Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:11 am BST

PDB ID	:	2I6A
Title	:	Human Adenosine Kinase in Complex With 5'-Deoxy-5-Iodotubercidin
Authors	:	Muchmore, S.W.
Deposited on	:	2006-08-28
Resolution	:	2.20 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*
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 ①) were used in the production of this report:

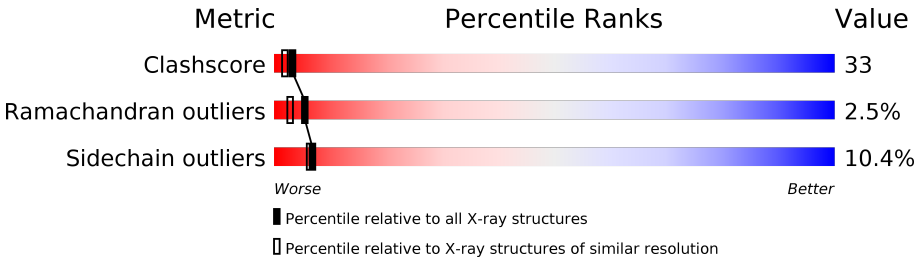
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	54% 39% 7%
1	B	345	54% 37% 8%
1	C	345	56% 34% 9%
1	D	345	51% 43% 6%

2 Entry composition

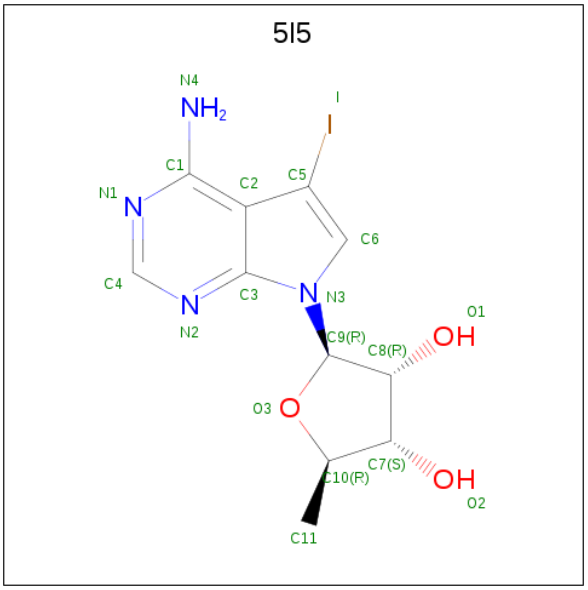
There are 3 unique types of molecules in this entry. The entry contains 11414 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Adenosine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2707	1721	461	511	14			
1	B	343	Total	C	N	O	S	0	0	0
			2707	1721	461	511	14			
1	C	343	Total	C	N	O	S	0	0	0
			2707	1721	461	511	14			
1	D	343	Total	C	N	O	S	0	0	0
			2707	1721	461	511	14			

- Molecule 2 is 7-(5-DEOXY-BETA-D-RIBOFURANOSYL)-5-IODO-7H-PYRROLO[2,3-D] PYRIMIDIN-4-AMINE (three-letter code: 5I5) (formula: $C_{11}H_{13}IN_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	I	N	O	0	0
			19	11	1	4	3		
2	B	1	Total	C	I	N	O	0	0
			19	11	1	4	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	I	N	O	0	0
			19	11	1	4	3		
2	D	1	Total	C	I	N	O	0	0
			19	11	1	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	125	Total	O	0	0
			125	125		
3	B	135	Total	O	0	0
			135	135		
3	C	109	Total	O	0	0
			109	109		
3	D	141	Total	O	0	0
			141	141		

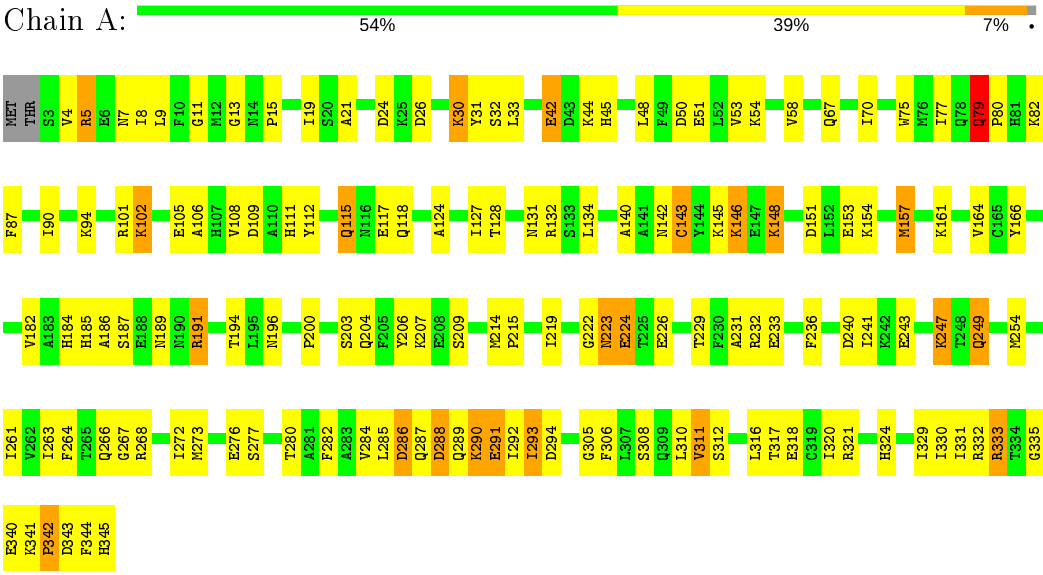
3 Residue-property plots (i)

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. 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.

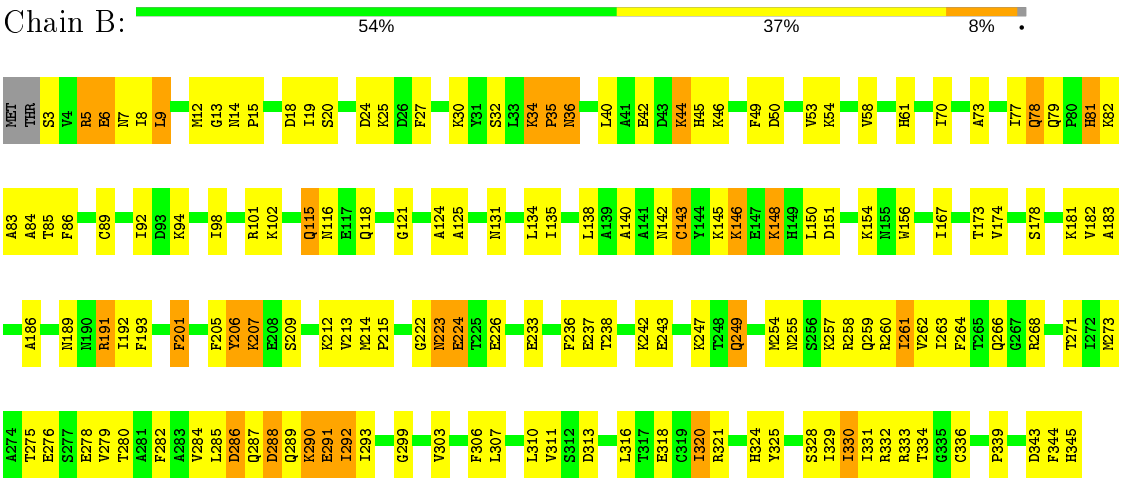
- Molecule 1: Adenosine kinase

Chain A:



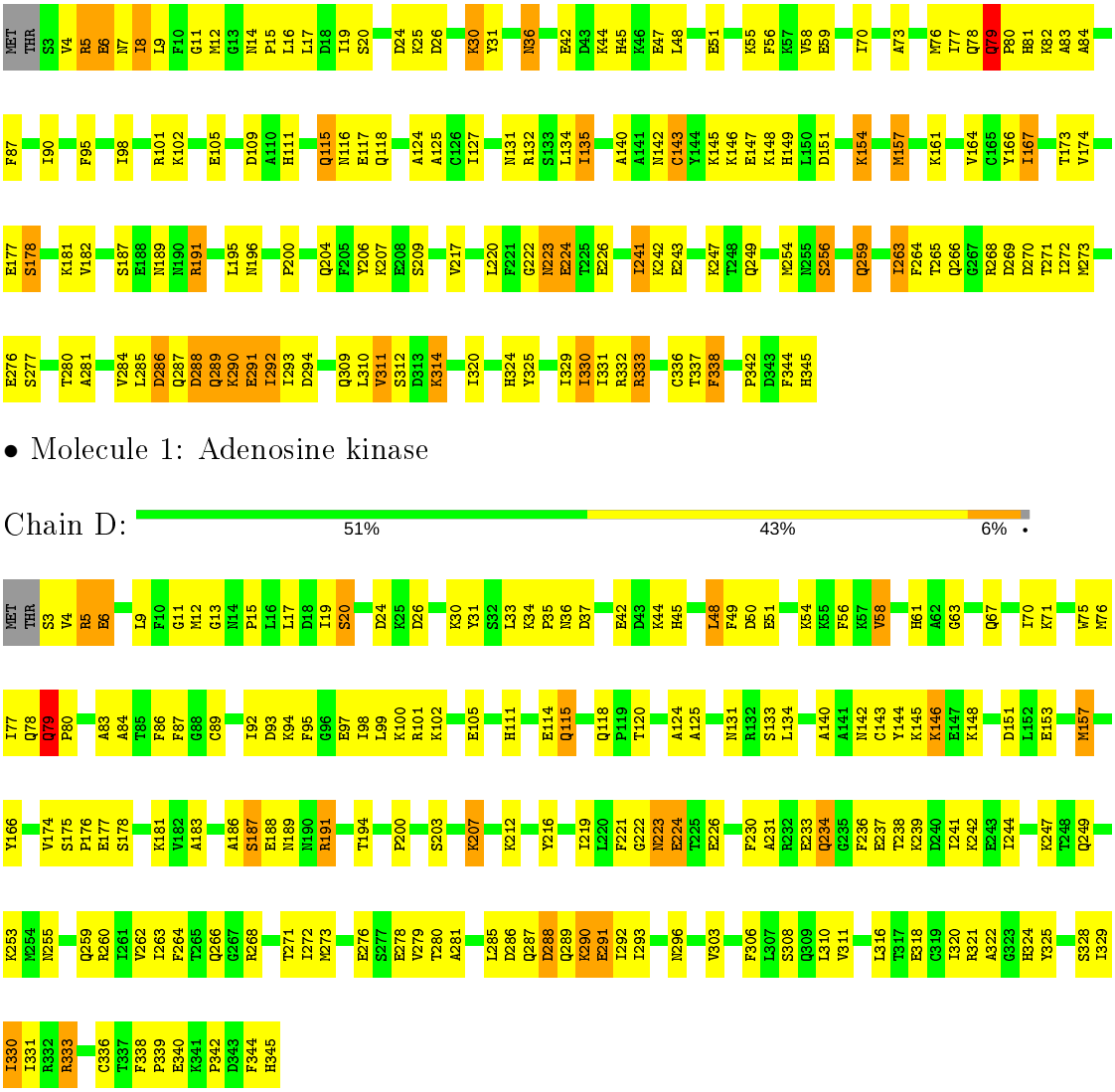
- Molecule 1: Adenosine kinase

Chain B:



- Molecule 1: Adenosine kinase

Chain C:



• Molecule 1: Adenosine kinase

Chain D:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.85Å 66.93Å 87.14Å 97.76° 103.70° 89.95°	Depositor
Resolution (Å)	50.00 – 2.20	Depositor
% Data completeness (in resolution range)	85.5 (50.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	BUSTER	Depositor
R, R_{free}	0.181 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11414	wwPDB-VP
Average B, all atoms (Å^2)	32.0	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: 5I5

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	0.65	0/2761	0.77	0/3722
1	B	0.68	0/2761	0.82	3/3722 (0.1%)
1	C	0.64	0/2761	0.77	0/3722
1	D	0.73	0/2761	0.83	0/3722
All	All	0.68	0/11044	0.80	3/14888 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	258	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	B	81	HIS	O-C-N	-6.41	112.44	122.70
1	B	34	LYS	C-N-CD	-5.40	108.72	120.60

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	2707	0	2690	229	0
1	B	2707	0	2690	168	0
1	C	2707	0	2690	170	0
1	D	2707	0	2690	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	19	0	13	0	0
2	B	19	0	13	0	0
2	C	19	0	13	1	0
2	D	19	0	13	0	0
3	A	125	0	0	20	0
3	B	135	0	0	23	0
3	C	109	0	0	15	0
3	D	141	0	0	19	0
All	All	11414	0	10812	716	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 33.

All (716) 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:C:273:MET:HE3	1:C:320:ILE:HD11	1.20	1.20
1:A:333:ARG:NH2	1:D:333:ARG:HH22	1.45	1.14
1:C:259:GLN:HG2	1:C:276:GLU:HB2	1.24	1.14
1:C:8:ILE:HD13	1:C:311:VAL:HG22	1.31	1.10
1:D:79:GLN:HB3	1:D:80:PRO:HD3	1.34	1.08
1:C:79:GLN:HB3	1:C:80:PRO:HD3	1.29	1.07
1:A:259:GLN:HG2	1:A:276:GLU:HB2	1.36	1.07
1:A:5:ARG:HD2	1:A:5:ARG:H	1.14	1.06
1:D:259:GLN:HG2	1:D:276:GLU:HB2	1.39	1.04
1:A:7:ASN:HB2	1:A:161:LYS:HE2	1.42	1.01
1:A:273:MET:HE1	1:A:316:LEU:HB3	1.43	1.00
1:A:115:GLN:HE22	1:A:118:GLN:H	1.01	1.00
1:B:19:ILE:HG22	1:B:58:VAL:HG21	1.41	0.99
1:C:115:GLN:HE22	1:C:118:GLN:H	1.05	0.99
1:B:290:LYS:HD3	1:B:293:ILE:HG12	1.45	0.98
1:C:263:ILE:HD11	1:C:273:MET:HE2	1.47	0.97
1:A:79:GLN:HB3	1:A:80:PRO:HD3	1.46	0.97
1:B:259:GLN:HG2	1:B:276:GLU:HB2	1.48	0.95
1:B:115:GLN:HE22	1:B:118:GLN:H	1.03	0.95
1:B:345:HIS:HA	3:B:607:HOH:O	1.66	0.95
1:C:79:GLN:HB3	1:C:80:PRO:CD	1.97	0.94
1:A:42:GLU:H	1:A:45:HIS:HD2	1.00	0.94
1:C:42:GLU:H	1:C:45:HIS:HD2	1.00	0.93
1:A:19:ILE:HG23	1:A:58:VAL:HG21	1.51	0.93
1:C:333:ARG:NH1	1:C:333:ARG:HB3	1.84	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:GLN:HE22	1:D:118:GLN:H	1.00	0.92
1:C:19:ILE:HG23	1:C:58:VAL:HG21	1.50	0.92
1:A:345:HIS:HB2	1:D:321:ARG:HH22	1.35	0.92
1:A:333:ARG:HH22	1:D:333:ARG:HH22	0.97	0.92
1:A:207:LYS:HG3	3:A:609:HOH:O	1.69	0.92
1:C:115:GLN:NE2	1:C:118:GLN:H	1.68	0.91
1:B:42:GLU:H	1:B:45:HIS:HD2	1.15	0.89
1:D:89:CYS:SG	1:D:143:CYS:HB2	2.12	0.89
1:D:187:SER:OG	1:D:255:ASN:HB2	1.72	0.89
1:A:345:HIS:HB2	1:D:321:ARG:NH2	1.87	0.88
1:B:290:LYS:HB2	1:B:293:ILE:HG21	1.56	0.87
1:D:288:ASP:HA	3:D:618:HOH:O	1.75	0.86
1:A:291:GLU:HG3	1:A:292:ILE:H	1.39	0.86
1:A:42:GLU:H	1:A:45:HIS:CD2	1.91	0.85
1:A:333:ARG:HH22	1:D:333:ARG:NH2	1.73	0.85
1:C:77:ILE:O	1:C:79:GLN:N	2.10	0.85
1:B:115:GLN:NE2	1:B:118:GLN:H	1.73	0.85
1:D:94:LYS:HG2	3:D:635:HOH:O	1.77	0.85
1:D:42:GLU:H	1:D:45:HIS:HD2	1.18	0.84
1:A:338:PHE:CE1	1:D:330:ILE:HG23	2.12	0.84
1:D:291:GLU:HG3	1:D:292:ILE:H	1.42	0.84
1:A:290:LYS:HE3	1:A:293:ILE:HD11	1.59	0.84
1:D:118:GLN:HG3	3:D:604:HOH:O	1.78	0.84
1:A:115:GLN:NE2	1:A:118:GLN:H	1.75	0.84
1:C:42:GLU:H	1:C:45:HIS:CD2	1.93	0.83
1:D:259:GLN:CG	1:D:276:GLU:HB2	2.06	0.83
1:A:145:LYS:HB2	1:A:148:LYS:HG2	1.61	0.83
1:B:42:GLU:H	1:B:45:HIS:CD2	1.98	0.82
1:A:333:ARG:HB3	1:A:333:ARG:NH1	1.93	0.82
1:D:5:ARG:HH11	1:D:5:ARG:HG3	1.44	0.82
1:C:273:MET:CE	1:C:320:ILE:HD11	2.06	0.82
1:A:341:LYS:NZ	1:D:78:GLN:NE2	2.28	0.81
1:D:115:GLN:NE2	1:D:118:GLN:H	1.76	0.81
1:A:338:PHE:CD1	1:D:330:ILE:HD12	2.15	0.81
1:A:8:ILE:CD1	1:A:311:VAL:HG22	2.11	0.81
1:A:243:GLU:O	1:A:247:LYS:HG3	1.81	0.80
1:A:340:GLU:HB3	3:A:551:HOH:O	1.81	0.80
1:D:79:GLN:HB3	1:D:80:PRO:CD	2.08	0.80
1:C:30:LYS:HE3	3:C:558:HOH:O	1.82	0.80
1:D:115:GLN:HE22	1:D:118:GLN:N	1.78	0.80
1:C:291:GLU:HG3	1:C:292:ILE:H	1.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:HE	1:A:290:LYS:HZ1	1.31	0.79
1:D:345:HIS:O	3:D:531:HOH:O	2.00	0.79
1:B:290:LYS:HB2	1:B:293:ILE:CG2	2.13	0.79
1:C:115:GLN:HE22	1:C:118:GLN:N	1.81	0.78
1:B:115:GLN:HE22	1:B:118:GLN:N	1.80	0.78
1:B:178:SER:O	1:B:182:VAL:HG23	1.83	0.78
1:B:261:ILE:HD13	1:B:275:THR:HG22	1.65	0.78
1:C:20:SER:HB3	1:C:125:ALA:HB3	1.65	0.78
1:C:268:ARG:HE	1:C:290:LYS:NZ	1.81	0.78
1:B:19:ILE:HG22	1:B:58:VAL:CG2	2.14	0.77
1:D:79:GLN:CB	1:D:80:PRO:HD3	2.14	0.77
1:A:273:MET:CE	1:A:316:LEU:HB3	2.13	0.77
1:C:256:SER:HA	3:C:570:HOH:O	1.83	0.77
1:D:290:LYS:HD2	1:D:291:GLU:N	2.00	0.77
1:B:78:GLN:HG2	3:B:592:HOH:O	1.84	0.77
1:D:157:MET:HG2	3:D:527:HOH:O	1.84	0.77
1:C:145:LYS:HB2	1:C:148:LYS:HG2	1.66	0.76
1:D:231:ALA:HB2	1:D:244:ILE:HG12	1.68	0.76
1:C:145:LYS:HB2	1:C:148:LYS:CG	2.16	0.76
1:A:140:ALA:HA	1:A:143:CYS:SG	2.27	0.75
1:A:5:ARG:N	1:A:5:ARG:HD2	1.91	0.75
1:B:223:ASN:ND2	1:B:226:GLU:H	1.85	0.75
1:D:146:LYS:HE2	1:D:181:LYS:HD2	1.68	0.75
1:A:8:ILE:HD13	1:A:311:VAL:HG22	1.67	0.75
1:A:344:PHE:CE1	1:D:321:ARG:HB3	2.22	0.75
1:A:79:GLN:CB	1:A:80:PRO:HD3	2.16	0.75
1:D:54:LYS:HG3	3:D:603:HOH:O	1.87	0.75
1:A:339:PRO:HD2	1:D:329:ILE:CG2	2.17	0.75
1:B:5:ARG:HG3	1:B:5:ARG:HH11	1.52	0.74
1:A:285:LEU:HD11	3:A:574:HOH:O	1.88	0.74
1:B:3:SER:N	3:B:614:HOH:O	2.20	0.74
1:A:31:TYR:CE2	1:A:48:LEU:HB2	2.23	0.73
1:A:268:ARG:HE	1:A:290:LYS:NZ	1.85	0.73
1:B:273:MET:HE2	1:B:320:ILE:HD11	1.68	0.73
1:B:42:GLU:N	1:B:45:HIS:HD2	1.86	0.73
1:B:125:ALA:HA	1:B:134:LEU:HD23	1.70	0.73
1:B:268:ARG:HE	1:B:290:LYS:HE2	1.54	0.73
1:D:333:ARG:HB3	1:D:333:ARG:NH1	2.04	0.73
1:C:5:ARG:HG3	1:C:5:ARG:HH11	1.52	0.73
1:B:145:LYS:HB2	1:B:148:LYS:HG3	1.69	0.73
1:B:191:ARG:HH11	1:B:191:ARG:HG3	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:GLU:HG2	3:D:641:HOH:O	1.88	0.73
1:D:98:ILE:HG13	3:D:635:HOH:O	1.87	0.73
1:A:11:GLY:O	1:A:86:PHE:HA	1.89	0.72
1:C:12:MET:CG	1:C:167:ILE:HD13	2.19	0.72
1:A:287:GLN:O	1:A:290:LYS:HG3	1.88	0.72
1:D:259:GLN:HG2	1:D:276:GLU:CB	2.18	0.72
1:A:341:LYS:HZ1	1:D:78:GLN:NE2	1.85	0.72
1:C:243:GLU:HG3	1:C:247:LYS:HE2	1.70	0.72
1:A:146:LYS:NZ	1:A:151:ASP:OD2	2.23	0.71
1:A:291:GLU:HG2	3:A:591:HOH:O	1.89	0.71
1:A:19:ILE:HG23	1:A:58:VAL:CG2	2.20	0.71
1:B:209:SER:O	1:B:213:VAL:HG23	1.90	0.71
1:D:328:SER:O	1:D:331:ILE:HD11	1.91	0.71
1:B:278:GLU:HA	3:B:543:HOH:O	1.90	0.71
1:C:140:ALA:HA	1:C:143:CYS:SG	2.30	0.71
1:D:333:ARG:HB3	1:D:333:ARG:HH11	1.56	0.71
1:B:145:LYS:HB2	1:B:148:LYS:CG	2.21	0.71
1:C:146:LYS:HE2	1:C:181:LYS:HD2	1.71	0.71
1:A:257:LYS:HE2	3:A:619:HOH:O	1.91	0.71
1:A:342:PRO:HA	1:D:75:TRP:CH2	2.26	0.71
1:C:56:PHE:HB3	3:C:561:HOH:O	1.91	0.71
1:C:285:LEU:O	1:C:287:GLN:N	2.21	0.70
1:C:47:GLU:HB2	3:C:594:HOH:O	1.89	0.70
1:B:140:ALA:HA	1:B:143:CYS:SG	2.31	0.70
1:A:115:GLN:HE22	1:A:118:GLN:N	1.85	0.70
1:D:5:ARG:HD2	1:D:5:ARG:H	1.56	0.70
1:B:243:GLU:HG2	3:B:596:HOH:O	1.90	0.70
1:D:191:ARG:HH11	1:D:191:ARG:HG3	1.57	0.70
1:A:184:HIS:HB2	3:A:623:HOH:O	1.91	0.70
1:C:263:ILE:HD11	1:C:273:MET:CE	2.20	0.70
1:A:333:ARG:NH2	1:D:333:ARG:NH2	2.30	0.70
1:A:50:ASP:HB3	1:A:54:LYS:NZ	2.07	0.70
1:A:79:GLN:HB3	1:A:80:PRO:CD	2.21	0.70
1:B:273:MET:CE	1:B:320:ILE:HD11	2.22	0.69
1:A:339:PRO:HD2	1:D:329:ILE:HG23	1.74	0.69
1:A:344:PHE:HB2	1:D:76:MET:HE1	1.73	0.69
1:D:101:ARG:O	1:D:105:GLU:HG3	1.93	0.69
1:B:291:GLU:HG3	1:B:292:ILE:H	1.58	0.69
1:C:4:VAL:O	1:C:80:PRO:HG3	1.93	0.69
1:C:333:ARG:HH11	1:C:333:ARG:HB3	1.57	0.68
1:A:267:GLY:HA3	3:A:587:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:SER:O	1:B:331:ILE:HD11	1.93	0.68
1:B:146:LYS:NZ	1:B:151:ASP:OD2	2.26	0.68
1:C:223:ASN:ND2	1:C:226:GLU:H	1.91	0.68
1:A:82:LYS:HB3	1:A:109:ASP:HB2	1.74	0.68
1:A:77:ILE:O	1:A:79:GLN:N	2.25	0.68
1:A:290:LYS:CE	1:A:293:ILE:HD11	2.22	0.68
1:B:318:GLU:OE2	1:B:321:ARG:NH1	2.27	0.67
1:B:325:TYR:CZ	1:B:329:ILE:HG13	2.29	0.67
1:A:19:ILE:CG2	1:A:58:VAL:HG21	2.22	0.67
1:C:12:MET:HG2	1:C:167:ILE:HD13	1.75	0.67
1:A:200:PRO:O	1:A:204:GLN:HG3	1.94	0.67
1:C:287:GLN:NE2	3:C:583:HOH:O	2.28	0.67
1:C:259:GLN:CG	1:C:276:GLU:HB2	2.15	0.67
1:C:117:GLU:N	1:C:117:GLU:OE2	2.24	0.67
1:C:101:ARG:HH12	1:C:102:LYS:HZ1	1.42	0.67
1:D:5:ARG:HG3	1:D:5:ARG:NH1	2.10	0.66
1:B:25:LYS:HB2	3:B:564:HOH:O	1.96	0.66
1:C:5:ARG:NH1	1:C:5:ARG:HG3	2.10	0.66
1:D:20:SER:HB2	1:D:125:ALA:HB3	1.78	0.66
1:D:35:PRO:O	1:D:131:ASN:HB3	1.96	0.66
1:C:191:ARG:HG3	1:C:191:ARG:HH11	1.60	0.66
1:B:242:LYS:HB3	1:B:279:VAL:HG11	1.78	0.66
1:C:36:ASN:HA	1:C:132:ARG:O	1.95	0.65
1:D:318:GLU:OE2	1:D:321:ARG:NH1	2.28	0.65
1:B:5:ARG:HD2	1:B:5:ARG:H	1.62	0.65
1:C:135:ILE:N	1:C:135:ILE:HD12	2.11	0.65
1:A:259:GLN:CG	1:A:276:GLU:HB2	2.22	0.65
1:C:263:ILE:CD1	1:C:273:MET:HE2	2.24	0.65
1:B:73:ALA:O	1:B:77:ILE:HG13	1.97	0.65
1:C:268:ARG:HE	1:C:290:LYS:HZ1	1.44	0.65
1:A:223:ASN:ND2	1:A:226:GLU:H	1.93	0.65
1:B:249:GLN:NE2	1:B:260:ARG:O	2.29	0.65
1:C:333:ARG:CZ	1:C:333:ARG:HB3	2.25	0.65
1:B:291:GLU:O	1:B:293:ILE:N	2.29	0.65
1:D:153:GLU:HG2	1:D:157:MET:CE	2.27	0.65
1:D:242:LYS:HD3	1:D:279:VAL:CG1	2.27	0.65
1:B:223:ASN:HD22	1:B:223:ASN:C	2.00	0.64
1:A:317:THR:HB	3:A:514:HOH:O	1.96	0.64
1:D:268:ARG:NH2	3:D:618:HOH:O	2.22	0.64
1:B:140:ALA:O	1:B:143:CYS:SG	2.53	0.64
1:B:290:LYS:HD2	1:B:291:GLU:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:LYS:HB2	1:D:148:LYS:CG	2.27	0.64
1:D:76:MET:HE1	1:D:325:TYR:HD2	1.62	0.64
1:C:288:ASP:HA	3:C:605:HOH:O	1.97	0.64
1:D:290:LYS:HD2	1:D:291:GLU:H	1.63	0.64
1:D:63:GLY:O	1:D:67:GLN:NE2	2.31	0.64
1:B:12:MET:O	1:B:167:ILE:HG23	1.98	0.64
1:B:299:GLY:HA3	3:B:612:HOH:O	1.98	0.64
1:A:285:LEU:HD21	3:A:583:HOH:O	1.97	0.64
1:A:140:ALA:C	1:A:143:CYS:HG	2.02	0.63
1:B:345:HIS:HE1	3:B:552:HOH:O	1.80	0.63
1:C:101:ARG:O	1:C:105:GLU:HG3	1.98	0.63
1:C:79:GLN:CB	1:C:80:PRO:CD	2.76	0.63
1:A:31:TYR:CD2	1:A:48:LEU:HB2	2.33	0.63
1:C:26:ASP:O	1:C:30:LYS:HD3	1.98	0.63
1:A:178:SER:O	1:A:182:VAL:HG23	1.98	0.63
1:A:344:PHE:CD1	1:D:322:ALA:HA	2.34	0.63
1:A:42:GLU:N	1:A:45:HIS:HD2	1.85	0.63
1:C:173:THR:HG22	1:C:206:TYR:CE2	2.33	0.63
1:D:207:LYS:NZ	1:D:233:GLU:OE2	2.25	0.63
1:A:339:PRO:HG2	1:D:329:ILE:HD12	1.80	0.63
1:C:73:ALA:O	1:C:77:ILE:HD12	1.98	0.63
1:B:77:ILE:O	1:B:78:GLN:CB	2.45	0.62
1:C:146:LYS:NZ	1:C:151:ASP:OD2	2.29	0.62
1:C:223:ASN:HD22	1:C:223:ASN:C	2.02	0.62
1:C:268:ARG:HE	1:C:290:LYS:CE	2.12	0.62
1:B:81:HIS:HB3	3:B:533:HOH:O	1.99	0.62
1:C:243:GLU:O	1:C:247:LYS:HG3	1.99	0.62
1:C:290:LYS:HE3	1:C:293:ILE:HD11	1.80	0.62
1:A:344:PHE:HE1	1:D:321:ARG:HB3	1.63	0.62
1:A:290:LYS:HG2	1:A:293:ILE:HD13	1.81	0.62
1:D:273:MET:CE	1:D:316:LEU:HB3	2.29	0.62
1:A:336:CYS:HB3	1:D:336:CYS:SG	2.40	0.62
1:A:94:LYS:NZ	3:A:620:HOH:O	2.30	0.62
1:A:285:LEU:O	1:A:287:GLN:N	2.27	0.61
1:A:333:ARG:HB3	1:A:333:ARG:HH11	1.64	0.61
1:B:223:ASN:HD21	1:B:226:GLU:H	1.48	0.61
1:A:339:PRO:CD	1:D:329:ILE:HG23	2.31	0.61
1:C:241:ILE:HG23	1:C:242:LYS:N	2.14	0.61
1:A:8:ILE:HG23	1:A:311:VAL:HG21	1.83	0.61
1:A:268:ARG:HE	1:A:290:LYS:CE	2.13	0.61
1:A:332:ARG:O	1:A:333:ARG:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLN:NE2	1:A:260:ARG:O	2.34	0.61
1:A:173:THR:HG22	1:A:206:TYR:CE2	2.36	0.61
1:C:290:LYS:HB2	1:C:293:ILE:CG2	2.31	0.61
1:D:273:MET:HE2	1:D:316:LEU:HB3	1.83	0.61
1:A:341:LYS:HZ2	1:D:78:GLN:NE2	1.97	0.61
1:A:285:LEU:O	1:A:287:GLN:HG2	2.01	0.60
1:A:336:CYS:HB3	3:A:624:HOH:O	2.01	0.60
1:C:19:ILE:CG2	1:C:58:VAL:HG21	2.27	0.60
1:B:290:LYS:HD3	1:B:293:ILE:CG1	2.26	0.60
1:D:288:ASP:O	1:D:289:GLN:HG2	2.01	0.60
1:D:51:GLU:HB2	3:D:586:HOH:O	2.01	0.60
1:C:290:LYS:HB2	1:C:293:ILE:HG21	1.83	0.60
1:C:290:LYS:HD2	1:C:291:GLU:N	2.15	0.60
1:D:290:LYS:HE3	1:D:293:ILE:HD11	1.84	0.60
1:D:48:LEU:HD23	1:D:48:LEU:C	2.21	0.60
1:B:293:ILE:HG13	1:B:293:ILE:O	2.00	0.60
1:D:203:SER:O	1:D:207:LYS:HG2	2.01	0.60
1:A:344:PHE:O	1:D:321:ARG:NH2	2.35	0.60
1:C:24:ASP:OD2	1:C:26:ASP:HB2	2.01	0.60
1:B:268:ARG:HE	1:B:290:LYS:CE	2.15	0.59
1:D:42:GLU:H	1:D:45:HIS:CD2	2.09	0.59
1:D:145:LYS:HB2	1:D:148:LYS:HG3	1.84	0.59
1:A:286:ASP:HB2	3:A:517:HOH:O	2.03	0.59
1:C:101:ARG:HH12	1:C:102:LYS:NZ	1.99	0.59
1:A:223:ASN:HD21	1:A:226:GLU:H	1.50	0.59
1:C:36:ASN:OD1	1:C:131:ASN:HA	2.03	0.59
1:D:280:THR:HG22	1:D:281:ALA:N	2.16	0.59
1:A:338:PHE:CD1	1:D:330:ILE:HG23	2.37	0.59
1:C:272:ILE:HD12	1:C:272:ILE:N	2.18	0.59
1:A:291:GLU:HG3	1:A:292:ILE:N	2.14	0.59
1:B:46:LYS:HB2	3:B:542:HOH:O	2.02	0.59
1:C:285:LEU:O	1:C:287:GLN:HG2	2.02	0.59
1:A:186:ALA:HA	1:A:191:ARG:HB2	1.85	0.59
1:B:5:ARG:NH1	1:B:5:ARG:HG3	2.18	0.59
1:D:79:GLN:CB	1:D:80:PRO:CD	2.76	0.59
1:A:241:ILE:HG12	1:A:272:ILE:HD13	1.84	0.58
1:A:344:PHE:O	1:A:345:HIS:HB2	2.03	0.58
1:D:296:ASN:ND2	3:D:592:HOH:O	2.29	0.58
1:B:290:LYS:HD3	1:B:293:ILE:CG2	2.32	0.58
1:A:261:ILE:HD13	1:A:316:LEU:CD1	2.34	0.58
1:A:284:VAL:HG22	1:A:324:HIS:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:LEU:HB2	3:C:583:HOH:O	2.03	0.58
1:A:290:LYS:HB2	1:A:293:ILE:HG21	1.86	0.58
1:D:36:ASN:ND2	3:D:552:HOH:O	2.37	0.57
1:D:194:THR:HG22	1:D:219:ILE:HB	1.87	0.57
1:A:166:TYR:OH	1:A:196:ASN:ND2	2.28	0.57
1:B:124:ALA:O	1:B:134:LEU:HA	2.04	0.57
1:A:185:HIS:CE1	1:A:189:ASN:ND2	2.73	0.57
1:A:332:ARG:C	1:A:333:ARG:HG2	2.23	0.57
1:D:70:ILE:HG23	1:D:84:ALA:HB1	1.87	0.57
1:B:183:ALA:HB2	1:B:193:PHE:CE2	2.39	0.57
1:B:285:LEU:HD23	3:B:568:HOH:O	2.04	0.57
1:B:78:GLN:OE1	1:C:342:PRO:HD3	2.04	0.57
1:A:257:LYS:HG3	3:A:619:HOH:O	2.05	0.57
1:B:49:PHE:O	1:B:53:VAL:HG23	2.05	0.57
1:D:242:LYS:HB3	1:D:279:VAL:HG11	1.86	0.56
1:B:285:LEU:O	1:B:287:GLN:HG2	2.05	0.56
1:A:333:ARG:NH1	3:A:569:HOH:O	2.39	0.56
1:A:223:ASN:C	1:A:223:ASN:HD22	2.09	0.56
1:C:290:LYS:HD2	1:C:291:GLU:H	1.71	0.56
1:B:330:ILE:HD12	1:C:338:PHE:CD1	2.41	0.56
1:B:36:ASN:OD1	1:B:131:ASN:HA	2.06	0.56
1:B:81:HIS:O	1:B:82:LYS:HB2	2.06	0.56
1:B:92:ILE:HD12	1:B:116:ASN:OD1	2.05	0.56
1:A:13:GLY:O	1:A:15:PRO:HD3	2.06	0.56
1:D:242:LYS:HD3	1:D:279:VAL:HG12	1.86	0.56
1:B:262:VAL:O	1:B:273:MET:HA	2.06	0.56
1:B:290:LYS:CB	1:B:293:ILE:HG21	2.33	0.55
1:D:77:ILE:O	1:D:79:GLN:N	2.37	0.55
1:A:203:SER:O	1:A:207:LYS:HG2	2.06	0.55
1:B:288:ASP:O	1:B:290:LYS:N	2.38	0.55
1:C:224:GLU:HG3	1:C:266:GLN:HA	1.87	0.55
1:D:50:ASP:HB3	1:D:54:LYS:NZ	2.21	0.55
1:A:261:ILE:HD13	1:A:316:LEU:HD11	1.88	0.55
1:A:343:ASP:OD2	1:A:343:ASP:O	2.25	0.55
1:A:50:ASP:HB3	1:A:54:LYS:HZ2	1.71	0.55
1:A:8:ILE:HD13	1:A:311:VAL:CG2	2.35	0.55
1:B:183:ALA:HB2	1:B:193:PHE:CZ	2.41	0.55
1:B:263:ILE:CD1	1:B:306:PHE:CE2	2.90	0.55
1:C:287:GLN:O	1:C:288:ASP:O	2.23	0.55
1:A:342:PRO:HB3	1:D:76:MET:SD	2.47	0.55
1:A:344:PHE:HB2	1:D:76:MET:CE	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LEU:HA	3:B:568:HOH:O	2.07	0.55
1:C:268:ARG:NE	1:C:290:LYS:CE	2.70	0.55
1:D:13:GLY:O	1:D:15:PRO:HD3	2.07	0.55
1:A:284:VAL:HG12	1:A:285:LEU:N	2.21	0.55
1:C:268:ARG:NE	1:C:290:LYS:HE2	2.21	0.55
1:D:223:ASN:C	1:D:223:ASN:HD22	2.10	0.55
1:D:231:ALA:CB	1:D:244:ILE:HG12	2.36	0.55
1:A:333:ARG:HB3	1:A:333:ARG:CZ	2.37	0.55
1:B:25:LYS:O	1:B:25:LYS:HG3	2.07	0.55
1:A:338:PHE:HB3	1:D:330:ILE:CD1	2.37	0.55
1:D:87:PHE:HA	1:D:111:HIS:O	2.07	0.55
1:D:285:LEU:O	1:D:287:GLN:N	2.38	0.55
1:A:184:HIS:CD2	3:A:623:HOH:O	2.60	0.54
1:B:255:ASN:OD1	1:B:257:LYS:HB2	2.07	0.54
1:D:291:GLU:HG3	1:D:292:ILE:N	2.19	0.54
1:B:206:TYR:CD1	1:B:206:TYR:N	2.75	0.54
1:B:292:ILE:O	1:B:292:ILE:HG22	2.07	0.54
1:C:191:ARG:CG	1:C:191:ARG:HH11	2.20	0.54
1:B:186:ALA:HA	1:B:191:ARG:HB2	1.90	0.54
1:B:290:LYS:HZ2	1:B:293:ILE:HD13	1.72	0.54
1:D:290:LYS:HD3	1:D:293:ILE:CD1	2.38	0.54
1:D:54:LYS:HE3	3:D:603:HOH:O	2.08	0.54
1:A:335:GLY:O	1:D:333:ARG:HG3	2.07	0.54
1:B:333:ARG:NH2	1:C:333:ARG:HH22	2.05	0.54
1:B:224:GLU:HG3	1:B:266:GLN:HA	1.90	0.54
1:B:53:VAL:HG13	1:B:58:VAL:HG11	1.89	0.54
1:B:214:MET:HB3	1:B:215:PRO:HD3	1.89	0.54
1:D:31:TYR:HB2	1:D:33:LEU:CD1	2.37	0.53
1:D:333:ARG:HB2	1:D:336:CYS:SG	2.48	0.53
1:C:70:ILE:HG23	1:C:84:ALA:HB1	1.90	0.53
1:B:284:VAL:HG12	1:B:285:LEU:N	2.22	0.53
1:B:19:ILE:CG2	1:B:58:VAL:HG21	2.28	0.53
1:A:224:GLU:HG2	1:A:266:GLN:HG2	1.91	0.53
1:B:325:TYR:CE1	1:B:329:ILE:HG13	2.43	0.53
1:D:186:ALA:HA	1:D:191:ARG:HB2	1.91	0.53
1:C:271:THR:C	1:C:272:ILE:HD12	2.28	0.53
1:D:280:THR:CG2	1:D:281:ALA:N	2.72	0.53
1:A:101:ARG:NE	3:A:554:HOH:O	2.33	0.53
1:A:31:TYR:CZ	1:A:48:LEU:HA	2.43	0.53
1:B:285:LEU:O	1:B:287:GLN:N	2.37	0.53
1:D:263:ILE:CD1	1:D:306:PHE:CE2	2.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:CD1	1:A:132:ARG:HH12	2.21	0.52
1:D:338:PHE:N	1:D:338:PHE:CD2	2.74	0.52
1:C:164:VAL:HG21	1:C:310:LEU:HD13	1.91	0.52
1:D:224:GLU:HG3	1:D:266:GLN:HA	1.91	0.52
1:D:290:LYS:HD3	1:D:293:ILE:HD13	1.91	0.52
1:A:263:ILE:HD11	1:A:273:MET:HE3	1.91	0.52
1:A:4:VAL:O	1:A:80:PRO:HG3	2.09	0.52
1:A:127:ILE:HD11	1:A:132:ARG:HH12	1.75	0.52
1:B:156:TRP:CE3	1:B:181:LYS:HE2	2.45	0.52
1:D:142:ASN:HD22	1:D:174:VAL:HG22	1.75	0.52
1:D:166:TYR:CZ	1:D:303:VAL:HG11	2.45	0.52
1:A:241:ILE:CG1	1:A:272:ILE:HD13	2.40	0.52
1:A:290:LYS:HD3	1:A:293:ILE:HG12	1.91	0.52
1:D:290:LYS:CD	1:D:293:ILE:HD13	2.40	0.52
1:C:290:LYS:HG2	1:C:293:ILE:HD13	1.92	0.51
1:D:329:ILE:HG22	1:D:330:ILE:N	2.25	0.51
1:B:135:ILE:HD12	1:B:135:ILE:N	2.25	0.51
1:A:344:PHE:HE1	1:D:321:ARG:CB	2.22	0.51
1:A:127:ILE:HG23	1:A:131:ASN:O	2.09	0.51
1:C:259:GLN:HG2	1:C:276:GLU:CB	2.17	0.51
1:B:280:THR:HG22	1:B:282:PHE:CE2	2.45	0.51
1:B:259:GLN:CG	1:B:276:GLU:HB2	2.32	0.51
1:B:34:LYS:HB3	1:B:35:PRO:HD2	1.91	0.51
1:C:125:ALA:O	1:C:127:ILE:HD12	2.10	0.51
1:C:291:GLU:O	1:C:293:ILE:N	2.43	0.51
1:A:333:ARG:CZ	1:D:333:ARG:HH22	2.20	0.51
1:B:284:VAL:CG1	1:B:285:LEU:N	2.73	0.51
1:C:324:HIS:HD2	3:C:542:HOH:O	1.93	0.51
1:B:207:LYS:NZ	1:B:233:GLU:OE2	2.42	0.51
1:A:79:GLN:CB	1:A:80:PRO:CD	2.83	0.51
1:B:332:ARG:HG2	3:B:613:HOH:O	2.10	0.51
1:A:338:PHE:CD2	1:A:338:PHE:N	2.78	0.51
1:C:154:LYS:HA	1:C:157:MET:HE2	1.93	0.51
1:C:55:LYS:HB2	1:C:56:PHE:CE1	2.46	0.51
1:D:273:MET:HE3	1:D:320:ILE:HD11	1.92	0.51
1:A:344:PHE:CZ	1:D:321:ARG:HB3	2.46	0.51
1:D:4:VAL:O	1:D:80:PRO:HG3	2.11	0.51
1:A:344:PHE:CE1	1:D:322:ALA:N	2.80	0.50
3:B:578:HOH:O	1:C:344:PHE:HB3	2.10	0.50
1:D:124:ALA:O	1:D:134:LEU:HA	2.11	0.50
1:A:241:ILE:CG2	1:A:272:ILE:HD13	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ARG:HH11	1:A:258:ARG:HG2	1.76	0.50
1:B:101:ARG:HH11	1:B:101:ARG:HG2	1.75	0.50
1:D:222:GLY:O	1:D:264:PHE:HA	2.11	0.50
1:D:92:ILE:O	1:D:92:ILE:HG22	2.11	0.50
1:A:48:LEU:C	1:A:48:LEU:HD23	2.31	0.50
1:B:290:LYS:O	1:B:293:ILE:HG23	2.12	0.50
1:C:55:LYS:HB2	1:C:56:PHE:CD1	2.47	0.50
1:D:153:GLU:CG	1:D:157:MET:CE	2.90	0.50
1:C:31:TYR:OH	1:C:51:GLU:OE1	2.30	0.50
1:A:24:ASP:OD2	1:A:26:ASP:HB2	2.11	0.50
1:B:303:VAL:O	1:B:307:LEU:HG	2.11	0.50
1:C:173:THR:HG22	1:C:206:TYR:CD2	2.45	0.50
1:C:142:ASN:HD22	1:C:174:VAL:HG22	1.76	0.50
1:A:261:ILE:CD1	1:A:316:LEU:HD11	2.42	0.50
1:B:254:MET:HA	1:B:254:MET:HE2	1.94	0.50
1:C:11:GLY:HA2	1:C:166:TYR:O	2.12	0.50
1:A:214:MET:N	1:A:215:PRO:CD	2.74	0.49
1:A:318:GLU:OE1	1:A:321:ARG:NH1	2.44	0.49
1:C:217:VAL:HG11	1:C:220:LEU:HB2	1.93	0.49
1:C:90:ILE:HA	3:C:512:HOH:O	2.11	0.49
1:A:215:PRO:HB3	1:A:254:MET:CE	2.41	0.49
1:B:336:CYS:SG	1:C:336:CYS:SG	3.09	0.49
1:B:205:PHE:HB2	1:B:206:TYR:CE1	2.47	0.49
1:C:265:THR:HB	3:C:602:HOH:O	2.12	0.49
1:B:94:LYS:O	1:B:98:ILE:HG13	2.13	0.49
1:C:147:GLU:HA	1:C:151:ASP:OD2	2.12	0.49
1:B:343:ASP:N	1:C:325:TYR:OH	2.37	0.49
1:C:338:PHE:CD2	1:C:338:PHE:N	2.79	0.49
1:B:6:GLU:O	1:B:7:ASN:HB2	2.13	0.49
1:C:58:VAL:CG2	1:C:59:GLU:N	2.74	0.49
1:A:243:GLU:HA	1:A:243:GLU:OE2	2.11	0.49
1:A:50:ASP:HB3	1:A:54:LYS:HZ3	1.75	0.49
1:B:286:ASP:HB3	3:B:631:HOH:O	2.11	0.49
1:C:290:LYS:CD	1:C:291:GLU:N	2.76	0.49
1:A:341:LYS:HB3	1:A:342:PRO:HD2	1.94	0.49
1:B:271:THR:OG1	1:B:324:HIS:HE1	1.96	0.49
1:C:195:LEU:HG	1:C:196:ASN:N	2.28	0.49
1:A:232:ARG:O	1:A:232:ARG:HG2	2.12	0.49
1:A:67:GLN:HG3	1:A:86:PHE:CE2	2.48	0.49
1:B:273:MET:CE	1:B:320:ILE:CD1	2.91	0.49
1:B:344:PHE:HB2	1:C:325:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ILE:O	1:B:78:GLN:HB3	2.12	0.49
1:D:67:GLN:O	1:D:71:LYS:HG3	2.12	0.49
1:D:271:THR:OG1	1:D:324:HIS:HE1	1.95	0.49
1:D:19:ILE:CG2	1:D:58:VAL:HG21	2.43	0.49
1:B:118:GLN:HG3	3:B:509:HOH:O	2.13	0.48
1:C:95:PHE:HA	1:C:98:ILE:HD12	1.95	0.48
1:A:189:ASN:HB2	1:A:191:ARG:HD3	1.94	0.48
1:A:286:ASP:N	3:A:517:HOH:O	2.47	0.48
1:D:237:GLU:O	1:D:238:THR:HB	2.13	0.48
1:D:339:PRO:O	1:D:340:GLU:C	2.51	0.48
1:A:333:ARG:HB2	1:A:336:CYS:SG	2.54	0.48
1:B:191:ARG:HH11	1:B:191:ARG:CG	2.18	0.48
1:B:261:ILE:CD1	1:B:316:LEU:HD11	2.43	0.48
1:C:87:PHE:HA	1:C:111:HIS:O	2.14	0.48
1:D:238:THR:HG23	1:D:244:ILE:HG13	1.95	0.48
1:A:102:LYS:HD2	3:A:614:HOH:O	2.13	0.48
1:B:121:GLY:HA3	1:B:138:LEU:O	2.14	0.48
1:B:243:GLU:O	1:B:247:LYS:HG3	2.13	0.48
1:C:58:VAL:HG22	1:C:59:GLU:N	2.28	0.48
1:A:240:ASP:OD1	1:A:243:GLU:HB2	2.13	0.47
1:A:291:GLU:CG	1:A:292:ILE:H	2.21	0.47
1:A:291:GLU:HG3	1:A:292:ILE:HG13	1.96	0.47
1:B:24:ASP:O	1:B:27:PHE:N	2.47	0.47
1:C:178:SER:O	1:C:182:VAL:HG23	2.13	0.47
1:C:266:GLN:O	1:C:269:ASP:HB2	2.14	0.47
1:A:70:ILE:HG23	1:A:84:ALA:HB1	1.97	0.47
1:C:268:ARG:NH2	3:C:605:HOH:O	2.20	0.47
1:D:19:ILE:HG22	1:D:58:VAL:CG2	2.44	0.47
1:B:263:ILE:O	1:B:263:ILE:HG22	2.13	0.47
1:C:344:PHE:O	1:C:345:HIS:HB2	2.14	0.47
1:A:142:ASN:HD22	1:A:174:VAL:HG22	1.78	0.47
1:A:173:THR:HG22	1:A:206:TYR:CZ	2.49	0.47
1:D:93:ASP:HB2	3:D:523:HOH:O	2.14	0.47
1:C:288:ASP:O	1:C:289:GLN:CG	2.63	0.47
1:C:290:LYS:CE	1:C:293:ILE:HD11	2.43	0.47
1:C:8:ILE:HG23	1:C:311:VAL:CG2	2.44	0.47
1:D:151:ASP:OD1	1:D:181:LYS:HE3	2.14	0.47
1:D:11:GLY:O	1:D:86:PHE:HA	2.14	0.47
1:B:288:ASP:C	1:B:290:LYS:H	2.18	0.47
1:C:284:VAL:HG12	1:C:285:LEU:N	2.29	0.47
1:C:77:ILE:O	1:C:79:GLN:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ASN:ND2	1:B:223:ASN:C	2.67	0.47
1:C:291:GLU:HG3	1:C:292:ILE:HG13	1.97	0.47
1:D:67:GLN:HG3	1:D:86:PHE:CE2	2.50	0.47
1:A:127:ILE:CD1	1:A:132:ARG:NH1	2.78	0.47
1:D:223:ASN:C	1:D:223:ASN:ND2	2.68	0.47
1:A:164:VAL:HG21	1:A:310:LEU:HD12	1.96	0.47
1:B:70:ILE:HG23	1:B:84:ALA:HB1	1.97	0.47
1:D:189:ASN:HB2	1:D:191:ARG:HD3	1.95	0.47
1:D:263:ILE:HA	1:D:272:ILE:O	2.15	0.46
1:A:101:ARG:HH11	1:A:101:ARG:HG2	1.80	0.46
1:A:215:PRO:HB3	1:A:254:MET:HE2	1.97	0.46
1:A:290:LYS:HD2	1:A:290:LYS:N	2.31	0.46
1:D:92:ILE:HG13	1:D:114:GLU:HB3	1.97	0.46
1:A:30:LYS:HG2	3:A:605:HOH:O	2.15	0.46
1:D:285:LEU:O	1:D:287:GLN:HG2	2.15	0.46
1:A:154:LYS:HA	1:A:157:MET:HE3	1.97	0.46
1:A:284:VAL:CG1	1:A:285:LEU:N	2.79	0.46
1:B:92:ILE:O	1:B:92:ILE:HG22	2.14	0.46
1:C:290:LYS:CE	1:C:293:ILE:CD1	2.94	0.46
1:A:7:ASN:CB	1:A:161:LYS:HE2	2.30	0.46
1:C:5:ARG:H	1:C:5:ARG:HD2	1.81	0.46
1:A:285:LEU:HD23	1:A:285:LEU:N	2.31	0.46
1:A:341:LYS:O	1:A:342:PRO:O	2.34	0.46
1:C:291:GLU:HG3	1:C:292:ILE:N	2.23	0.46
1:D:241:ILE:HD13	1:D:266:GLN:NE2	2.30	0.46
1:A:53:VAL:HG13	1:A:58:VAL:HG11	1.98	0.46
1:D:318:GLU:HA	1:D:318:GLU:OE1	2.16	0.46
1:A:189:ASN:O	1:A:191:ARG:HD2	2.16	0.46
1:A:224:GLU:HG3	1:A:266:GLN:HA	1.98	0.46
1:D:140:ALA:HA	1:D:143:CYS:SG	2.56	0.46
1:A:293:ILE:HG22	1:A:331:ILE:HD13	1.97	0.46
1:B:191:ARG:NH1	1:B:191:ARG:CG	2.76	0.46
1:B:222:GLY:O	1:B:264:PHE:HA	2.15	0.46
1:C:12:MET:HG3	1:C:167:ILE:HD13	1.96	0.46
1:C:191:ARG:CG	1:C:191:ARG:NH1	2.78	0.46
1:C:280:THR:HG22	1:C:281:ALA:N	2.31	0.46
1:D:191:ARG:NH1	1:D:191:ARG:HG3	2.27	0.46
1:D:344:PHE:O	1:D:345:HIS:O	2.34	0.46
1:B:287:GLN:O	1:B:290:LYS:HG3	2.16	0.45
1:D:290:LYS:CE	1:D:293:ILE:CD1	2.94	0.45
1:D:76:MET:HB2	1:D:308:SER:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:LYS:HB2	1:A:293:ILE:CG2	2.46	0.45
1:B:18:ASP:CB	1:B:332:ARG:HH22	2.28	0.45
1:A:258:ARG:HH11	1:A:258:ARG:CG	2.29	0.45
1:B:13:GLY:O	1:B:15:PRO:HD3	2.17	0.45
1:B:290:LYS:HD2	3:B:569:HOH:O	2.15	0.45
1:C:173:THR:HG22	1:C:206:TYR:CZ	2.52	0.45
1:A:268:ARG:NE	1:A:290:LYS:CE	2.80	0.45
1:D:236:PHE:O	1:D:237:GLU:HB2	2.17	0.45
1:B:150:LEU:O	1:B:156:TRP:HB2	2.17	0.45
1:B:290:LYS:NZ	1:B:293:ILE:CD1	2.80	0.45
1:C:101:ARG:NH1	1:C:102:LYS:NZ	2.64	0.45
1:B:25:LYS:HB3	3:B:619:HOH:O	2.17	0.45
1:B:5:ARG:CG	1:B:5:ARG:NH1	2.80	0.45
1:B:191:ARG:NH1	1:B:191:ARG:HG3	2.28	0.45
1:B:173:THR:HG22	1:B:206:TYR:CE2	2.52	0.45
1:D:19:ILE:HG22	1:D:58:VAL:HG21	1.99	0.45
1:D:329:ILE:O	1:D:331:ILE:HD12	2.16	0.45
1:C:223:ASN:HD22	1:C:226:GLU:H	1.64	0.45
1:B:339:PRO:HD2	1:C:329:ILE:CG2	2.47	0.45
1:D:24:ASP:OD2	1:D:26:ASP:HB2	2.17	0.45
1:A:241:ILE:HD11	1:A:264:PHE:CD2	2.52	0.44
1:A:338:PHE:HE2	1:D:331:ILE:O	2.00	0.44
1:C:134:LEU:HD23	1:C:134:LEU:N	2.31	0.44
1:C:222:GLY:O	1:C:264:PHE:HA	2.17	0.44
1:C:6:GLU:O	1:C:7:ASN:HB2	2.17	0.44
1:D:17:LEU:HD22	1:D:95:PHE:CD1	2.51	0.44
1:D:268:ARG:HE	1:D:290:LYS:NZ	2.15	0.44
1:D:287:GLN:O	1:D:290:LYS:HG3	2.16	0.44
1:A:338:PHE:HB3	1:D:330:ILE:HD13	1.99	0.44
1:D:97:GLU:HB3	3:D:617:HOH:O	2.17	0.44
1:A:344:PHE:O	1:A:345:HIS:CB	2.65	0.44
1:B:101:ARG:HH12	1:B:102:LYS:HE2	1.82	0.44
1:B:5:ARG:CD	1:B:5:ARG:H	2.24	0.44
1:B:61:HIS:HB2	1:B:332:ARG:CZ	2.48	0.44
1:C:76:MET:CE	1:C:325:TYR:HD2	2.30	0.44
1:A:50:ASP:CB	1:A:54:LYS:NZ	2.80	0.44
1:B:12:MET:HG2	1:B:167:ILE:HG12	1.99	0.44
1:B:189:ASN:HB3	1:B:191:ARG:HE	1.81	0.44
1:C:200:PRO:O	1:C:204:GLN:HG3	2.16	0.44
1:A:127:ILE:HD13	1:A:132:ARG:NH1	2.32	0.44
1:C:12:MET:HG2	1:C:167:ILE:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LYS:HA	1:D:102:LYS:HD3	1.89	0.44
1:D:76:MET:HE2	1:D:322:ALA:HB1	1.99	0.44
1:C:331:ILE:HG22	1:C:331:ILE:O	2.17	0.44
1:D:223:ASN:ND2	1:D:226:GLU:H	2.16	0.44
1:A:344:PHE:HB2	1:D:325:TYR:CD2	2.53	0.44
1:A:101:ARG:O	1:A:105:GLU:HG3	2.17	0.44
1:A:268:ARG:NE	1:A:290:LYS:HZ1	2.08	0.44
1:A:90:ILE:HG12	1:A:112:TYR:HB3	1.99	0.44
1:C:280:THR:CG2	1:C:281:ALA:N	2.81	0.44
1:D:36:ASN:OD1	1:D:131:ASN:HA	2.18	0.44
1:A:140:ALA:CA	1:A:143:CYS:HG	2.31	0.44
1:B:40:LEU:HG	1:B:201:PHE:CZ	2.52	0.44
1:C:8:ILE:HG23	1:C:311:VAL:HG21	1.99	0.44
1:C:7:ASN:HB2	1:C:161:LYS:HE2	1.99	0.43
1:D:288:ASP:O	1:D:289:GLN:CG	2.66	0.43
1:A:101:ARG:HG2	1:A:101:ARG:NH1	2.33	0.43
1:B:290:LYS:CD	1:B:293:ILE:HG12	2.31	0.43
1:C:268:ARG:CZ	1:C:290:LYS:HE2	2.48	0.43
1:C:6:GLU:HA	1:C:83:ALA:HA	2.00	0.43
1:A:140:ALA:O	1:A:143:CYS:SG	2.59	0.43
1:C:167:ILE:O	1:C:195:LEU:HA	2.18	0.43
1:C:272:ILE:CD1	1:C:272:ILE:N	2.81	0.43
1:D:12:MET:HE1	1:D:144:TYR:CE2	2.54	0.43
1:B:329:ILE:O	1:B:331:ILE:HD12	2.18	0.43
1:B:50:ASP:O	1:B:54:LYS:HG3	2.18	0.43
1:C:288:ASP:C	1:C:290:LYS:H	2.22	0.43
1:D:239:LYS:HD2	3:D:619:HOH:O	2.17	0.43
1:D:17:LEU:HD12	1:D:61:HIS:O	2.19	0.43
1:A:153:GLU:HG2	1:A:157:MET:HE2	2.01	0.43
1:D:241:ILE:CD1	1:D:266:GLN:NE2	2.82	0.43
1:A:288:ASP:O	1:A:290:LYS:N	2.51	0.43
1:B:154:LYS:HB3	3:B:545:HOH:O	2.18	0.43
1:B:6:GLU:HA	1:B:83:ALA:HA	2.01	0.43
1:C:30:LYS:HA	1:C:30:LYS:HD2	1.68	0.43
1:D:194:THR:HB	1:D:221:PHE:HE1	1.83	0.43
1:A:21:ALA:HB2	1:A:58:VAL:HA	2.01	0.43
1:B:15:PRO:HG2	1:B:89:CYS:O	2.18	0.43
1:C:45:HIS:O	1:C:48:LEU:HB3	2.19	0.43
1:A:336:CYS:CB	1:D:336:CYS:SG	3.07	0.43
1:B:254:MET:CE	1:B:254:MET:CA	2.97	0.43
1:C:241:ILE:CG2	1:C:242:LYS:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:LYS:HD3	1:C:293:ILE:HG12	2.01	0.43
1:D:5:ARG:NH1	1:D:5:ARG:CG	2.76	0.43
1:A:127:ILE:HG22	1:A:128:THR:N	2.34	0.43
1:A:153:GLU:HG2	1:A:157:MET:CE	2.48	0.43
1:B:290:LYS:HD2	1:B:290:LYS:C	2.39	0.43
1:C:314:LYS:HD3	1:C:314:LYS:HA	1.68	0.43
1:B:336:CYS:CB	1:C:336:CYS:HG	2.32	0.43
1:D:271:THR:OG1	1:D:324:HIS:CE1	2.71	0.43
1:C:124:ALA:O	1:C:134:LEU:HA	2.18	0.42
1:D:20:SER:CB	1:D:125:ALA:HB3	2.47	0.42
1:A:26:ASP:O	1:A:30:LYS:HD3	2.19	0.42
1:A:344:PHE:CB	1:D:76:MET:CE	2.96	0.42
1:B:9:LEU:HD13	1:B:70:ILE:HD13	2.00	0.42
1:A:260:ARG:HG2	1:A:261:ILE:N	2.35	0.42
1:B:142:ASN:HD22	1:B:174:VAL:HG22	1.83	0.42
1:B:332:ARG:HB3	3:B:613:HOH:O	2.19	0.42
1:C:177:GLU:H	1:C:177:GLU:CD	2.23	0.42
1:D:290:LYS:HE2	3:D:618:HOH:O	2.20	0.42
1:A:305:GLY:O	1:A:308:SER:OG	2.24	0.42
1:B:329:ILE:HD11	3:C:566:HOH:O	2.19	0.42
1:A:140:ALA:CA	1:A:143:CYS:SG	3.04	0.42
1:A:87:PHE:HA	1:A:111:HIS:O	2.20	0.42
1:B:101:ARG:NH1	1:B:101:ARG:HG2	2.34	0.42
1:B:290:LYS:HZ2	1:B:293:ILE:CD1	2.33	0.42
1:D:253:LYS:HZ2	1:D:253:LYS:HG2	1.58	0.42
1:D:278:GLU:HB3	1:D:279:VAL:H	1.53	0.42
1:B:236:PHE:HB3	1:B:238:THR:HG22	2.01	0.42
1:C:25:LYS:O	1:C:25:LYS:HG3	2.19	0.42
1:D:239:LYS:HB2	3:D:620:HOH:O	2.19	0.42
1:A:5:ARG:N	1:A:5:ARG:CD	2.74	0.42
1:D:175:SER:OG	1:D:178:SER:OG	2.37	0.42
1:A:140:ALA:HA	1:A:143:CYS:HG	1.85	0.42
1:A:229:THR:O	1:A:233:GLU:HG2	2.20	0.42
1:A:4:VAL:HG23	1:A:4:VAL:O	2.19	0.42
1:C:290:LYS:HZ2	1:C:293:ILE:HD13	1.85	0.42
1:D:318:GLU:CD	1:D:321:ARG:NH1	2.73	0.42
1:D:48:LEU:HD23	1:D:49:PHE:N	2.34	0.42
1:A:223:ASN:ND2	1:A:223:ASN:C	2.72	0.42
1:A:231:ALA:HB1	1:A:236:PHE:HB2	2.02	0.42
1:A:268:ARG:NE	1:A:290:LYS:HE2	2.35	0.42
1:A:344:PHE:CD1	1:A:344:PHE:O	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:PHE:HD1	3:B:547:HOH:O	2.02	0.42
1:B:284:VAL:HG13	3:B:603:HOH:O	2.19	0.42
1:B:34:LYS:CB	1:B:35:PRO:HD2	2.48	0.42
1:C:15:PRO:O	1:C:16:LEU:HD23	2.20	0.42
1:C:288:ASP:O	1:C:289:GLN:HG2	2.20	0.42
1:C:329:ILE:HG22	1:C:330:ILE:N	2.33	0.42
1:C:82:LYS:HB3	1:C:109:ASP:HB2	2.01	0.42
1:D:99:LEU:HD12	1:D:120:THR:HG21	2.02	0.42
1:A:31:TYR:O	1:A:32:SER:OG	2.32	0.41
1:B:236:PHE:O	1:B:237:GLU:HB2	2.19	0.41
1:D:176:PRO:HD2	1:D:177:GLU:OE1	2.20	0.41
1:A:124:ALA:O	1:A:134:LEU:HA	2.20	0.41
1:A:224:GLU:H	1:A:224:GLU:HG3	1.58	0.41
1:B:20:SER:O	1:B:58:VAL:HG23	2.20	0.41
1:B:78:GLN:HB2	3:B:529:HOH:O	2.19	0.41
1:C:189:ASN:HB3	1:C:191:ARG:NE	2.35	0.41
1:A:290:LYS:CE	1:A:293:ILE:CD1	2.97	0.41
1:A:45:HIS:O	1:A:48:LEU:HB3	2.20	0.41
1:B:290:LYS:HD3	1:B:293:ILE:HG21	2.00	0.41
1:B:44:LYS:HB2	1:B:44:LYS:HE2	1.43	0.41
1:C:81:HIS:O	1:C:82:LYS:HB2	2.20	0.41
1:D:223:ASN:ND2	1:D:226:GLU:CD	2.74	0.41
1:C:286:ASP:C	1:C:288:ASP:H	2.24	0.41
1:D:290:LYS:CE	1:D:293:ILE:HD11	2.50	0.41
1:D:76:MET:HE1	1:D:325:TYR:CD2	2.50	0.41
1:A:290:LYS:CD	1:A:293:ILE:CD1	2.98	0.41
1:B:224:GLU:CG	1:B:266:GLN:HG2	2.50	0.41
1:B:260:ARG:HG2	1:B:261:ILE:N	2.34	0.41
1:C:241:ILE:HG23	1:C:242:LYS:H	1.84	0.41
1:C:17:LEU:CD2	1:C:95:PHE:CG	3.03	0.41
1:C:223:ASN:C	1:C:223:ASN:ND2	2.68	0.41
1:D:183:ALA:HB1	1:D:216:TYR:HB3	2.02	0.41
1:D:290:LYS:HB2	1:D:293:ILE:HG23	2.03	0.41
1:D:56:PHE:HA	3:D:624:HOH:O	2.21	0.41
1:C:19:ILE:HG23	1:C:58:VAL:CG2	2.35	0.41
1:C:332:ARG:NH2	3:C:517:HOH:O	2.53	0.41
1:A:285:LEU:HA	3:A:549:HOH:O	2.19	0.41
1:C:154:LYS:O	1:C:157:MET:HE3	2.20	0.41
1:D:19:ILE:CG2	1:D:58:VAL:CG2	2.98	0.41
1:A:106:ALA:CB	1:A:108:VAL:HG23	2.50	0.41
1:A:329:ILE:O	1:A:331:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:GLU:HA	1:D:83:ALA:HA	2.03	0.41
1:A:215:PRO:HB2	1:A:254:MET:HE3	2.02	0.41
1:A:8:ILE:CG1	1:A:311:VAL:HG22	2.51	0.41
1:A:285:LEU:HG	1:A:324:HIS:HB3	2.03	0.41
1:A:344:PHE:CB	1:D:76:MET:HE3	2.51	0.41
1:A:194:THR:HG22	1:A:219:ILE:HB	2.02	0.41
1:A:222:GLY:O	1:A:264:PHE:HA	2.21	0.41
1:A:280:THR:HG22	1:A:282:PHE:CE2	2.55	0.41
1:D:183:ALA:HB1	1:D:216:TYR:CB	2.51	0.41
1:A:164:VAL:HG21	1:A:310:LEU:CD1	2.50	0.40
1:B:224:GLU:HG2	1:B:266:GLN:HG2	2.04	0.40
1:C:309:GLN:HB3	1:C:314:LYS:HB2	2.01	0.40
1:D:262:VAL:O	1:D:273:MET:HA	2.21	0.40
1:D:31:TYR:HB2	1:D:33:LEU:HD12	2.03	0.40
1:A:117:GLU:OE2	1:A:117:GLU:N	2.46	0.40
1:B:85:THR:HG22	1:B:86:PHE:N	2.36	0.40
1:A:75:TRP:CZ2	1:D:342:PRO:HB3	2.56	0.40
1:D:34:LYS:HE2	1:D:37:ASP:OD2	2.21	0.40
1:A:215:PRO:CB	1:A:254:MET:CE	2.99	0.40
1:A:261:ILE:HD13	1:A:316:LEU:HD13	2.02	0.40
1:A:273:MET:HE3	1:A:320:ILE:HD11	2.02	0.40
1:B:121:GLY:CA	1:B:138:LEU:O	2.69	0.40
1:B:14:ASN:HA	1:B:15:PRO:HD2	1.96	0.40
1:C:116:ASN:HA	3:C:601:HOH:O	2.20	0.40
1:A:263:ILE:HD12	1:A:306:PHE:CE2	2.56	0.40
1:A:33:LEU:HD11	1:A:48:LEU:HD11	2.03	0.40
1:D:273:MET:HE1	1:D:316:LEU:HB3	2.02	0.40
1:D:45:HIS:O	1:D:48:LEU:HB3	2.22	0.40
1:D:99:LEU:HD12	1:D:120:THR:CG2	2.52	0.40
1:A:241:ILE:HG12	1:A:272:ILE:CD1	2.49	0.40
1:A:241:ILE:HG21	1:A:272:ILE:CD1	2.52	0.40
1:C:14:ASN:HB2	2:C:500:5I5:H4	2.04	0.40
1:C:276:GLU:HG3	3:C:595:HOH:O	2.21	0.40
1:C:332:ARG:C	1:C:333:ARG:HG2	2.40	0.40
1:D:230:PHE:O	1:D:234:GLN:HB2	2.21	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	341/345 (99%)	313 (92%)	20 (6%)	8 (2%)	6	3
1	B	341/345 (99%)	314 (92%)	19 (6%)	8 (2%)	6	3
1	C	341/345 (99%)	315 (92%)	15 (4%)	11 (3%)	4	2
1	D	341/345 (99%)	314 (92%)	20 (6%)	7 (2%)	7	4
All	All	1364/1380 (99%)	1256 (92%)	74 (5%)	34 (2%)	5	3

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	286	ASP
1	A	288	ASP
1	A	291	GLU
1	A	342	PRO
1	B	289	GLN
1	B	292	ILE
1	C	78	GLN
1	C	79	GLN
1	C	286	ASP
1	C	288	ASP
1	D	79	GLN
1	D	291	GLU
1	A	289	GLN
1	A	294	ASP
1	A	330	ILE
1	B	286	ASP
1	B	288	ASP
1	B	291	GLU
1	C	291	GLU
1	C	292	ILE
1	C	330	ILE

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Mol	Chain	Res	Type
1	D	286	ASP
1	B	78	GLN
1	D	188	GLU
1	D	288	ASP
1	B	330	ILE
1	C	149	HIS
1	C	270	ASP
1	C	289	GLN
1	C	294	ASP
1	D	330	ILE
1	D	260	ARG
1	B	35	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/292 (99%)	262 (90%)	28 (10%)	8	7
1	B	290/292 (99%)	261 (90%)	29 (10%)	7	7
1	C	290/292 (99%)	255 (88%)	35 (12%)	5	4
1	D	290/292 (99%)	261 (90%)	29 (10%)	7	7
All	All	1160/1168 (99%)	1039 (90%)	121 (10%)	7	6

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	9	LEU
1	A	30	LYS
1	A	42	GLU
1	A	44	LYS
1	A	51	GLU
1	A	79	GLN
1	A	102	LYS
1	A	115	GLN

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Mol	Chain	Res	Type
1	A	143	CYS
1	A	146	LYS
1	A	148	LYS
1	A	157	MET
1	A	187	SER
1	A	191	ARG
1	A	209	SER
1	A	223	ASN
1	A	224	GLU
1	A	247	LYS
1	A	249	GLN
1	A	258	ARG
1	A	277	SER
1	A	290	LYS
1	A	293	ILE
1	A	311	VAL
1	A	312	SER
1	A	333	ARG
1	A	337	THR
1	B	5	ARG
1	B	6	GLU
1	B	8	ILE
1	B	9	LEU
1	B	30	LYS
1	B	32	SER
1	B	36	ASN
1	B	44	LYS
1	B	79	GLN
1	B	115	GLN
1	B	143	CYS
1	B	146	LYS
1	B	148	LYS
1	B	191	ARG
1	B	192	ILE
1	B	201	PHE
1	B	206	TYR
1	B	207	LYS
1	B	212	LYS
1	B	223	ASN
1	B	224	GLU
1	B	249	GLN
1	B	261	ILE

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Mol	Chain	Res	Type
1	B	290	LYS
1	B	310	LEU
1	B	311	VAL
1	B	313	ASP
1	B	320	ILE
1	B	334	THR
1	C	5	ARG
1	C	6	GLU
1	C	8	ILE
1	C	9	LEU
1	C	30	LYS
1	C	36	ASN
1	C	44	LYS
1	C	79	GLN
1	C	115	GLN
1	C	135	ILE
1	C	143	CYS
1	C	154	LYS
1	C	157	MET
1	C	167	ILE
1	C	178	SER
1	C	187	SER
1	C	191	ARG
1	C	207	LYS
1	C	209	SER
1	C	223	ASN
1	C	224	GLU
1	C	241	ILE
1	C	249	GLN
1	C	254	MET
1	C	256	SER
1	C	259	GLN
1	C	263	ILE
1	C	277	SER
1	C	290	LYS
1	C	311	VAL
1	C	312	SER
1	C	314	LYS
1	C	333	ARG
1	C	337	THR
1	C	338	PHE
1	D	3	SER

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Mol	Chain	Res	Type
1	D	5	ARG
1	D	6	GLU
1	D	9	LEU
1	D	20	SER
1	D	30	LYS
1	D	44	LYS
1	D	48	LEU
1	D	58	VAL
1	D	79	GLN
1	D	100	LYS
1	D	115	GLN
1	D	133	SER
1	D	146	LYS
1	D	157	MET
1	D	187	SER
1	D	191	ARG
1	D	200	PRO
1	D	207	LYS
1	D	212	LYS
1	D	223	ASN
1	D	224	GLU
1	D	234	GLN
1	D	247	LYS
1	D	249	GLN
1	D	290	LYS
1	D	310	LEU
1	D	311	VAL
1	D	333	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	61	HIS
1	A	107	HIS
1	A	115	GLN
1	A	118	GLN
1	A	137	ASN
1	A	142	ASN
1	A	155	ASN
1	A	184	HIS
1	A	185	HIS

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Mol	Chain	Res	Type
1	A	189	ASN
1	A	223	ASN
1	A	259	GLN
1	A	266	GLN
1	A	324	HIS
1	B	45	HIS
1	B	115	GLN
1	B	142	ASN
1	B	155	ASN
1	B	184	HIS
1	B	185	HIS
1	B	223	ASN
1	B	249	GLN
1	B	259	GLN
1	B	287	GLN
1	B	296	ASN
1	B	324	HIS
1	B	345	HIS
1	C	45	HIS
1	C	61	HIS
1	C	78	GLN
1	C	115	GLN
1	C	142	ASN
1	C	184	HIS
1	C	185	HIS
1	C	223	ASN
1	C	249	GLN
1	C	259	GLN
1	C	324	HIS
1	D	45	HIS
1	D	61	HIS
1	D	78	GLN
1	D	115	GLN
1	D	142	ASN
1	D	155	ASN
1	D	184	HIS
1	D	223	ASN
1	D	266	GLN
1	D	324	HIS

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

4 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	5I5	D	500	-	19,21,21	0.88	1 (5%)	17,32,32	1.69	5 (29%)
2	5I5	B	500	-	19,21,21	1.37	2 (10%)	17,32,32	1.87	6 (35%)
2	5I5	C	500	-	19,21,21	1.20	1 (5%)	17,32,32	1.78	6 (35%)
2	5I5	A	500	-	19,21,21	1.22	2 (10%)	17,32,32	1.80	4 (23%)

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	5I5	D	500	-	-	0/0/20/20	0/3/3/3
2	5I5	B	500	-	-	0/0/20/20	0/3/3/3
2	5I5	C	500	-	-	0/0/20/20	0/3/3/3
2	5I5	A	500	-	-	0/0/20/20	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	5I5	C5-C2	3.91	1.47	1.42
2	C	500	5I5	C5-C2	3.88	1.47	1.42
2	A	500	5I5	C5-I	-3.11	2.04	2.10
2	B	500	5I5	C4-N2	3.02	1.37	1.32
2	A	500	5I5	C5-C2	2.56	1.45	1.42
2	D	500	5I5	C5-I	-2.44	2.06	2.10

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	5I5	O3-C9-C8	-4.04	101.03	106.93
2	B	500	5I5	N2-C4-N1	-3.83	122.69	128.68
2	D	500	5I5	C11-C10-C7	-3.72	111.80	115.70
2	B	500	5I5	O3-C9-C8	-3.62	101.64	106.93
2	C	500	5I5	N2-C4-N1	-3.44	123.30	128.68
2	A	500	5I5	N2-C4-N1	-3.40	123.37	128.68
2	A	500	5I5	C11-C10-C7	-3.28	112.26	115.70
2	B	500	5I5	N4-C1-N1	-3.20	111.94	118.57
2	D	500	5I5	N2-C4-N1	-2.84	124.24	128.68
2	C	500	5I5	C11-C10-C7	-2.80	112.76	115.70
2	C	500	5I5	C5-C6-N3	2.73	111.22	108.22
2	D	500	5I5	C7-C8-C9	2.67	105.00	100.98
2	C	500	5I5	N4-C1-N1	-2.59	113.19	118.57
2	C	500	5I5	O3-C9-C8	-2.53	103.22	106.93
2	A	500	5I5	N4-C1-N1	-2.52	113.35	118.57
2	B	500	5I5	C5-C6-N3	2.49	110.95	108.22
2	B	500	5I5	C7-C8-C9	2.48	104.71	100.98
2	D	500	5I5	C5-C6-N3	2.32	110.77	108.22
2	D	500	5I5	O3-C9-C8	-2.27	103.61	106.93
2	C	500	5I5	C7-C8-C9	2.15	104.21	100.98
2	B	500	5I5	C2-C1-N4	2.00	126.28	122.67

There are no chirality outliers.

There are no torsion outliers.

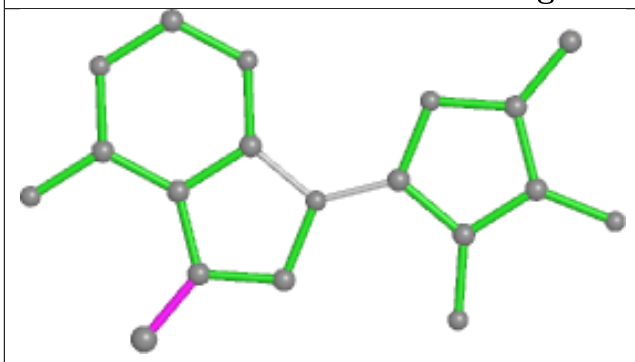
There are no ring outliers.

1 monomer is involved in 1 short contact:

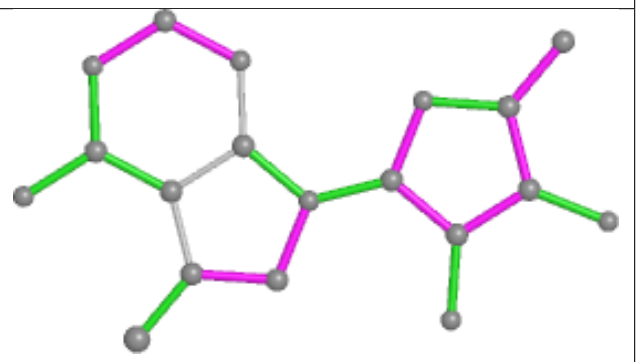
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	5I5	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

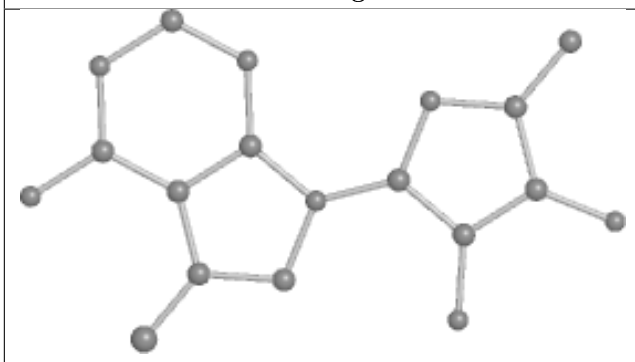
Ligand 5I5 D 500



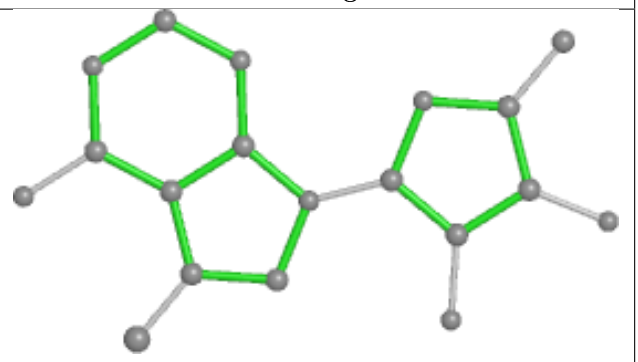
Bond lengths



Bond angles

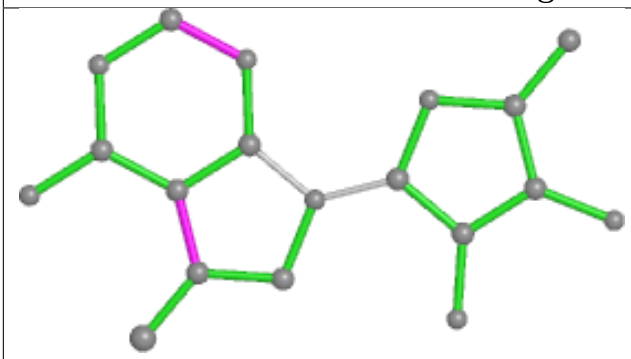


Torsions

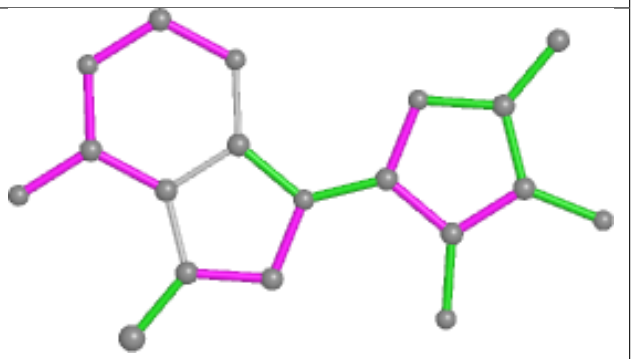


Rings

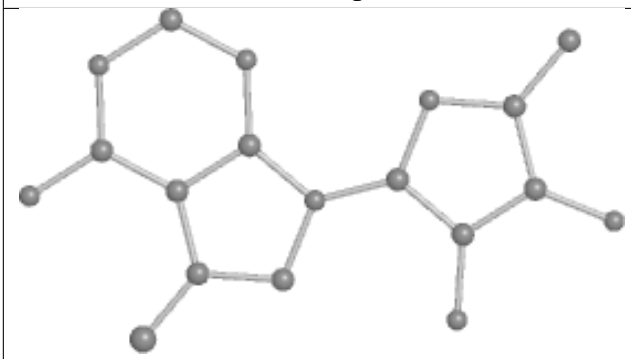
Ligand 5I5 B 500



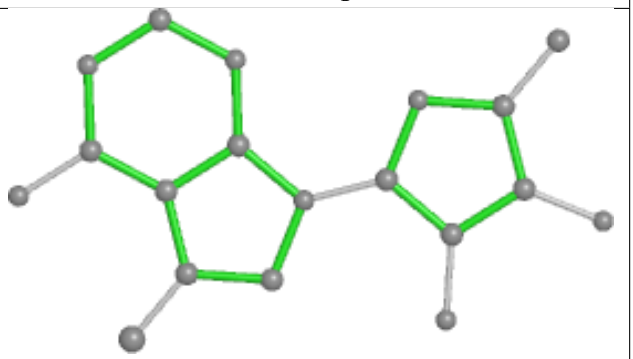
Bond lengths



Bond angles

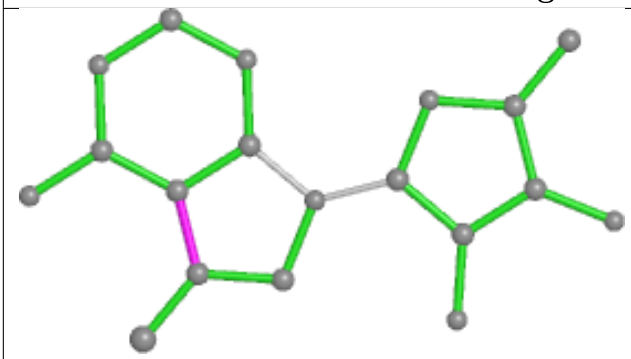


Torsions

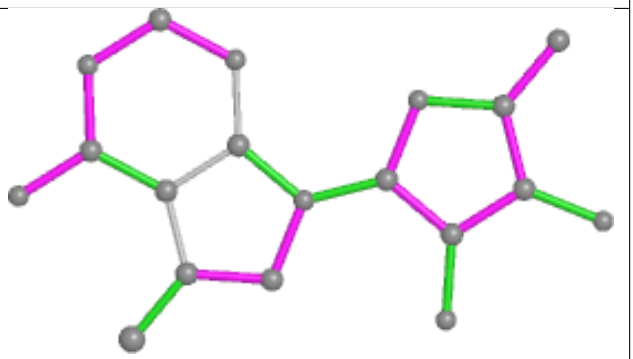


Rings

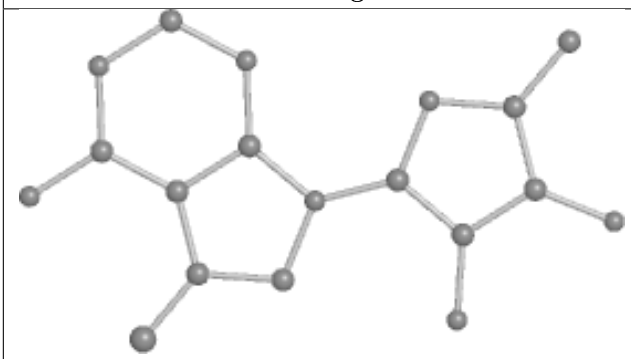
Ligand 5I5 C 500



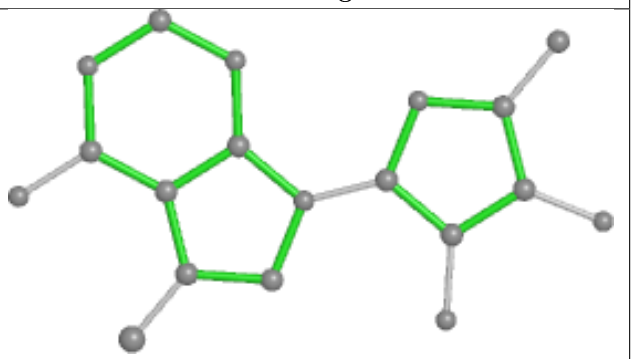
Bond lengths



Bond angles

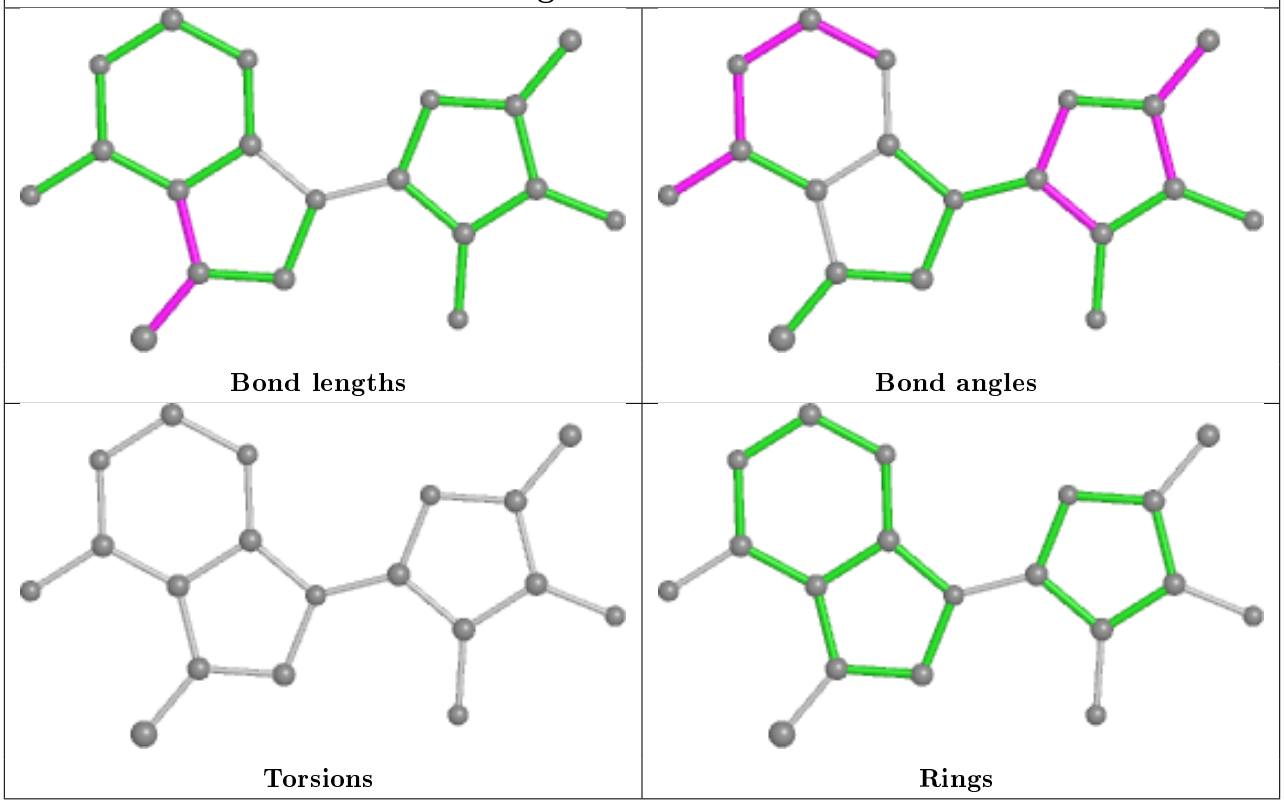


Torsions



Rings

Ligand 5I5 A 500



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.