



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2024 – 01:55 AM EST

PDB ID : 3AKL
Title : Crystal structure of A Helicobacter pylori proinflammatory kinase CtkA
Authors : Kim, D.J.; Suh, S.W.
Deposited on : 2010-07-14
Resolution : 2.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

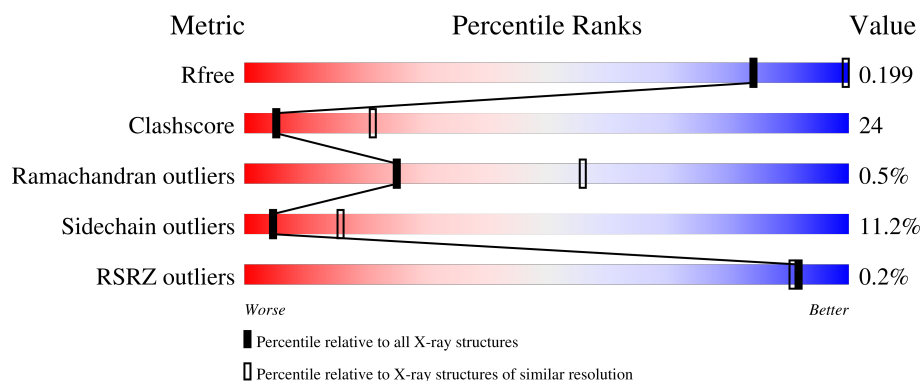
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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 ≥ 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	325	
1	B	325	
1	C	325	
1	D	325	

2 Entry composition [i](#)

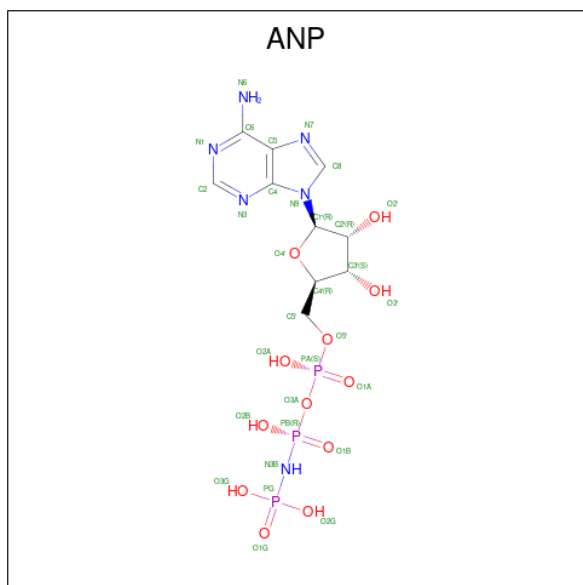
There are 5 unique types of molecules in this entry. The entry contains 9276 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CtkA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2282	1467	375	425	15			
1	B	281	Total	C	N	O	S	0	0	0
			2282	1467	375	425	15			
1	C	279	Total	C	N	O	S	0	0	0
			2263	1456	370	422	15			
1	D	279	Total	C	N	O	S	0	0	0
			2263	1456	370	422	15			

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

Continued on next page...

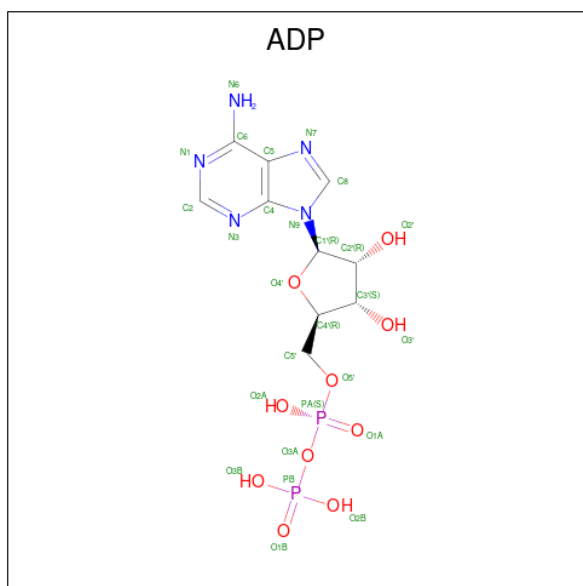
Continued from previous page...

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	C	1	Total	Mg	0	0
			1	1		
3	D	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



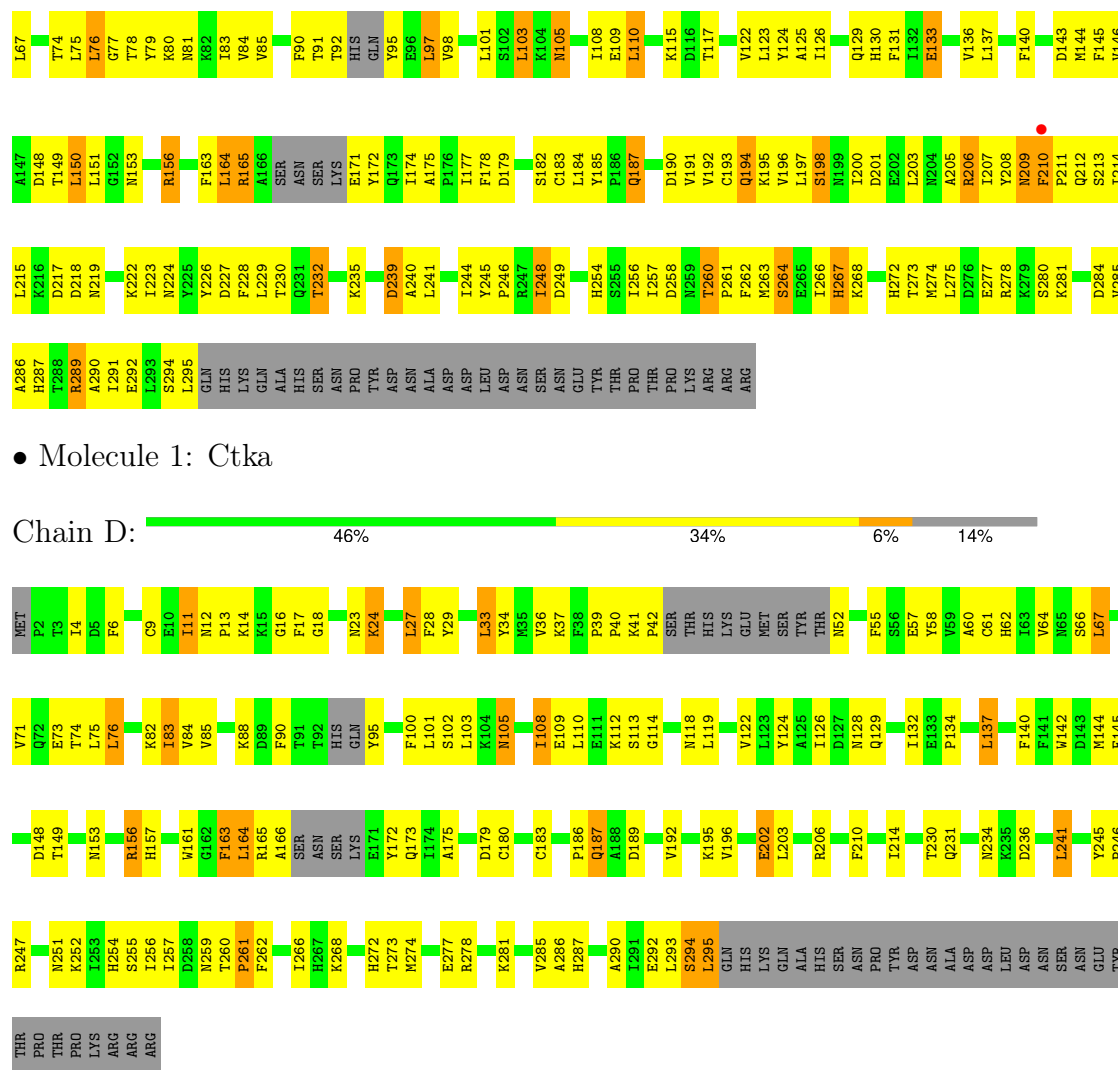
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	13	Total 13	O 13	0	0
5	B	16	Total 16	O 16	0	0
5	C	10	Total 10	O 10	0	0
5	D	20	Total 20	O 20	0	0

- Molecule 1: Ctka





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.13Å 74.83Å 75.81Å 78.84° 71.36° 85.44°	Depositor
Resolution (Å)	19.94 – 2.90 19.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.7 (19.94-2.90) 98.2 (19.94-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.88Å)	Xtriage
Refinement program	REFMAC, PHENIX 1.5_2	Depositor
R, R_{free}	0.189 , 0.280 0.196 , 0.199	Depositor DCC
R_{free} test set	2678 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.0	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 19.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9276	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ADP, ANP, MG

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	0.73	0/2333	0.73	1/3153 (0.0%)
1	B	0.51	0/2333	0.63	0/3153
1	C	0.48	0/2312	0.62	0/3123
1	D	0.56	0/2312	0.65	1/3123 (0.0%)
All	All	0.58	0/9290	0.66	2/12552 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	261	PRO	N-CA-C	6.05	127.82	112.10
1	A	219	ASN	N-CA-C	-5.27	96.76	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2282	0	2242	96	0
1	B	2282	0	2244	76	0
1	C	2263	0	2228	167	0
1	D	2263	0	2228	109	0
2	A	31	0	13	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	13	3	0
2	D	31	0	13	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	C	27	0	12	5	0
5	A	13	0	0	0	0
5	B	16	0	0	1	0
5	C	10	0	0	3	0
5	D	20	0	0	2	0
All	All	9276	0	8993	435	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 24.

All (435) 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:208:TYR:C	1:C:209:ASN:HD22	1.38	1.24
1:C:208:TYR:C	1:C:209:ASN:ND2	1.97	1.15
4:C:500:ADP:H8	4:C:500:ADP:H5'2	1.09	1.11
1:C:210:PHE:HB2	1:C:211:PRO:HD3	1.23	1.10
1:D:40:PRO:C	1:D:42:PRO:HD2	1.72	1.09
1:A:30:ASN:O	1:A:31:ASN:HB2	1.57	1.05
4:C:500:ADP:H5'2	4:C:500:ADP:C8	1.98	0.98
1:C:257:ILE:O	1:C:260:THR:OG1	1.80	0.97
1:D:254:HIS:CD2	1:D:272:HIS:HD2	1.82	0.97
1:C:210:PHE:N	1:C:210:PHE:HD2	1.66	0.94
1:C:206:ARG:HH11	1:C:206:ARG:HG3	1.34	0.93
1:D:254:HIS:HD2	1:D:272:HIS:HD2	1.10	0.93
1:D:109:GLU:OE1	1:D:124:TYR:OH	1.85	0.92
1:D:255:SER:O	1:D:259:ASN:ND2	2.03	0.91
1:A:14:LYS:NZ	1:B:171:GLU:HB2	1.85	0.91
1:C:210:PHE:N	1:C:210:PHE:CD2	2.34	0.91
1:D:37:LYS:NZ	1:D:57:GLU:OE2	2.04	0.91
1:A:80:LYS:O	1:A:81:ASN:HB2	1.71	0.89
1:A:254:HIS:CD2	1:A:272:HIS:HD2	1.91	0.89
1:B:6:PHE:CE1	1:B:77:GLY:HA3	2.09	0.87
1:C:208:TYR:O	1:C:209:ASN:ND2	2.05	0.85
1:D:254:HIS:HD2	1:D:272:HIS:CD2	1.94	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:PHE:HE1	1:B:77:GLY:HA3	1.40	0.85
1:C:126:ILE:HG23	1:C:137:LEU:HD12	1.58	0.84
1:A:254:HIS:HD2	1:A:272:HIS:HD2	1.23	0.84
1:B:254:HIS:CD2	1:B:272:HIS:HD2	1.94	0.84
1:D:105:ASN:ND2	1:D:114:GLY:H	1.76	0.83
1:A:103:LEU:HG	1:A:131:PHE:CE1	2.14	0.83
1:C:254:HIS:CD2	1:C:272:HIS:CD2	2.66	0.83
1:C:164:LEU:HD13	1:C:175:ALA:HB2	1.62	0.81
1:C:6:PHE:CE1	1:C:77:GLY:HA3	2.16	0.81
1:C:245:TYR:HA	1:C:248:ILE:HD12	1.63	0.80
1:C:206:ARG:HH11	1:C:206:ARG:CG	1.93	0.79
1:B:105:ASN:ND2	1:B:114:GLY:H	1.79	0.79
1:A:18:GLY:O	1:A:24:LYS:HE3	1.83	0.78
1:A:165:ARG:HD2	1:A:172:TYR:CE1	2.18	0.78
1:A:254:HIS:CD2	1:A:272:HIS:CD2	2.72	0.78
1:C:210:PHE:CB	1:C:211:PRO:HD3	2.07	0.77
1:B:210:PHE:CZ	1:D:195:LYS:HD3	2.20	0.77
1:C:254:HIS:CD2	1:C:272:HIS:HD2	2.02	0.77
1:B:76:LEU:HD23	1:B:261:PRO:HD2	1.66	0.76
1:C:254:HIS:HD2	1:C:272:HIS:CD2	2.04	0.76
1:D:41:LYS:N	1:D:42:PRO:CD	2.49	0.75
1:A:290:ALA:O	1:A:293:LEU:HB2	1.87	0.75
1:B:148:ASP:OD2	1:B:156:ARG:HD2	1.87	0.75
1:B:144:MET:SD	1:B:156:ARG:HD3	2.26	0.75
1:A:101:LEU:HG	1:A:114:GLY:O	1.86	0.74
1:A:133:GLU:O	1:A:133:GLU:HG3	1.83	0.74
1:A:30:ASN:O	1:A:31:ASN:CB	2.30	0.73
1:D:41:LYS:N	1:D:42:PRO:HD2	1.94	0.73
1:C:210:PHE:HB2	1:C:211:PRO:CD	2.12	0.72
1:A:186:PRO:HD2	1:A:187:GLN:OE1	1.90	0.71
1:C:18:GLY:O	1:C:24:LYS:HE3	1.91	0.71
1:C:177:ILE:HA	5:C:332:HOH:O	1.89	0.71
1:D:165:ARG:HB3	1:D:172:TYR:CE1	2.26	0.71
1:A:14:LYS:HZ3	1:B:171:GLU:HB2	1.54	0.70
1:C:217:ASP:C	1:C:217:ASP:OD2	2.30	0.70
1:C:207:ILE:HD11	1:C:277:GLU:HB3	1.72	0.70
1:C:214:ILE:HD12	1:C:222:LYS:HE2	1.74	0.70
1:A:105:ASN:O	1:B:23:ASN:HB3	1.92	0.69
1:C:133:GLU:HG3	1:C:133:GLU:O	1.89	0.69
1:A:27:LEU:HD12	1:A:27:LEU:C	2.13	0.69
1:A:202:GLU:HG3	1:A:206:ARG:HH12	1.57	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:TYR:HA	1:C:248:ILE:CD1	2.23	0.69
1:C:97:LEU:HD12	1:C:98:VAL:N	2.08	0.68
1:C:179:ASP:OD2	4:C:500:ADP:O2A	2.11	0.68
1:A:5:ASP:OD2	1:A:7:THR:HB	1.93	0.68
1:A:58:TYR:CG	1:A:76:LEU:HD22	2.28	0.68
1:D:148:ASP:OD2	1:D:156:ARG:HD2	1.93	0.68
1:C:6:PHE:HE1	1:C:77:GLY:HA3	1.58	0.68
1:C:130:HIS:O	1:D:14:LYS:HE2	1.95	0.67
1:C:17:PHE:HE2	1:C:26:SER:HB2	1.59	0.67
1:A:189:ASP:OD1	1:A:189:ASP:C	2.30	0.67
1:C:149:THR:O	1:C:278:ARG:NH2	2.24	0.67
1:C:280:SER:HA	1:C:284:ASP:OD2	1.94	0.66
1:C:209:ASN:ND2	1:C:209:ASN:N	2.30	0.66
1:C:285:VAL:HB	5:C:326:HOH:O	1.94	0.66
1:D:40:PRO:O	1:D:42:PRO:HD2	1.95	0.66
1:D:41:LYS:O	1:D:42:PRO:C	2.33	0.66
1:D:179:ASP:OD2	2:D:602:ANP:O2G	2.14	0.66
1:C:4:ILE:HG22	1:C:5:ASP:N	2.11	0.65
1:C:174:ILE:HG22	1:C:175:ALA:O	1.96	0.65
1:C:248:ILE:HG22	1:C:248:ILE:O	1.96	0.64
1:C:294:SER:HA	1:C:295:LEU:C	2.18	0.64
1:B:253:ILE:O	1:B:257:ILE:HG13	1.97	0.64
1:C:60:ALA:O	1:C:64:VAL:HG23	1.97	0.64
1:C:192:VAL:HA	1:C:195:LYS:HB3	1.80	0.64
1:A:237:CYS:O	1:A:240:ALA:HB3	1.98	0.64
1:D:40:PRO:HB2	1:D:42:PRO:CD	2.27	0.64
1:B:254:HIS:CD2	1:B:272:HIS:CD2	2.83	0.64
1:D:153:ASN:HB2	1:D:183:CYS:SG	2.37	0.64
1:C:217:ASP:OD2	1:C:219:ASN:N	2.28	0.63
1:B:156:ARG:NH2	1:B:178:PHE:O	2.32	0.63
1:D:254:HIS:CD2	1:D:272:HIS:CD2	2.74	0.63
1:D:66:SER:HB2	1:D:252:LYS:HE3	1.81	0.63
1:C:110:LEU:HD21	1:C:124:TYR:CD2	2.34	0.62
1:C:264:SER:OG	1:C:267:HIS:HB2	1.98	0.62
1:C:126:ILE:HG23	1:C:137:LEU:CD1	2.28	0.62
1:B:254:HIS:HD2	1:B:272:HIS:CD2	2.18	0.62
1:C:23:ASN:HB3	1:D:108:ILE:HG22	1.80	0.62
1:C:79:TYR:HE2	1:C:80:LYS:HE2	1.65	0.62
1:D:186:PRO:HG2	1:D:187:GLN:OE1	1.99	0.62
1:C:235:LYS:O	1:C:235:LYS:HD3	1.99	0.62
1:C:192:VAL:O	1:C:196:VAL:HG23	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ILE:HD11	1:D:262:PHE:CD1	2.35	0.61
1:A:125:ALA:O	1:A:129:GLN:HG3	2.01	0.61
1:A:58:TYR:CB	1:A:76:LEU:HD22	2.31	0.61
1:D:64:VAL:CG1	1:D:71:VAL:HB	2.31	0.61
1:A:206:ARG:HA	1:A:210:PHE:O	2.01	0.60
1:A:6:PHE:CE1	1:A:77:GLY:HA3	2.35	0.60
1:A:252:LYS:O	1:A:255:SER:HB3	2.01	0.60
1:B:66:SER:HB2	1:B:252:LYS:HE3	1.84	0.60
1:D:40:PRO:C	1:D:42:PRO:CD	2.60	0.59
1:C:63:ILE:O	1:C:67:LEU:HD13	2.02	0.59
1:C:274:MET:O	1:C:278:ARG:HG3	2.01	0.59
1:D:27:LEU:HG	1:D:36:VAL:HG21	1.84	0.59
1:A:149:THR:HG21	1:A:229:LEU:HD22	1.85	0.59
1:B:27:LEU:HD12	1:B:27:LEU:O	2.03	0.59
1:C:212:GLN:HG2	1:C:223:ILE:O	2.02	0.59
1:B:58:TYR:O	1:B:62:HIS:HD2	1.84	0.59
1:A:154:PHE:HB3	1:A:211:PRO:HB3	1.84	0.59
1:B:212:GLN:HE21	1:B:224:ASN:HD22	1.51	0.59
1:C:207:ILE:CD1	1:C:277:GLU:HB3	2.32	0.59
1:A:210:PHE:HA	1:A:211:PRO:C	2.23	0.58
1:D:164:LEU:HD13	1:D:175:ALA:HB2	1.84	0.58
1:A:17:PHE:HB2	1:A:24:LYS:HG3	1.84	0.58
1:A:179:ASP:HB2	2:A:601:ANP:O2A	2.02	0.58
1:C:146:VAL:O	1:C:149:THR:HB	2.03	0.58
1:C:105:ASN:O	1:D:23:ASN:HB3	2.02	0.58
1:A:17:PHE:O	1:B:102:SER:HA	2.04	0.58
1:D:192:VAL:O	1:D:196:VAL:HG23	2.04	0.58
1:D:214:ILE:O	1:D:214:ILE:HG13	2.03	0.57
1:A:253:ILE:HG21	1:A:275:LEU:HD22	1.87	0.57
1:C:58:TYR:CE1	1:C:260:THR:HG23	2.39	0.57
1:B:263:MET:HG2	1:B:268:LYS:HG3	1.86	0.57
1:C:144:MET:CE	1:C:156:ARG:HD3	2.35	0.57
1:D:95:TYR:N	5:D:337:HOH:O	2.36	0.57
1:C:289:ARG:O	1:C:289:ARG:HG3	2.05	0.56
1:C:78:THR:HG22	1:C:83:ILE:HG13	1.87	0.56
1:A:165:ARG:HD2	1:A:172:TYR:CZ	2.41	0.56
1:C:226:TYR:CE1	1:C:230:THR:HG21	2.41	0.56
1:C:264:SER:HG	1:C:267:HIS:HB2	1.71	0.56
1:B:11:ILE:O	1:B:11:ILE:HG13	2.02	0.56
1:C:123:LEU:HD23	1:C:126:ILE:HD12	1.88	0.56
1:C:151:LEU:HB3	1:C:183:CYS:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:PHE:HB2	5:D:341:HOH:O	2.05	0.56
1:D:52:ASN:HA	1:D:55:PHE:HD1	1.70	0.56
1:C:213:SER:OG	1:C:215:LEU:HB2	2.06	0.56
1:C:206:ARG:O	1:C:211:PRO:HD2	2.05	0.56
1:C:203:LEU:O	1:C:203:LEU:HD23	2.06	0.55
1:B:245:TYR:HB3	1:B:246:PRO:HD3	1.88	0.55
1:C:38:PHE:CD1	1:C:38:PHE:N	2.75	0.55
1:B:23:ASN:C	1:B:24:LYS:HD3	2.27	0.55
1:C:206:ARG:CG	1:C:206:ARG:NH1	2.59	0.55
1:A:133:GLU:HG2	1:A:136:VAL:HG23	1.88	0.55
1:C:57:GLU:O	1:C:61:CYS:HB2	2.07	0.55
1:D:105:ASN:HD21	1:D:114:GLY:H	1.50	0.55
1:D:245:TYR:HB3	1:D:246:PRO:HD3	1.88	0.55
1:C:6:PHE:O	1:C:8:PHE:N	2.40	0.55
1:C:79:TYR:CE2	1:C:80:LYS:HE2	2.41	0.55
1:C:185:TYR:C	1:C:187:GLN:H	2.10	0.54
1:B:150:LEU:O	1:B:278:ARG:HD3	2.06	0.54
1:A:94:GLN:O	1:A:94:GLN:HG3	2.06	0.54
1:B:210:PHE:CE1	1:D:195:LYS:HD3	2.41	0.54
1:A:199:ASN:HB3	1:A:202:GLU:HB2	1.89	0.54
1:A:185:TYR:CE1	1:A:206:ARG:HB3	2.43	0.53
1:C:103:LEU:HD12	1:C:163:PHE:CZ	2.43	0.53
1:B:202:GLU:HG3	1:B:206:ARG:NH1	2.23	0.53
1:C:178:PHE:O	1:C:179:ASP:C	2.46	0.53
1:C:192:VAL:HG13	1:C:195:LYS:HE2	1.90	0.53
1:A:14:LYS:HA	1:B:131:PHE:CE2	2.43	0.53
1:B:79:TYR:CE2	1:B:80:LYS:HD2	2.43	0.53
1:D:126:ILE:HG23	1:D:137:LEU:HD12	1.90	0.53
1:B:137:LEU:HD23	1:B:174:ILE:HD11	1.90	0.53
1:D:83:ILE:HD11	1:D:262:PHE:CG	2.44	0.53
1:C:286:ALA:N	5:C:326:HOH:O	2.41	0.53
1:D:67:LEU:O	1:D:247:ARG:HD2	2.08	0.53
1:C:273:THR:O	1:C:277:GLU:HG2	2.08	0.53
1:C:36:VAL:HG12	1:C:84:VAL:HG21	1.90	0.53
1:D:273:THR:O	1:D:277:GLU:HG2	2.08	0.53
1:C:27:LEU:C	1:C:27:LEU:HD12	2.30	0.53
1:C:240:ALA:O	1:C:244:ILE:HG12	2.09	0.53
1:B:245:TYR:HA	1:B:248:ILE:HD12	1.90	0.52
1:A:62:HIS:CD2	1:A:74:THR:HG1	2.27	0.52
1:C:210:PHE:CB	1:C:211:PRO:CD	2.82	0.52
1:D:277:GLU:OE1	1:D:281:LYS:HE3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:LEU:HD21	1:C:273:THR:OG1	2.09	0.52
1:C:29:TYR:O	1:C:32:GLU:HB2	2.10	0.52
1:C:156:ARG:HG3	1:C:156:ARG:O	2.09	0.52
1:C:287:HIS:O	1:C:290:ALA:HB3	2.10	0.52
1:D:61:CYS:O	1:D:71:VAL:HG11	2.09	0.52
1:B:202:GLU:HG3	1:B:206:ARG:HH12	1.74	0.52
1:D:58:TYR:O	1:D:62:HIS:HD2	1.92	0.52
1:B:18:GLY:O	1:B:24:LYS:CE	2.58	0.52
1:B:58:TYR:CG	1:B:76:LEU:HD22	2.45	0.52
1:B:264:SER:OG	1:B:266:ILE:HG23	2.10	0.52
1:D:165:ARG:NH1	1:D:166:ALA:O	2.43	0.52
1:D:187:GLN:H	1:D:187:GLN:CD	2.14	0.51
1:B:93:HIS:O	1:B:94:GLN:HB2	2.10	0.51
1:D:18:GLY:O	1:D:24:LYS:HE3	2.11	0.51
1:C:185:TYR:C	1:C:187:GLN:N	2.64	0.51
1:C:192:VAL:HG22	1:C:195:LYS:NZ	2.26	0.51
1:D:9:CYS:HB3	1:D:28:PHE:O	2.11	0.51
1:B:126:ILE:O	1:B:129:GLN:HG3	2.11	0.51
1:B:287:HIS:CE1	1:B:291:ILE:HD12	2.44	0.51
1:C:140:PHE:HE1	1:C:177:ILE:HD11	1.76	0.51
1:B:7:THR:HG23	1:B:80:LYS:HG3	1.93	0.51
1:B:17:PHE:HB2	1:B:24:LYS:HG3	1.92	0.51
1:C:191:VAL:O	1:C:195:LYS:HB2	2.10	0.51
1:A:14:LYS:HA	1:B:131:PHE:HE2	1.76	0.51
1:A:23:ASN:HB3	1:B:105:ASN:O	2.10	0.50
1:A:207:ILE:HD13	1:A:278:ARG:HG2	1.93	0.50
1:D:17:PHE:HB2	1:D:24:LYS:HG3	1.94	0.50
1:C:192:VAL:HA	1:C:195:LYS:CB	2.40	0.50
1:C:164:LEU:HD22	1:C:175:ALA:HA	1.93	0.50
1:D:74:THR:O	1:D:75:LEU:HD23	2.12	0.50
1:A:171:GLU:HB2	1:B:14:LYS:NZ	2.27	0.50
1:D:105:ASN:HD22	1:D:114:GLY:H	1.57	0.50
1:A:179:ASP:OD2	2:A:601:ANP:O1G	2.29	0.50
1:A:217:ASP:OD1	1:A:219:ASN:O	2.29	0.50
1:C:190:ASP:HA	1:C:193:CYS:HB2	1.93	0.50
1:A:103:LEU:HD12	1:A:163:PHE:CE2	2.47	0.50
1:A:287:HIS:CE1	1:A:291:ILE:HD11	2.47	0.50
1:A:144:MET:SD	1:A:156:ARG:HD3	2.52	0.49
1:C:38:PHE:H	1:C:38:PHE:HD1	1.60	0.49
1:C:228:PHE:O	1:C:232:THR:HG22	2.12	0.49
1:D:144:MET:CE	1:D:156:ARG:HD3	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ILE:HG13	1:D:12:ASN:N	2.26	0.49
1:A:217:ASP:O	1:A:219:ASN:O	2.30	0.49
4:C:500:ADP:H8	4:C:500:ADP:C5'	2.01	0.49
1:D:105:ASN:ND2	1:D:114:GLY:N	2.52	0.49
1:B:106:THR:O	1:B:108:ILE:HG23	2.12	0.49
1:C:62:HIS:HB3	1:C:256:ILE:HD13	1.95	0.49
1:A:126:ILE:HG23	1:A:137:LEU:HD12	1.94	0.49
1:A:62:HIS:CD2	1:A:74:THR:OG1	2.66	0.49
1:C:22:GLY:N	1:C:40:PRO:HG3	2.28	0.49
1:C:115:LYS:O	1:C:115:LYS:HG2	2.12	0.49
1:D:230:THR:HG22	1:D:286:ALA:HA	1.95	0.49
1:C:22:GLY:CA	1:C:40:PRO:HG3	2.43	0.48
1:C:52:ASN:HA	1:C:55:PHE:CD1	2.47	0.48
1:C:150:LEU:O	1:C:278:ARG:NE	2.40	0.48
1:D:64:VAL:HG11	1:D:71:VAL:HB	1.94	0.48
1:D:287:HIS:O	1:D:290:ALA:HB3	2.13	0.48
1:A:254:HIS:HE1	1:A:276:ASP:OD1	1.97	0.48
1:A:34:TYR:CE1	1:A:75:LEU:HD12	2.49	0.48
1:B:111:GLU:N	5:B:333:HOH:O	2.45	0.48
1:C:56:SER:O	1:C:60:ALA:HB3	2.13	0.48
1:A:248:ILE:HG21	1:A:279:LYS:CE	2.44	0.48
1:C:194:GLN:O	1:C:198:SER:OG	2.25	0.48
1:A:254:HIS:CE1	1:A:276:ASP:OD1	2.67	0.48
1:C:193:CYS:HB3	1:C:266:ILE:HG13	1.96	0.48
1:C:208:TYR:O	1:C:224:ASN:ND2	2.47	0.48
1:B:76:LEU:HD12	1:B:76:LEU:HA	1.74	0.48
1:D:105:ASN:HD22	1:D:105:ASN:HA	1.51	0.48
1:A:67:LEU:O	1:A:247:ARG:HD2	2.14	0.48
1:D:196:VAL:HG13	1:D:203:LEU:HA	1.95	0.48
1:A:185:TYR:HE1	1:A:206:ARG:HB3	1.78	0.47
1:C:261:PRO:HB2	1:C:262:PHE:CD2	2.49	0.47
1:C:17:PHE:CE1	1:C:35:MET:HB2	2.50	0.47
1:C:97:LEU:HD12	1:C:97:LEU:C	2.34	0.47
1:C:165:ARG:O	1:C:165:ARG:HG3	2.13	0.47
1:C:165:ARG:NH2	1:C:171:GLU:OE2	2.47	0.47
1:D:261:PRO:HB2	1:D:262:PHE:CD2	2.50	0.47
2:B:600:ANP:H8	2:B:600:ANP:O5'	2.14	0.47
1:C:264:SER:HG	1:C:267:HIS:H	1.56	0.47
1:D:29:TYR:HB3	1:D:34:TYR:CE2	2.50	0.47
1:B:105:ASN:HD21	1:B:114:GLY:H	1.58	0.47
1:C:277:GLU:O	1:C:281:LYS:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ARG:O	1:C:292:GLU:HB3	2.13	0.47
1:D:60:ALA:CB	1:D:180:CYS:HB3	2.44	0.47
1:C:91:THR:HB	1:C:95:TYR:O	2.14	0.47
1:C:117:THR:HB	1:C:215:LEU:HD23	1.96	0.47
1:D:76:LEU:HD12	1:D:76:LEU:HA	1.79	0.47
1:D:257:ILE:O	1:D:268:LYS:HD3	2.15	0.47
1:A:110:LEU:C	1:A:112:LYS:H	2.19	0.47
1:B:21:ASN:ND2	2:B:600:ANP:O1G	2.47	0.47
1:D:163:PHE:N	1:D:163:PHE:CD2	2.83	0.47
1:A:19:GLY:CA	2:A:601:ANP:HNB1	2.28	0.47
1:A:100:PHE:CE2	1:A:122:VAL:HG13	2.50	0.47
1:A:118:ASN:O	1:A:122:VAL:HG23	2.15	0.47
1:A:245:TYR:N	1:A:246:PRO:HD2	2.30	0.47
1:A:248:ILE:HG21	1:A:279:LYS:HE2	1.97	0.47
1:C:23:ASN:CB	1:D:108:ILE:HG22	2.45	0.47
1:C:28:PHE:CE1	1:C:33:LEU:HD13	2.50	0.47
1:C:217:ASP:OD2	1:C:218:ASP:N	2.48	0.47
1:B:27:LEU:O	1:B:27:LEU:CD1	2.63	0.46
1:B:105:ASN:HD22	1:B:114:GLY:H	1.61	0.46
1:C:258:ASP:O	1:C:268:LYS:NZ	2.34	0.46
1:D:144:MET:SD	1:D:156:ARG:HD3	2.55	0.46
1:A:103:LEU:HG	1:A:131:PHE:CD1	2.51	0.46
1:A:103:LEU:HD12	1:A:163:PHE:CZ	2.50	0.46
1:C:108:ILE:HG13	1:C:109:GLU:N	2.29	0.46
1:C:140:PHE:HE1	1:C:177:ILE:CD1	2.29	0.46
1:A:217:ASP:OD2	1:A:221:LYS:CE	2.64	0.46
1:C:280:SER:O	1:C:284:ASP:HB2	2.16	0.46
1:B:206:ARG:HA	1:B:210:PHE:O	2.16	0.46
1:C:133:GLU:HG2	1:C:136:VAL:HG23	1.97	0.46
1:B:4:ILE:HG22	1:B:5:ASP:N	2.30	0.46
1:C:90:PHE:CE1	4:C:500:ADP:N6	2.83	0.46
1:C:140:PHE:CE1	1:C:177:ILE:HD11	2.50	0.46
1:B:260:THR:HG21	1:B:263:MET:HE3	1.97	0.46
1:D:85:VAL:HG13	1:D:85:VAL:O	2.16	0.46
1:B:12:ASN:HA	1:B:13:PRO:HD3	1.79	0.46
1:C:92:THR:H	1:C:95:TYR:HB2	1.80	0.46
1:C:291:ILE:H	1:C:291:ILE:HG13	1.58	0.46
1:D:64:VAL:HG12	1:D:71:VAL:HB	1.96	0.46
1:D:73:GLU:HB2	1:D:88:LYS:HB2	1.98	0.46
1:A:17:PHE:CE2	1:A:35:MET:HG3	2.51	0.45
1:A:131:PHE:O	1:A:132:ILE:HD13	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LYS:HE2	1:A:216:LYS:HB2	1.57	0.45
1:B:58:TYR:CE2	1:B:62:HIS:NE2	2.84	0.45
1:C:146:VAL:HG11	1:C:244:ILE:HG13	1.98	0.45
1:D:206:ARG:HA	1:D:210:PHE:O	2.16	0.45
1:D:260:THR:HA	1:D:261:PRO:HD3	1.65	0.45
1:A:140:PHE:O	1:A:143:ASP:HB2	2.16	0.45
1:A:229:LEU:HA	1:A:229:LEU:HD12	1.73	0.45
1:A:29:TYR:O	1:A:30:ASN:HB2	2.16	0.45
1:A:148:ASP:OD2	1:A:156:ARG:HD2	2.16	0.45
1:B:149:THR:HG21	1:B:229:LEU:HD22	1.97	0.45
1:D:189:ASP:OD1	1:D:189:ASP:C	2.54	0.45
1:A:99:ASP:HA	1:A:162:GLY:HA3	1.97	0.45
1:A:105:ASN:ND2	1:A:114:GLY:H	2.14	0.45
1:B:6:PHE:HE1	1:B:77:GLY:CA	2.20	0.45
1:B:133:GLU:OE1	1:B:134:PRO:HD2	2.17	0.45
1:C:36:VAL:HG12	1:C:84:VAL:CG2	2.46	0.45
1:D:262:PHE:CD2	1:D:262:PHE:N	2.85	0.45
1:B:131:PHE:O	1:B:132:ILE:HD13	2.16	0.45
1:C:4:ILE:HG22	1:C:5:ASP:H	1.79	0.45
1:C:58:TYR:HB2	1:C:76:LEU:HD13	1.98	0.45
1:D:261:PRO:HB2	1:D:262:PHE:CE2	2.51	0.45
1:C:17:PHE:O	1:D:102:SER:HA	2.16	0.45
1:C:235:LYS:O	1:C:239:ASP:HB2	2.17	0.45
1:C:105:ASN:ND2	1:D:23:ASN:HA	2.31	0.45
1:D:27:LEU:HD12	1:D:27:LEU:C	2.36	0.45
1:A:131:PHE:CE2	1:B:14:LYS:HA	2.52	0.45
1:C:4:ILE:CG2	1:C:5:ASP:N	2.77	0.45
1:C:257:ILE:HD12	1:C:272:HIS:CD2	2.52	0.45
1:A:58:TYR:O	1:A:62:HIS:HD2	1.98	0.44
1:A:187:GLN:H	1:A:187:GLN:CD	2.19	0.44
1:C:12:ASN:HB3	1:C:26:SER:O	2.17	0.44
1:D:90:PHE:CE1	2:D:602:ANP:N6	2.85	0.44
1:A:17:PHE:CD2	1:A:35:MET:HG3	2.52	0.44
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.58	0.44
1:C:6:PHE:HE1	1:C:77:GLY:CA	2.25	0.44
1:C:129:GLN:OE1	1:C:131:PHE:N	2.49	0.44
1:A:217:ASP:OD2	1:A:221:LYS:HE2	2.17	0.44
1:C:80:LYS:O	1:C:81:ASN:HB2	2.17	0.44
1:C:245:TYR:HB3	1:C:246:PRO:HD3	1.99	0.44
1:D:294:SER:HA	1:D:295:LEU:HA	1.66	0.44
1:D:100:PHE:CD1	1:D:161:TRP:CH2	3.05	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ILE:HD13	1:C:29:TYR:OH	2.16	0.44
1:D:145:PHE:O	1:D:149:THR:N	2.49	0.44
1:D:234:ASN:OD1	1:D:236:ASP:HB2	2.17	0.44
2:B:600:ANP:O2A	2:B:600:ANP:H3'	2.17	0.44
1:C:257:ILE:HD11	1:C:275:LEU:HD12	2.00	0.44
1:D:27:LEU:C	1:D:27:LEU:CD1	2.86	0.44
1:D:40:PRO:HB2	1:D:42:PRO:HD2	1.99	0.44
1:A:58:TYR:CE2	1:A:62:HIS:NE2	2.86	0.43
1:C:249:ASP:OD1	1:C:249:ASP:C	2.57	0.43
1:D:124:TYR:C	1:D:124:TYR:CD2	2.92	0.43
1:A:29:TYR:O	1:A:30:ASN:CB	2.62	0.43
1:C:149:THR:HG21	1:C:229:LEU:HD22	1.99	0.43
1:D:101:LEU:C	1:D:101:LEU:HD23	2.38	0.43
1:D:118:ASN:O	1:D:119:LEU:C	2.56	0.43
1:D:122:VAL:O	1:D:126:ILE:HG13	2.18	0.43
1:C:15:LYS:NZ	1:C:91:THR:O	2.50	0.43
1:C:122:VAL:O	1:C:125:ALA:HB3	2.18	0.43
1:D:161:TRP:CD1	1:D:161:TRP:N	2.87	0.43
1:A:253:ILE:CG2	1:A:275:LEU:HD22	2.49	0.43
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.66	0.43
1:B:27:LEU:CD1	1:B:27:LEU:C	2.86	0.43
1:A:15:LYS:HG3	1:A:16:GLY:N	2.33	0.43
1:C:143:ASP:OD1	1:C:244:ILE:HD11	2.17	0.43
1:D:12:ASN:HA	1:D:13:PRO:HD3	1.64	0.43
1:D:157:HIS:CD2	1:D:157:HIS:H	2.36	0.43
1:C:58:TYR:HE1	1:C:260:THR:HG23	1.82	0.43
1:D:124:TYR:CZ	1:D:128:ASN:OD1	2.72	0.43
1:D:274:MET:O	1:D:278:ARG:HG3	2.18	0.43
1:B:107:MET:HG3	1:B:125:ALA:HB2	2.00	0.43
1:A:113:SER:HA	1:B:23:ASN:HD21	1.84	0.43
1:C:200:ILE:O	1:C:200:ILE:HG23	2.18	0.43
1:D:109:GLU:H	1:D:109:GLU:HG3	1.35	0.43
1:C:52:ASN:HA	1:C:55:PHE:HD1	1.84	0.42
1:C:74:THR:O	1:C:75:LEU:HD23	2.18	0.42
1:C:260:THR:HA	1:C:261:PRO:HD3	1.83	0.42
1:B:126:ILE:HG12	1:B:137:LEU:HD13	2.02	0.42
1:B:4:ILE:CG2	1:B:5:ASP:N	2.82	0.42
1:B:66:SER:HB2	1:B:252:LYS:CE	2.47	0.42
1:C:33:LEU:HD12	1:C:33:LEU:HA	1.55	0.42
1:C:153:ASN:OD1	1:C:182:SER:HB2	2.19	0.42
1:D:16:GLY:C	1:D:17:PHE:CD2	2.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:THR:HG22	1:D:286:ALA:CA	2.50	0.42
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.84	0.42
1:C:245:TYR:HB3	1:C:246:PRO:CD	2.49	0.42
1:D:142:TRP:CD1	1:D:236:ASP:HB3	2.54	0.42
1:D:241:LEU:HA	1:D:241:LEU:HD23	1.79	0.42
1:D:33:LEU:HD12	1:D:33:LEU:HA	1.79	0.42
1:B:41:LYS:HA	1:B:42:PRO:HD3	1.62	0.42
1:D:202:GLU:OE2	1:D:202:GLU:HA	2.20	0.42
1:A:133:GLU:HA	1:A:134:PRO:HD3	1.86	0.42
1:B:18:GLY:O	1:B:24:LYS:HE2	2.20	0.42
1:B:263:MET:HG3	1:B:267:HIS:HB3	2.02	0.42
1:C:197:LEU:HD23	1:C:197:LEU:HA	1.88	0.42
1:D:126:ILE:O	1:D:129:GLN:HG3	2.19	0.42
1:D:4:ILE:HG21	1:D:6:PHE:CE2	2.55	0.41
1:C:18:GLY:O	1:C:24:LYS:CE	2.66	0.41
1:A:19:GLY:HA3	2:A:601:ANP:HNB1	1.86	0.41
1:D:230:THR:O	1:D:231:GLN:HG3	2.21	0.41
1:A:110:LEU:HD21	1:A:124:TYR:CD2	2.55	0.41
1:D:163:PHE:HB3	1:D:173:GLN:O	2.20	0.41
1:B:100:PHE:HD2	1:B:158:ASN:ND2	2.19	0.41
1:A:7:THR:OG1	1:A:79:TYR:HA	2.21	0.41
1:C:145:PHE:O	1:C:148:ASP:HB2	2.20	0.41
1:A:27:LEU:C	1:A:27:LEU:CD1	2.85	0.41
1:A:125:ALA:O	1:A:129:GLN:CG	2.68	0.41
1:B:64:VAL:O	1:B:67:LEU:HB2	2.21	0.41
1:C:84:VAL:HG22	1:C:85:VAL:N	2.35	0.41
1:C:254:HIS:HD2	1:C:272:HIS:CG	2.36	0.41
1:C:257:ILE:C	1:C:260:THR:HG1	2.01	0.41
1:D:40:PRO:HB2	1:D:42:PRO:CG	2.51	0.41
1:D:132:ILE:O	1:D:134:PRO:HD3	2.21	0.41
1:C:131:PHE:CE1	1:C:172:TYR:CZ	3.09	0.41
1:C:257:ILE:C	1:C:260:THR:OG1	2.55	0.40
1:D:27:LEU:HG	1:D:36:VAL:CG2	2.51	0.40
1:A:97:LEU:HD12	1:A:163:PHE:O	2.20	0.40
1:C:226:TYR:O	1:C:230:THR:HG23	2.21	0.40
1:B:107:MET:HG3	1:B:125:ALA:CB	2.52	0.40
1:C:6:PHE:O	1:C:7:THR:C	2.60	0.40
1:C:26:SER:HA	1:C:34:TYR:O	2.21	0.40
1:C:280:SER:HA	1:C:284:ASP:CG	2.41	0.40
1:B:64:VAL:HG12	1:B:71:VAL:HG22	2.02	0.40
1:B:200:ILE:HD12	1:B:200:ILE:HA	1.83	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:HD23	1:B:275:LEU:HA	1.86	0.40
1:C:205:ALA:O	1:C:207:ILE:N	2.55	0.40
1:D:62:HIS:HB3	1:D:256:ILE:HD13	2.03	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	275/325 (85%)	250 (91%)	25 (9%)	0	100	100
1	B	275/325 (85%)	252 (92%)	23 (8%)	0	100	100
1	C	271/325 (83%)	236 (87%)	33 (12%)	2 (1%)	19	49
1	D	271/325 (83%)	247 (91%)	21 (8%)	3 (1%)	12	37
All	All	1092/1300 (84%)	985 (90%)	102 (9%)	5 (0%)	25	56

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	7	THR
1	D	293	LEU
1	C	248	ILE
1	D	39	PRO
1	D	285	VAL

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	257/299 (86%)	229 (89%)	28 (11%)	5	17
1	B	257/299 (86%)	230 (90%)	27 (10%)	5	18
1	C	255/299 (85%)	222 (87%)	33 (13%)	3	11
1	D	255/299 (85%)	228 (89%)	27 (11%)	5	18
All	All	1024/1196 (86%)	909 (89%)	115 (11%)	5	16

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	15	LYS
1	A	24	LYS
1	A	25	ILE
1	A	31	ASN
1	A	32	GLU
1	A	76	LEU
1	A	83	ILE
1	A	84	VAL
1	A	103	LEU
1	A	105	ASN
1	A	110	LEU
1	A	112	LYS
1	A	133	GLU
1	A	137	LEU
1	A	156	ARG
1	A	164	LEU
1	A	180	CYS
1	A	187	GLN
1	A	202	GLU
1	A	220	ASP
1	A	221	LYS
1	A	241	LEU
1	A	260	THR
1	A	264	SER
1	A	275	LEU
1	A	292	GLU
1	A	294	SER
1	B	11	ILE
1	B	24	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	25	ILE
1	B	27	LEU
1	B	31	ASN
1	B	71	VAL
1	B	76	LEU
1	B	78	THR
1	B	84	VAL
1	B	96	GLU
1	B	103	LEU
1	B	108	ILE
1	B	113	SER
1	B	118	ASN
1	B	137	LEU
1	B	156	ARG
1	B	164	LEU
1	B	187	GLN
1	B	198	SER
1	B	220	ASP
1	B	231	GLN
1	B	241	LEU
1	B	247	ARG
1	B	266	ILE
1	B	280	SER
1	B	291	ILE
1	B	295	LEU
1	C	14	LYS
1	C	24	LYS
1	C	33	LEU
1	C	41	LYS
1	C	66	SER
1	C	76	LEU
1	C	97	LEU
1	C	101	LEU
1	C	103	LEU
1	C	105	ASN
1	C	110	LEU
1	C	133	GLU
1	C	150	LEU
1	C	156	ARG
1	C	164	LEU
1	C	165	ARG
1	C	184	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	187	GLN
1	C	194	GLN
1	C	198	SER
1	C	201	ASP
1	C	206	ARG
1	C	209	ASN
1	C	210	PHE
1	C	227	ASP
1	C	232	THR
1	C	239	ASP
1	C	241	LEU
1	C	260	THR
1	C	263	MET
1	C	264	SER
1	C	267	HIS
1	C	289	ARG
1	D	11	ILE
1	D	24	LYS
1	D	27	LEU
1	D	33	LEU
1	D	67	LEU
1	D	76	LEU
1	D	82	LYS
1	D	83	ILE
1	D	84	VAL
1	D	103	LEU
1	D	105	ASN
1	D	108	ILE
1	D	110	LEU
1	D	112	LYS
1	D	113	SER
1	D	137	LEU
1	D	156	ARG
1	D	163	PHE
1	D	164	LEU
1	D	187	GLN
1	D	202	GLU
1	D	241	LEU
1	D	251	ASN
1	D	266	ILE
1	D	292	GLU
1	D	294	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	295	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	105	ASN
1	A	158	ASN
1	A	212	GLN
1	A	254	HIS
1	A	267	HIS
1	A	272	HIS
1	A	287	HIS
1	B	21	ASN
1	B	31	ASN
1	B	94	GLN
1	B	105	ASN
1	B	158	ASN
1	B	187	GLN
1	B	194	GLN
1	B	212	GLN
1	B	254	HIS
1	B	267	HIS
1	B	272	HIS
1	B	287	HIS
1	C	105	ASN
1	C	128	ASN
1	C	158	ASN
1	C	187	GLN
1	C	209	ASN
1	C	254	HIS
1	C	267	HIS
1	C	272	HIS
1	D	23	ASN
1	D	31	ASN
1	D	62	HIS
1	D	105	ASN
1	D	120	ASN
1	D	128	ASN
1	D	157	HIS
1	D	158	ASN
1	D	219	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	254	HIS
1	D	272	HIS
1	D	287	HIS

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](#)

Of 11 ligands modelled in this entry, 7 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADP	C	500	3	24,29,29	0.93	0	29,45,45	1.50	5 (17%)
2	ANP	A	601	3	29,33,33	1.86	7 (24%)	31,52,52	1.54	6 (19%)
2	ANP	D	602	3	29,33,33	1.75	6 (20%)	31,52,52	1.71	6 (19%)
2	ANP	B	600	3	29,33,33	1.53	3 (10%)	31,52,52	1.55	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	C	500	3	-	3/12/32/32	0/3/3/3
2	ANP	A	601	3	-	4/14/38/38	0/3/3/3
2	ANP	D	602	3	-	3/14/38/38	0/3/3/3
2	ANP	B	600	3	-	2/14/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	ANP	PB-O3A	4.86	1.65	1.59
2	B	600	ANP	PG-O2G	4.62	1.69	1.56
2	A	601	ANP	PG-O3G	4.33	1.68	1.56
2	A	601	ANP	PB-O3A	4.30	1.64	1.59
2	A	601	ANP	O4'-C1'	4.22	1.46	1.40
2	D	602	ANP	O4'-C1'	3.99	1.46	1.40
2	B	600	ANP	PB-O3A	3.44	1.63	1.59
2	D	602	ANP	PB-O2B	-3.37	1.47	1.56
2	A	601	ANP	PB-O2B	-3.25	1.48	1.56
2	A	601	ANP	PG-O2G	2.78	1.64	1.56
2	B	600	ANP	PB-O2B	-2.64	1.49	1.56
2	A	601	ANP	PA-O3A	2.45	1.62	1.59
2	D	602	ANP	PG-O3G	2.38	1.63	1.56
2	D	602	ANP	PG-O2G	2.37	1.63	1.56
2	A	601	ANP	PA-O2A	-2.25	1.44	1.55
2	D	602	ANP	PA-O3A	2.11	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	ANP	N3-C2-N1	-4.81	122.15	128.67
2	B	600	ANP	N3-C2-N1	-4.59	122.44	128.67
2	A	601	ANP	N3-C2-N1	-4.55	122.49	128.67
2	B	600	ANP	O2B-PB-O1B	4.27	119.04	109.87
2	A	601	ANP	O2B-PB-O1B	4.13	118.73	109.87
2	D	602	ANP	O2B-PB-O1B	3.77	117.95	109.87
4	C	500	ADP	N3-C2-N1	-3.47	123.97	128.67
2	D	602	ANP	O4'-C1'-N9	-3.05	104.70	108.75
4	C	500	ADP	C5'-C4'-C3'	-2.89	104.81	115.21
2	D	602	ANP	O2A-PA-O3A	2.87	115.03	107.27
4	C	500	ADP	PA-O5'-C5'	-2.67	106.04	121.35
2	A	601	ANP	C4-C5-N7	-2.31	106.90	109.34
2	B	600	ANP	O4'-C4'-C5'	-2.22	102.24	109.33
2	D	602	ANP	C4-C5-N7	-2.21	107.01	109.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	ANP	O4'-C1'-N9	2.18	111.63	108.75
4	C	500	ADP	O2B-PB-O3A	-2.17	97.35	104.64
2	D	602	ANP	O3A-PA-O1A	-2.12	104.34	110.70
2	A	601	ANP	O2A-PA-O3A	2.10	112.94	107.27
4	C	500	ADP	C4-C5-N7	-2.07	107.15	109.34
2	A	601	ANP	O1G-PG-N3B	2.06	114.80	111.77

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	ANP	PA-O3A-PB-O1B
2	A	601	ANP	PA-O3A-PB-O2B
2	A	601	ANP	C5'-O5'-PA-O1A
2	B	600	ANP	PG-N3B-PB-O1B
2	B	600	ANP	PG-N3B-PB-O3A
2	D	602	ANP	PB-N3B-PG-O1G
2	D	602	ANP	PG-N3B-PB-O1B
4	C	500	ADP	C5'-O5'-PA-O1A
4	C	500	ADP	C5'-O5'-PA-O3A
4	C	500	ADP	PB-O3A-PA-O1A
2	A	601	ANP	O4'-C4'-C5'-O5'
2	D	602	ANP	PB-O3A-PA-O2A

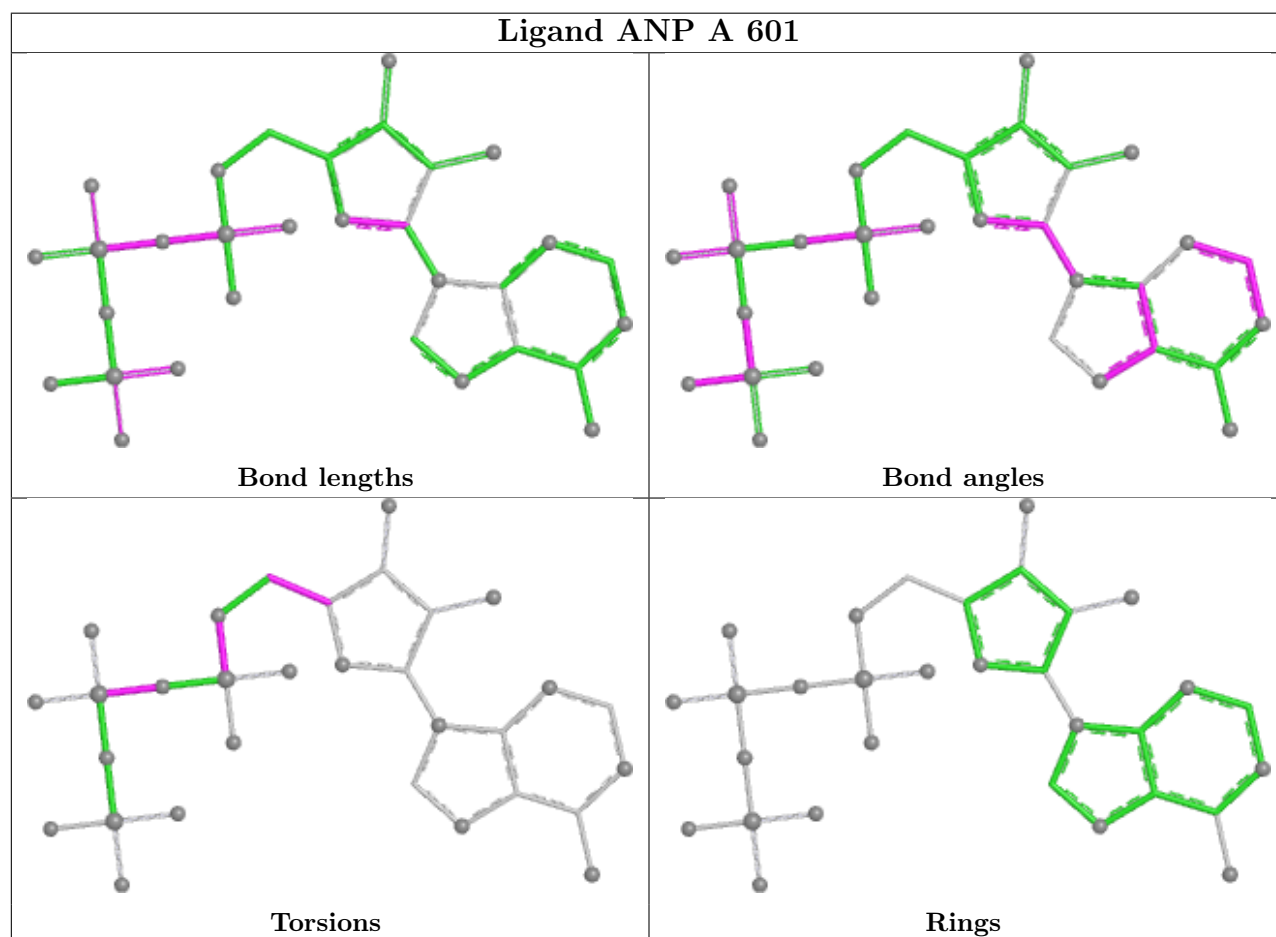
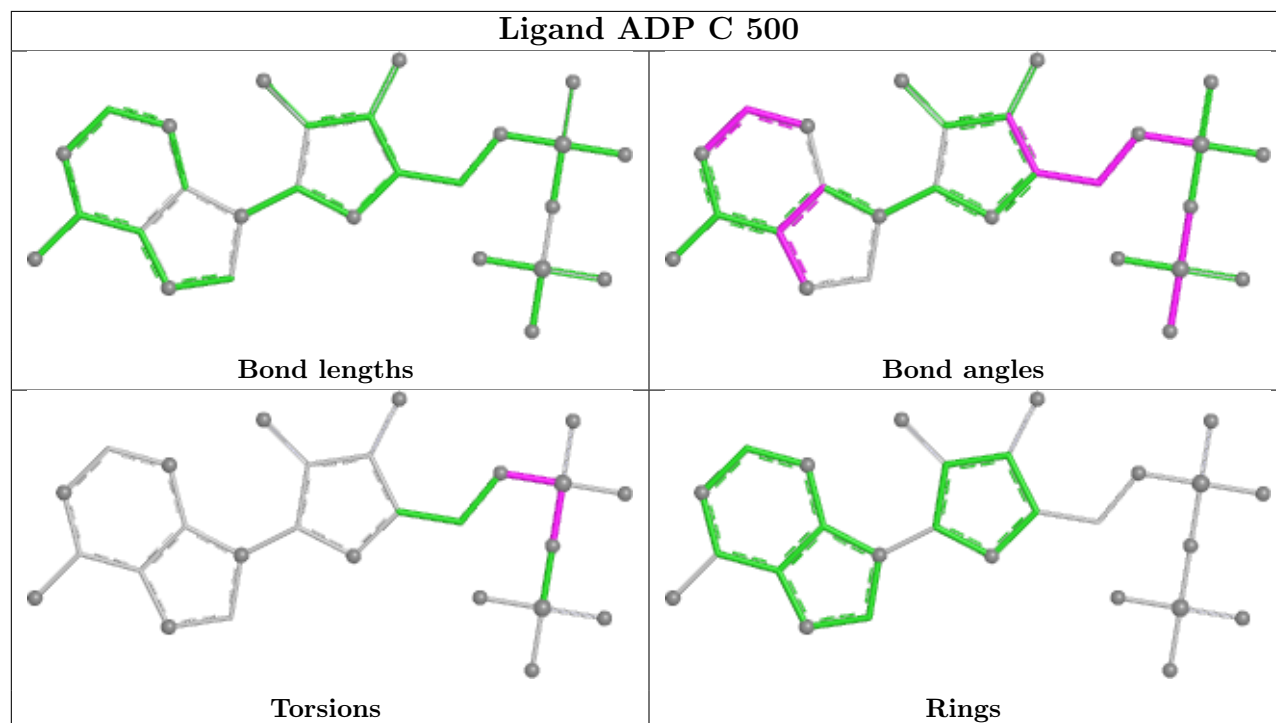
There are no ring outliers.

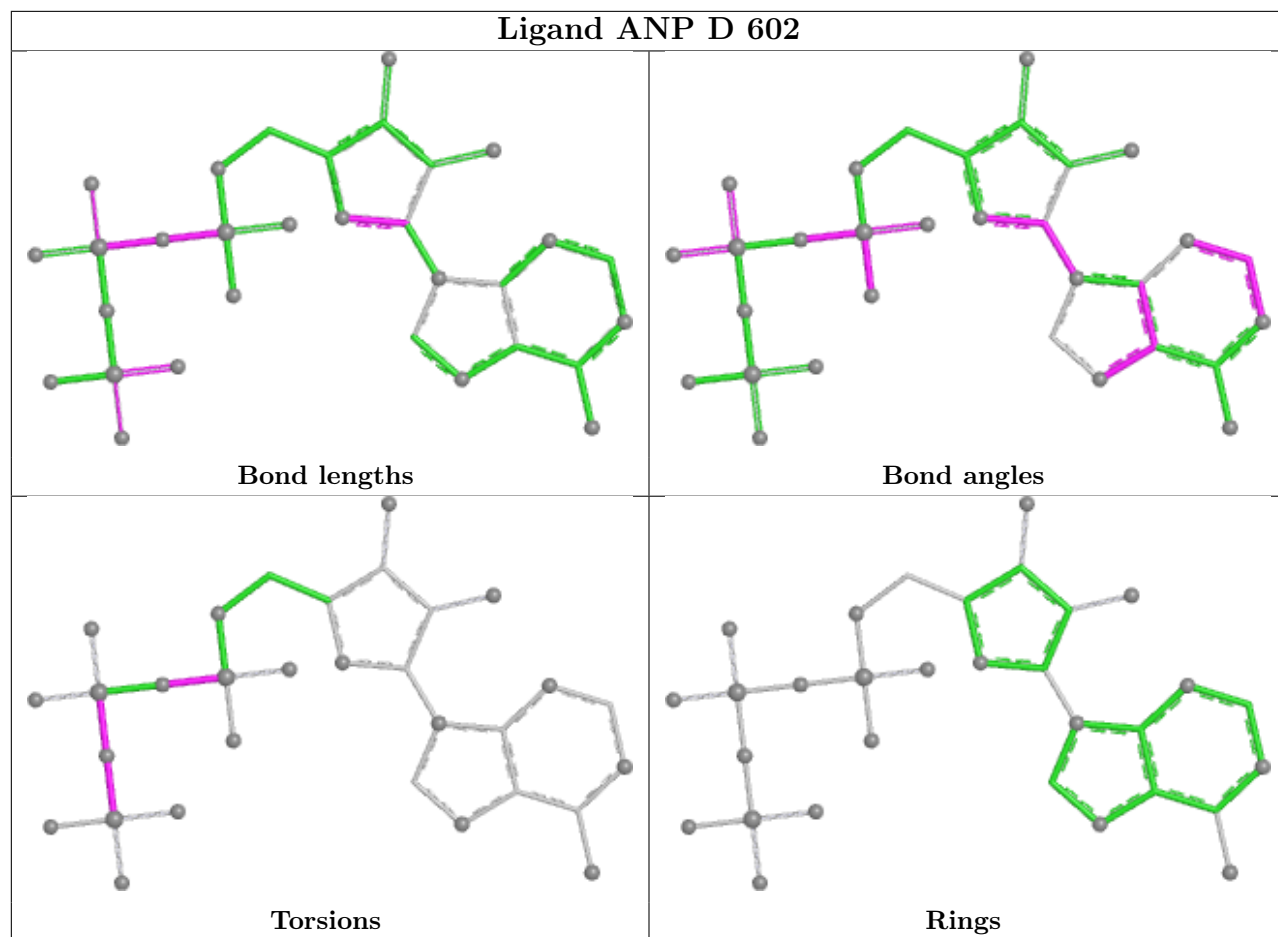
4 monomers are involved in 14 short contacts:

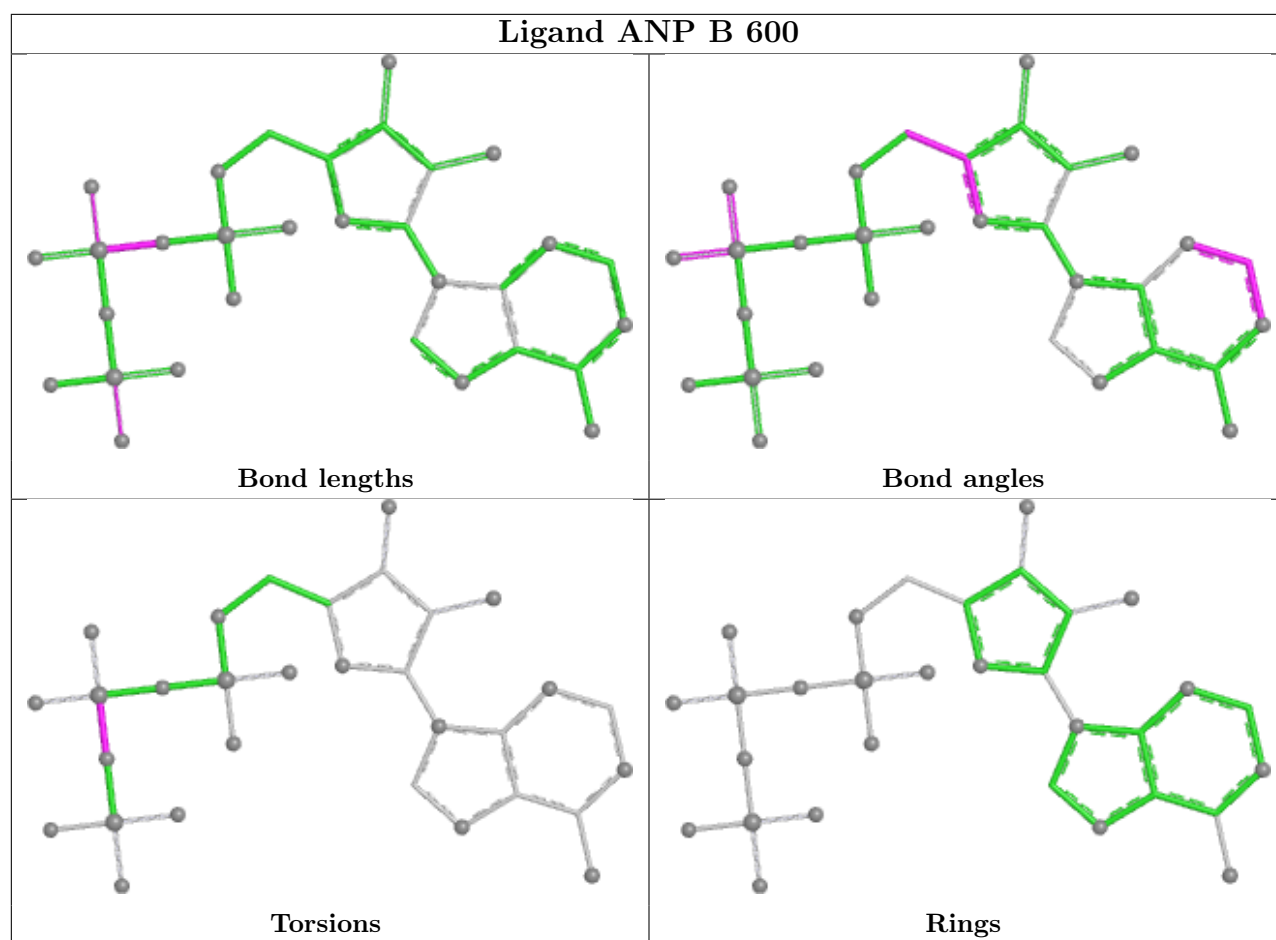
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	500	ADP	5	0
2	A	601	ANP	4	0
2	D	602	ANP	2	0
2	B	600	ANP	3	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	281/325 (86%)	-0.76	0 100 100	40, 52, 76, 110	0
1	B	281/325 (86%)	-0.84	1 (0%) 89 86	39, 52, 80, 109	0
1	C	279/325 (85%)	-0.45	1 (0%) 89 86	50, 78, 113, 122	0
1	D	279/325 (85%)	-0.79	0 100 100	41, 57, 74, 97	0
All	All	1120/1300 (86%)	-0.71	2 (0%) 92 91	39, 58, 101, 122	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	210	PHE	2.4
1	B	295	LEU	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](#)

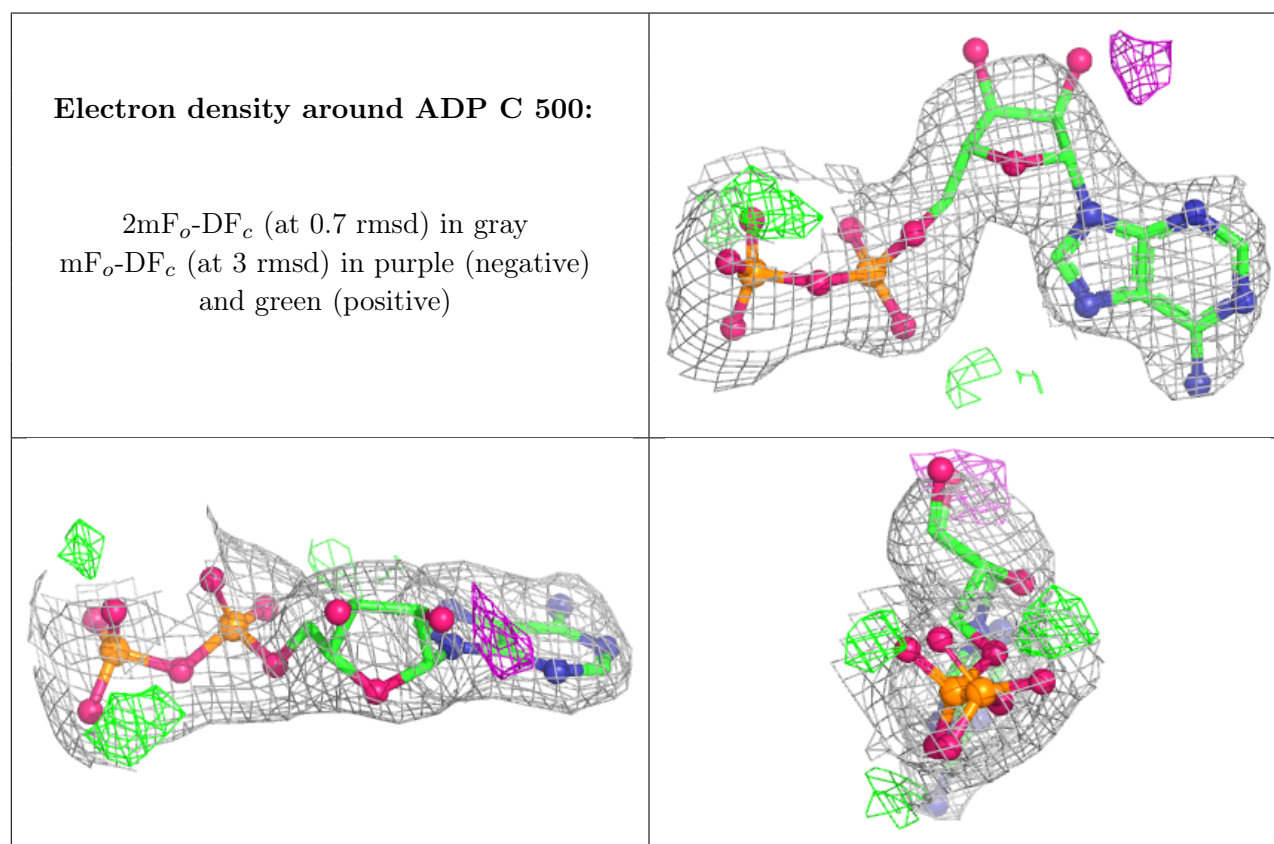
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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.

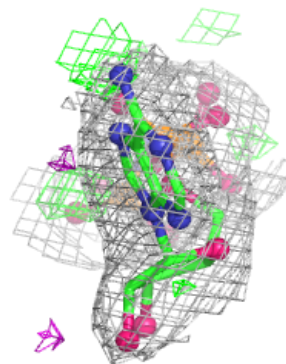
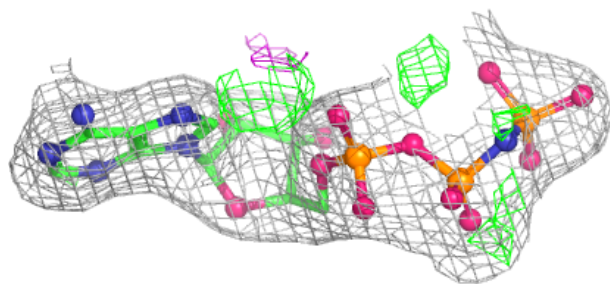
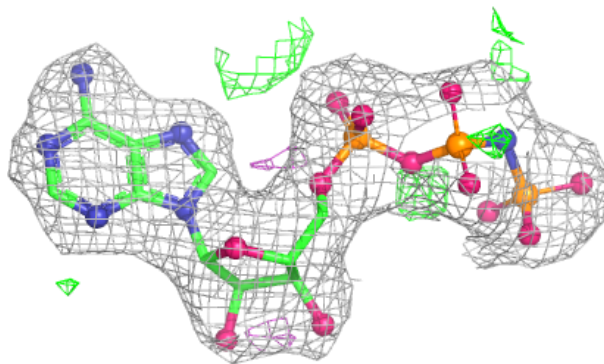
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	B	401	1/1	0.79	0.10	60,60,60,60	0
3	MG	D	403	1/1	0.86	0.21	68,68,68,68	0
4	ADP	C	500	27/27	0.92	0.08	55,64,75,78	0
3	MG	D	406	1/1	0.94	0.12	51,51,51,51	0
3	MG	B	404	1/1	0.95	0.08	48,48,48,48	0
3	MG	A	402	1/1	0.95	0.05	61,61,61,61	0
2	ANP	D	602	31/31	0.96	0.07	40,46,64,68	0
2	ANP	A	601	31/31	0.97	0.06	37,46,56,71	0
2	ANP	B	600	31/31	0.97	0.06	34,42,54,67	0
3	MG	C	400	1/1	0.97	0.09	57,57,57,57	0
3	MG	A	405	1/1	0.98	0.05	38,38,38,38	0

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

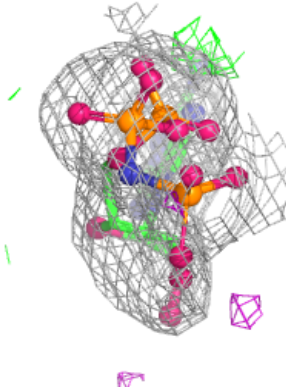
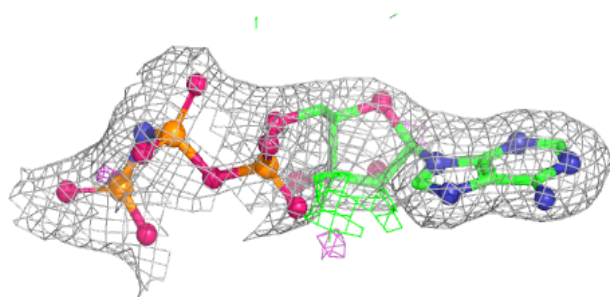
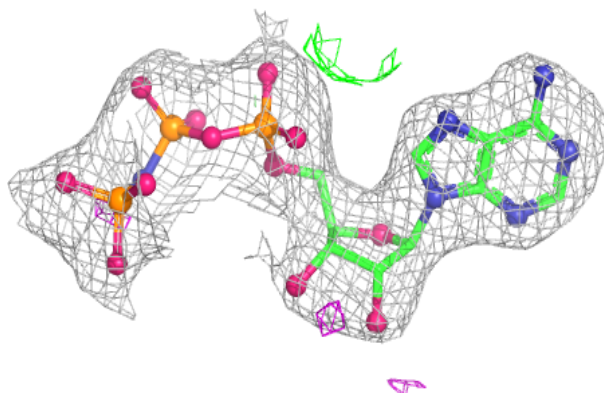


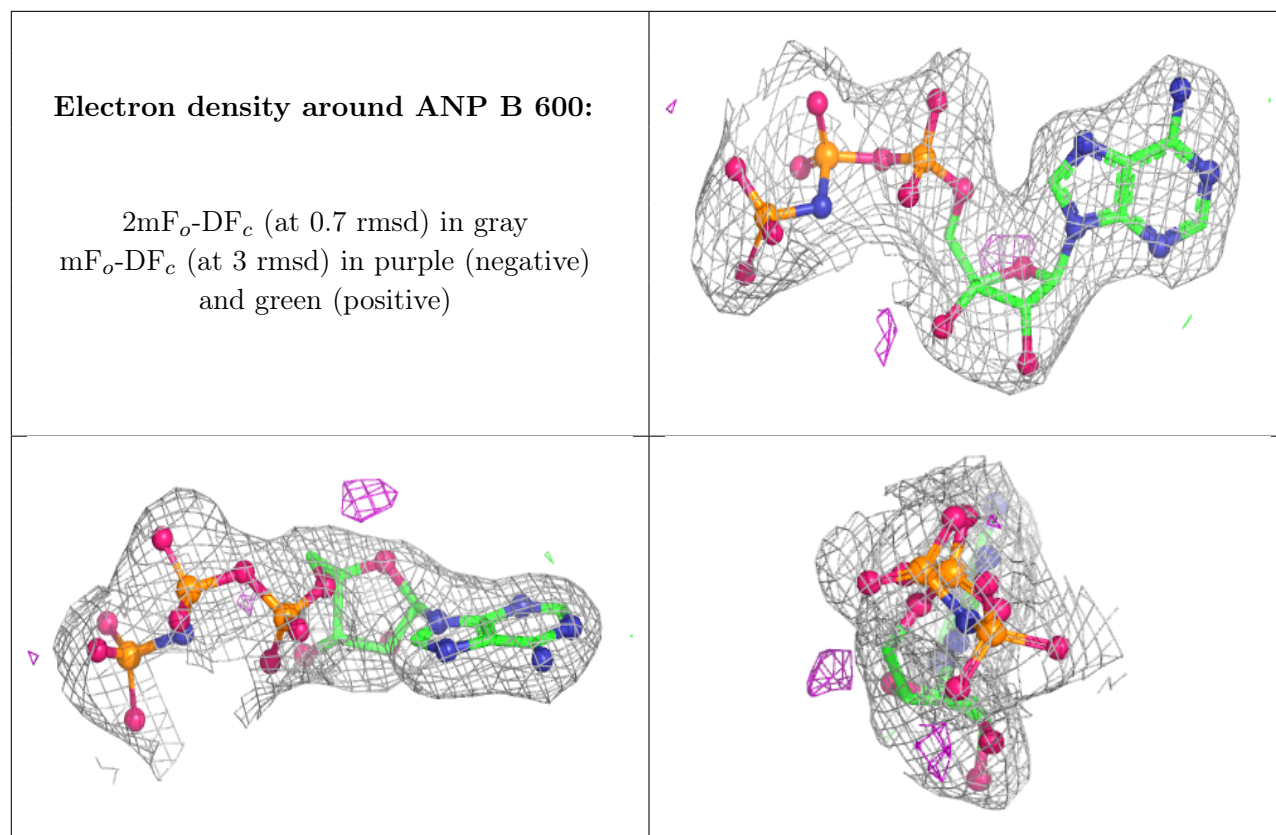
Electron density around ANP D 602:

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

**Electron density around ANP A 601:**

$2mF_o-DF_c$ (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.