



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 08:01 PM EDT

PDB ID : 1HI1  
Title : RNA dependent RNA polymerase from dsRNA bacteriophage phi6 plus bound NTP  
Authors : Grimes, J.M.; Butcher, S.J.; Makeyev, E.V.; Bamford, D.H.; Stuart, D.I.  
Deposited on : 2001-01-01  
Resolution : 3.00 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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

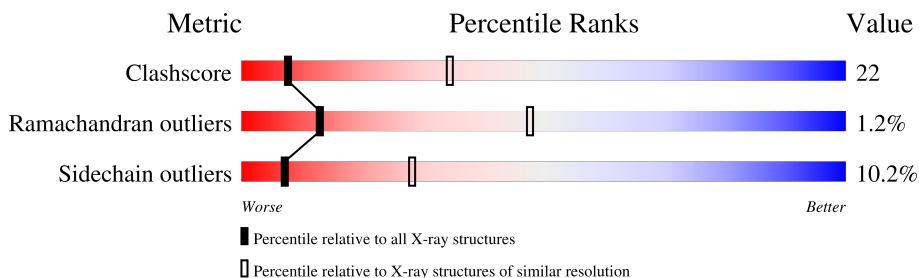
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	664	
1	B	664	
1	C	664	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 15888 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.

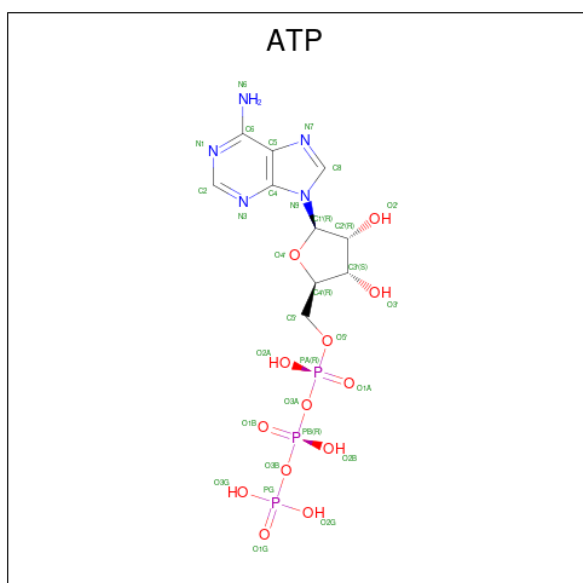
- Molecule 1 is a protein called P2 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	B	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			
1	C	664	Total	C	N	O	S	0	0	0
			5265	3342	914	977	32			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	456	MET	ILE	conflict	UNP P11124
B	456	MET	ILE	conflict	UNP P11124
C	456	MET	ILE	conflict	UNP P11124

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



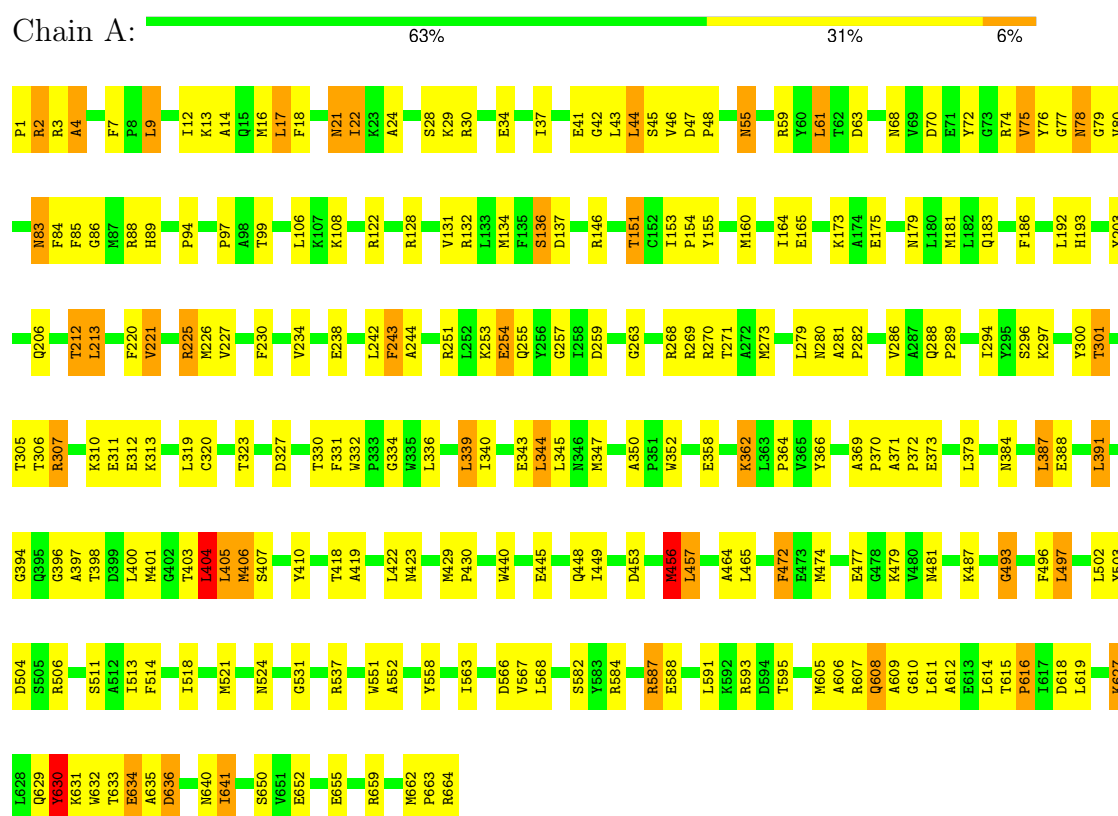
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

### 3 Residue-property plots

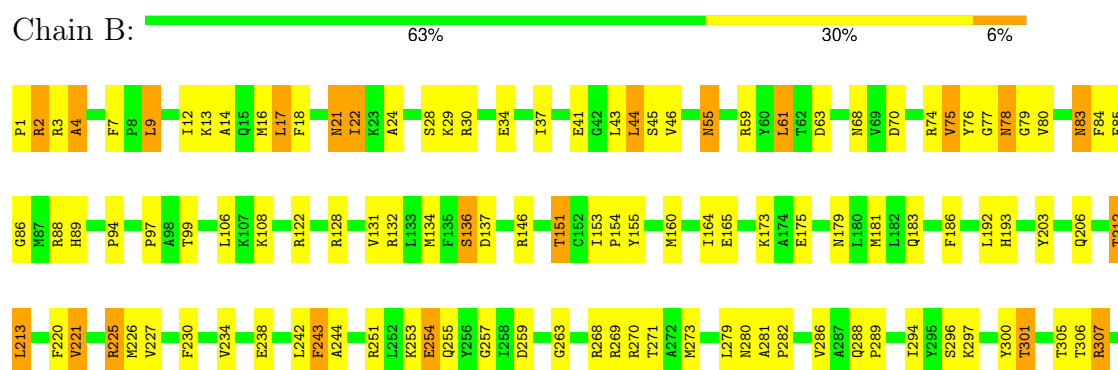
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: P2 PROTEIN



#### • Molecule 1: P2 PROTEIN





## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.65Å 92.70Å 140.79Å 90.00° 101.09° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program		Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15888	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.70	0/5396	0.87	5/7297 (0.1%)
1	B	0.70	0/5396	0.87	5/7297 (0.1%)
1	C	0.70	0/5396	0.87	5/7297 (0.1%)
All	All	0.70	0/16188	0.87	15/21891 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	GLN	N-CA-C	-6.97	92.17	111.00
1	B	206	GLN	N-CA-C	-6.97	92.19	111.00
1	C	206	GLN	N-CA-C	-6.96	92.20	111.00
1	B	339	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	339	LEU	CA-CB-CG	5.86	128.78	115.30
1	C	339	LEU	CA-CB-CG	5.85	128.75	115.30
1	C	493	GLY	N-CA-C	-5.40	99.61	113.10
1	B	493	GLY	N-CA-C	-5.38	99.65	113.10
1	A	493	GLY	N-CA-C	-5.38	99.66	113.10
1	A	404	LEU	CA-CB-CG	5.37	127.66	115.30
1	B	404	LEU	CA-CB-CG	5.37	127.65	115.30
1	C	404	LEU	CA-CB-CG	5.36	127.62	115.30
1	C	456	MET	N-CA-C	-5.22	96.89	111.00
1	B	456	MET	N-CA-C	-5.22	96.92	111.00
1	A	456	MET	N-CA-C	-5.21	96.93	111.00

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	5265	0	5164	237	3
1	B	5265	0	5164	238	0
1	C	5265	0	5164	225	3
2	A	31	0	9	7	0
2	B	31	0	9	7	0
2	C	31	0	9	7	0
All	All	15888	0	15519	689	3

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 22.

All (689) 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:270:ARG:NH1	2:A:665:ATP:O3'	1.59	1.35
1:B:270:ARG:NH1	2:B:665:ATP:O3'	1.59	1.34
1:C:270:ARG:NH1	2:C:665:ATP:O3'	1.59	1.31
1:A:270:ARG:HH22	2:A:665:ATP:PA	1.66	1.19
1:B:270:ARG:HH22	2:B:665:ATP:PA	1.66	1.18
1:C:270:ARG:HH22	2:C:665:ATP:PA	1.66	1.17
1:B:22:ILE:HD12	1:B:22:ILE:H	1.16	1.11
1:C:405:LEU:HG	1:C:406:MET:H	1.15	1.10
1:B:405:LEU:HG	1:B:406:MET:H	1.14	1.08
1:C:22:ILE:HD12	1:C:22:ILE:H	1.16	1.06
1:A:405:LEU:HG	1:A:406:MET:H	1.14	1.06
1:A:22:ILE:HD12	1:A:22:ILE:H	1.16	1.03
1:A:270:ARG:NH2	2:A:665:ATP:PA	2.35	1.00
1:A:251:ARG:HH11	1:A:255:GLN:HE22	1.10	1.00
1:C:270:ARG:NH2	2:C:665:ATP:PA	2.35	0.99
1:B:270:ARG:NH2	2:B:665:ATP:PA	2.35	0.99
1:C:122:ARG:HH11	1:C:423:ASN:HD21	1.02	0.99
1:A:122:ARG:HH11	1:A:423:ASN:HD21	1.02	0.98
1:C:225:ARG:HG3	1:C:225:ARG:HH11	1.27	0.98
1:C:122:ARG:HH11	1:C:423:ASN:ND2	1.63	0.97
1:C:251:ARG:HH11	1:C:255:GLN:HE22	1.10	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:HG3	1:A:225:ARG:HH11	1.27	0.97
1:A:226:MET:HE1	1:A:244:ALA:HB2	1.46	0.96
1:B:225:ARG:HG3	1:B:225:ARG:HH11	1.27	0.96
1:B:122:ARG:HH11	1:B:423:ASN:ND2	1.63	0.96
1:B:270:ARG:NH2	2:B:665:ATP:O1A	1.98	0.96
1:A:270:ARG:NH2	2:A:665:ATP:O1A	1.98	0.96
1:A:122:ARG:HH11	1:A:423:ASN:ND2	1.63	0.95
1:A:593:ARG:NH1	1:B:608:GLN:HE22	1.65	0.95
1:C:270:ARG:NH2	2:C:665:ATP:O1A	1.98	0.95
1:B:122:ARG:HH11	1:B:423:ASN:HD21	1.02	0.95
1:B:251:ARG:HH11	1:B:255:GLN:HE22	1.10	0.94
1:A:122:ARG:NH1	1:A:423:ASN:HD21	1.67	0.93
1:C:226:MET:HE1	1:C:244:ALA:HB2	1.48	0.93
1:C:122:ARG:NH1	1:C:423:ASN:HD21	1.67	0.92
1:B:226:MET:HE1	1:B:244:ALA:HB2	1.48	0.92
1:B:427:LYS:HE3	1:C:12:ILE:HG21	1.52	0.91
1:B:122:ARG:NH1	1:B:423:ASN:HD21	1.67	0.91
1:C:83:ASN:HD22	1:C:85:PHE:H	1.20	0.90
1:C:22:ILE:H	1:C:22:ILE:CD1	1.83	0.90
1:A:83:ASN:HD22	1:A:85:PHE:H	1.20	0.88
1:B:83:ASN:HD22	1:B:85:PHE:H	1.20	0.88
1:A:22:ILE:H	1:A:22:ILE:CD1	1.83	0.87
1:A:405:LEU:HG	1:A:406:MET:N	1.90	0.87
1:A:68:ASN:ND2	1:A:78:ASN:H	1.73	0.87
1:C:68:ASN:ND2	1:C:78:ASN:H	1.73	0.86
1:B:364:PRO:HA	1:B:387:LEU:CD2	2.06	0.86
1:A:364:PRO:HA	1:A:387:LEU:CD2	2.06	0.86
1:B:68:ASN:ND2	1:B:78:ASN:H	1.73	0.86
1:B:405:LEU:HG	1:B:406:MET:N	1.90	0.85
1:C:364:PRO:HA	1:C:387:LEU:CD2	2.06	0.85
1:C:405:LEU:HG	1:C:406:MET:N	1.90	0.85
1:B:270:ARG:NH2	2:B:665:ATP:O2A	2.10	0.84
1:C:270:ARG:NH2	2:C:665:ATP:O2A	2.10	0.84
1:A:593:ARG:CD	1:B:608:GLN:OE1	2.24	0.83
1:A:270:ARG:NH2	2:A:665:ATP:O2A	2.10	0.82
1:B:55:ASN:HD21	1:B:59:ARG:HD2	1.44	0.82
1:C:55:ASN:HD21	1:C:59:ARG:HD2	1.44	0.82
1:C:78:ASN:HD22	1:C:79:GLY:N	1.78	0.82
1:A:83:ASN:ND2	1:A:85:PHE:H	1.78	0.82
1:B:132:ARG:HA	1:B:347:MET:CE	2.10	0.82
1:A:78:ASN:HD22	1:A:79:GLY:N	1.78	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ASN:ND2	1:B:85:PHE:H	1.78	0.81
1:C:132:ARG:HA	1:C:347:MET:CE	2.10	0.81
1:C:606:ALA:HB3	1:C:609:ALA:HB2	1.62	0.81
1:A:55:ASN:HD21	1:A:59:ARG:HD2	1.44	0.81
1:C:281:ALA:HB3	1:C:282:PRO:HD3	1.63	0.81
1:A:68:ASN:HD22	1:A:78:ASN:H	1.28	0.81
1:A:132:ARG:HA	1:A:347:MET:CE	2.10	0.80
1:B:78:ASN:HD22	1:B:79:GLY:N	1.78	0.80
1:C:83:ASN:ND2	1:C:85:PHE:H	1.78	0.80
1:A:281:ALA:HB3	1:A:282:PRO:HD3	1.63	0.80
1:A:606:ALA:HB3	1:A:609:ALA:HB2	1.62	0.80
1:B:22:ILE:H	1:B:22:ILE:CD1	1.83	0.80
1:B:606:ALA:HB3	1:B:609:ALA:HB2	1.62	0.80
1:B:281:ALA:HB3	1:B:282:PRO:HD3	1.63	0.79
1:B:131:VAL:HG12	1:B:347:MET:CE	2.13	0.78
1:A:42:GLY:HA2	1:B:593:ARG:HG3	1.66	0.78
1:C:251:ARG:HH11	1:C:255:GLN:NE2	1.81	0.78
1:B:68:ASN:HD22	1:B:78:ASN:H	1.28	0.78
1:C:68:ASN:HD22	1:C:78:ASN:H	1.28	0.78
1:C:131:VAL:HG12	1:C:347:MET:HE3	1.66	0.78
1:A:131:VAL:HG12	1:A:347:MET:CE	2.13	0.77
1:C:270:ARG:NH1	2:C:665:ATP:C3'	2.48	0.77
1:B:251:ARG:HH11	1:B:255:GLN:NE2	1.81	0.77
1:B:270:ARG:NH1	2:B:665:ATP:C3'	2.48	0.77
1:B:427:LYS:HE3	1:C:12:ILE:CG2	2.14	0.77
1:C:131:VAL:HG12	1:C:347:MET:CE	2.13	0.77
1:A:270:ARG:NH1	2:A:665:ATP:C3'	2.48	0.76
1:A:251:ARG:HH11	1:A:255:GLN:NE2	1.81	0.76
1:C:34:GLU:OE1	1:C:251:ARG:NH2	2.17	0.76
1:C:78:ASN:ND2	1:C:80:VAL:H	1.84	0.76
1:B:34:GLU:OE1	1:B:251:ARG:NH2	2.17	0.75
1:A:78:ASN:ND2	1:A:80:VAL:H	1.84	0.75
1:B:131:VAL:HG12	1:B:347:MET:HE3	1.68	0.75
1:B:650:SER:HB2	1:B:652:GLU:OE1	1.87	0.74
1:B:78:ASN:ND2	1:B:80:VAL:H	1.84	0.74
1:A:650:SER:HB2	1:A:652:GLU:OE1	1.87	0.74
1:A:131:VAL:HG12	1:A:347:MET:HE3	1.68	0.73
1:B:610:GLY:C	1:B:612:ALA:H	1.91	0.73
1:B:243:PHE:HD1	1:B:243:PHE:H	1.37	0.73
1:C:610:GLY:C	1:C:612:ALA:H	1.91	0.73
1:C:650:SER:HB2	1:C:652:GLU:OE1	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLU:OE1	1:A:251:ARG:NH2	2.17	0.72
1:A:610:GLY:C	1:A:612:ALA:H	1.91	0.72
1:C:55:ASN:ND2	1:C:59:ARG:HD2	2.05	0.72
1:C:226:MET:CE	1:C:244:ALA:HB2	2.20	0.71
1:B:3:ARG:O	1:B:4:ALA:HB3	1.90	0.71
1:A:55:ASN:ND2	1:A:59:ARG:HD2	2.05	0.71
1:A:405:LEU:O	1:A:407:SER:N	2.24	0.71
1:C:3:ARG:O	1:C:4:ALA:HB3	1.90	0.71
1:B:364:PRO:HA	1:B:387:LEU:HD22	1.73	0.70
1:A:3:ARG:O	1:A:4:ALA:HB3	1.90	0.70
1:A:243:PHE:HD1	1:A:243:PHE:H	1.37	0.70
1:B:405:LEU:O	1:B:407:SER:N	2.24	0.70
1:C:364:PRO:HA	1:C:387:LEU:HD22	1.73	0.70
1:B:55:ASN:ND2	1:B:59:ARG:HD2	2.05	0.70
1:B:226:MET:CE	1:B:244:ALA:HB2	2.20	0.70
1:C:405:LEU:O	1:C:407:SER:N	2.24	0.69
1:A:364:PRO:HA	1:A:387:LEU:HD22	1.73	0.69
1:B:74:ARG:HB3	1:B:503:TYR:CD2	2.27	0.69
1:C:74:ARG:HB3	1:C:503:TYR:CD2	2.27	0.69
1:C:173:LYS:HG2	1:C:193:HIS:CE1	2.28	0.69
1:A:173:LYS:HG2	1:A:193:HIS:CE1	2.28	0.69
1:A:74:ARG:HB3	1:A:503:TYR:CD2	2.27	0.69
1:A:226:MET:CE	1:A:244:ALA:HB2	2.20	0.69
1:C:419:ALA:HB1	1:C:422:LEU:HD12	1.76	0.68
1:A:593:ARG:HD3	1:B:608:GLN:OE1	1.94	0.68
1:B:173:LYS:HG2	1:B:193:HIS:CE1	2.28	0.68
1:A:22:ILE:HD12	1:A:22:ILE:N	2.01	0.68
1:B:270:ARG:NH1	2:B:665:ATP:H3'	2.09	0.68
1:A:212:THR:HG22	1:A:221:VAL:HG13	1.76	0.68
1:B:21:ASN:C	1:B:21:ASN:HD22	1.97	0.68
1:A:34:GLU:HG3	1:A:94:PRO:HD2	1.75	0.68
1:A:270:ARG:NH1	2:A:665:ATP:H3'	2.09	0.68
1:A:419:ALA:HB1	1:A:422:LEU:HD12	1.76	0.68
1:C:132:ARG:HA	1:C:347:MET:HE1	1.76	0.67
1:C:270:ARG:NH1	2:C:665:ATP:H3'	2.09	0.67
1:B:34:GLU:HG3	1:B:94:PRO:HD2	1.75	0.67
1:B:203:TYR:HE1	1:B:271:THR:HG22	1.60	0.67
1:C:34:GLU:HG3	1:C:94:PRO:HD2	1.75	0.67
1:A:21:ASN:C	1:A:21:ASN:HD22	1.97	0.67
1:A:552:ALA:HB3	1:A:619:LEU:HD13	1.77	0.67
1:A:68:ASN:HD22	1:A:77:GLY:HA3	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ASN:C	1:C:21:ASN:HD22	1.97	0.67
1:C:203:TYR:HE1	1:C:271:THR:HG22	1.60	0.67
1:B:419:ALA:HB1	1:B:422:LEU:HD12	1.76	0.66
1:A:203:TYR:HE1	1:A:271:THR:HG22	1.60	0.66
1:C:68:ASN:HD22	1:C:77:GLY:HA3	1.60	0.66
1:C:212:THR:HG22	1:C:221:VAL:HG13	1.76	0.66
1:C:243:PHE:HD1	1:C:243:PHE:H	1.37	0.66
1:C:552:ALA:HB3	1:C:619:LEU:HD13	1.77	0.66
1:B:22:ILE:HD12	1:B:22:ILE:N	2.01	0.65
1:B:212:THR:HG22	1:B:221:VAL:HG13	1.76	0.65
1:A:181:MET:HG2	1:A:186:PHE:CD2	2.31	0.65
1:C:225:ARG:HG3	1:C:225:ARG:NH1	2.05	0.65
1:C:22:ILE:HD12	1:C:22:ILE:N	2.01	0.65
1:B:552:ALA:HB3	1:B:619:LEU:HD13	1.77	0.65
1:C:181:MET:HG2	1:C:186:PHE:CD2	2.31	0.65
1:B:68:ASN:HD22	1:B:77:GLY:HA3	1.60	0.65
1:B:181:MET:HG2	1:B:186:PHE:CD2	2.31	0.65
1:A:21:ASN:ND2	1:A:24:ALA:H	1.96	0.64
1:B:21:ASN:ND2	1:B:24:ALA:H	1.96	0.64
1:A:593:ARG:CZ	1:B:608:GLN:HE22	2.11	0.63
1:C:301:THR:HG23	1:C:440:TRP:O	1.99	0.63
1:C:445:GLU:OE2	1:C:464:ALA:N	2.29	0.63
1:A:615:THR:HB	1:A:618:ASP:H	1.64	0.63
1:C:21:ASN:ND2	1:C:24:ALA:H	1.96	0.63
1:B:301:THR:HG23	1:B:440:TRP:O	1.99	0.63
1:A:407:SER:HA	1:A:448:GLN:HE22	1.64	0.62
1:A:17:LEU:HG	1:A:153:ILE:HD13	1.82	0.62
1:A:132:ARG:HA	1:A:347:MET:HE2	1.81	0.62
1:B:21:ASN:HD21	1:B:24:ALA:H	1.48	0.62
1:A:288:GLN:HB3	1:A:289:PRO:HD3	1.82	0.62
1:A:664:ARG:HA	1:A:664:ARG:NE	2.15	0.62
1:C:615:THR:HB	1:C:618:ASP:H	1.64	0.62
1:A:301:THR:HG23	1:A:440:TRP:O	1.99	0.61
1:B:407:SER:HA	1:B:448:GLN:HE22	1.65	0.61
1:A:225:ARG:HG3	1:A:225:ARG:NH1	2.05	0.61
1:A:243:PHE:CD1	1:A:243:PHE:N	2.66	0.61
1:B:615:THR:HB	1:B:618:ASP:H	1.64	0.61
1:B:288:GLN:HB3	1:B:289:PRO:HD3	1.82	0.61
1:C:407:SER:HA	1:C:448:GLN:HE22	1.65	0.61
1:A:405:LEU:CG	1:A:406:MET:H	2.03	0.61
1:C:181:MET:HG2	1:C:186:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:664:ARG:NE	1:C:664:ARG:HA	2.15	0.61
1:B:243:PHE:CD1	1:B:243:PHE:N	2.66	0.61
1:B:132:ARG:HA	1:B:347:MET:HE1	1.82	0.61
1:B:664:ARG:HA	1:B:664:ARG:NE	2.15	0.61
1:C:288:GLN:HB3	1:C:289:PRO:HD3	1.82	0.61
1:A:593:ARG:NH1	1:B:608:GLN:NE2	2.43	0.61
1:B:225:ARG:HG3	1:B:225:ARG:NH1	2.05	0.61
1:A:21:ASN:HD21	1:A:24:ALA:H	1.48	0.60
1:B:181:MET:HG2	1:B:186:PHE:CE2	2.35	0.60
1:C:17:LEU:HG	1:C:153:ILE:HD13	1.82	0.60
1:A:181:MET:HG2	1:A:186:PHE:CE2	2.35	0.60
1:A:251:ARG:NH1	1:A:255:GLN:HE22	1.92	0.60
1:A:253:LYS:HD2	1:A:253:LYS:O	2.02	0.60
1:B:160:MET:O	1:B:164:ILE:HG12	2.01	0.60
1:A:132:ARG:HA	1:A:347:MET:HE1	1.82	0.60
1:C:160:MET:O	1:C:164:ILE:HG12	2.01	0.60
1:B:427:LYS:CE	1:C:12:ILE:HG21	2.28	0.60
1:C:481:ASN:HD21	1:C:487:LYS:HA	1.66	0.60
1:A:160:MET:O	1:A:164:ILE:HG12	2.01	0.60
1:B:17:LEU:HG	1:B:153:ILE:HD13	1.82	0.60
1:C:391:LEU:HD13	1:C:398:THR:HG23	1.84	0.60
1:B:132:ARG:HA	1:B:347:MET:HE2	1.81	0.60
1:B:655:GLU:HG2	1:B:659:ARG:NH1	2.17	0.60
1:A:655:GLU:HG2	1:A:659:ARG:NH1	2.17	0.59
1:B:68:ASN:HD22	1:B:78:ASN:N	1.98	0.59
1:B:481:ASN:HD21	1:B:487:LYS:HA	1.66	0.59
1:C:68:ASN:HD22	1:C:78:ASN:N	1.98	0.59
1:A:251:ARG:HB2	1:A:255:GLN:HE21	1.68	0.59
1:A:481:ASN:HD21	1:A:487:LYS:HA	1.67	0.59
1:C:21:ASN:HD21	1:C:24:ALA:H	1.48	0.59
1:B:225:ARG:HH11	1:B:225:ARG:CG	2.08	0.59
1:A:391:LEU:HD13	1:A:398:THR:HG23	1.84	0.59
1:B:253:LYS:HD2	1:B:253:LYS:O	2.02	0.59
1:B:251:ARG:HB2	1:B:255:GLN:HE21	1.68	0.59
1:C:151:THR:HG21	1:C:155:TYR:HB2	1.85	0.59
1:C:655:GLU:HG2	1:C:659:ARG:NH1	2.17	0.59
1:B:151:THR:HG21	1:B:155:TYR:HB2	1.85	0.59
1:C:253:LYS:HD2	1:C:253:LYS:O	2.01	0.59
1:A:1:PRO:HG2	1:A:238:GLU:CD	2.23	0.59
1:A:524:ASN:OD1	1:A:627:LYS:NZ	2.33	0.59
1:A:151:THR:HG21	1:A:155:TYR:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:PRO:HG2	1:C:238:GLU:CD	2.23	0.59
1:B:1:PRO:HG2	1:B:238:GLU:CD	2.23	0.58
1:B:524:ASN:OD1	1:B:627:LYS:NZ	2.33	0.58
1:C:405:LEU:CG	1:C:406:MET:H	2.03	0.58
1:B:391:LEU:HD13	1:B:398:THR:HG23	1.84	0.58
1:A:225:ARG:HH11	1:A:225:ARG:CG	2.08	0.58
1:B:652:GLU:CD	1:B:652:GLU:H	2.07	0.58
1:C:251:ARG:HB2	1:C:255:GLN:HE21	1.68	0.57
1:B:179:ASN:O	1:B:183:GLN:HG3	2.04	0.57
1:B:122:ARG:NH1	1:B:423:ASN:ND2	2.37	0.57
1:A:21:ASN:C	1:A:21:ASN:ND2	2.58	0.57
1:B:429:MET:HB2	1:B:430:PRO:HD3	1.86	0.57
1:A:68:ASN:HD22	1:A:78:ASN:N	1.98	0.57
1:A:179:ASN:O	1:A:183:GLN:HG3	2.04	0.57
1:A:429:MET:HB2	1:A:430:PRO:HD3	1.86	0.57
1:C:652:GLU:H	1:C:652:GLU:CD	2.07	0.57
1:A:663:PRO:O	1:A:664:ARG:CZ	2.53	0.57
1:B:21:ASN:C	1:B:21:ASN:ND2	2.58	0.57
1:C:132:ARG:HA	1:C:347:MET:HE2	1.87	0.57
1:C:179:ASN:O	1:C:183:GLN:HG3	2.04	0.57
1:B:663:PRO:O	1:B:664:ARG:CZ	2.53	0.57
1:A:122:ARG:NH1	1:A:423:ASN:ND2	2.37	0.56
1:C:21:ASN:C	1:C:21:ASN:ND2	2.58	0.56
1:C:663:PRO:O	1:C:664:ARG:CZ	2.53	0.56
1:A:68:ASN:ND2	1:A:77:GLY:HA3	2.21	0.56
1:C:429:MET:HB2	1:C:430:PRO:HD3	1.86	0.56
1:A:652:GLU:CD	1:A:652:GLU:H	2.07	0.55
1:B:301:THR:HG21	1:B:440:TRP:HA	1.89	0.55
1:B:251:ARG:NH1	1:B:255:GLN:HE22	1.92	0.55
1:C:14:ALA:O	1:C:17:LEU:HB2	2.06	0.55
1:C:305:THR:OG1	1:C:306:THR:N	2.39	0.55
1:A:14:ALA:O	1:A:17:LEU:HB2	2.06	0.55
1:A:78:ASN:HD22	1:A:78:ASN:C	2.09	0.55
1:B:254:GLU:CD	1:B:254:GLU:H	2.09	0.55
1:A:301:THR:HG21	1:A:440:TRP:HA	1.88	0.55
1:B:68:ASN:ND2	1:B:77:GLY:HA3	2.21	0.55
1:C:254:GLU:H	1:C:254:GLU:CD	2.09	0.55
1:B:14:ALA:O	1:B:17:LEU:HB2	2.06	0.55
1:C:524:ASN:OD1	1:C:627:LYS:NZ	2.33	0.55
1:A:254:GLU:H	1:A:254:GLU:CD	2.09	0.55
1:B:404:LEU:C	1:B:405:LEU:O	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLU:OE2	1:B:464:ALA:N	2.29	0.55
1:C:404:LEU:C	1:C:405:LEU:O	2.44	0.55
1:A:410:TYR:HB3	1:A:457:LEU:HD11	1.89	0.55
1:B:305:THR:OG1	1:B:306:THR:N	2.39	0.55
1:A:445:GLU:OE2	1:A:464:ALA:N	2.29	0.54
1:C:68:ASN:ND2	1:C:77:GLY:HA3	2.21	0.54
1:C:243:PHE:CD1	1:C:243:PHE:N	2.66	0.54
1:C:78:ASN:HD22	1:C:78:ASN:C	2.09	0.54
1:B:203:TYR:CE1	1:B:271:THR:HG22	2.42	0.54
1:C:88:ARG:HD3	1:C:263:GLY:O	2.08	0.54
1:C:175:GLU:HA	1:C:352:TRP:CE3	2.42	0.54
1:C:301:THR:HG21	1:C:440:TRP:HA	1.89	0.54
1:A:310:LYS:HB3	1:A:514:PHE:CE1	2.43	0.54
1:B:175:GLU:HA	1:B:352:TRP:CE3	2.42	0.54
1:B:410:TYR:HB3	1:B:457:LEU:HD11	1.89	0.54
1:B:584:ARG:O	1:B:588:GLU:HG3	2.07	0.54
1:B:663:PRO:HG2	1:B:664:ARG:H	1.73	0.54
1:C:410:TYR:HB3	1:C:457:LEU:HD11	1.90	0.54
1:A:175:GLU:HA	1:A:352:TRP:CE3	2.42	0.54
1:A:131:VAL:O	1:A:347:MET:HE1	2.08	0.54
1:A:584:ARG:O	1:A:588:GLU:HG3	2.08	0.54
1:A:663:PRO:HG2	1:A:664:ARG:H	1.73	0.54
1:B:88:ARG:HD3	1:B:263:GLY:O	2.08	0.54
1:C:310:LYS:HB3	1:C:514:PHE:CE1	2.43	0.54
1:A:593:ARG:HD2	1:B:608:GLN:OE1	2.06	0.54
1:B:14:ALA:HA	1:B:17:LEU:HD22	1.90	0.54
1:C:3:ARG:O	1:C:4:ALA:CB	2.56	0.54
1:A:14:ALA:HA	1:A:17:LEU:HD22	1.90	0.53
1:B:310:LYS:HB3	1:B:514:PHE:CE1	2.43	0.53
1:C:37:ILE:HG22	1:C:45:SER:HB3	1.89	0.53
1:C:131:VAL:O	1:C:347:MET:HE1	2.08	0.53
1:C:213:LEU:HG	1:C:220:PHE:CE1	2.43	0.53
1:A:203:TYR:CE1	1:A:271:THR:HG22	2.42	0.53
1:A:593:ARG:CZ	1:B:608:GLN:NE2	2.71	0.53
1:B:78:ASN:HD22	1:B:78:ASN:C	2.09	0.53
1:B:615:THR:HG22	1:B:616:PRO:HD2	1.90	0.53
1:C:225:ARG:HH11	1:C:225:ARG:CG	2.08	0.53
1:C:364:PRO:HA	1:C:387:LEU:HD23	1.90	0.53
1:C:663:PRO:HG2	1:C:664:ARG:H	1.73	0.53
1:A:37:ILE:HG22	1:A:45:SER:HB3	1.89	0.53
1:A:88:ARG:HD3	1:A:263:GLY:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ASN:HD22	1:C:85:PHE:N	1.98	0.53
1:C:301:THR:HB	1:C:448:GLN:O	2.09	0.53
1:A:213:LEU:HG	1:A:220:PHE:CE1	2.43	0.53
1:C:320:CYS:SG	1:C:456:MET:HG3	2.49	0.53
1:A:301:THR:HB	1:A:448:GLN:O	2.09	0.53
1:A:521:MET:HG3	1:A:558:TYR:CE1	2.44	0.53
1:B:37:ILE:HG22	1:B:45:SER:HB3	1.90	0.53
1:B:131:VAL:O	1:B:347:MET:HE1	2.08	0.53
1:B:213:LEU:HG	1:B:220:PHE:CE1	2.43	0.53
1:B:629:GLN:O	1:B:630:TYR:HB3	2.08	0.53
1:C:584:ARG:O	1:C:588:GLU:HG3	2.08	0.53
1:C:629:GLN:O	1:C:630:TYR:HB3	2.08	0.53
1:A:364:PRO:HA	1:A:387:LEU:HD23	1.90	0.53
1:B:301:THR:HB	1:B:448:GLN:O	2.09	0.53
1:B:481:ASN:ND2	1:B:487:LYS:HA	2.24	0.53
1:C:615:THR:HG22	1:C:616:PRO:HD2	1.90	0.52
1:B:320:CYS:SG	1:B:456:MET:HG3	2.49	0.52
1:C:481:ASN:ND2	1:C:487:LYS:HA	2.24	0.52
1:C:251:ARG:NH1	1:C:255:GLN:HE22	1.92	0.52
1:A:83:ASN:HD22	1:A:85:PHE:N	1.98	0.52
1:A:615:THR:HG22	1:A:616:PRO:HD2	1.90	0.52
1:B:83:ASN:HD22	1:B:85:PHE:N	1.98	0.52
1:A:83:ASN:HD22	1:A:83:ASN:C	2.13	0.52
1:B:465:LEU:HD12	1:B:465:LEU:O	2.10	0.52
1:C:521:MET:HG3	1:C:558:TYR:CE1	2.44	0.52
1:A:629:GLN:O	1:A:630:TYR:HB3	2.08	0.52
1:B:521:MET:HG3	1:B:558:TYR:CE1	2.44	0.52
1:C:83:ASN:HD22	1:C:83:ASN:C	2.13	0.52
1:C:122:ARG:NH1	1:C:423:ASN:ND2	2.37	0.52
1:C:465:LEU:HD12	1:C:465:LEU:O	2.10	0.52
1:A:305:THR:OG1	1:A:306:THR:N	2.39	0.52
1:A:320:CYS:SG	1:A:456:MET:HG3	2.49	0.52
1:B:254:GLU:CD	1:B:254:GLU:N	2.64	0.52
1:C:14:ALA:HA	1:C:17:LEU:HD22	1.90	0.52
1:C:203:TYR:CE1	1:C:271:THR:HG22	2.42	0.52
1:A:404:LEU:C	1:A:405:LEU:O	2.44	0.51
1:A:481:ASN:ND2	1:A:487:LYS:HA	2.24	0.51
1:A:465:LEU:HD12	1:A:465:LEU:O	2.10	0.51
1:C:254:GLU:CD	1:C:254:GLU:N	2.64	0.51
1:A:311:GLU:OE1	1:A:513:ILE:HB	2.11	0.51
1:A:664:ARG:HG2	1:A:664:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:PRO:HB3	1:B:269:ARG:HD3	1.93	0.51
1:B:83:ASN:HD22	1:B:83:ASN:C	2.13	0.51
1:B:364:PRO:HA	1:B:387:LEU:HD23	1.90	0.51
1:C:664:ARG:HG2	1:C:664:ARG:HH11	1.76	0.51
1:C:477:GLU:HB3	1:C:479:LYS:HD3	1.94	0.50
1:A:12:ILE:O	1:A:16:MET:HG2	2.12	0.50
1:B:12:ILE:O	1:B:16:MET:HG2	2.12	0.50
1:A:254:GLU:CD	1:A:254:GLU:N	2.64	0.50
1:B:227:VAL:O	1:B:242:LEU:HD12	2.12	0.50
1:C:61:LEU:HB3	1:C:84:PHE:CD1	2.46	0.50
1:A:61:LEU:HB3	1:A:84:PHE:CD1	2.46	0.50
1:A:319:LEU:HD12	1:A:320:CYS:H	1.77	0.50
1:A:477:GLU:HB3	1:A:479:LYS:HD3	1.94	0.50
1:B:61:LEU:HB3	1:B:84:PHE:CD1	2.46	0.50
1:A:301:THR:CG2	1:A:440:TRP:O	2.60	0.50
1:B:301:THR:CG2	1:B:440:TRP:O	2.60	0.49
1:B:477:GLU:HB3	1:B:479:LYS:HD3	1.94	0.49
1:A:227:VAL:O	1:A:242:LEU:HD12	2.12	0.49
1:B:664:ARG:HG2	1:B:664:ARG:HH11	1.76	0.49
1:C:12:ILE:O	1:C:16:MET:HG2	2.12	0.49
1:C:173:LYS:CG	1:C:193:HIS:CE1	2.95	0.49
1:C:227:VAL:O	1:C:242:LEU:HD12	2.12	0.49
1:C:311:GLU:OE1	1:C:513:ILE:HB	2.11	0.49
1:C:403:THR:O	1:C:405:LEU:O	2.30	0.49
1:B:311:GLU:OE1	1:B:513:ILE:HB	2.11	0.49
1:C:94:PRO:HB3	1:C:269:ARG:HD3	1.93	0.49
1:C:301:THR:CG2	1:C:440:TRP:O	2.60	0.49
1:A:94:PRO:HB3	1:A:269:ARG:HD3	1.93	0.49
1:A:253:LYS:O	1:A:257:GLY:HA2	2.12	0.49
1:A:595:THR:HG23	1:A:611:LEU:HD21	1.95	0.49
1:B:86:GLY:O	1:B:89:HIS:HD2	1.96	0.49
1:B:173:LYS:CG	1:B:193:HIS:CE1	2.95	0.49
1:C:86:GLY:O	1:C:89:HIS:HD2	1.96	0.49
1:B:253:LYS:O	1:B:257:GLY:HA2	2.12	0.49
1:B:319:LEU:HD12	1:B:320:CYS:H	1.77	0.49
1:C:75:VAL:HG12	1:C:493:GLY:HA2	1.94	0.49
1:C:253:LYS:O	1:C:257:GLY:HA2	2.12	0.49
1:C:319:LEU:HD12	1:C:320:CYS:H	1.77	0.49
1:A:75:VAL:HG12	1:A:493:GLY:HA2	1.94	0.49
1:B:3:ARG:O	1:B:4:ALA:CB	2.56	0.49
1:B:75:VAL:HG12	1:B:493:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ASN:HD22	1:C:84:PHE:N	2.11	0.49
1:C:136:SER:O	1:C:662:MET:HE1	2.12	0.49
1:A:403:THR:O	1:A:405:LEU:O	2.31	0.48
1:A:332:TRP:CZ2	1:A:401:MET:HB3	2.48	0.48
1:B:136:SER:O	1:B:662:MET:HE1	2.12	0.48
1:B:83:ASN:HD22	1:B:84:PHE:N	2.11	0.48
1:A:86:GLY:O	1:A:89:HIS:HD2	1.96	0.48
1:B:230:PHE:O	1:B:234:VAL:HG22	2.14	0.48
1:B:403:THR:O	1:B:405:LEU:O	2.31	0.48
1:A:173:LYS:CG	1:A:193:HIS:CE1	2.95	0.48
1:B:332:TRP:CZ2	1:B:401:MET:HB3	2.48	0.48
1:C:332:TRP:CZ2	1:C:401:MET:HB3	2.48	0.48
1:C:595:THR:HG23	1:C:611:LEU:HD21	1.94	0.48
1:A:83:ASN:HD22	1:A:84:PHE:N	2.11	0.48
1:A:230:PHE:O	1:A:234:VAL:HG22	2.14	0.48
1:B:610:GLY:C	1:B:612:ALA:N	2.63	0.48
1:B:37:ILE:HD12	1:B:37:ILE:HA	1.69	0.48
1:C:37:ILE:HD12	1:C:37:ILE:HA	1.69	0.48
1:C:387:LEU:HD12	1:C:387:LEU:HA	1.57	0.48
1:A:134:MET:HG2	1:A:294:ILE:HG21	1.96	0.47
1:A:136:SER:O	1:A:662:MET:HE1	2.14	0.47
1:C:55:ASN:O	1:C:59:ARG:HG3	2.14	0.47
1:C:83:ASN:ND2	1:C:85:PHE:N	2.57	0.47
1:B:595:THR:HG23	1:B:611:LEU:HD21	1.95	0.47
1:C:70:ASP:OD1	1:C:74:ARG:NH1	2.48	0.47
1:B:55:ASN:O	1:B:59:ARG:HG3	2.14	0.47
1:B:83:ASN:ND2	1:B:83:ASN:C	2.68	0.47
1:B:134:MET:HG2	1:B:294:ILE:HG21	1.96	0.47
1:C:551:TRP:CZ3	1:C:587:ARG:HG3	2.49	0.47
1:A:327:ASP:OD1	1:A:330:THR:OG1	2.31	0.47
1:A:83:ASN:ND2	1:A:83:ASN:C	2.68	0.47
1:A:551:TRP:CZ3	1:A:587:ARG:HG3	2.49	0.47
1:B:307:ARG:HG3	1:B:307:ARG:HH11	1.80	0.47
1:B:551:TRP:CZ3	1:B:587:ARG:HG3	2.49	0.47
1:B:606:ALA:O	1:B:608:GLN:N	2.42	0.47
1:C:83:ASN:ND2	1:C:83:ASN:C	2.68	0.47
1:A:568:LEU:HD23	1:A:568:LEU:HA	1.68	0.47
1:C:99:THR:HB	1:C:227:VAL:HG12	1.97	0.47
1:C:230:PHE:O	1:C:234:VAL:HG22	2.14	0.47
1:A:55:ASN:O	1:A:59:ARG:HG3	2.14	0.47
1:B:323:THR:HG21	1:B:457:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:GLU:O	1:C:312:GLU:C	2.54	0.47
1:B:99:THR:HB	1:B:227:VAL:HG12	1.97	0.46
1:B:568:LEU:HA	1:B:568:LEU:HD23	1.68	0.46
1:A:358:GLU:HG2	1:A:362:LYS:HD3	1.98	0.46
1:B:273:MET:O	1:B:394:GLY:HA3	2.15	0.46
1:A:273:MET:O	1:A:394:GLY:HA3	2.15	0.46
1:B:327:ASP:OD1	1:B:330:THR:OG1	2.31	0.46
1:B:358:GLU:HG2	1:B:362:LYS:HD3	1.98	0.46
1:C:21:ASN:HD22	1:C:22:ILE:N	2.14	0.46
1:C:37:ILE:HG13	1:C:531:GLY:CA	2.45	0.46
1:C:134:MET:HG2	1:C:294:ILE:HG21	1.96	0.46
1:A:323:THR:HG21	1:A:457:LEU:HD22	1.97	0.46
1:B:37:ILE:HG13	1:B:531:GLY:CA	2.46	0.46
1:C:212:THR:HG22	1:C:221:VAL:CG1	2.45	0.46
1:A:9:LEU:HG	1:A:366:TYR:OH	2.16	0.46
1:A:37:ILE:HG13	1:A:531:GLY:CA	2.46	0.46
1:A:70:ASP:OD1	1:A:74:ARG:NH1	2.48	0.46
1:C:663:PRO:O	1:C:664:ARG:NH2	2.49	0.46
1:A:419:ALA:CB	1:A:422:LEU:HD12	2.45	0.46
1:C:9:LEU:HG	1:C:366:TYR:OH	2.16	0.46
1:A:497:LEU:HA	1:A:497:LEU:HD12	1.65	0.46
1:A:614:LEU:HD21	1:A:641:ILE:HD11	1.98	0.46
1:A:663:PRO:O	1:A:664:ARG:NH2	2.49	0.46
1:B:614:LEU:HD21	1:B:641:ILE:HD11	1.98	0.46
1:C:323:THR:HG21	1:C:457:LEU:HD22	1.97	0.46
1:C:664:ARG:HG2	1:C:664:ARG:NH1	2.30	0.46
1:C:340:ILE:O	1:C:344:LEU:HD22	2.16	0.46
1:C:474:MET:HB2	1:C:474:MET:HE2	1.76	0.46
1:A:86:GLY:O	1:A:89:HIS:CD2	2.69	0.46
1:A:606:ALA:O	1:A:608:GLN:N	2.42	0.46
1:B:86:GLY:O	1:B:89:HIS:CD2	2.69	0.46
1:B:243:PHE:HD1	1:B:243:PHE:N	2.10	0.46
1:B:453:ASP:OD2	1:B:453:ASP:N	2.37	0.46
1:C:327:ASP:OD1	1:C:330:THR:OG1	2.31	0.46
1:A:453:ASP:N	1:A:453:ASP:OD2	2.37	0.45
1:B:664:ARG:HG2	1:B:664:ARG:NH1	2.30	0.45
1:A:94:PRO:HB3	1:A:269:ARG:CD	2.47	0.45
1:A:99:THR:HB	1:A:227:VAL:HG12	1.97	0.45
1:A:350:ALA:HB1	1:A:352:TRP:NE1	2.31	0.45
1:B:94:PRO:HB3	1:B:269:ARG:CD	2.47	0.45
1:C:350:ALA:HB1	1:C:352:TRP:NE1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:614:LEU:HD21	1:C:641:ILE:HD11	1.98	0.45
1:C:632:TRP:HB3	1:C:636:ASP:OD2	2.17	0.45
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.80	0.45
1:A:340:ILE:O	1:A:344:LEU:HD22	2.16	0.45
1:B:21:ASN:HD22	1:B:22:ILE:N	2.14	0.45
1:C:55:ASN:CG	1:C:88:ARG:HH22	2.20	0.45
1:C:307:ARG:HG3	1:C:307:ARG:HH11	1.80	0.45
1:C:358:GLU:HG2	1:C:362:LYS:HD3	1.98	0.45
1:A:21:ASN:HD22	1:A:22:ILE:N	2.14	0.45
1:A:29:LYS:O	1:A:30:ARG:C	2.55	0.45
1:A:311:GLU:O	1:A:312:GLU:C	2.54	0.45
1:B:268:ARG:NH2	1:B:270:ARG:HH21	2.15	0.45
1:B:350:ALA:HB1	1:B:352:TRP:NE1	2.31	0.45
1:C:94:PRO:HB3	1:C:269:ARG:CD	2.47	0.45
1:C:273:MET:O	1:C:394:GLY:HA3	2.15	0.45
1:A:122:ARG:HD3	1:A:423:ASN:HD22	1.81	0.45
1:B:663:PRO:O	1:B:664:ARG:NH2	2.49	0.45
1:C:86:GLY:O	1:C:89:HIS:CD2	2.69	0.45
1:A:474:MET:HE2	1:A:474:MET:HB2	1.74	0.45
1:A:655:GLU:HG2	1:A:659:ARG:HH12	1.81	0.45
1:B:340:ILE:O	1:B:344:LEU:HD22	2.16	0.45
1:C:630:TYR:CD1	1:C:630:TYR:C	2.90	0.45
1:A:55:ASN:CG	1:A:88:ARG:HH22	2.20	0.45
1:A:132:ARG:CG	1:A:347:MET:HE2	2.47	0.45
1:A:664:ARG:HG2	1:A:664:ARG:NH1	2.30	0.45
1:B:70:ASP:OD1	1:B:74:ARG:NH1	2.48	0.45
1:C:655:GLU:HG2	1:C:659:ARG:HH12	1.81	0.45
1:B:9:LEU:HG	1:B:366:TYR:OH	2.16	0.45
1:B:311:GLU:O	1:B:312:GLU:C	2.54	0.45
1:B:405:LEU:CG	1:B:406:MET:H	2.03	0.45
1:A:253:LYS:HD2	1:A:257:GLY:HA2	1.98	0.45
1:B:336:LEU:O	1:B:340:ILE:HG13	2.16	0.45
1:C:311:GLU:OE1	1:C:513:ILE:CB	2.65	0.45
1:B:55:ASN:CG	1:B:88:ARG:HH22	2.20	0.44
1:B:83:ASN:ND2	1:B:85:PHE:N	2.57	0.44
1:B:55:ASN:C	1:B:55:ASN:HD22	2.21	0.44
1:B:323:THR:CG2	1:B:457:LEU:HD22	2.48	0.44
1:C:336:LEU:O	1:C:340:ILE:HG13	2.16	0.44
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.68	0.44
1:A:311:GLU:OE1	1:A:513:ILE:CB	2.65	0.44
1:C:253:LYS:HD2	1:C:257:GLY:HA2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:THR:CG2	1:C:457:LEU:HD22	2.48	0.44
1:C:453:ASP:OD2	1:C:453:ASP:N	2.37	0.44
1:A:632:TRP:HB3	1:A:636:ASP:OD2	2.17	0.44
1:B:632:TRP:HB3	1:B:636:ASP:OD2	2.17	0.44
1:C:122:ARG:HD3	1:C:423:ASN:HD22	1.81	0.44
1:A:323:THR:CG2	1:A:457:LEU:HD22	2.48	0.44
1:B:132:ARG:CG	1:B:347:MET:HE2	2.47	0.44
1:B:311:GLU:OE1	1:B:513:ILE:CB	2.65	0.44
1:C:595:THR:HG23	1:C:611:LEU:CD2	2.48	0.44
1:C:633:THR:O	1:C:634:GLU:C	2.55	0.44
1:A:212:THR:HG22	1:A:221:VAL:CG1	2.45	0.44
1:A:595:THR:HG23	1:A:611:LEU:CD2	2.48	0.44
1:B:29:LYS:O	1:B:30:ARG:C	2.55	0.44
1:B:253:LYS:HD2	1:B:257:GLY:HA2	1.98	0.44
1:B:630:TYR:CD1	1:B:630:TYR:C	2.90	0.44
1:C:225:ARG:NH1	1:C:225:ARG:CG	2.73	0.44
1:A:268:ARG:NH2	1:A:270:ARG:HH21	2.15	0.44
1:A:83:ASN:ND2	1:A:85:PHE:N	2.57	0.44
1:A:336:LEU:O	1:A:340:ILE:HG13	2.16	0.44
1:A:630:TYR:CD1	1:A:630:TYR:C	2.90	0.44
1:B:122:ARG:HD3	1:B:423:ASN:HD22	1.81	0.44
1:B:633:THR:O	1:B:634:GLU:C	2.55	0.44
1:C:319:LEU:HD12	1:C:320:CYS:N	2.33	0.44
1:C:449:ILE:HD12	1:C:496:PHE:CE2	2.53	0.44
1:A:7:PHE:CE2	1:A:13:LYS:HD2	2.53	0.43
1:A:131:VAL:HG12	1:A:347:MET:HE1	1.99	0.43
1:B:286:VAL:O	1:B:289:PRO:HD2	2.18	0.43
1:B:595:THR:HG23	1:B:611:LEU:CD2	2.48	0.43
1:C:55:ASN:C	1:C:55:ASN:HD22	2.21	0.43
1:A:334:GLY:HA3	1:A:388:GLU:OE1	2.19	0.43
1:B:449:ILE:HD12	1:B:496:PHE:CE2	2.53	0.43
1:C:334:GLY:HA3	1:C:388:GLU:OE1	2.19	0.43
1:A:37:ILE:HA	1:A:37:ILE:HD12	1.69	0.43
1:A:253:LYS:HB3	1:A:254:GLU:OE2	2.18	0.43
1:A:633:THR:O	1:A:634:GLU:C	2.55	0.43
1:B:131:VAL:HG12	1:B:347:MET:HE1	1.99	0.43
1:B:319:LEU:HD12	1:B:320:CYS:N	2.33	0.43
1:C:419:ALA:CB	1:C:422:LEU:HD12	2.45	0.43
1:B:18:PHE:CG	1:B:28:SER:HB3	2.54	0.43
1:C:587:ARG:HA	1:C:587:ARG:HD2	1.87	0.43
1:C:606:ALA:O	1:C:608:GLN:N	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PHE:CG	1:A:28:SER:HB3	2.54	0.43
1:A:286:VAL:O	1:A:289:PRO:HD2	2.18	0.43
1:A:449:ILE:HD12	1:A:496:PHE:CE2	2.53	0.43
1:A:610:GLY:C	1:A:612:ALA:N	2.63	0.43
1:B:253:LYS:HB3	1:B:254:GLU:OE2	2.18	0.43
1:C:29:LYS:O	1:C:30:ARG:C	2.55	0.43
1:C:286:VAL:O	1:C:289:PRO:HD2	2.18	0.43
1:A:55:ASN:HD22	1:A:55:ASN:C	2.21	0.43
1:A:7:PHE:CD1	1:A:7:PHE:N	2.87	0.43
1:B:7:PHE:CE2	1:B:13:LYS:HD2	2.53	0.43
1:B:44:LEU:HA	1:B:44:LEU:HD12	1.68	0.43
1:B:334:GLY:HA3	1:B:388:GLU:OE1	2.19	0.43
1:C:268:ARG:NH2	1:C:270:ARG:HH21	2.15	0.43
1:A:319:LEU:HD12	1:A:320:CYS:N	2.33	0.43
1:B:387:LEU:HD12	1:B:387:LEU:HA	1.57	0.43
1:C:7:PHE:CE2	1:C:13:LYS:HD2	2.53	0.43
1:C:253:LYS:HB3	1:C:254:GLU:OE2	2.18	0.43
1:A:300:TYR:HA	1:A:313:LYS:HE2	2.01	0.43
1:A:633:THR:O	1:A:635:ALA:N	2.52	0.43
1:C:397:ALA:O	1:C:398:THR:C	2.57	0.43
1:A:132:ARG:NH1	1:A:343:GLU:OE2	2.46	0.42
1:A:419:ALA:HB1	1:A:422:LEU:CD1	2.47	0.42
1:B:655:GLU:HG2	1:B:659:ARG:HH12	1.81	0.42
1:C:18:PHE:CG	1:C:28:SER:HB3	2.54	0.42
1:C:300:TYR:HA	1:C:313:LYS:HE2	2.01	0.42
1:B:7:PHE:CD1	1:B:7:PHE:N	2.87	0.42
1:B:132:ARG:NH1	1:B:343:GLU:OE2	2.46	0.42
1:B:563:ILE:HG13	1:B:567:VAL:HG23	2.01	0.42
1:A:55:ASN:CG	1:A:88:ARG:NH2	2.73	0.42
1:A:563:ILE:HG13	1:A:567:VAL:HG23	2.01	0.42
1:B:55:ASN:CG	1:B:88:ARG:NH2	2.73	0.42
1:B:539:ARG:HH11	1:B:539:ARG:HD2	1.69	0.42
1:C:504:ASP:OD2	1:C:511:SER:HB2	2.19	0.42
1:A:3:ARG:O	1:A:4:ALA:CB	2.56	0.42
1:B:128:ARG:HG3	1:B:339:LEU:HD11	2.02	0.42
1:B:212:THR:HG22	1:B:221:VAL:CG1	2.45	0.42
1:B:300:TYR:HA	1:B:313:LYS:HE2	2.01	0.42
1:B:633:THR:O	1:B:635:ALA:N	2.52	0.42
1:C:633:THR:O	1:C:635:ALA:N	2.52	0.42
1:B:76:TYR:HA	1:B:502:LEU:HD12	2.01	0.42
1:B:280:ASN:ND2	1:B:396:GLY:H	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:TYR:HA	1:C:502:LEU:HD12	2.01	0.42
1:C:407:SER:OG	1:C:448:GLN:NE2	2.53	0.42
1:C:615:THR:HG22	1:C:616:PRO:CD	2.50	0.42
1:A:225:ARG:NH1	1:A:225:ARG:CG	2.73	0.42
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.65	0.42
1:C:128:ARG:HG3	1:C:339:LEU:HD11	2.02	0.42
1:C:132:ARG:CG	1:C:347:MET:HE2	2.49	0.42
1:B:132:ARG:CA	1:B:347:MET:HE2	2.48	0.42
1:B:504:ASP:OD2	1:B:511:SER:HB2	2.20	0.42
1:C:280:ASN:ND2	1:C:396:GLY:H	2.18	0.42
1:A:407:SER:OG	1:A:448:GLN:NE2	2.53	0.42
1:B:419:ALA:CB	1:B:422:LEU:HD12	2.45	0.42
1:A:279:LEU:O	1:A:282:PRO:HD2	2.20	0.42
1:B:631:LYS:HG2	1:B:632:TRP:CE2	2.55	0.42
1:C:7:PHE:CD1	1:C:7:PHE:N	2.87	0.42
1:C:279:LEU:O	1:C:282:PRO:HD2	2.20	0.42
1:C:429:MET:CB	1:C:430:PRO:HD3	2.50	0.42
1:C:522:LEU:HA	1:C:522:LEU:HD23	1.85	0.42
1:C:631:LYS:HG2	1:C:632:TRP:CE2	2.55	0.42
1:B:587:ARG:HA	1:B:587:ARG:HD2	1.87	0.41
1:C:44:LEU:HD12	1:C:44:LEU:HA	1.68	0.41
1:C:55:ASN:CG	1:C:88:ARG:NH2	2.73	0.41
1:C:563:ILE:HG13	1:C:567:VAL:HG23	2.01	0.41
1:A:281:ALA:HB3	1:A:282:PRO:CD	2.42	0.41
1:B:226:MET:CE	1:B:244:ALA:CB	2.96	0.41
1:B:281:ALA:HB3	1:B:282:PRO:CD	2.43	0.41
1:B:602:VAL:HB	1:B:605:MET:HB2	2.02	0.41
1:A:128:ARG:HG3	1:A:339:LEU:HD11	2.02	0.41
1:A:504:ASP:OD2	1:A:511:SER:HB2	2.20	0.41
1:A:615:THR:HG22	1:A:616:PRO:CD	2.50	0.41
1:B:407:SER:OG	1:B:448:GLN:NE2	2.53	0.41
1:A:132:ARG:CA	1:A:347:MET:HE2	2.48	0.41
1:C:254:GLU:N	1:C:254:GLU:OE2	2.51	0.41
1:C:602:VAL:HB	1:C:605:MET:HB2	2.02	0.41
1:A:76:TYR:HA	1:A:502:LEU:HD12	2.01	0.41
1:A:631:LYS:HG2	1:A:632:TRP:CE2	2.55	0.41
1:A:641:ILE:N	1:A:641:ILE:CD1	2.84	0.41
1:C:419:ALA:HB1	1:C:422:LEU:CD1	2.47	0.41
1:A:268:ARG:HH22	1:A:270:ARG:HH21	1.69	0.41
1:A:371:ALA:HB1	1:A:372:PRO:HD2	2.03	0.41
1:A:406:MET:HE3	1:A:406:MET:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LEU:HD12	1:A:457:LEU:HA	1.84	0.41
1:B:192:LEU:HB3	1:B:193:HIS:CD2	2.56	0.41
1:B:279:LEU:O	1:B:282:PRO:HD2	2.20	0.41
1:B:615:THR:HG22	1:B:616:PRO:CD	2.50	0.41
1:B:13:LYS:NZ	1:B:383:SER:OG	2.54	0.41
1:B:108:LYS:HE3	1:B:331:PHE:CZ	2.56	0.41
1:B:369:ALA:HA	1:B:370:PRO:HD2	1.81	0.41
1:C:108:LYS:HE3	1:C:331:PHE:CZ	2.55	0.41
1:A:132:ARG:CA	1:A:347:MET:CE	2.93	0.41
1:A:280:ASN:ND2	1:A:396:GLY:H	2.18	0.41
1:B:99:THR:HA	1:B:227:VAL:HB	2.03	0.41
1:B:253:LYS:HD2	1:B:253:LYS:C	2.41	0.41
1:B:641:ILE:N	1:B:641:ILE:CD1	2.84	0.41
1:C:72:TYR:HB3	1:C:472:PHE:CZ	2.56	0.41
1:C:99:THR:HA	1:C:227:VAL:HB	2.03	0.41
1:A:47:ASP:HA	1:A:48:PRO:HD3	1.98	0.41
1:A:72:TYR:HB3	1:A:472:PHE:CZ	2.56	0.41
1:A:253:LYS:HD2	1:A:253:LYS:C	2.41	0.41
1:A:254:GLU:N	1:A:254:GLU:OE2	2.51	0.41
1:A:429:MET:CB	1:A:430:PRO:HD3	2.50	0.41
1:A:504:ASP:OD1	1:A:506:ARG:N	2.53	0.41
1:A:633:THR:HG23	1:A:635:ALA:HB3	2.03	0.41
1:B:273:MET:HE2	1:B:392:SER:HB3	2.03	0.41
1:B:397:ALA:O	1:B:398:THR:C	2.57	0.41
1:C:43:LEU:HD23	1:C:43:LEU:HA	1.88	0.41
1:C:192:LEU:HB3	1:C:193:HIS:CD2	2.56	0.41
1:A:296:SER:OG	1:A:297:LYS:N	2.54	0.40
1:A:418:THR:O	1:A:464:ALA:HA	2.21	0.40
1:B:364:PRO:HB3	1:B:379:LEU:O	2.22	0.40
1:C:407:SER:CA	1:C:448:GLN:HE22	2.34	0.40
1:C:641:ILE:N	1:C:641:ILE:CD1	2.84	0.40
1:A:364:PRO:HB3	1:A:379:LEU:O	2.21	0.40
1:A:397:ALA:O	1:A:398:THR:C	2.57	0.40
1:C:131:VAL:C	1:C:347:MET:HE1	2.41	0.40
1:C:364:PRO:HB3	1:C:379:LEU:O	2.22	0.40
1:A:78:ASN:HD22	1:A:79:GLY:H	1.63	0.40
1:A:108:LYS:HE3	1:A:331:PHE:CZ	2.56	0.40
1:A:369:ALA:HA	1:A:370:PRO:HD2	1.81	0.40
1:B:296:SER:OG	1:B:297:LYS:N	2.54	0.40
1:B:549:LEU:HA	1:B:549:LEU:HD23	1.84	0.40
1:C:419:ALA:N	1:C:420:PRO:CD	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:LEU:HA	1:C:497:LEU:HD12	1.65	0.40
1:C:602:VAL:HB	1:C:605:MET:HG3	2.04	0.40
1:C:615:THR:HG22	1:C:617:ILE:H	1.87	0.40
1:A:192:LEU:HB3	1:A:193:HIS:CD2	2.56	0.40
1:B:134:MET:HG2	1:B:294:ILE:CG2	2.51	0.40
1:B:371:ALA:HB1	1:B:372:PRO:HD2	2.03	0.40
1:C:449:ILE:HG13	1:C:456:MET:HB2	2.04	0.40
1:A:286:VAL:C	1:A:289:PRO:HD2	2.42	0.40
1:B:418:THR:O	1:B:464:ALA:HA	2.21	0.40
1:B:429:MET:CB	1:B:430:PRO:HD3	2.50	0.40
1:B:449:ILE:HG13	1:B:456:MET:HB2	2.04	0.40
1:C:134:MET:HG2	1:C:294:ILE:CG2	2.51	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ARG:NH2	1:C:582:SER:O[1_655]	1.34	0.86
1:A:537:ARG:NH1	1:C:586:TYR:N[1_655]	1.73	0.47
1:A:537:ARG:NH2	1:C:582:SER:C[1_655]	2.10	0.10

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	662/664 (100%)	613 (93%)	41 (6%)	8 (1%)	13	48
1	B	662/664 (100%)	613 (93%)	41 (6%)	8 (1%)	13	48
1	C	662/664 (100%)	613 (93%)	41 (6%)	8 (1%)	13	48
All	All	1986/1992 (100%)	1839 (93%)	123 (6%)	24 (1%)	13	48

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	406	MET
1	A	608	GLN
1	A	630	TYR
1	B	2	ARG
1	B	406	MET
1	B	608	GLN
1	B	630	TYR
1	C	2	ARG
1	C	406	MET
1	C	608	GLN
1	C	630	TYR
1	A	405	LEU
1	A	607	ARG
1	B	405	LEU
1	B	607	ARG
1	C	405	LEU
1	C	607	ARG
1	A	4	ALA
1	A	634	GLU
1	B	4	ALA
1	B	634	GLU
1	C	4	ALA
1	C	634	GLU

### 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	557/557 (100%)	500 (90%)	57 (10%)	7	28
1	B	557/557 (100%)	500 (90%)	57 (10%)	7	28
1	C	557/557 (100%)	500 (90%)	57 (10%)	7	28
All	All	1671/1671 (100%)	1500 (90%)	171 (10%)	7	28

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	9	LEU
1	A	17	LEU
1	A	21	ASN
1	A	22	ILE
1	A	41	GLU
1	A	43	LEU
1	A	44	LEU
1	A	46	VAL
1	A	55	ASN
1	A	61	LEU
1	A	63	ASP
1	A	75	VAL
1	A	78	ASN
1	A	83	ASN
1	A	97	PRO
1	A	106	LEU
1	A	136	SER
1	A	137	ASP
1	A	146	ARG
1	A	151	THR
1	A	154	PRO
1	A	165	GLU
1	A	212	THR
1	A	213	LEU
1	A	221	VAL
1	A	225	ARG
1	A	243	PHE
1	A	254	GLU
1	A	259	ASP
1	A	301	THR
1	A	307	ARG
1	A	344	LEU
1	A	345	LEU
1	A	362	LYS
1	A	373	GLU
1	A	384	ASN
1	A	387	LEU
1	A	391	LEU
1	A	400	LEU
1	A	404	LEU
1	A	456	MET
1	A	457	LEU

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Mol	Chain	Res	Type
1	A	472	PHE
1	A	497	LEU
1	A	518	ILE
1	A	566	ASP
1	A	582	SER
1	A	587	ARG
1	A	591	LEU
1	A	605	MET
1	A	616	PRO
1	A	627	LYS
1	A	630	TYR
1	A	636	ASP
1	A	640	ASN
1	A	641	ILE
1	B	2	ARG
1	B	9	LEU
1	B	17	LEU
1	B	21	ASN
1	B	22	ILE
1	B	41	GLU
1	B	43	LEU
1	B	44	LEU
1	B	46	VAL
1	B	55	ASN
1	B	61	LEU
1	B	63	ASP
1	B	75	VAL
1	B	78	ASN
1	B	83	ASN
1	B	97	PRO
1	B	106	LEU
1	B	136	SER
1	B	137	ASP
1	B	146	ARG
1	B	151	THR
1	B	154	PRO
1	B	165	GLU
1	B	212	THR
1	B	213	LEU
1	B	221	VAL
1	B	225	ARG
1	B	243	PHE

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Mol	Chain	Res	Type
1	B	254	GLU
1	B	259	ASP
1	B	301	THR
1	B	307	ARG
1	B	344	LEU
1	B	345	LEU
1	B	362	LYS
1	B	373	GLU
1	B	384	ASN
1	B	387	LEU
1	B	391	LEU
1	B	400	LEU
1	B	404	LEU
1	B	456	MET
1	B	457	LEU
1	B	472	PHE
1	B	497	LEU
1	B	518	ILE
1	B	566	ASP
1	B	582	SER
1	B	587	ARG
1	B	591	LEU
1	B	605	MET
1	B	616	PRO
1	B	627	LYS
1	B	630	TYR
1	B	636	ASP
1	B	640	ASN
1	B	641	ILE
1	C	2	ARG
1	C	9	LEU
1	C	17	LEU
1	C	21	ASN
1	C	22	ILE
1	C	41	GLU
1	C	43	LEU
1	C	44	LEU
1	C	46	VAL
1	C	55	ASN
1	C	61	LEU
1	C	63	ASP
1	C	75	VAL

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Mol	Chain	Res	Type
1	C	78	ASN
1	C	83	ASN
1	C	97	PRO
1	C	106	LEU
1	C	136	SER
1	C	137	ASP
1	C	146	ARG
1	C	151	THR
1	C	154	PRO
1	C	165	GLU
1	C	212	THR
1	C	213	LEU
1	C	221	VAL
1	C	225	ARG
1	C	243	PHE
1	C	254	GLU
1	C	259	ASP
1	C	301	THR
1	C	307	ARG
1	C	344	LEU
1	C	345	LEU
1	C	362	LYS
1	C	373	GLU
1	C	384	ASN
1	C	387	LEU
1	C	391	LEU
1	C	400	LEU
1	C	404	LEU
1	C	456	MET
1	C	457	LEU
1	C	472	PHE
1	C	497	LEU
1	C	518	ILE
1	C	566	ASP
1	C	582	SER
1	C	587	ARG
1	C	591	LEU
1	C	605	MET
1	C	616	PRO
1	C	627	LYS
1	C	630	TYR
1	C	636	ASP

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Mol	Chain	Res	Type
1	C	640	ASN
1	C	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	26	GLN
1	A	55	ASN
1	A	68	ASN
1	A	78	ASN
1	A	83	ASN
1	A	89	HIS
1	A	191	GLN
1	A	193	HIS
1	A	255	GLN
1	A	280	ASN
1	A	309	ASN
1	A	328	HIS
1	A	384	ASN
1	A	423	ASN
1	A	448	GLN
1	A	577	ASN
1	B	21	ASN
1	B	26	GLN
1	B	55	ASN
1	B	68	ASN
1	B	78	ASN
1	B	83	ASN
1	B	89	HIS
1	B	191	GLN
1	B	193	HIS
1	B	255	GLN
1	B	280	ASN
1	B	309	ASN
1	B	328	HIS
1	B	384	ASN
1	B	423	ASN
1	B	448	GLN
1	B	577	ASN
1	C	21	ASN
1	C	26	GLN

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Mol	Chain	Res	Type
1	C	55	ASN
1	C	68	ASN
1	C	78	ASN
1	C	83	ASN
1	C	89	HIS
1	C	191	GLN
1	C	193	HIS
1	C	255	GLN
1	C	280	ASN
1	C	309	ASN
1	C	328	HIS
1	C	384	ASN
1	C	423	ASN
1	C	448	GLN
1	C	577	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

3 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
2	ATP	A	665	-	28,33,33	2.78	7 (25%)	34,52,52	2.93	13 (38%)
2	ATP	C	665	-	28,33,33	2.79	7 (25%)	34,52,52	2.94	13 (38%)
2	ATP	B	665	-	28,33,33	2.79	7 (25%)	34,52,52	2.93	13 (38%)

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
2	ATP	A	665	-	-	3/18/38/38	0/3/3/3
2	ATP	C	665	-	-	3/18/38/38	0/3/3/3
2	ATP	B	665	-	-	3/18/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	665	ATP	PA-O3A	-8.84	1.50	1.59
2	B	665	ATP	PA-O3A	-8.80	1.50	1.59
2	A	665	ATP	PA-O3A	-8.75	1.50	1.59
2	A	665	ATP	PB-O3A	-8.09	1.50	1.59
2	B	665	ATP	PB-O3A	-8.06	1.50	1.59
2	C	665	ATP	PB-O3A	-8.05	1.50	1.59
2	B	665	ATP	C2-N3	4.06	1.38	1.32
2	A	665	ATP	C2-N3	4.06	1.38	1.32
2	C	665	ATP	C2-N3	4.05	1.38	1.32
2	B	665	ATP	C6-N6	3.59	1.46	1.34
2	C	665	ATP	C6-N6	3.58	1.46	1.34
2	A	665	ATP	C6-N6	3.57	1.46	1.34
2	C	665	ATP	C2-N1	3.10	1.39	1.33
2	B	665	ATP	C2-N1	3.10	1.39	1.33
2	A	665	ATP	C2-N1	3.09	1.39	1.33
2	C	665	ATP	C8-N7	2.88	1.40	1.34
2	B	665	ATP	C8-N7	2.88	1.40	1.34
2	A	665	ATP	C8-N7	2.85	1.39	1.34
2	C	665	ATP	O4'-C1'	2.74	1.44	1.40
2	B	665	ATP	O4'-C1'	2.71	1.44	1.40
2	A	665	ATP	O4'-C1'	2.67	1.44	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	665	ATP	C4'-O4'-C1'	-8.18	102.43	109.92
2	B	665	ATP	C4'-O4'-C1'	-8.18	102.44	109.92
2	A	665	ATP	C4'-O4'-C1'	-8.17	102.44	109.92
2	A	665	ATP	O4'-C1'-N9	7.83	119.13	108.75
2	C	665	ATP	O4'-C1'-N9	7.83	119.13	108.75
2	B	665	ATP	O4'-C1'-N9	7.82	119.12	108.75
2	C	665	ATP	C6-C5-C4	6.63	130.80	117.90
2	B	665	ATP	C6-C5-C4	6.62	130.77	117.90
2	A	665	ATP	C6-C5-C4	6.60	130.74	117.90
2	C	665	ATP	O4'-C4'-C3'	5.01	115.10	105.15
2	B	665	ATP	O4'-C4'-C3'	5.00	115.08	105.15
2	A	665	ATP	O4'-C4'-C3'	4.99	115.07	105.15
2	C	665	ATP	O3G-PG-O3B	3.67	116.95	104.64
2	B	665	ATP	O3G-PG-O3B	3.66	116.92	104.64
2	A	665	ATP	O3G-PG-O3B	3.65	116.88	104.64
2	B	665	ATP	C5'-C4'-C3'	3.60	128.18	115.21
2	A	665	ATP	C5'-C4'-C3'	3.60	128.17	115.21
2	C	665	ATP	C5'-C4'-C3'	3.59	128.15	115.21
2	B	665	ATP	O3'-C3'-C4'	3.30	120.55	111.08
2	A	665	ATP	O3'-C3'-C4'	3.30	120.55	111.08
2	C	665	ATP	O3'-C3'-C4'	3.28	120.51	111.08
2	A	665	ATP	C5-C6-N1	-2.51	114.23	120.23
2	C	665	ATP	C5-C6-N1	-2.51	114.25	120.23
2	B	665	ATP	C5-C6-N1	-2.50	114.26	120.23
2	C	665	ATP	C1'-N9-C4	-2.31	122.59	126.64
2	B	665	ATP	C1'-N9-C4	-2.29	122.62	126.64
2	A	665	ATP	C1'-N9-C4	-2.28	122.64	126.64
2	A	665	ATP	C5-C6-N6	2.28	123.78	120.31
2	C	665	ATP	C5-C6-N6	2.27	123.78	120.31
2	B	665	ATP	C5-C6-N6	2.27	123.76	120.31
2	A	665	ATP	C4-C5-N7	2.10	111.55	109.34
2	A	665	ATP	O2B-PB-O3B	2.08	112.90	107.27
2	C	665	ATP	O2B-PB-O3B	2.08	112.90	107.27
2	B	665	ATP	O2B-PB-O3B	2.08	112.90	107.27
2	B	665	ATP	C4-C5-N7	2.07	111.52	109.34
2	C	665	ATP	O2G-PG-O3B	2.05	111.50	104.64
2	B	665	ATP	O2G-PG-O3B	2.04	111.49	104.64
2	C	665	ATP	C4-C5-N7	2.04	111.50	109.34
2	A	665	ATP	O2G-PG-O3B	2.04	111.47	104.64

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	665	ATP	O4'-C4'-C5'-O5'
2	B	665	ATP	O4'-C4'-C5'-O5'
2	C	665	ATP	O4'-C4'-C5'-O5'
2	A	665	ATP	PB-O3B-PG-O1G
2	B	665	ATP	PB-O3B-PG-O1G
2	C	665	ATP	PB-O3B-PG-O1G
2	A	665	ATP	PA-O3A-PB-O1B
2	B	665	ATP	PA-O3A-PB-O1B
2	C	665	ATP	PA-O3A-PB-O1B

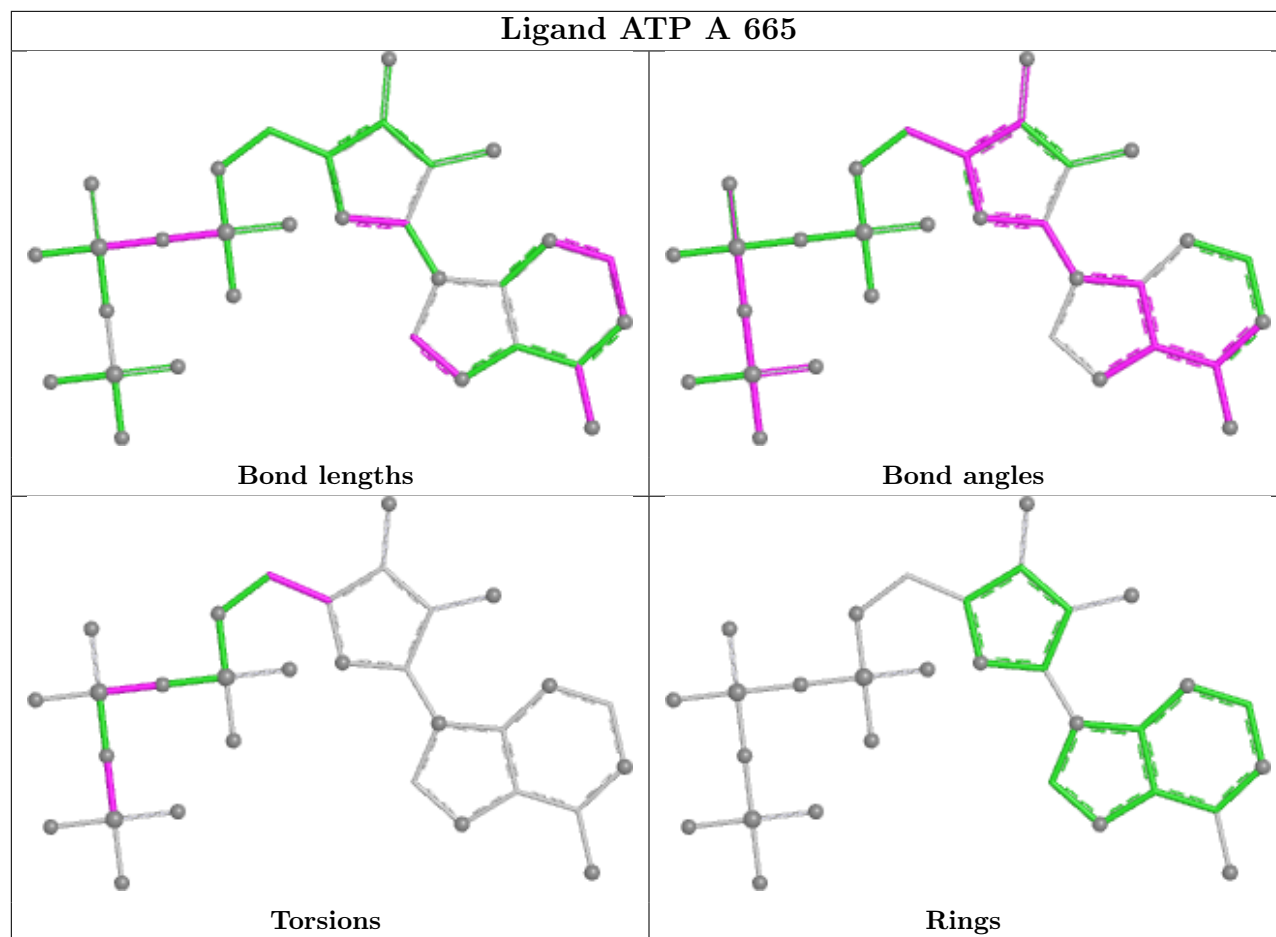
There are no ring outliers.

3 monomers are involved in 21 short contacts:

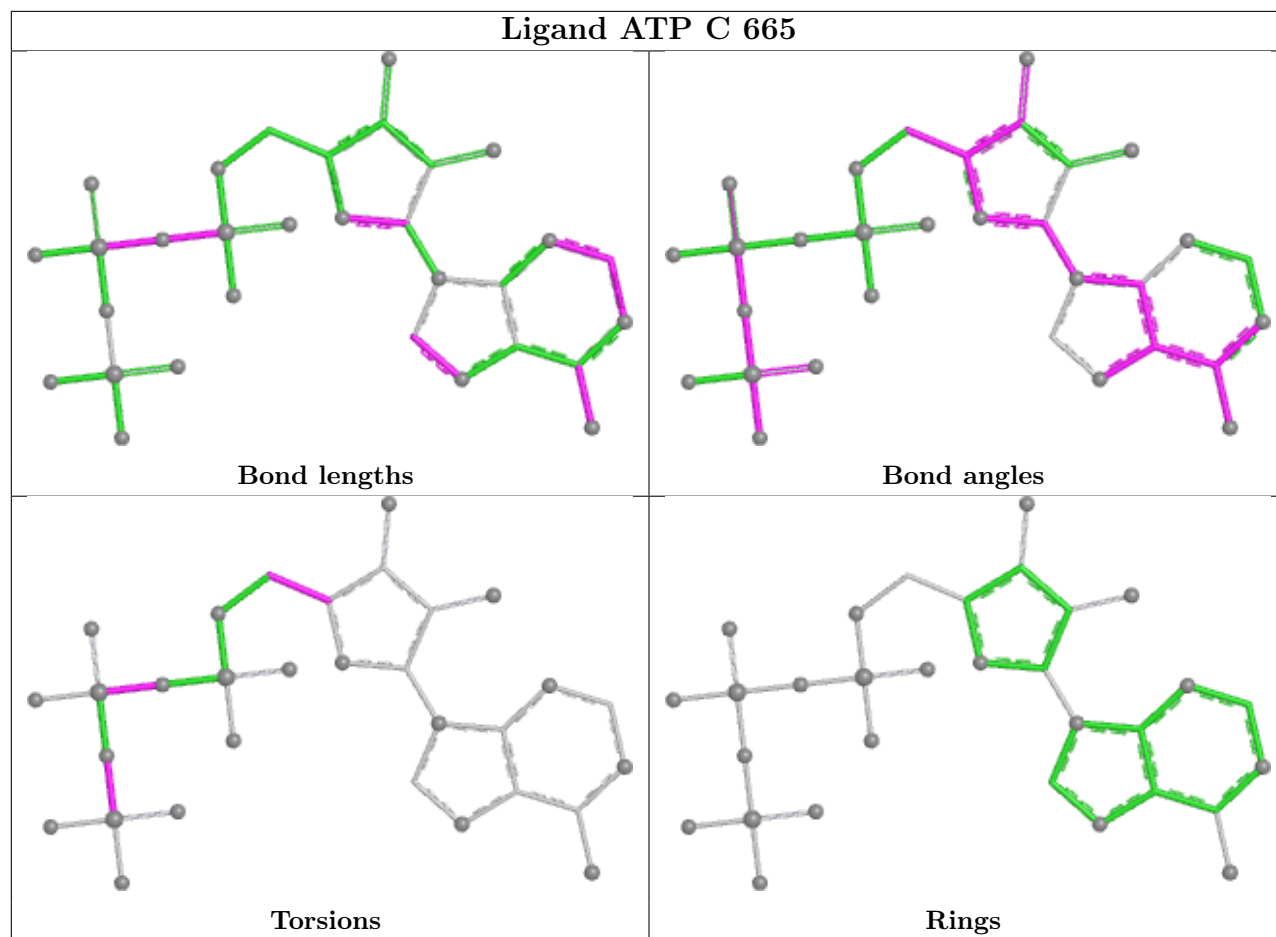
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	665	ATP	7	0
2	C	665	ATP	7	0
2	B	665	ATP	7	0

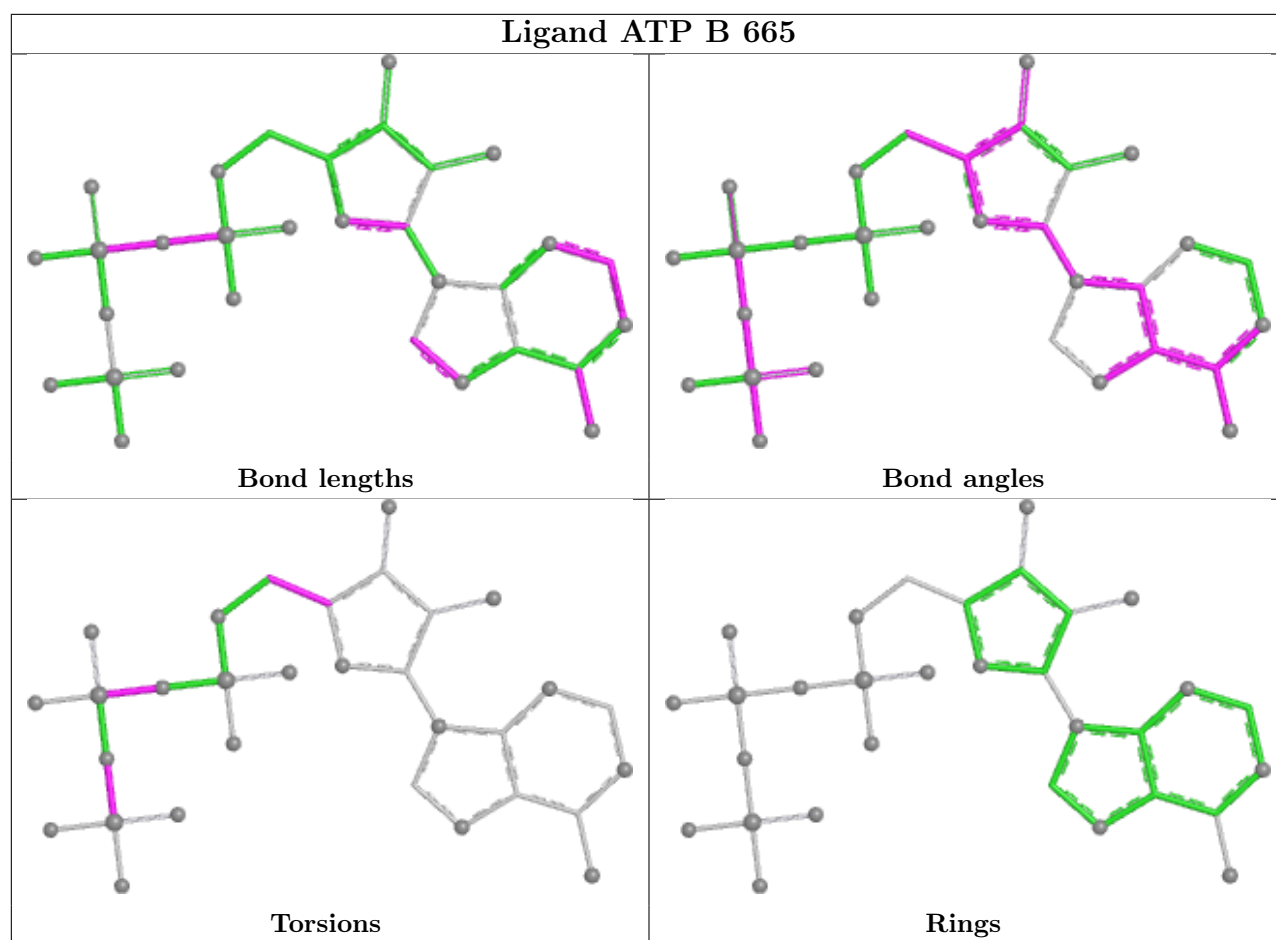
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand ATP A 665



## Ligand ATP C 665





## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.