ARG:N	2.53	0.42
1:A:204:TYR:HB2	1:A:222:ILE:HD11	2.01	0.42
1:A:118:GLU:CB	1:A:171:LYS:HE3	2.49	0.42
1:A:184:ILE:HG12	1:A:199:SER:CB	2.50	0.42
1:A:339:VAL:HG12	1:A:339:VAL:O	2.20	0.42
1:A:121:THR:HG23	1:A:124:ARG:HD2	2.02	0.42
1:A:99:GLY:CA	1:A:252:GLN:HG2	2.48	0.41
2:B:64:LEU:O	2:B:65:GLU:HB2	2.20	0.41
1:A:21:ASN:C	1:A:21:ASN:HD22	2.23	0.41
1:A:167:TRP:CH2	1:A:232:ALA:HB1	2.55	0.41
1:A:257:GLN:O	1:A:260:GLY:N	2.48	0.41
1:A:347:ILE:HG23	1:A:367:ASP:OD1	2.19	0.41
2:B:13:LEU:HD22	2:B:17:MET:SD	2.61	0.41
3:T:718:DA:H1'	3:T:719:DG:C5'	2.48	0.41
1:A:138:LEU:HB2	1:A:140:MSE:HE2	2.02	0.41
1:A:255:MET:HE3	1:A:278:ILE:CG2	2.47	0.41
1:A:337:PHE:H	1:A:338:PRO:HD2	1.85	0.41
1:A:75:ILE:HD13	1:A:137:PRO:HG3	2.03	0.41
1:A:322:GLY:HA3	2:B:5:GLN:HB3	2.03	0.41
1:A:261:LEU:HB3	1:A:262:PRO:HD2	2.01	0.41
1:A:285:SER:OG	1:A:286:SER:N	2.54	0.41
1:A:433:LEU:O	1:A:436:GLU:N	2.50	0.41
2:B:20:VAL:HG11	2:B:66:LEU:HD21	2.02	0.41
1:A:74:ARG:HB3	1:A:137:PRO:HB3	2.03	0.41
1:A:197:SER:HB2	1:A:198:GLN:H	1.67	0.41
1:A:255:MET:CG	1:A:315:PHE:HB2	2.50	0.41
1:A:312:ALA:C	1:A:314:ASN:H	2.23	0.41
1:A:352:LEU:O	1:A:353:ALA:C	2.58	0.41
1:A:363:LYS:NZ	5:A:833:SO4:O4	2.53	0.41
3:T:703:DT:C2	3:T:704:DC:C5	3.09	0.41
1:A:200:VAL:HG13	1:A:231:LEU:CB	2.48	0.41
1:A:297:LYS:HA	1:A:391:ILE:HG21	2.02	0.41
1:A:411:PRO:C	1:A:413:ASP:N	2.74	0.41
1:A:418:VAL:O	1:A:422:VAL:HG23	2.21	0.41
1:A:70:ILE:HD12	1:A:70:ILE:N	2.36	0.41
1:A:79:TYR:CE2	1:A:148:ARG:NE	2.89	0.41
1:A:83:SER:OG	1:A:85:GLN:N	2.45	0.41
1:A:85:GLN:O	1:A:86:PRO:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:TYR:O	1:A:371:PRO:C	2.59	0.41
1:A:27:LYS:HG2	1:A:28:TYR:O	2.21	0.41
1:A:257:GLN:O	1:A:258:THR:C	2.59	0.41
1:A:314:ASN:ND2	1:A:332:ASP:OD2	2.50	0.41
2:B:31:LEU:O	2:B:35:ILE:HG12	2.21	0.41
1:A:13:VAL:HG13	1:A:32:TRP:CE2	2.56	0.40
1:A:42:SER:C	1:A:44:SER:H	2.24	0.40
1:A:75:ILE:HD13	1:A:137:PRO:CG	2.50	0.40
2:B:14:ALA:HB2	2:B:49:PRO:HG3	2.02	0.40
1:A:120:LEU:CD2	1:A:124:ARG:HB3	2.50	0.40
1:A:132:TYR:HB3	1:A:156:GLU:HG2	2.02	0.40
1:A:175:PRO:CB	1:A:249:ARG:HE	2.30	0.40
3:T:708:DT:H2''	3:T:709:DT:C6	2.56	0.40
1:A:217:VAL:O	1:A:217:VAL:HG23	2.21	0.40
1:A:224:LYS:HE2	1:A:224:LYS:HB3	1.88	0.40
1:A:430:HIS:O	1:A:433:LEU:HB2	2.22	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	417/440 (95%)	316 (76%)	80 (19%)	21 (5%)	2	11
2	B	69/88 (78%)	64 (93%)	4 (6%)	1 (1%)	11	41
All	All	486/528 (92%)	380 (78%)	84 (17%)	22 (4%)	2	13

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	GLU
1	A	110	VAL

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Mol	Chain	Res	Type
1	A	313	LYS
1	A	347	ILE
1	A	212	GLU
1	A	276	ALA
1	A	77	LYS
1	A	332	ASP
1	A	342	GLY
1	A	416	GLU
1	A	111	THR
1	A	142	ARG
1	A	227	ASN
1	A	384	PRO
2	B	53	THR
1	A	38	ALA
1	A	412	THR
1	A	21	ASN
1	A	310	GLY
1	A	337	PHE
1	A	275	ILE
1	A	338	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	360/371 (97%)	329 (91%)	31 (9%)	10	35
2	B	64/80 (80%)	53 (83%)	11 (17%)	2	9
All	All	424/451 (94%)	382 (90%)	42 (10%)	8	28

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	21	ASN
1	A	36	ARG

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Mol	Chain	Res	Type
1	A	73	ASP
1	A	78	ARG
1	A	79	TYR
1	A	80	HIS
1	A	85	GLN
1	A	95	ARG
1	A	157	LYS
1	A	176	THR
1	A	182	LEU
1	A	198	GLN
1	A	216	ASN
1	A	243	ARG
1	A	244	ARG
1	A	266	LYS
1	A	283	MSE
1	A	289	LEU
1	A	305	ILE
1	A	327	LEU
1	A	332	ASP
1	A	346	HIS
1	A	356	LEU
1	A	371	PRO
1	A	386	VAL
1	A	387	GLN
1	A	393	SER
1	A	397	ARG
1	A	416	GLU
1	A	427	LEU
2	B	5	GLN
2	B	13	LEU
2	B	19	LEU
2	B	23	GLN
2	B	39	GLN
2	B	44	ASN
2	B	61	LEU
2	B	66	LEU
2	B	68	MET
2	B	69	THR
2	B	72	ASP

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	21	ASN
1	A	112	HIS
1	A	216	ASN
1	A	309	GLN
1	A	387	GLN
1	A	430	HIS
2	B	12	GLN
2	B	15	ASN
2	B	22	GLN
2	B	23	GLN
2	B	39	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	SO4	A	833	-	4,4,4	0.76	0	6,6,6	0.39	0
5	SO4	A	879	-	4,4,4	0.39	0	6,6,6	0.15	0
5	SO4	A	834	-	4,4,4	0.39	0	6,6,6	0.45	0
5	SO4	A	837	-	4,4,4	0.23	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SO4	A	878	-	4,4,4	0.35	0	6,6,6	0.41	0
5	SO4	A	835	-	4,4,4	0.63	0	6,6,6	0.33	0
5	SO4	A	836	-	4,4,4	0.42	0	6,6,6	0.32	0
4	ATP	A	500	-	26,33,33	1.58	3 (11%)	31,52,52	1.46	4 (12%)
5	SO4	A	838	-	4,4,4	0.31	0	6,6,6	0.33	0
5	SO4	B	640	-	4,4,4	0.66	0	6,6,6	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	500	-	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	500	ATP	C2-N3	4.40	1.39	1.32
4	A	500	ATP	C4-N3	4.29	1.41	1.35
4	A	500	ATP	O4'-C1'	2.65	1.44	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	500	ATP	C3'-C2'-C1'	4.50	107.75	100.98
4	A	500	ATP	O2B-PB-O1B	4.15	132.76	112.24
4	A	500	ATP	PB-O3B-PG	-2.31	124.89	132.83
4	A	500	ATP	PA-O3A-PB	2.21	140.40	132.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	500	ATP	PB-O3B-PG-O1G
4	A	500	ATP	O4'-C4'-C5'-O5'
4	A	500	ATP	C3'-C4'-C5'-O5'

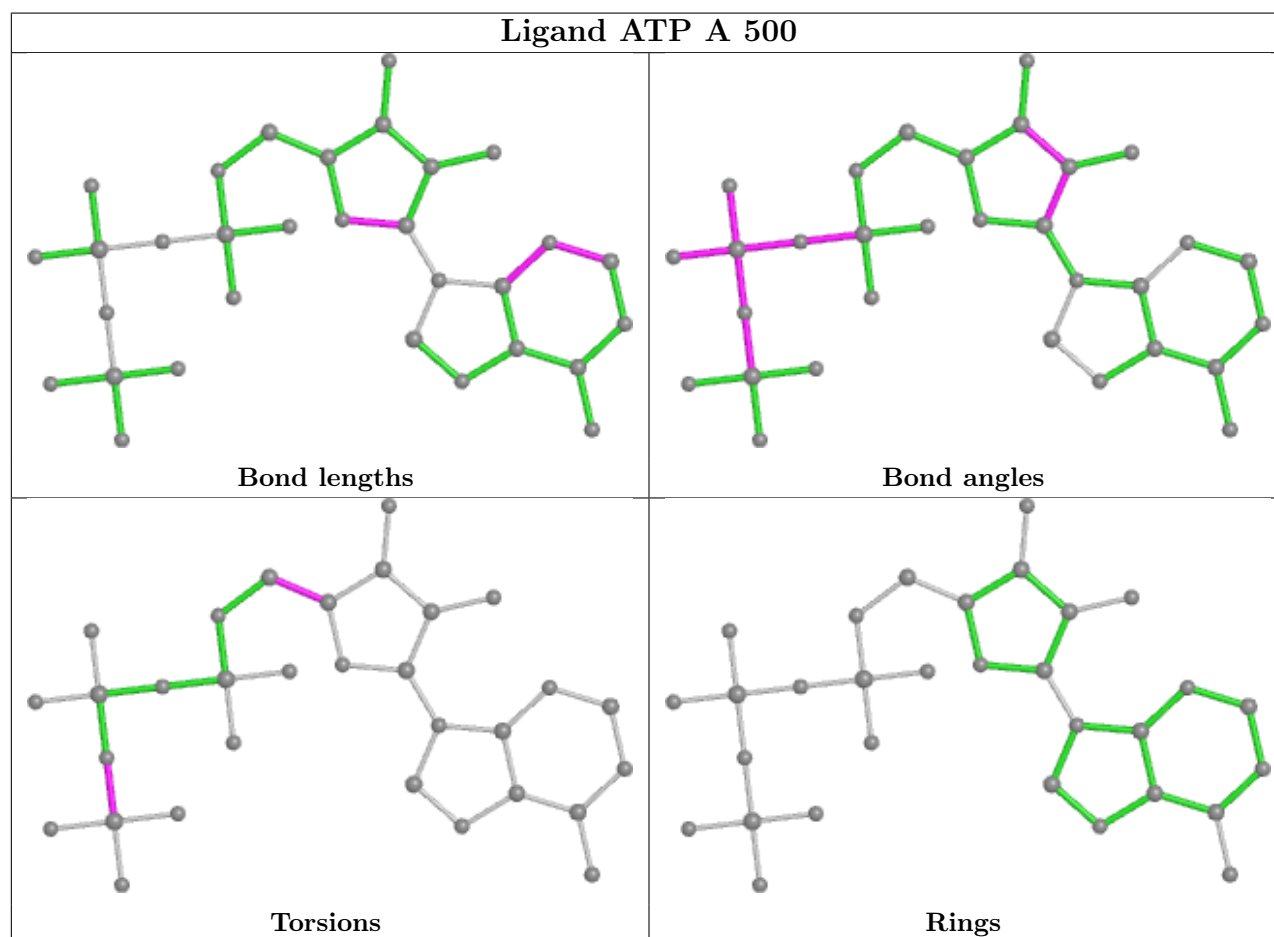
There are no ring outliers.

6 monomers are involved in 18 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	833	SO4	4	0
5	A	834	SO4	4	0
5	A	878	SO4	2	0
5	A	836	SO4	2	0
4	A	500	ATP	2	0
5	B	640	SO4	4	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

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	420/440 (95%)	0.81	55 (13%) <b>3</b> <b>1</b>	39, 81, 133, 146	0
2	B	71/88 (80%)	0.45	2 (2%) 53 34	33, 58, 92, 122	0
3	T	21/21 (100%)	-0.16	0 <b>100</b> <b>100</b>	63, 90, 112, 114	0
All	All	512/549 (93%)	0.72	57 (11%) <b>5</b> <b>3</b>	33, 77, 131, 146	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	PHE	7.2
1	A	163	ILE	6.2
1	A	149	ILE	6.1
1	A	87	PHE	6.1
1	A	233	VAL	5.6
1	A	120	LEU	5.5
1	A	167	TRP	4.8
1	A	179	ILE	3.7
1	A	196	LEU	3.7
1	A	139	GLY	3.6
1	A	119	LYS	3.5
1	A	358	ALA	3.5
1	A	117	TRP	3.4
1	A	141	ILE	3.2
1	A	111	THR	3.2
1	A	433	LEU	3.1
1	A	168	CYS	3.0
1	A	345	ILE	2.9
1	A	340	LEU	2.9
1	A	366	ILE	2.8
1	A	414	PHE	2.8
1	A	110	VAL	2.8
1	A	368	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	90	LEU	2.8
1	A	227	ASN	2.7
1	A	342	GLY	2.7
1	A	19	LEU	2.7
1	A	86	PRO	2.6
1	A	419	VAL	2.6
1	A	61	PHE	2.6
1	A	148	ARG	2.5
1	A	347	ILE	2.5
1	A	341	GLY	2.4
1	A	93	ILE	2.4
1	A	209	LEU	2.4
1	A	138	LEU	2.3
1	A	200	VAL	2.3
1	A	92	GLU	2.3
1	A	215	LEU	2.3
2	B	5	GLN	2.2
1	A	118	GLU	2.2
1	A	89	LEU	2.2
1	A	184	ILE	2.2
1	A	103	LEU	2.2
1	A	125	LEU	2.1
1	A	437	TYR	2.1
1	A	410	LEU	2.1
2	B	45	PHE	2.1
1	A	218	PRO	2.1
1	A	95	ARG	2.1
1	A	356	LEU	2.1
1	A	203	GLU	2.1
1	A	259	PHE	2.1
1	A	41	LEU	2.1
1	A	99	GLY	2.1
1	A	13	VAL	2.0
1	A	43	LEU	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 [i](#)

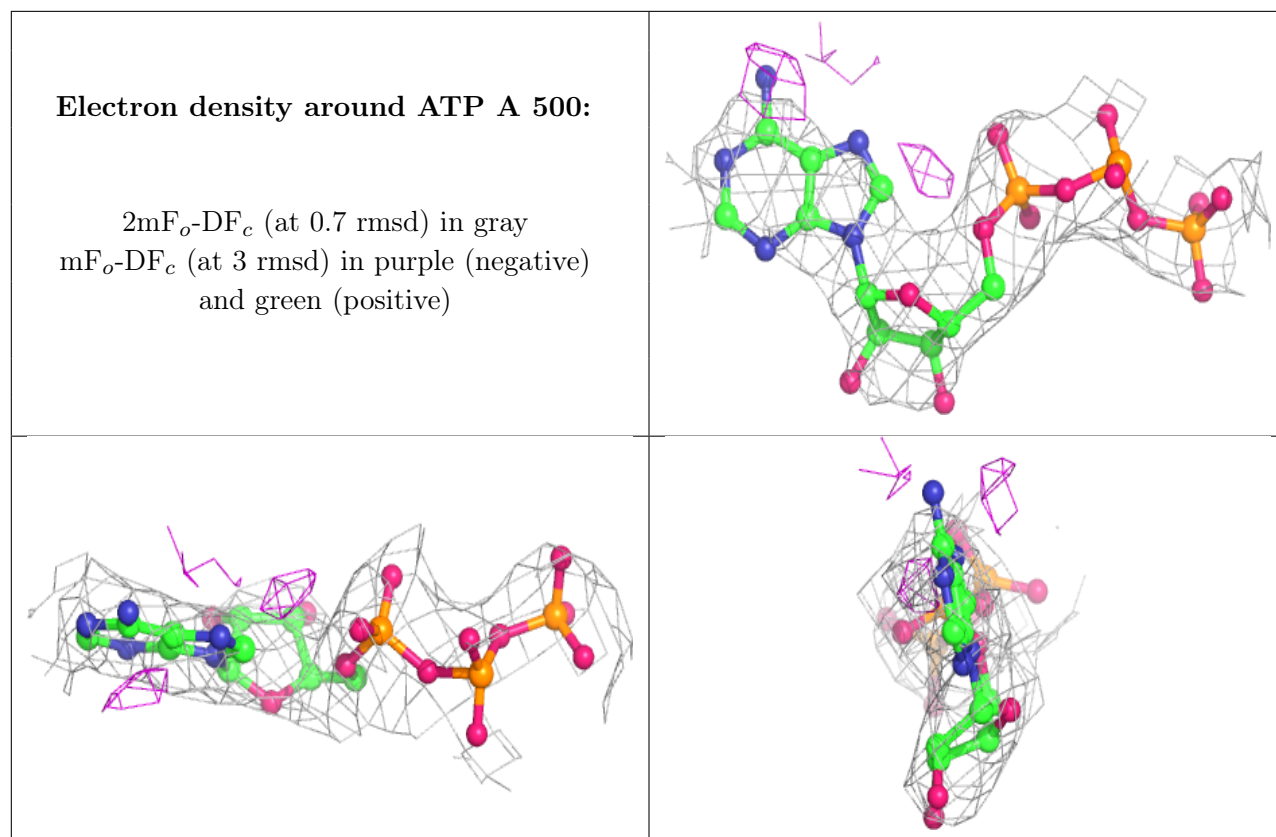
There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	SO4	A	835	5/5	0.67	0.22	119,120,123,137	0
5	SO4	B	640	5/5	0.71	0.41	100,100,106,126	0
5	SO4	A	833	5/5	0.76	0.25	92,98,103,127	0
5	SO4	A	878	5/5	0.84	0.20	121,122,126,129	0
5	SO4	A	838	5/5	0.86	0.29	101,102,108,117	0
5	SO4	A	879	5/5	0.89	0.18	134,135,136,140	0
5	SO4	A	834	5/5	0.89	0.21	103,104,108,122	0
4	ATP	A	500	31/31	0.90	0.36	88,108,147,150	0
5	SO4	A	836	5/5	0.93	0.27	120,121,125,131	0
5	SO4	A	837	5/5	0.94	0.20	115,119,122,122	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.