



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:24 PM UTC

PDB ID : 2E21 / pdb\_00002e21  
Title : Crystal structure of TilS in a complex with AMPPNP from Aquifex aeolicus.  
Authors : Kuratani, M.; Yoshikawa, Y.; Sekine, S.; Ishii, T.; Shibata, R.; Bessho, Y.;  
Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2006-11-06  
Resolution : 2.70 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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

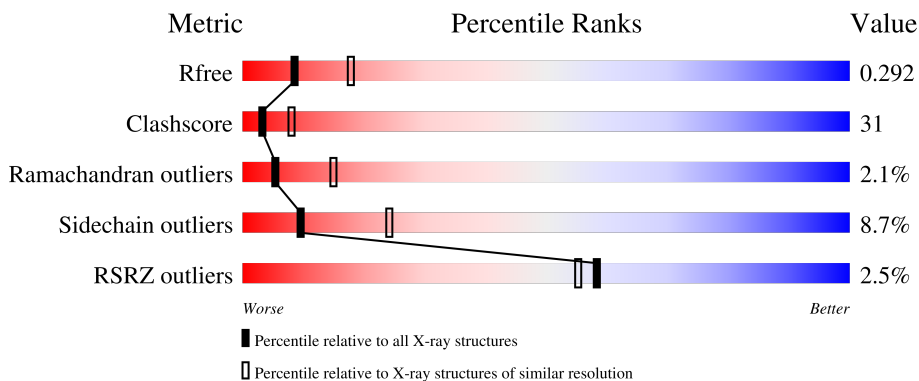
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	317	
1	B	317	
1	C	317	
1	D	317	

## 2 Entry composition [i](#)

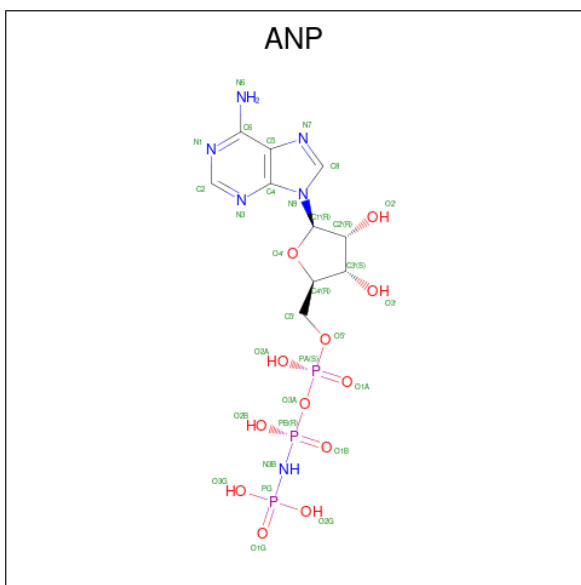
There are 3 unique types of molecules in this entry. The entry contains 10690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 tRNA(Ile)-lysidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	317	Total 2630	C 1682	N 467	O 472	S 9	0	0	0
1	B	314	Total 2606	C 1667	N 464	O 466	S 9	0	0	0
1	C	314	Total 2606	C 1667	N 464	O 466	S 9	0	0	0
1	D	314	Total 2606	C 1667	N 464	O 466	S 9	0	0	0

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	C	1	Total 31	C 10	N 6	O 12	P 3	0	0

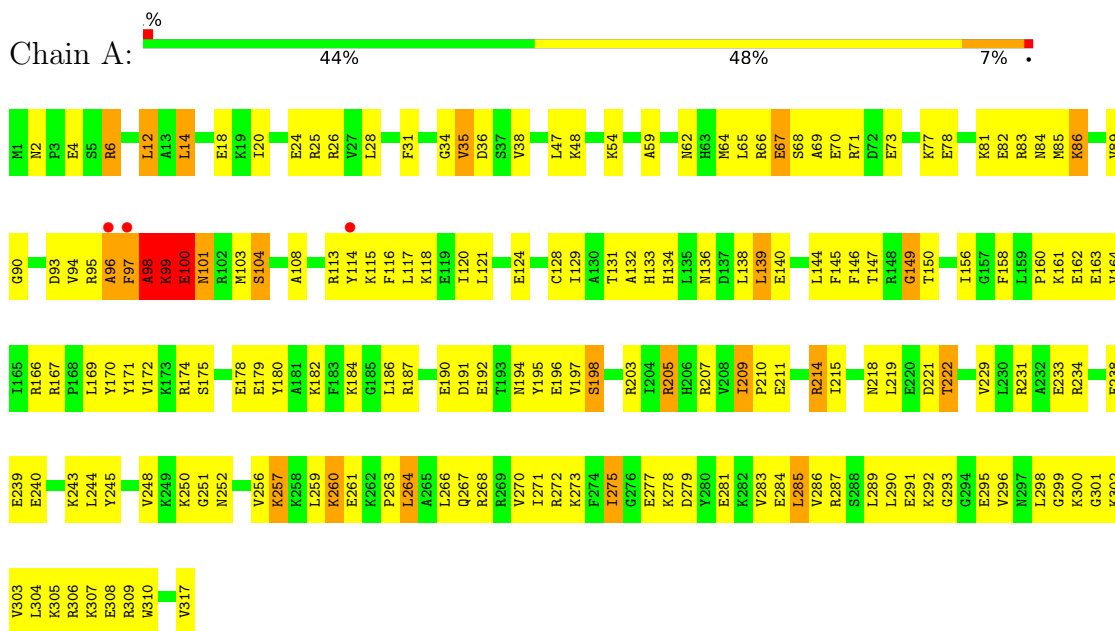
- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
3	A	49	Total O 49 49	0	0
3	B	43	Total O 43 43	0	0
3	C	59	Total O 59 59	0	0
3	D	29	Total O 29 29	0	0

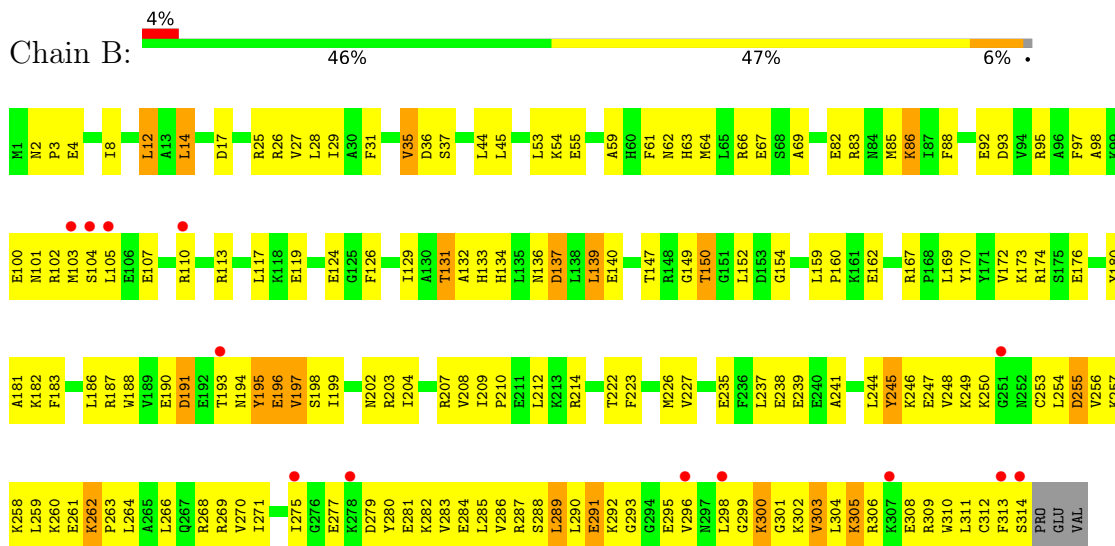
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: tRNA(Ile)-lysidine synthase



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- Molecule 1: tRNA(Ile)-lysidine synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.46Å 82.23Å 109.43Å 90.00° 105.85° 90.00°	Depositor
Resolution (Å)	49.01 – 2.70 49.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.01-2.70) 99.4 (49.01-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 2.61Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.294 0.221 , 0.292	Depositor DCC
$R_{free}$ test set	2303 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtrriage
Anisotropy	0.515	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10690	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.67	2/2672 (0.1%)	1.11	21/3569 (0.6%)
1	B	0.50	0/2647	0.98	13/3535 (0.4%)
1	C	0.53	0/2647	1.05	17/3535 (0.5%)
1	D	0.42	0/2647	0.90	8/3535 (0.2%)
All	All	0.54	2/10613 (0.0%)	1.01	59/14174 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	ALA	CA-CB	-20.53	1.18	1.53
1	A	98	ALA	CA-C	-5.47	1.45	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	GLU	N-CA-C	-19.84	89.08	113.28
1	A	97	PHE	N-CA-C	-15.06	92.47	111.75
1	B	196	GLU	N-CA-C	-10.68	92.12	108.67
1	A	97	PHE	CA-C-O	9.64	130.99	120.20
1	C	308	GLU	N-CA-C	9.57	122.92	111.82
1	C	307	LYS	N-CA-C	-9.36	96.02	109.31
1	C	215	ILE	N-CA-C	-8.35	105.13	111.90
1	A	205	ARG	N-CA-C	7.70	119.37	110.97
1	C	256	VAL	N-CA-C	7.29	120.17	111.05
1	D	215	ILE	N-CA-C	-7.25	106.03	111.90
1	C	165	ILE	N-CA-C	7.17	119.39	108.71
1	C	310	TRP	N-CA-C	7.08	121.07	109.24
1	A	214	ARG	N-CA-C	-7.05	104.49	113.23
1	A	167	ARG	CA-C-N	6.91	126.61	119.56
1	A	167	ARG	C-N-CA	6.91	126.61	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	ASP	N-CA-C	-6.91	103.68	111.07
1	C	252	ASN	N-CA-C	-6.87	104.89	112.72
1	A	115	LYS	N-CA-C	-6.74	103.86	111.14
1	A	209	ILE	CB-CA-C	-6.67	107.36	113.70
1	A	99	LYS	N-CA-CB	-6.38	102.53	112.41
1	B	31	PHE	N-CA-C	6.34	119.14	107.99
1	A	96	ALA	N-CA-C	6.22	119.26	111.24
1	B	208	VAL	N-CA-C	6.05	116.10	110.42
1	A	215	ILE	N-CA-C	-5.98	105.89	111.45
1	C	306	ARG	N-CA-C	5.92	118.54	108.90
1	B	150	THR	N-CA-C	5.81	116.08	107.88
1	C	209	ILE	CB-CA-C	-5.79	108.20	113.70
1	D	192	GLU	N-CA-C	5.79	123.12	110.80
1	C	214	ARG	N-CA-C	-5.73	106.05	113.16
1	A	98	ALA	CA-C-N	-5.72	114.07	123.05
1	A	98	ALA	C-N-CA	-5.72	114.07	123.05
1	D	167	ARG	CA-C-N	5.71	126.10	119.47
1	D	167	ARG	C-N-CA	5.71	126.10	119.47
1	B	86	LYS	N-CA-C	-5.70	101.85	110.28
1	C	2	ASN	CA-C-N	5.65	125.50	119.28
1	C	2	ASN	C-N-CA	5.65	125.50	119.28
1	A	101	ASN	N-CA-C	-5.53	106.42	112.72
1	D	214	ARG	N-CA-C	-5.52	106.55	113.28
1	A	172	VAL	N-CA-C	5.50	116.70	109.21
1	C	33	GLY	N-CA-C	-5.50	107.77	114.92
1	C	234	ARG	N-CA-C	-5.47	105.31	111.28
1	A	31	PHE	N-CA-C	5.47	117.61	107.99
1	D	203	ARG	N-CA-C	-5.41	105.39	111.28
1	A	98	ALA	CB-CA-C	-5.33	99.82	110.42
1	C	198	SER	N-CA-C	-5.31	105.60	111.71
1	C	110	ARG	N-CA-C	-5.29	105.20	110.97
1	A	100	GLU	CB-CA-C	5.25	119.81	109.72
1	B	195	TYR	CA-C-N	-5.24	114.18	121.99
1	B	195	TYR	C-N-CA	-5.24	114.18	121.99
1	B	263	PRO	N-CA-C	5.21	119.06	111.03
1	D	206	HIS	N-CA-C	5.18	119.69	112.90
1	A	67	GLU	N-CA-C	-5.15	105.74	111.36
1	B	17	ASP	N-CA-C	5.15	116.98	111.36
1	B	291	GLU	N-CA-C	-5.15	107.06	113.55
1	B	262	LYS	CA-C-N	5.14	125.38	119.83
1	B	262	LYS	C-N-CA	5.14	125.38	119.83
1	C	163	GLU	CB-CA-C	-5.09	110.68	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	308	GLU	CB-CA-C	-5.06	110.76	116.63
1	A	146	PHE	N-CA-C	-5.06	105.66	111.07

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	2630	0	2722	194	0
1	B	2606	0	2700	168	0
1	C	2606	0	2700	159	0
1	D	2606	0	2700	178	0
2	A	31	0	12	3	0
2	C	31	0	13	0	0
3	A	49	0	0	7	0
3	B	43	0	0	6	0
3	C	59	0	0	7	0
3	D	29	0	0	3	0
All	All	10690	0	10847	656	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 31.

All (656) 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:95:ARG:C	1:A:98:ALA:HB2	1.64	1.21
1:A:99:LYS:HG2	1:A:103:MET:H	1.09	1.18
1:A:95:ARG:O	1:A:98:ALA:CB	1.93	1.16
1:B:105:LEU:HD21	3:B:359:HOH:O	1.51	1.11
1:D:121:LEU:HD21	1:D:164:VAL:HG21	1.32	1.10
1:B:95:ARG:HA	3:B:359:HOH:O	1.60	1.00
1:A:6:ARG:HG2	1:A:6:ARG:HH11	1.27	1.00
1:B:295:GLU:HB3	1:B:305:LYS:HG3	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:THR:HG21	1:C:133:HIS:ND1	1.77	0.99
1:C:194:ASN:HD22	1:C:194:ASN:H	1.02	0.96
1:A:95:ARG:C	1:A:98:ALA:CB	2.39	0.94
1:C:292:LYS:HG2	1:C:293:GLY:H	1.33	0.93
1:A:131:THR:HG22	1:A:133:HIS:H	1.33	0.93
1:C:252:ASN:HD21	1:C:313:PHE:HB2	1.32	0.93
1:C:62:ASN:ND2	1:C:64:MET:H	1.68	0.92
1:C:254:LEU:O	1:C:310:TRP:CE3	2.23	0.92
1:A:99:LYS:HG3	1:A:103:MET:O	1.71	0.90
1:B:181:ALA:HA	1:B:186:LEU:HD12	1.53	0.89
1:B:244:LEU:HD11	1:B:262:LYS:HG3	1.56	0.88
1:A:96:ALA:C	1:A:98:ALA:N	2.22	0.87
1:C:254:LEU:O	1:C:310:TRP:HE3	1.58	0.86
1:B:139:LEU:HD13	1:B:209:ILE:HD12	1.57	0.86
1:C:256:VAL:CG2	1:C:290:LEU:HD23	2.07	0.84
1:D:14:LEU:HD13	1:D:20:ILE:HD11	1.59	0.83
1:C:20:ILE:HG23	1:C:166:ARG:HG3	1.61	0.83
1:D:14:LEU:HD11	1:D:170:TYR:HB3	1.61	0.83
1:C:194:ASN:HD22	1:C:194:ASN:N	1.74	0.83
1:C:256:VAL:HG22	1:C:290:LEU:HD23	1.61	0.82
1:D:131:THR:HG22	1:D:133:HIS:H	1.45	0.81
1:A:190:GLU:HB3	1:D:71:ARG:HH12	1.43	0.81
1:A:131:THR:HG21	1:A:133:HIS:CE1	2.15	0.81
1:D:29:ILE:HD11	1:D:44:LEU:HD12	1.64	0.80
1:B:26:ARG:HG3	1:B:55:GLU:HB3	1.61	0.79
1:A:6:ARG:HH11	1:A:6:ARG:CG	1.93	0.79
1:A:99:LYS:CG	1:A:103:MET:H	1.92	0.79
1:D:272:ARG:HD3	1:D:278:LYS:HZ2	1.48	0.79
1:B:62:ASN:HD21	1:B:69:ALA:HB1	1.48	0.79
1:D:257:LYS:HE2	1:D:257:LYS:N	1.97	0.78
1:C:256:VAL:O	1:C:260:LYS:HB2	1.82	0.78
1:B:191:ASP:HB3	1:B:194:ASN:HD22	1.49	0.78
1:D:202:ASN:N	1:D:202:ASN:HD22	1.82	0.78
1:A:65:LEU:HA	1:A:95:ARG:NH1	1.99	0.77
1:C:292:LYS:HG2	1:C:293:GLY:N	1.98	0.77
1:B:275:ILE:HG23	1:B:277:GLU:H	1.50	0.77
1:A:302:LYS:HG2	3:A:546:HOH:O	1.85	0.77
1:A:162:GLU:OE1	3:A:544:HOH:O	2.02	0.76
1:B:303:VAL:HG13	1:B:314:SER:HB3	1.67	0.76
1:B:266:LEU:O	1:B:269:ARG:HB2	1.86	0.76
1:A:260:LYS:HD2	1:A:261:GLU:HG3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:VAL:HG11	1:A:207:ARG:NH2	2.01	0.76
1:A:131:THR:HG21	1:A:133:HIS:ND1	2.02	0.75
1:C:275:ILE:HG21	1:C:286:VAL:HG21	1.69	0.75
1:A:95:ARG:O	1:A:98:ALA:HB3	1.88	0.74
1:C:254:LEU:HD23	1:C:311:LEU:HD23	1.70	0.74
1:A:234:ARG:HD3	1:A:238:GLU:OE1	1.89	0.73
1:D:272:ARG:HD3	1:D:278:LYS:NZ	2.04	0.73
1:D:1:MET:HB2	1:D:5:SER:OG	1.88	0.73
1:A:305:LYS:HE2	1:A:307:LYS:HE3	1.69	0.73
1:C:306:ARG:HG2	1:C:307:LYS:O	1.88	0.73
1:D:257:LYS:HE2	1:D:257:LYS:H	1.52	0.73
1:A:99:LYS:HG2	1:A:103:MET:N	1.95	0.72
1:B:187:ARG:HG2	1:C:196:GLU:HG2	1.69	0.72
1:C:207:ARG:HG2	1:D:211:GLU:CD	2.13	0.72
1:B:255:ASP:OD1	1:B:257:LYS:HB3	1.89	0.72
1:B:45:LEU:HD21	1:B:85:MET:HE3	1.70	0.72
1:C:298:LEU:HB2	1:C:302:LYS:HB2	1.72	0.71
1:A:197:VAL:HG23	1:A:203:ARG:HA	1.72	0.71
1:C:256:VAL:HG22	1:C:290:LEU:CD2	2.20	0.71
1:A:100:GLU:C	1:A:100:GLU:OE2	2.33	0.71
1:C:62:ASN:HD22	1:C:64:MET:H	1.36	0.71
1:A:94:VAL:O	1:A:98:ALA:HB2	1.91	0.70
1:A:229:VAL:HA	1:B:268:ARG:NH1	2.06	0.70
1:B:191:ASP:CB	1:B:194:ASN:HD22	2.04	0.70
1:C:205:ARG:HA	1:C:209:ILE:HD13	1.72	0.70
1:B:93:ASP:OD1	1:B:95:ARG:HB3	1.91	0.70
1:B:275:ILE:HD12	1:B:286:VAL:HG21	1.73	0.70
1:C:131:THR:HG23	1:C:133:HIS:H	1.55	0.70
1:C:14:LEU:HD13	1:C:20:ILE:HG13	1.74	0.70
1:A:139:LEU:HD13	1:A:209:ILE:HD12	1.73	0.70
1:D:139:LEU:HD13	1:D:209:ILE:HD12	1.74	0.69
1:B:35:VAL:HG13	1:B:188:TRP:CE2	2.27	0.69
1:C:36:ASP:HB2	1:C:132:ALA:HB1	1.74	0.69
1:B:14:LEU:HD11	1:B:170:TYR:HB3	1.73	0.69
1:C:306:ARG:CG	1:C:307:LYS:O	2.41	0.69
1:D:134:HIS:HD2	1:D:136:ASN:H	1.40	0.69
1:C:296:VAL:O	1:C:303:VAL:HA	1.93	0.69
1:B:29:ILE:HD11	1:B:44:LEU:HD12	1.75	0.69
1:C:255:ASP:HA	1:C:309:ARG:O	1.92	0.68
1:A:131:THR:HG22	1:A:133:HIS:N	2.07	0.68
1:B:131:THR:HG21	1:B:133:HIS:ND1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:ASN:H	1:C:194:ASN:ND2	1.80	0.68
1:D:257:LYS:HD2	1:D:309:ARG:HB2	1.75	0.68
1:A:95:ARG:O	1:A:98:ALA:HB2	1.68	0.68
1:D:209:ILE:HB	1:D:210:PRO:HD3	1.74	0.68
1:A:96:ALA:C	1:A:98:ALA:H	1.93	0.68
1:A:66:ARG:HD2	1:D:187:ARG:NH1	2.08	0.67
1:A:209:ILE:HB	1:A:210:PRO:HD3	1.75	0.67
1:C:35:VAL:HG23	3:C:551:HOH:O	1.94	0.67
1:A:77:LYS:O	1:A:81:LYS:HG3	1.95	0.67
1:D:197:VAL:HG21	1:D:207:ARG:NH2	2.10	0.67
1:A:121:LEU:HD11	1:A:164:VAL:HG21	1.75	0.67
1:A:128:CYS:HA	1:A:164:VAL:HG22	1.76	0.67
1:A:293:GLY:HA2	1:A:306:ARG:HD3	1.76	0.67
1:B:62:ASN:ND2	1:B:64:MET:H	1.93	0.67
1:B:88:PHE:CZ	1:B:124:GLU:HG2	2.29	0.67
1:C:104:SER:OG	1:C:107:GLU:HG2	1.95	0.67
1:C:62:ASN:ND2	1:C:69:ALA:HB1	2.10	0.67
1:A:99:LYS:HG3	1:A:103:MET:C	2.19	0.67
1:B:253:CYS:O	1:B:254:LEU:HD12	1.95	0.67
1:C:131:THR:CG2	1:C:133:HIS:H	2.09	0.66
1:D:121:LEU:CD2	1:D:164:VAL:HG21	2.18	0.66
1:B:248:VAL:HG11	1:B:259:LEU:HG	1.76	0.66
1:C:296:VAL:HB	1:C:304:LEU:H	1.60	0.66
1:D:308:GLU:HG3	1:D:309:ARG:H	1.59	0.66
1:A:65:LEU:HD21	1:A:94:VAL:HB	1.78	0.66
1:A:260:LYS:HD3	1:A:291:GLU:OE1	1.96	0.66
1:D:49:ASN:O	1:D:52:SER:N	2.27	0.65
1:D:292:LYS:HG2	1:D:293:GLY:H	1.62	0.65
1:B:305:LYS:NZ	1:B:305:LYS:HB3	2.12	0.65
1:C:62:ASN:HD22	1:C:62:ASN:C	2.03	0.65
1:D:14:LEU:HB3	1:D:20:ILE:HD11	1.78	0.65
1:A:266:LEU:O	1:A:270:VAL:HG23	1.97	0.65
1:A:156:ILE:HD12	1:A:234:ARG:NE	2.13	0.64
1:B:25:ARG:HG3	1:B:54:LYS:NZ	2.12	0.64
1:D:63:HIS:HB3	1:D:65:LEU:HG	1.80	0.64
1:A:86:LYS:HB2	1:A:86:LYS:NZ	2.12	0.64
1:A:275:ILE:CD1	1:A:286:VAL:HG21	2.27	0.64
1:A:275:ILE:HD11	1:A:286:VAL:HG21	1.78	0.64
1:D:289:LEU:HD23	1:D:311:LEU:HD11	1.78	0.64
1:D:110:ARG:NH1	1:D:113:ARG:HH22	1.96	0.64
1:D:121:LEU:HD12	1:D:126:PHE:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLU:CD	1:A:190:GLU:H	2.03	0.63
1:C:222:THR:HG22	3:D:345:HOH:O	1.97	0.63
1:B:196:GLU:HG2	1:B:198:SER:OG	1.99	0.63
1:A:285:LEU:HD12	1:A:296:VAL:CG1	2.29	0.63
1:B:260:LYS:HG3	1:B:291:GLU:OE1	1.98	0.63
1:A:78:GLU:O	1:A:82:GLU:HG3	1.98	0.63
1:C:204:ILE:HG22	1:C:209:ILE:CD1	2.28	0.63
1:C:256:VAL:HG21	1:C:290:LEU:HA	1.81	0.62
1:B:281:GLU:HA	1:B:281:GLU:OE2	1.98	0.62
1:B:300:LYS:HG3	1:B:300:LYS:O	1.97	0.62
1:A:248:VAL:HG11	1:A:259:LEU:HB2	1.80	0.62
1:B:190:GLU:HG3	1:C:207:ARG:NH2	2.14	0.62
1:B:62:ASN:C	1:B:62:ASN:HD22	2.05	0.62
1:C:131:THR:CG2	1:C:133:HIS:ND1	2.58	0.62
1:A:28:LEU:HD11	1:A:59:ALA:HB2	1.81	0.62
1:B:159:LEU:HB2	1:B:162:GLU:HG3	1.81	0.62
1:C:306:ARG:HB3	3:C:559:HOH:O	2.00	0.61
1:B:55:GLU:OE1	1:B:86:LYS:HE2	2.01	0.61
1:D:234:ARG:HH11	1:D:234:ARG:HB3	1.66	0.61
1:A:203:ARG:HH12	1:B:214:ARG:HH11	1.46	0.61
1:A:257:LYS:HE3	1:A:306:ARG:NH1	2.15	0.61
1:B:35:VAL:HG13	1:B:188:TRP:CD2	2.36	0.61
1:C:259:LEU:HD22	1:C:267:GLN:HG2	1.82	0.61
1:B:62:ASN:ND2	1:B:69:ALA:HB1	2.15	0.61
1:D:161:LYS:HG3	1:D:166:ARG:HD3	1.81	0.61
1:A:218:ASN:ND2	3:A:549:HOH:O	2.32	0.61
1:C:256:VAL:CG2	1:C:290:LEU:HA	2.31	0.61
1:D:14:LEU:HD11	1:D:170:TYR:CB	2.30	0.61
1:C:20:ILE:CG2	1:C:166:ARG:HG3	2.30	0.61
1:C:149:GLY:HA2	1:D:222:THR:HG23	1.82	0.61
1:D:65:LEU:HA	1:D:95:ARG:HH22	1.66	0.60
1:A:222:THR:HG23	1:B:149:GLY:HA2	1.83	0.60
1:C:304:LEU:HA	1:C:312:CYS:O	2.01	0.60
1:A:267:GLN:O	1:A:271:ILE:HG12	2.01	0.60
1:B:289:LEU:HD12	1:B:292:LYS:O	2.00	0.60
1:A:36:ASP:HB3	1:A:132:ALA:HB1	1.84	0.60
1:D:15:GLN:HE22	1:D:21:PHE:HB2	1.65	0.60
1:C:14:LEU:HD13	1:C:20:ILE:CG1	2.31	0.60
1:B:139:LEU:CD1	1:B:209:ILE:HD12	2.30	0.60
1:B:173:LYS:HG2	1:B:176:GLU:HG3	1.84	0.60
1:C:306:ARG:HG3	1:C:310:TRP:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:VAL:O	1:C:11:VAL:HG23	2.03	0.59
1:B:271:ILE:O	1:B:275:ILE:HG22	2.02	0.59
1:D:271:ILE:O	1:D:275:ILE:HG12	2.02	0.59
1:B:194:ASN:O	1:B:195:TYR:HB2	2.01	0.59
1:A:93:ASP:HB3	1:A:96:ALA:HB3	1.84	0.59
1:C:62:ASN:HD22	1:C:63:HIS:N	2.01	0.59
1:D:65:LEU:HD21	1:D:94:VAL:HB	1.84	0.59
1:D:63:HIS:O	1:D:64:MET:HB2	2.02	0.59
1:C:268:ARG:HD2	3:C:553:HOH:O	2.01	0.59
1:A:26:ARG:HH22	1:A:54:LYS:HD2	1.67	0.59
1:A:131:THR:HG21	1:A:133:HIS:CG	2.38	0.59
1:A:150:THR:O	1:B:226:MET:HG3	2.02	0.59
1:C:204:ILE:HG22	1:C:209:ILE:HD11	1.85	0.59
1:D:173:LYS:HG2	1:D:176:GLU:OE1	2.02	0.59
1:B:83:ARG:HH11	1:B:83:ARG:HG3	1.67	0.58
1:A:95:ARG:O	1:A:98:ALA:HB1	1.99	0.58
1:A:97:PHE:HE2	1:A:103:MET:CE	2.16	0.58
1:B:296:VAL:O	1:B:303:VAL:HG23	2.03	0.58
1:C:62:ASN:ND2	1:C:64:MET:N	2.47	0.58
1:D:29:ILE:CD1	1:D:44:LEU:HD12	2.33	0.58
1:B:83:ARG:NE	3:B:351:HOH:O	2.32	0.58
1:A:174:ARG:O	1:A:178:GLU:HG3	2.04	0.58
1:A:83:ARG:HB2	1:A:85:MET:HG3	1.85	0.58
1:A:131:THR:HG23	2:A:500:ANP:O2'	2.03	0.58
1:D:87:ILE:HD13	1:D:87:ILE:C	2.29	0.58
1:A:73:GLU:CD	1:A:89:VAL:HG21	2.29	0.58
1:A:99:LYS:CG	1:A:103:MET:O	2.49	0.58
1:D:93:ASP:OD2	1:D:96:ALA:HB3	2.03	0.58
1:D:298:LEU:HB2	1:D:302:LYS:HB3	1.86	0.58
1:A:289:LEU:O	1:A:306:ARG:HD2	2.04	0.58
1:A:6:ARG:HG2	1:A:6:ARG:NH1	2.05	0.57
1:B:66:ARG:HA	1:B:66:ARG:NE	2.19	0.57
1:C:62:ASN:HD21	1:C:69:ALA:HB1	1.68	0.57
1:A:233:GLU:HB3	1:B:237:LEU:HD11	1.87	0.57
1:B:209:ILE:HB	1:B:210:PRO:HD3	1.87	0.57
1:A:121:LEU:HD12	1:A:129:ILE:HG13	1.85	0.57
1:D:86:LYS:HD3	1:D:87:ILE:H	1.69	0.57
1:A:191:ASP:O	1:A:192:GLU:HB2	2.05	0.57
1:A:275:ILE:HD11	1:A:286:VAL:CG2	2.34	0.57
1:A:275:ILE:HG22	1:A:277:GLU:H	1.69	0.57
1:B:124:GLU:HB3	1:B:126:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:GLU:N	1:C:281:GLU:OE1	2.38	0.57
1:C:173:LYS:HE3	3:C:525:HOH:O	2.04	0.56
1:C:149:GLY:CA	1:D:222:THR:HG23	2.35	0.56
1:A:187:ARG:N	1:A:187:ARG:HD2	2.20	0.56
1:C:256:VAL:O	1:C:260:LYS:CB	2.53	0.56
1:A:64:MET:O	1:A:65:LEU:HD23	2.06	0.56
1:A:257:LYS:HD2	1:A:309:ARG:HB2	1.86	0.56
1:B:134:HIS:HD2	1:B:136:ASN:H	1.52	0.56
1:C:66:ARG:HG3	1:C:66:ARG:HH11	1.70	0.56
1:B:197:VAL:HG22	1:B:203:ARG:HA	1.88	0.56
1:D:131:THR:HG21	1:D:133:HIS:ND1	2.20	0.56
1:A:285:LEU:HD12	1:A:296:VAL:HG11	1.88	0.56
1:B:280:TYR:CZ	1:B:284:GLU:HG3	2.41	0.56
1:C:28:LEU:HD11	1:C:59:ALA:HB2	1.87	0.56
1:D:101:ASN:CB	1:D:103:MET:HE3	2.35	0.56
1:D:161:LYS:HG3	1:D:166:ARG:CD	2.36	0.56
1:D:86:LYS:HD3	1:D:87:ILE:N	2.20	0.56
1:D:292:LYS:HG2	1:D:293:GLY:N	2.21	0.56
1:C:280:TYR:CZ	1:C:284:GLU:HG3	2.41	0.56
1:D:38:VAL:HG12	1:D:186:LEU:HD13	1.88	0.56
1:D:101:ASN:HB3	1:D:103:MET:HE3	1.88	0.56
1:B:248:VAL:HG22	1:B:258:LYS:HB2	1.89	0.55
1:A:190:GLU:CB	1:D:71:ARG:HH12	2.18	0.55
1:B:190:GLU:HG3	1:C:207:ARG:CZ	2.36	0.55
1:C:140:GLU:OE2	1:C:174:ARG:NH2	2.36	0.55
1:B:150:THR:OG1	1:B:154:GLY:HA3	2.07	0.55
1:B:187:ARG:CZ	1:C:66:ARG:HD3	2.37	0.55
1:C:134:HIS:HD2	1:C:137:ASP:H	1.54	0.55
1:A:66:ARG:HD2	1:D:187:ARG:CZ	2.37	0.55
1:A:121:LEU:HD23	1:A:121:LEU:C	2.32	0.55
1:B:279:ASP:O	1:B:283:VAL:HG23	2.07	0.55
1:A:251:GLY:C	1:A:252:ASN:HD22	2.15	0.55
1:C:254:LEU:HB2	1:C:311:LEU:HB3	1.88	0.55
1:C:135:LEU:HD21	1:C:220:GLU:O	2.06	0.55
1:D:204:ILE:O	1:D:209:ILE:HG12	2.06	0.55
1:B:25:ARG:HG3	1:B:54:LYS:HZ3	1.71	0.55
1:B:199:ILE:HB	1:B:202:ASN:ND2	2.21	0.55
1:B:25:ARG:NH2	3:B:319:HOH:O	2.39	0.55
1:D:254:LEU:HD13	1:D:274:PHE:CE1	2.41	0.55
1:A:67:GLU:OE1	1:D:81:LYS:HG2	2.07	0.54
1:A:94:VAL:O	1:A:98:ALA:CA	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ARG:O	1:B:290:LEU:HG	2.08	0.54
1:B:308:GLU:OE1	1:B:308:GLU:HA	2.06	0.54
1:D:235:GLU:O	1:D:239:GLU:HG3	2.06	0.54
1:B:304:LEU:HA	1:B:313:PHE:HA	1.89	0.54
1:D:29:ILE:HG12	1:D:130:ALA:HB3	1.88	0.54
1:D:255:ASP:HB3	1:D:258:LYS:HE3	1.90	0.54
1:D:255:ASP:OD2	1:D:258:LYS:HE2	2.07	0.54
1:C:86:LYS:HD2	1:C:87:ILE:H	1.74	0.53
1:C:152:LEU:HD21	1:D:152:LEU:HD21	1.89	0.53
1:A:83:ARG:CB	1:A:85:MET:HG3	2.38	0.53
1:A:190:GLU:HB3	1:D:71:ARG:NH1	2.19	0.53
1:C:88:PHE:CZ	1:C:124:GLU:HG2	2.43	0.53
1:B:187:ARG:HG2	1:C:196:GLU:CG	2.39	0.53
1:A:178:GLU:O	1:A:182:LYS:HG3	2.09	0.53
1:C:292:LYS:CG	1:C:293:GLY:H	2.16	0.53
1:B:300:LYS:O	1:B:302:LYS:N	2.42	0.53
1:D:308:GLU:OE2	1:D:308:GLU:HA	2.08	0.53
1:A:194:ASN:ND2	1:D:190:GLU:CG	2.71	0.53
1:C:1:MET:HG3	1:C:5:SER:OG	2.09	0.53
1:C:207:ARG:NH1	3:C:550:HOH:O	2.22	0.53
1:C:248:VAL:HG13	1:C:255:ASP:HB3	1.91	0.53
1:A:275:ILE:HG23	1:A:277:GLU:HB2	1.91	0.53
1:C:238:GLU:O	1:C:242:GLN:HG2	2.09	0.53
1:C:287:ARG:HG3	1:C:290:LEU:HD12	1.90	0.53
1:D:60:HIS:CD2	1:D:76:CYS:SG	3.01	0.53
1:A:6:ARG:CG	1:A:6:ARG:NH1	2.63	0.53
1:B:235:GLU:HG2	1:B:239:GLU:OE2	2.09	0.53
1:B:253:CYS:HA	1:B:311:LEU:O	2.09	0.53
1:C:204:ILE:O	1:C:209:ILE:HD12	2.08	0.53
1:D:308:GLU:HG3	1:D:309:ARG:N	2.22	0.52
1:A:116:PHE:O	1:A:120:ILE:HG12	2.09	0.52
1:B:139:LEU:HD13	1:B:209:ILE:CD1	2.34	0.52
1:B:308:GLU:HG3	1:B:309:ARG:H	1.74	0.52
1:C:222:THR:HG23	1:D:149:GLY:CA	2.39	0.52
1:D:39:VAL:HG13	1:D:180:TYR:CD2	2.45	0.52
1:A:244:LEU:HD23	1:A:266:LEU:HB3	1.90	0.52
1:B:104:SER:OG	1:B:107:GLU:HG2	2.10	0.52
1:A:175:SER:O	1:A:179:GLU:HG3	2.09	0.52
1:B:173:LYS:CG	1:B:176:GLU:HG3	2.40	0.52
1:B:223:PHE:O	1:B:227:VAL:HG23	2.10	0.52
1:A:134:HIS:HD2	1:A:136:ASN:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:VAL:HG21	1:C:304:LEU:HB2	1.92	0.52
1:B:35:VAL:HG22	3:B:322:HOH:O	2.09	0.52
1:B:160:PRO:HD3	1:B:170:TYR:CE1	2.45	0.52
1:A:131:THR:HG22	1:A:132:ALA:N	2.24	0.52
1:C:209:ILE:HB	1:C:210:PRO:HD3	1.91	0.52
1:B:62:ASN:ND2	1:B:62:ASN:C	2.68	0.51
1:C:222:THR:HG22	1:C:223:PHE:N	2.25	0.51
1:D:254:LEU:HD22	1:D:274:PHE:CD1	2.45	0.51
1:D:40:LEU:HB2	1:D:169:LEU:HD11	1.92	0.51
1:A:161:LYS:HG3	1:A:166:ARG:HD3	1.93	0.51
1:B:61:PHE:HB3	1:B:113:ARG:HG3	1.92	0.51
1:A:62:ASN:C	1:A:62:ASN:HD22	2.17	0.51
1:A:139:LEU:HD11	1:A:219:LEU:HD23	1.92	0.51
1:C:124:GLU:HB3	1:C:126:PHE:CE1	2.45	0.51
1:A:275:ILE:CG2	1:A:277:GLU:H	2.23	0.51
1:B:131:THR:CG2	1:B:133:HIS:H	2.24	0.51
1:C:303:VAL:CG1	1:C:314:SER:HB2	2.40	0.51
1:D:260:LYS:HE3	1:D:291:GLU:OE2	2.11	0.51
1:B:309:ARG:HG3	1:B:310:TRP:CD1	2.45	0.51
1:D:59:ALA:HA	1:D:88:PHE:O	2.10	0.51
1:C:62:ASN:ND2	1:C:62:ASN:C	2.69	0.51
1:C:306:ARG:HG3	1:C:307:LYS:O	2.11	0.51
1:D:14:LEU:HB3	1:D:20:ILE:CD1	2.41	0.51
1:B:2:ASN:HB2	1:B:3:PRO:CD	2.41	0.51
1:A:147:THR:OG1	1:B:212:LEU:HD22	2.10	0.51
1:D:190:GLU:H	1:D:190:GLU:CD	2.19	0.51
1:D:192:GLU:O	1:D:193:THR:HG22	2.10	0.51
1:D:300:LYS:HG3	1:D:300:LYS:O	2.11	0.51
1:C:4:GLU:OE2	1:C:184:LYS:NZ	2.44	0.50
1:A:68:SER:C	1:A:70:GLU:N	2.69	0.50
1:A:272:ARG:HD3	1:A:278:LYS:HD2	1.93	0.50
1:A:299:GLY:C	3:A:546:HOH:O	2.54	0.50
1:A:156:ILE:HD12	1:A:234:ARG:HE	1.76	0.50
1:B:180:TYR:C	1:B:180:TYR:CD2	2.89	0.50
1:B:308:GLU:HG3	1:B:309:ARG:N	2.26	0.50
1:C:144:LEU:HD22	1:C:148:ARG:HD2	1.93	0.50
1:A:68:SER:O	1:A:70:GLU:N	2.44	0.50
1:A:131:THR:CG2	1:A:132:ALA:N	2.75	0.50
1:A:281:GLU:O	1:A:285:LEU:HB2	2.12	0.50
1:A:138:LEU:HD13	1:A:158:PHE:CE1	2.46	0.50
1:B:207:ARG:CZ	1:D:195:TYR:HB3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:HD23	1:B:259:LEU:HD11	1.94	0.50
1:D:253:CYS:O	1:D:254:LEU:HD12	2.11	0.50
1:A:222:THR:HG23	1:B:149:GLY:CA	2.42	0.50
1:A:14:LEU:HD13	1:A:20:ILE:CG1	2.42	0.49
1:C:81:LYS:HD3	1:C:81:LYS:O	2.12	0.49
1:D:237:LEU:HD13	1:D:269:ARG:HH21	1.77	0.49
1:A:34:GLY:O	1:A:38:VAL:HG23	2.12	0.49
1:B:2:ASN:HB2	1:B:3:PRO:HD2	1.94	0.49
1:D:128:CYS:HA	1:D:164:VAL:HG22	1.95	0.49
1:D:164:VAL:O	1:D:164:VAL:HG22	2.13	0.49
1:C:222:THR:HG23	1:D:149:GLY:HA2	1.93	0.49
1:A:287:ARG:HG3	1:A:290:LEU:HD12	1.94	0.49
1:B:124:GLU:HB3	1:B:126:PHE:HE1	1.76	0.49
1:C:66:ARG:HG3	1:C:66:ARG:NH1	2.27	0.49
1:A:205:ARG:O	1:A:210:PRO:HD3	2.12	0.49
1:A:97:PHE:HE2	1:A:103:MET:HE1	1.78	0.49
1:A:194:ASN:HD21	1:D:190:GLU:HG2	1.76	0.49
1:A:256:VAL:HG13	1:A:290:LEU:HA	1.95	0.49
1:D:87:ILE:HD13	1:D:88:PHE:N	2.27	0.49
1:D:257:LYS:HD2	1:D:309:ARG:CB	2.43	0.49
1:A:214:ARG:HD2	1:B:203:ARG:NH2	2.27	0.49
1:A:257:LYS:HE2	1:A:257:LYS:HA	1.94	0.49
1:C:134:HIS:CD2	1:C:137:ASP:H	2.31	0.49
1:C:303:VAL:HG13	1:C:314:SER:HB2	1.95	0.48
1:D:2:ASN:HB2	1:D:3:PRO:CD	2.43	0.48
1:D:131:THR:CG2	1:D:133:HIS:H	2.22	0.48
1:D:191:ASP:O	1:D:193:THR:HG23	2.13	0.48
1:B:26:ARG:HB3	1:B:126:PHE:CD2	2.48	0.48
1:C:86:LYS:HD2	1:C:87:ILE:N	2.27	0.48
1:A:306:ARG:HG3	1:A:310:TRP:O	2.14	0.48
1:B:254:LEU:O	1:B:256:VAL:N	2.46	0.48
1:D:197:VAL:HG12	1:D:203:ARG:CZ	2.43	0.48
1:A:94:VAL:O	1:A:98:ALA:CB	2.60	0.48
1:A:156:ILE:CD1	1:A:231:ARG:HA	2.43	0.48
1:B:260:LYS:HD3	1:B:261:GLU:N	2.28	0.48
1:C:296:VAL:CG2	1:C:304:LEU:HB2	2.44	0.48
1:B:245:TYR:HD1	1:B:270:VAL:HG13	1.78	0.48
1:A:194:ASN:ND2	1:D:190:GLU:HG3	2.27	0.48
1:D:140:GLU:OE2	1:D:174:ARG:NH2	2.46	0.48
1:A:190:GLU:OE2	1:A:190:GLU:N	2.36	0.48
1:A:203:ARG:NH1	1:B:214:ARG:HH11	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LEU:HD21	1:D:148:ARG:NE	2.28	0.48
1:B:2:ASN:OD1	1:B:2:ASN:N	2.47	0.48
1:B:95:ARG:HG3	3:B:359:HOH:O	2.14	0.48
1:B:191:ASP:HB3	1:B:194:ASN:HB2	1.96	0.48
1:B:275:ILE:HD11	1:B:298:LEU:HD13	1.94	0.48
1:C:260:LYS:HE2	1:C:290:LEU:O	2.14	0.47
1:D:26:ARG:NH1	1:D:124:GLU:O	2.47	0.47
1:D:242:GLN:O	1:D:246:LYS:HG2	2.14	0.47
1:B:190:GLU:HG2	1:B:191:ASP:N	2.29	0.47
1:C:293:GLY:HA2	3:C:559:HOH:O	2.14	0.47
1:A:117:LEU:HB3	1:A:129:ILE:HD13	1.94	0.47
1:B:62:ASN:HD22	1:B:63:HIS:N	2.12	0.47
1:B:86:LYS:HG2	1:B:88:PHE:CZ	2.49	0.47
1:B:250:LYS:NZ	1:B:255:ASP:HB2	2.29	0.47
1:C:48:LYS:HG3	1:C:53:LEU:HB2	1.94	0.47
1:A:295:GLU:HG3	1:A:305:LYS:HB2	1.96	0.47
1:C:87:ILE:HG12	1:C:88:PHE:N	2.29	0.47
1:A:24:GLU:O	1:A:25:ARG:HD3	2.15	0.47
1:A:184:LYS:HB2	1:A:186:LEU:HG	1.96	0.47
1:C:150:THR:OG1	1:C:154:GLY:HA3	2.13	0.47
1:B:204:ILE:O	1:B:209:ILE:HG12	2.15	0.47
1:C:4:GLU:OE2	1:C:46:LYS:HE2	2.13	0.47
1:A:121:LEU:HD11	1:A:164:VAL:CG2	2.40	0.47
1:B:83:ARG:HG3	1:B:83:ARG:NH1	2.29	0.47
1:B:131:THR:HG23	1:B:133:HIS:H	1.80	0.47
1:C:203:ARG:HD3	1:D:211:GLU:OE1	2.14	0.47
1:D:48:LYS:O	1:D:53:LEU:HB2	2.13	0.47
1:B:134:HIS:CD2	1:B:137:ASP:H	2.33	0.47
1:B:187:ARG:CG	1:C:196:GLU:HG2	2.44	0.47
1:B:285:LEU:HG	1:B:296:VAL:HG11	1.96	0.47
1:C:197:VAL:O	1:C:197:VAL:CG1	2.63	0.47
1:A:14:LEU:HD13	1:A:20:ILE:HG13	1.97	0.47
1:A:229:VAL:HA	1:B:268:ARG:HH12	1.78	0.47
1:A:304:LEU:N	1:A:304:LEU:HD12	2.30	0.47
1:B:29:ILE:CD1	1:B:44:LEU:HD12	2.44	0.47
1:B:101:ASN:HB3	1:B:103:MET:HE3	1.98	0.46
1:C:143:LEU:HD21	1:C:212:LEU:HD11	1.97	0.46
1:D:28:LEU:O	1:D:129:ILE:HA	2.14	0.46
1:D:255:ASP:O	1:D:256:VAL:C	2.58	0.46
1:A:164:VAL:HG22	1:A:164:VAL:O	2.15	0.46
2:A:500:ANP:H8	2:A:500:ANP:H5'2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:LEU:N	1:C:289:LEU:HD22	2.30	0.46
1:C:303:VAL:O	1:C:313:PHE:HA	2.14	0.46
1:D:144:LEU:CD2	1:D:148:ARG:NE	2.78	0.46
1:B:275:ILE:HD12	1:B:286:VAL:CG2	2.42	0.46
1:D:252:ASN:O	1:D:312:CYS:SG	2.72	0.46
1:A:47:LEU:O	1:A:48:LYS:C	2.58	0.46
1:A:179:GLU:HG2	3:A:512:HOH:O	2.15	0.46
1:A:195:TYR:O	1:D:187:ARG:HB3	2.16	0.46
1:A:257:LYS:HE3	1:A:306:ARG:HH11	1.78	0.46
1:B:28:LEU:O	1:B:129:ILE:HA	2.14	0.46
1:B:187:ARG:NH1	1:C:66:ARG:HD3	2.31	0.46
1:B:133:HIS:ND1	1:B:167:ARG:NH1	2.64	0.46
1:D:150:THR:OG1	1:D:151:GLY:N	2.49	0.46
1:D:295:GLU:HG2	3:D:325:HOH:O	2.16	0.46
1:A:248:VAL:O	1:A:248:VAL:HG12	2.16	0.46
1:A:263:PRO:O	1:A:267:GLN:HG3	2.16	0.46
1:B:305:LYS:HB3	1:B:305:LYS:HZ2	1.81	0.46
1:C:60:HIS:O	1:C:89:VAL:HA	2.15	0.46
1:A:18:GLU:HG3	1:A:160:PRO:CG	2.45	0.46
1:D:202:ASN:N	1:D:202:ASN:ND2	2.55	0.46
1:C:36:ASP:OD2	1:C:36:ASP:N	2.48	0.46
1:C:135:LEU:HD23	1:C:220:GLU:HB3	1.98	0.46
1:D:4:GLU:HG3	1:D:184:LYS:HD2	1.97	0.46
1:C:244:LEU:HD21	1:C:262:LYS:HG3	1.97	0.46
1:D:299:GLY:O	1:D:301:GLY:N	2.48	0.46
1:A:221:ASP:HA	3:A:514:HOH:O	2.15	0.46
1:D:116:PHE:CE1	1:D:120:ILE:HD11	2.51	0.46
1:B:98:ALA:HB2	1:B:105:LEU:HD23	1.97	0.45
1:D:121:LEU:HD12	1:D:126:PHE:CB	2.45	0.45
1:B:98:ALA:CB	1:B:105:LEU:HD23	2.46	0.45
1:B:37:SER:HA	1:B:132:ALA:HB2	1.97	0.45
1:B:134:HIS:CD2	1:B:136:ASN:HB2	2.51	0.45
1:D:54:LYS:O	1:D:55:GLU:HB2	2.15	0.45
1:A:99:LYS:C	1:A:101:ASN:N	2.63	0.45
1:A:229:VAL:HA	1:B:268:ARG:HH11	1.81	0.45
1:A:302:LYS:O	1:A:302:LYS:HG3	2.16	0.45
1:D:65:LEU:HA	1:D:95:ARG:NH2	2.31	0.45
1:D:134:HIS:CD2	1:D:136:ASN:HB2	2.51	0.45
1:D:160:PRO:HD3	1:D:170:TYR:CE1	2.51	0.45
1:D:244:LEU:HD12	1:D:266:LEU:HB3	1.98	0.45
1:B:248:VAL:HG12	1:B:254:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:VAL:O	1:C:209:ILE:C	2.60	0.45
1:D:191:ASP:OD1	1:D:191:ASP:N	2.47	0.45
1:D:206:HIS:O	1:D:210:PRO:HG2	2.16	0.45
1:D:35:VAL:HG22	1:D:188:TRP:CD1	2.52	0.45
1:B:134:HIS:HD2	1:B:136:ASN:N	2.12	0.45
1:C:35:VAL:HG22	1:C:188:TRP:CD1	2.51	0.45
1:C:252:ASN:ND2	1:C:313:PHE:H	2.15	0.45
1:D:275:ILE:O	1:D:302:LYS:HE2	2.16	0.45
1:C:20:ILE:HD11	1:C:160:PRO:HB2	1.99	0.45
1:A:145:PHE:HB3	1:A:150:THR:HG21	1.98	0.45
1:A:271:ILE:O	1:A:275:ILE:HB	2.17	0.45
1:A:245:TYR:CE2	1:A:273:LYS:HD2	2.52	0.45
1:C:194:ASN:N	1:C:194:ASN:ND2	2.46	0.45
1:B:26:ARG:CB	1:B:126:PHE:HA	2.48	0.44
1:D:144:LEU:HD21	1:D:148:ARG:HE	1.82	0.44
1:D:156:ILE:HD11	1:D:234:ARG:HB2	1.99	0.44
1:D:166:ARG:O	1:D:168:PRO:HD3	2.17	0.44
1:C:272:ARG:HG3	1:C:278:LYS:HA	2.00	0.44
1:A:14:LEU:HD23	1:A:171:TYR:CZ	2.53	0.44
1:A:86:LYS:HB2	1:A:86:LYS:HZ3	1.81	0.44
1:C:63:HIS:C	1:C:65:LEU:H	2.26	0.44
1:C:165:ILE:HG21	1:C:167:ARG:NH1	2.32	0.44
1:D:166:ARG:C	1:D:168:PRO:HD3	2.42	0.44
1:D:228:LYS:HE2	3:D:327:HOH:O	2.15	0.44
1:D:300:LYS:C	1:D:302:LYS:H	2.25	0.44
1:A:35:VAL:O	1:A:36:ASP:C	2.60	0.44
1:A:68:SER:C	1:A:70:GLU:H	2.25	0.44
1:A:284:GLU:HG2	3:A:524:HOH:O	2.17	0.44
1:C:75:PHE:CZ	1:C:188:TRP:HA	2.51	0.44
1:C:140:GLU:HB3	1:C:201:ARG:HD2	2.00	0.44
1:C:296:VAL:HG23	1:C:304:LEU:O	2.17	0.44
1:C:299:GLY:C	1:C:301:GLY:H	2.24	0.44
1:A:26:ARG:NH2	1:A:54:LYS:HD2	2.32	0.44
1:B:45:LEU:CD1	1:B:83:ARG:HD3	2.48	0.44
1:C:209:ILE:HD12	1:C:209:ILE:H	1.82	0.44
1:D:78:GLU:O	1:D:82:GLU:HG3	2.17	0.44
1:D:157:GLY:O	1:D:158:PHE:C	2.61	0.44
1:D:196:GLU:HG3	1:D:198:SER:OG	2.17	0.44
1:A:279:ASP:O	1:A:283:VAL:HG23	2.18	0.44
1:B:61:PHE:CB	1:B:113:ARG:HG3	2.48	0.44
1:B:207:ARG:NH2	1:D:195:TYR:HB3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ILE:HB	1:D:58:LEU:HD23	1.99	0.44
1:A:86:LYS:HB2	1:A:86:LYS:HZ2	1.82	0.44
1:B:281:GLU:OE2	1:B:281:GLU:CA	2.65	0.44
1:C:177:ILE:O	1:C:180:TYR:HB3	2.17	0.44
1:A:2:ASN:OD1	1:A:2:ASN:C	2.60	0.44
1:A:149:GLY:O	1:A:150:THR:HB	2.18	0.44
1:B:260:LYS:HD3	1:B:260:LYS:C	2.41	0.44
1:C:245:TYR:CZ	1:C:273:LYS:HD2	2.52	0.44
1:A:196:GLU:C	1:A:198:SER:N	2.74	0.44
1:C:172:VAL:HG12	1:C:173:LYS:O	2.18	0.44
1:B:101:ASN:O	1:B:102:ARG:C	2.61	0.43
1:A:103:MET:HE3	1:A:108:ALA:HA	1.99	0.43
1:C:207:ARG:NH2	3:C:550:HOH:O	2.51	0.43
1:B:305:LYS:HB3	1:B:305:LYS:HZ3	1.84	0.43
1:C:209:ILE:O	1:C:213:LYS:HG3	2.19	0.43
1:A:191:ASP:O	1:A:192:GLU:CB	2.66	0.43
1:C:150:THR:O	1:D:226:MET:HG3	2.18	0.43
1:D:89:VAL:CG2	1:D:90:GLY:N	2.81	0.43
1:D:124:GLU:HB3	1:D:126:PHE:CE1	2.53	0.43
1:D:285:LEU:HD12	1:D:285:LEU:HA	1.91	0.43
1:D:300:LYS:C	1:D:302:LYS:N	2.76	0.43
1:B:134:HIS:HB2	1:B:172:VAL:O	2.19	0.43
1:C:58:LEU:HB2	1:C:87:ILE:HG13	2.00	0.43
1:D:37:SER:HA	1:D:132:ALA:HB2	2.01	0.43
1:A:89:VAL:HG22	1:A:90:GLY:N	2.34	0.43
1:D:229:VAL:O	1:D:233:GLU:HG3	2.19	0.43
1:A:160:PRO:HD3	1:A:170:TYR:CE1	2.53	0.43
1:A:194:ASN:ND2	1:D:190:GLU:HG2	2.33	0.43
1:B:36:ASP:HB3	1:B:132:ALA:HB1	2.00	0.43
1:B:117:LEU:HB3	1:B:129:ILE:HD13	2.01	0.43
1:D:7:VAL:HG21	1:D:180:TYR:HB2	2.00	0.43
1:D:31:PHE:CE2	1:D:33:GLY:HA2	2.54	0.43
1:D:279:ASP:O	1:D:283:VAL:HG23	2.18	0.43
1:D:289:LEU:CD2	1:D:296:VAL:HG23	2.49	0.43
1:A:197:VAL:HG11	1:A:207:ARG:CZ	2.47	0.43
1:A:103:MET:O	1:A:104:SER:C	2.62	0.43
1:A:149:GLY:HA3	1:B:222:THR:HB	2.01	0.43
1:A:156:ILE:HD11	1:A:231:ARG:HA	2.01	0.43
1:A:207:ARG:NH2	1:D:191:ASP:OD1	2.52	0.43
1:B:182:LYS:O	1:B:183:PHE:C	2.61	0.43
1:B:279:ASP:OD1	1:B:282:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:SER:HA	1:C:71:ARG:HD3	2.00	0.42
1:C:97:PHE:HE2	1:C:103:MET:HE1	1.84	0.42
1:D:2:ASN:O	1:D:6:ARG:HG3	2.19	0.42
1:D:12:LEU:O	1:D:13:ALA:C	2.61	0.42
1:D:270:VAL:O	1:D:271:ILE:C	2.62	0.42
1:A:250:LYS:O	1:A:251:GLY:C	2.63	0.42
1:B:249:LYS:O	1:B:249:LYS:HD3	2.19	0.42
1:B:288:SER:HB2	1:B:292:LYS:NZ	2.33	0.42
1:C:174:ARG:O	1:C:178:GLU:HG3	2.19	0.42
1:D:134:HIS:CD2	1:D:136:ASN:H	2.28	0.42
1:A:96:ALA:N	1:A:98:ALA:HB2	2.26	0.42
1:C:242:GLN:O	1:C:246:LYS:HG3	2.18	0.42
1:D:139:LEU:HA	1:D:223:PHE:CZ	2.54	0.42
1:D:294:GLY:O	1:D:305:LYS:HG3	2.19	0.42
1:A:211:GLU:OE1	1:B:203:ARG:HD2	2.19	0.42
1:B:4:GLU:O	1:B:8:ILE:HG12	2.18	0.42
1:C:197:VAL:O	1:C:197:VAL:HG12	2.19	0.42
1:C:244:LEU:O	1:C:248:VAL:HG23	2.19	0.42
1:D:49:ASN:C	1:D:51:PHE:N	2.76	0.42
1:D:217:GLU:HG3	1:D:218:ASN:ND2	2.34	0.42
1:A:196:GLU:C	1:A:198:SER:H	2.28	0.42
1:A:285:LEU:HD12	1:A:296:VAL:HG13	2.00	0.42
1:B:14:LEU:HD11	1:B:170:TYR:CB	2.44	0.42
1:B:254:LEU:HD23	1:B:259:LEU:CD1	2.49	0.42
1:D:103:MET:SD	1:D:108:ALA:HB2	2.60	0.42
1:D:204:ILE:HD13	1:D:208:VAL:HG21	2.02	0.42
1:A:307:LYS:O	1:A:308:GLU:HB2	2.19	0.42
1:B:97:PHE:O	1:B:101:ASN:HB2	2.20	0.42
1:B:289:LEU:HD12	1:B:289:LEU:HA	1.92	0.42
1:D:18:GLU:O	1:D:19:LYS:C	2.63	0.42
1:B:8:ILE:HG22	1:B:12:LEU:HD22	2.02	0.42
1:B:223:PHE:O	1:B:226:MET:HB3	2.19	0.42
1:C:248:VAL:CG1	1:C:255:ASP:HB3	2.49	0.42
1:B:131:THR:HG21	1:B:133:HIS:CE1	2.55	0.42
1:B:173:LYS:HG2	1:B:176:GLU:CG	2.46	0.42
1:B:275:ILE:HG23	1:B:277:GLU:N	2.27	0.42
1:D:254:LEU:HD13	1:D:274:PHE:CZ	2.55	0.42
1:D:285:LEU:O	1:D:288:SER:OG	2.34	0.42
1:A:140:GLU:OE2	1:A:174:ARG:NH2	2.53	0.42
1:C:143:LEU:HD21	1:C:212:LEU:CD1	2.49	0.42
1:D:202:ASN:HD22	1:D:202:ASN:H	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:VAL:O	1:D:257:LYS:C	2.62	0.42
1:C:139:LEU:O	1:C:139:LEU:HD22	2.19	0.41
1:C:281:GLU:O	1:C:285:LEU:HB2	2.20	0.41
1:A:4:GLU:OE1	1:A:184:LYS:NZ	2.48	0.41
1:A:62:ASN:C	1:A:62:ASN:ND2	2.78	0.41
1:A:97:PHE:HE2	1:A:103:MET:HE2	1.85	0.41
1:A:219:LEU:HD13	1:B:147:THR:HG23	2.01	0.41
1:B:59:ALA:HB3	1:B:117:LEU:CD2	2.50	0.41
1:B:152:LEU:HA	1:B:152:LEU:HD23	1.84	0.41
1:C:283:VAL:C	1:C:285:LEU:H	2.27	0.41
1:A:240:GLU:HB3	1:A:266:LEU:HD11	2.02	0.41
1:A:252:ASN:N	1:A:252:ASN:ND2	2.66	0.41
1:A:264:LEU:HD21	1:A:268:ARG:NE	2.35	0.41
1:B:279:ASP:OD2	1:B:281:GLU:HB2	2.20	0.41
1:C:200:PRO:O	1:C:201:ARG:C	2.63	0.41
1:D:192:GLU:C	1:D:193:THR:CG2	2.93	0.41
1:A:113:ARG:NH1	1:A:114:TYR:HE1	2.17	0.41
1:C:121:LEU:HD13	1:C:129:ILE:HG13	2.02	0.41
1:D:101:ASN:HB2	1:D:103:MET:HE3	2.01	0.41
1:D:275:ILE:HG22	1:D:304:LEU:HD21	2.02	0.41
1:A:12:LEU:HD12	1:A:12:LEU:HA	1.85	0.41
1:A:239:GLU:O	1:A:243:LYS:HG3	2.20	0.41
1:C:146:PHE:C	1:C:146:PHE:CD2	2.98	0.41
1:C:209:ILE:N	1:C:210:PRO:CD	2.84	0.41
1:B:140:GLU:OE2	1:B:174:ARG:NH1	2.53	0.41
1:C:41:THR:HG21	1:C:79:PHE:HE2	1.86	0.41
1:C:237:LEU:HD13	1:C:269:ARG:HH21	1.86	0.41
1:C:93:ASP:O	1:C:94:VAL:C	2.63	0.41
1:D:163:GLU:HB3	1:D:164:VAL:H	1.67	0.41
1:D:196:GLU:OE1	1:D:196:GLU:HA	2.21	0.41
1:A:83:ARG:O	1:A:84:ASN:HB2	2.20	0.41
1:C:95:ARG:HA	1:C:105:LEU:CD2	2.50	0.41
1:D:251:GLY:C	1:D:252:ASN:HD22	2.28	0.41
1:D:255:ASP:CG	1:D:258:LYS:HE2	2.46	0.41
1:D:286:VAL:O	1:D:289:LEU:HB2	2.20	0.41
1:A:131:THR:CG2	1:A:133:HIS:CG	3.03	0.41
1:A:180:TYR:C	1:A:180:TYR:CD2	2.99	0.41
1:A:197:VAL:HG21	1:A:207:ARG:NE	2.35	0.41
1:B:244:LEU:CD1	1:B:262:LYS:HG3	2.37	0.41
1:C:149:GLY:HA2	1:D:222:THR:CG2	2.51	0.41
1:D:62:ASN:HB3	1:D:91:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HD11	1:B:59:ALA:HB2	2.02	0.41
1:B:159:LEU:HD12	1:B:162:GLU:HG2	2.03	0.41
1:B:238:GLU:O	1:B:241:ALA:HB3	2.21	0.41
1:B:293:GLY:HA2	1:B:306:ARG:HD3	2.03	0.41
1:D:15:GLN:HA	1:D:15:GLN:OE1	2.21	0.41
1:D:34:GLY:O	1:D:38:VAL:HG23	2.21	0.41
1:D:242:GLN:C	1:D:244:LEU:N	2.77	0.41
1:D:245:TYR:C	1:D:247:GLU:H	2.29	0.41
1:A:96:ALA:O	1:A:98:ALA:N	2.53	0.40
1:A:97:PHE:CD2	1:A:97:PHE:C	2.98	0.40
1:B:26:ARG:HB3	1:B:126:PHE:HA	2.03	0.40
1:B:159:LEU:HB2	1:B:162:GLU:CG	2.50	0.40
1:D:49:ASN:O	1:D:50:TYR:C	2.64	0.40
1:D:121:LEU:HD21	1:D:164:VAL:CG2	2.24	0.40
1:A:113:ARG:HD3	2:A:500:ANP:C4	2.51	0.40
1:C:254:LEU:HD22	1:C:274:PHE:CE1	2.57	0.40
1:C:277:GLU:HG2	1:C:302:LYS:NZ	2.35	0.40
1:C:279:ASP:HB2	1:C:281:GLU:OE1	2.22	0.40
1:B:27:VAL:HG23	1:B:53:LEU:HD22	2.02	0.40
1:C:299:GLY:C	1:C:301:GLY:N	2.79	0.40
1:D:2:ASN:HB2	1:D:3:PRO:HD2	2.02	0.40
1:D:95:ARG:HH11	1:D:95:ARG:HG3	1.86	0.40
1:D:255:ASP:OD1	1:D:255:ASP:C	2.64	0.40
1:C:24:GLU:OE1	1:C:24:GLU:N	2.40	0.40
1:D:27:VAL:HG23	1:D:53:LEU:HD22	2.04	0.40
1:D:156:ILE:HD12	1:D:234:ARG:HG3	2.02	0.40
1:A:163:GLU:HB3	1:A:164:VAL:H	1.68	0.40
1:A:289:LEU:HA	1:A:292:LYS:O	2.21	0.40
1:A:298:LEU:HD12	1:A:302:LYS:HD2	2.04	0.40
1:B:249:LYS:HD3	1:B:249:LYS:C	2.47	0.40
1:C:2:ASN:HB2	1:C:3:PRO:HD2	2.04	0.40
1:C:2:ASN:OD1	1:C:4:GLU:HB3	2.22	0.40
1:D:273:LYS:HB3	1:D:273:LYS:HE2	1.84	0.40

There are no symmetry-related clashes.

## 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	315/317 (99%)	284 (90%)	24 (8%)	7 (2%)	5	14
1	B	312/317 (98%)	276 (88%)	29 (9%)	7 (2%)	5	14
1	C	312/317 (98%)	291 (93%)	19 (6%)	2 (1%)	21	44
1	D	312/317 (98%)	266 (85%)	36 (12%)	10 (3%)	3	7
All	All	1251/1268 (99%)	1117 (89%)	108 (9%)	26 (2%)	5	15

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ALA
1	B	255	ASP
1	B	300	LYS
1	D	69	ALA
1	D	192	GLU
1	A	69	ALA
1	B	247	GLU
1	B	301	GLY
1	D	158	PHE
1	D	194	ASN
1	D	196	GLU
1	A	300	LYS
1	D	193	THR
1	D	274	PHE
1	B	100	GLU
1	B	299	GLY
1	C	65	LEU
1	D	300	LYS
1	A	104	SER
1	A	260	LYS
1	A	301	GLY
1	B	245	TYR

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Mol	Chain	Res	Type
1	C	280	TYR
1	D	102	ARG
1	D	256	VAL
1	A	149	GLY

### 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	285/285 (100%)	264 (93%)	21 (7%)	13	32
1	B	282/285 (99%)	262 (93%)	20 (7%)	13	33
1	C	282/285 (99%)	250 (89%)	32 (11%)	5	14
1	D	282/285 (99%)	257 (91%)	25 (9%)	9	23
All	All	1131/1140 (99%)	1033 (91%)	98 (9%)	9	24

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	12	LEU
1	A	14	LEU
1	A	35	VAL
1	A	71	ARG
1	A	86	LYS
1	A	99	LYS
1	A	100	GLU
1	A	118	LYS
1	A	124	GLU
1	A	139	LEU
1	A	144	LEU
1	A	169	LEU
1	A	198	SER
1	A	222	THR
1	A	257	LYS
1	A	264	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	275	ILE
1	A	285	LEU
1	A	303	VAL
1	A	317	VAL
1	B	12	LEU
1	B	14	LEU
1	B	35	VAL
1	B	67	GLU
1	B	82	GLU
1	B	92	GLU
1	B	110	ARG
1	B	119	GLU
1	B	131	THR
1	B	139	LEU
1	B	169	LEU
1	B	191	ASP
1	B	193	THR
1	B	197	VAL
1	B	246	LYS
1	B	264	LEU
1	B	289	LEU
1	B	303	VAL
1	B	305	LYS
1	B	312	CYS
1	C	12	LEU
1	C	14	LEU
1	C	36	ASP
1	C	55	GLU
1	C	62	ASN
1	C	66	ARG
1	C	67	GLU
1	C	81	LYS
1	C	110	ARG
1	C	119	GLU
1	C	131	THR
1	C	139	LEU
1	C	143	LEU
1	C	144	LEU
1	C	164	VAL
1	C	166	ARG
1	C	175	SER
1	C	190	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	194	ASN
1	C	207	ARG
1	C	222	THR
1	C	234	ARG
1	C	239	GLU
1	C	254	LEU
1	C	256	VAL
1	C	259	LEU
1	C	264	LEU
1	C	281	GLU
1	C	305	LYS
1	C	307	LYS
1	C	309	ARG
1	C	312	CYS
1	D	14	LEU
1	D	35	VAL
1	D	86	LYS
1	D	87	ILE
1	D	89	VAL
1	D	124	GLU
1	D	127	ASP
1	D	131	THR
1	D	139	LEU
1	D	167	ARG
1	D	190	GLU
1	D	191	ASP
1	D	193	THR
1	D	196	GLU
1	D	202	ASN
1	D	217	GLU
1	D	222	THR
1	D	234	ARG
1	D	244	LEU
1	D	248	VAL
1	D	257	LYS
1	D	289	LEU
1	D	303	VAL
1	D	309	ARG
1	D	312	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	62	ASN
1	A	101	ASN
1	A	134	HIS
1	A	194	ASN
1	A	216	ASN
1	A	252	ASN
1	A	267	GLN
1	B	62	ASN
1	B	134	HIS
1	B	194	ASN
1	B	202	ASN
1	B	252	ASN
1	C	62	ASN
1	C	63	HIS
1	C	134	HIS
1	C	194	ASN
1	C	202	ASN
1	C	252	ASN
1	D	60	HIS
1	D	134	HIS
1	D	202	ASN
1	D	218	ASN
1	D	252	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

2 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	ANP	C	501	-	33,33,33	1.58	7 (21%)	45,52,52	2.30	13 (28%)
2	ANP	A	500	-	33,33,33	1.57	7 (21%)	45,52,52	2.55	12 (26%)

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	ANP	C	501	-	-	3/18/38/38	0/3/3/3
2	ANP	A	500	-	-	5/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	ANP	C1'-N9	-4.73	1.33	1.46
2	A	500	ANP	C1'-N9	-4.59	1.33	1.46
2	C	501	ANP	PB-O2B	-3.21	1.48	1.56
2	C	501	ANP	C5-N7	-3.16	1.33	1.39
2	A	500	ANP	C5-N7	-3.09	1.33	1.39
2	A	500	ANP	PB-O2B	-2.97	1.48	1.56
2	A	500	ANP	C8-N9	-2.32	1.33	1.37
2	A	500	ANP	O4'-C1'	-2.27	1.36	1.42
2	C	501	ANP	O4'-C1'	-2.12	1.37	1.42
2	A	500	ANP	PB-O3A	2.08	1.61	1.59
2	A	500	ANP	C4-N9	-2.04	1.33	1.37
2	C	501	ANP	C4-N9	-2.02	1.33	1.37
2	C	501	ANP	PG-O2G	2.00	1.62	1.56
2	C	501	ANP	C8-N9	-2.00	1.34	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	ANP	O4'-C1'-N9	9.91	127.12	108.09
2	C	501	ANP	C5-C4-N3	-6.15	118.24	126.72
2	C	501	ANP	C1'-N9-C8	-5.88	114.04	127.09
2	A	500	ANP	N3-C2-N1	-5.88	119.68	128.58
2	C	501	ANP	N3-C2-N1	-5.46	120.32	128.58
2	A	500	ANP	C5-C4-N3	-5.14	119.64	126.72
2	C	501	ANP	C2-N3-C4	4.45	122.69	111.83
2	A	500	ANP	O2B-PB-O1B	4.26	119.00	109.87
2	A	500	ANP	C2-N3-C4	4.23	122.15	111.83
2	C	501	ANP	C2'-C1'-N9	3.80	122.75	113.30
2	C	501	ANP	O2B-PB-O1B	3.56	117.50	109.87
2	A	500	ANP	O1B-PB-N3B	-3.42	106.74	111.77
2	A	500	ANP	N3-C4-N9	3.34	132.85	127.17
2	C	501	ANP	O2G-PG-O3G	-3.30	98.72	107.59
2	C	501	ANP	C4-N9-C1'	3.16	134.02	126.63
2	C	501	ANP	O1G-PG-N3B	2.99	116.17	111.77
2	C	501	ANP	O4'-C1'-N9	2.89	113.63	108.09
2	A	500	ANP	C2'-C1'-N9	2.81	120.28	113.30
2	A	500	ANP	N9-C8-N7	-2.77	110.00	113.94
2	A	500	ANP	C4-C5-N7	-2.73	107.46	110.58
2	A	500	ANP	C5-N7-C8	2.63	107.59	103.45
2	C	501	ANP	C5-C4-N9	2.61	108.66	105.81
2	C	501	ANP	O3'-C3'-C4'	-2.50	103.90	111.08
2	C	501	ANP	C4-C5-N7	-2.42	107.82	110.58
2	A	500	ANP	O4'-C1'-C2'	-2.42	101.45	106.62

There are no chirality outliers.

All (8) torsion outliers are listed below:

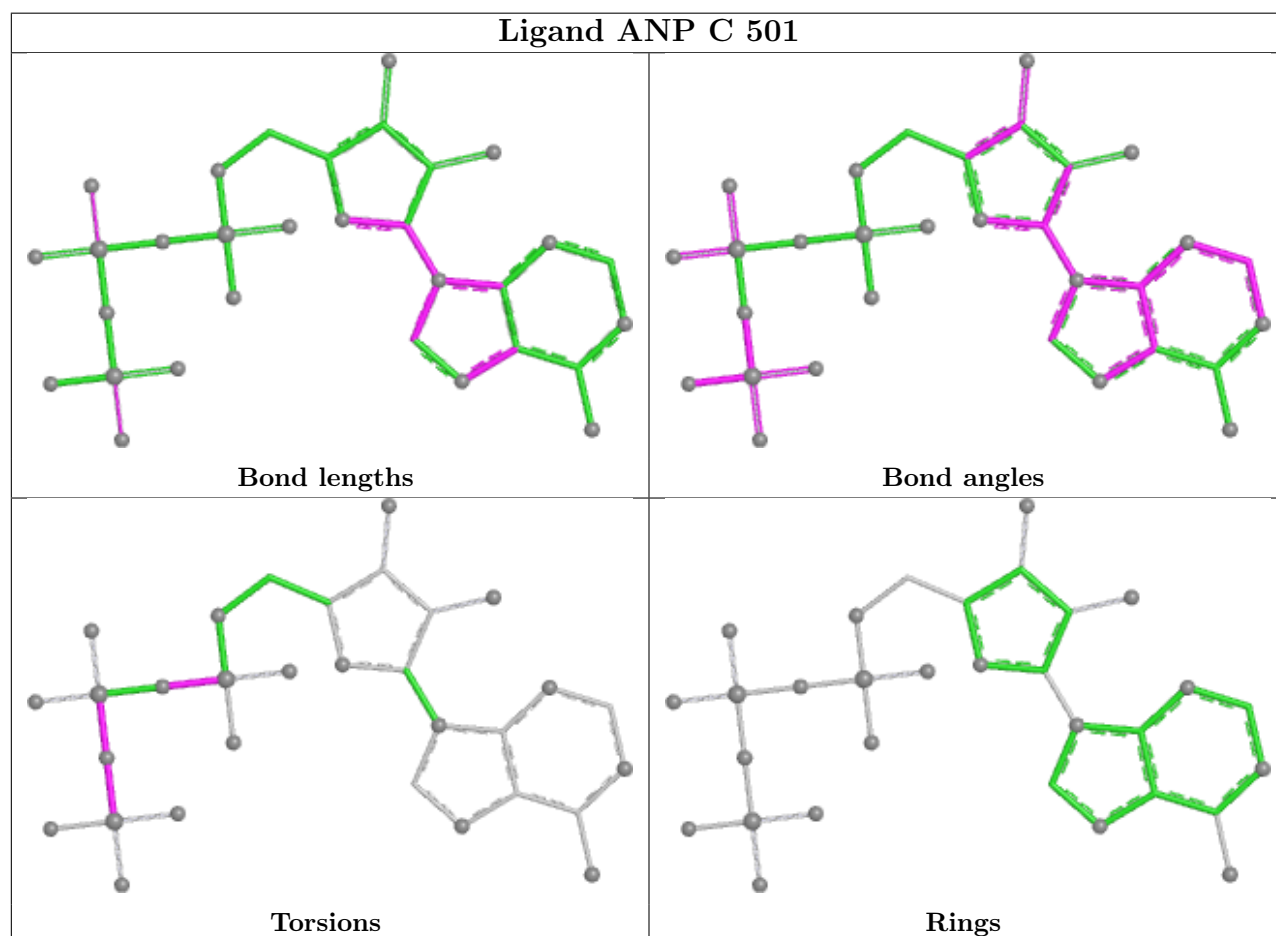
Mol	Chain	Res	Type	Atoms
2	A	500	ANP	PG-N3B-PB-O1B
2	A	500	ANP	PG-N3B-PB-O3A
2	A	500	ANP	PA-O3A-PB-O2B
2	C	501	ANP	PB-N3B-PG-O1G
2	A	500	ANP	C4'-C5'-O5'-PA
2	C	501	ANP	PG-N3B-PB-O3A
2	A	500	ANP	PA-O3A-PB-O1B
2	C	501	ANP	PB-O3A-PA-O1A

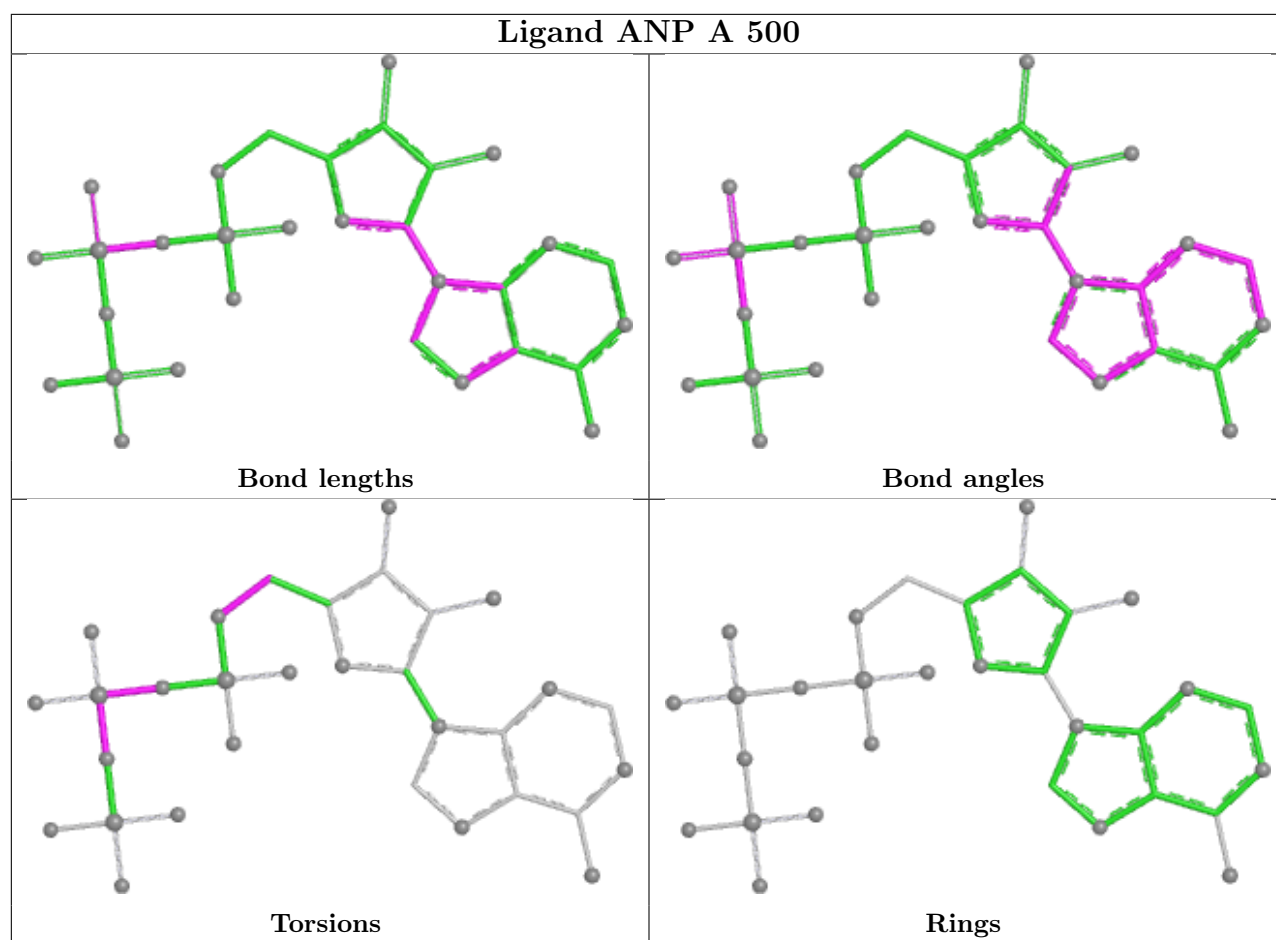
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	ANP	3	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	317/317 (100%)	-0.06	3 (0%) 81 80	23, 48, 88, 114	0
1	B	314/317 (99%)	0.04	13 (4%) 41 37	16, 44, 90, 100	0
1	C	314/317 (99%)	-0.13	8 (2%) 58 55	19, 41, 99, 112	0
1	D	314/317 (99%)	0.25	8 (2%) 58 55	27, 60, 109, 119	0
All	All	1259/1268 (99%)	0.02	32 (2%) 58 55	16, 48, 96, 119	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	SER	4.1
1	D	195	TYR	3.8
1	B	104	SER	3.6
1	D	314	SER	2.9
1	D	194	ASN	2.9
1	B	313	PHE	2.8
1	D	193	THR	2.7
1	D	191	ASP	2.7
1	C	294	GLY	2.6
1	D	114	TYR	2.6
1	C	298	LEU	2.5
1	C	314	SER	2.5
1	B	275	ILE	2.4
1	B	103	MET	2.4
1	A	114	TYR	2.4
1	B	298	LEU	2.4
1	B	110	ARG	2.4
1	B	193	THR	2.3
1	B	278	LYS	2.3
1	C	299	GLY	2.3
1	C	311	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	121	LEU	2.3
1	A	96	ALA	2.3
1	C	305	LYS	2.2
1	A	97	PHE	2.2
1	D	66	ARG	2.1
1	B	296	VAL	2.1
1	B	105	LEU	2.1
1	C	304	LEU	2.1
1	B	307	LYS	2.1
1	C	1	MET	2.1
1	B	251	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

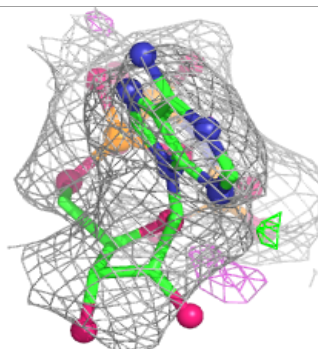
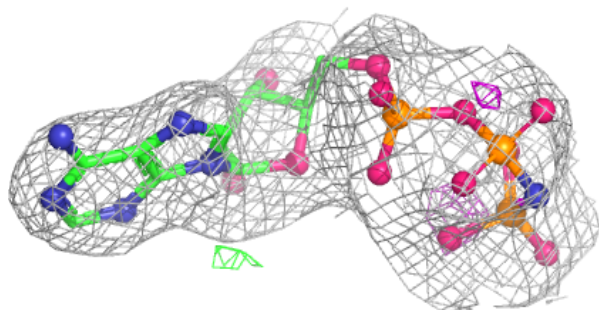
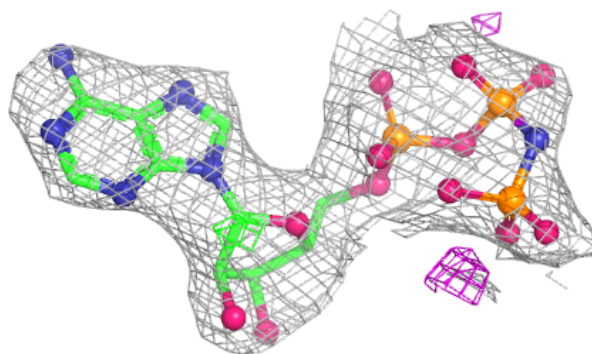
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ANP	A	500	31/31	0.82	0.13	94,100,117,118	0
2	ANP	C	501	31/31	0.87	0.15	32,38,47,49	21

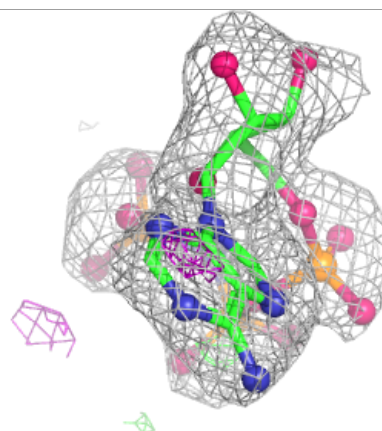
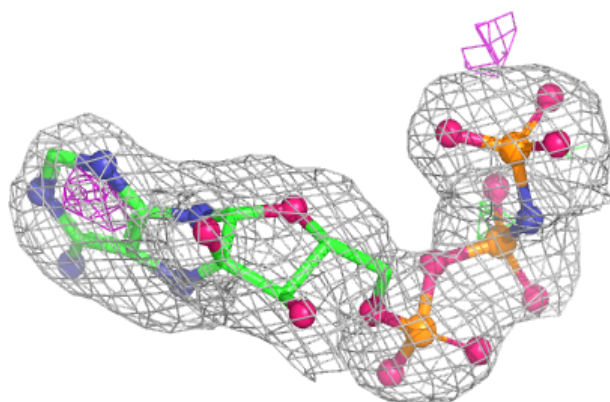
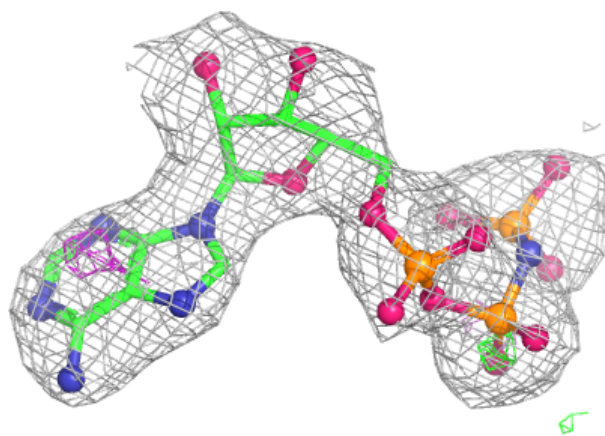
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around ANP A 500:**

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

**Electron density around ANP C 501:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.