



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:13 am BST

PDB ID : 3ALN
Title : Crystal Structure of human non-phosphorylated MKK4 kinase domain complexed with AMP-PNP
Authors : Matsumoto, T.; Kinoshita, T.; Kirii, Y.; Yokota, K.; Hamada, K.; Tada, T.
Deposited on : 2010-08-04
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

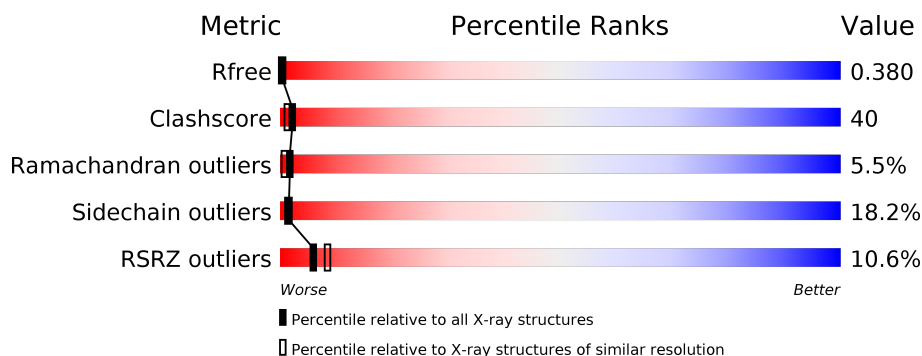
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	327	<div> <div>5%</div> <div>32% 39% 12% 17%</div> </div>
1	B	327	<div> <div>11%</div> <div>33% 35% 11% 20%</div> </div>
1	C	327	<div> <div>8%</div> <div>23% 25% 7% 44%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ANP	A	1	X	-	-	-
2	ANP	B	1	X	-	-	-
2	ANP	C	1	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5773 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 Dual specificity mitogen-activated protein kinase kinase 4.

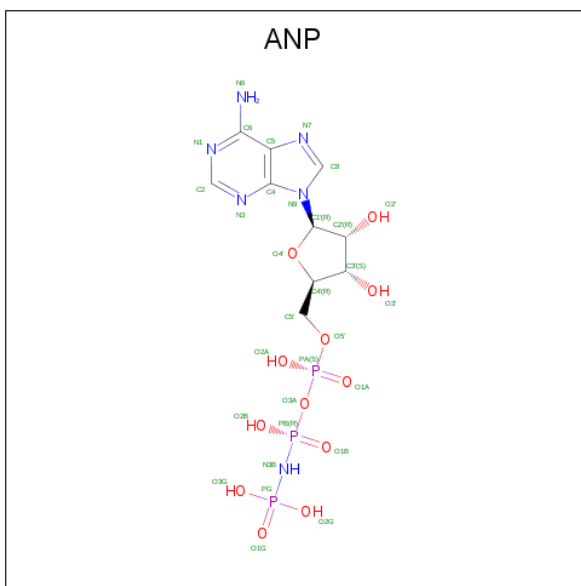
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2133	1368	355	395	15			
1	B	263	Total	C	N	O	S	0	0	0
			2090	1337	347	391	15			
1	C	183	Total	C	N	O	S	0	0	0
			1455	943	232	267	13			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	MET	-	INITIATING METHIONINE	UNP P45985
A	400	HIS	-	EXPRESSION TAG	UNP P45985
A	401	HIS	-	EXPRESSION TAG	UNP P45985
A	402	HIS	-	EXPRESSION TAG	UNP P45985
A	403	HIS	-	EXPRESSION TAG	UNP P45985
A	404	HIS	-	EXPRESSION TAG	UNP P45985
A	405	HIS	-	EXPRESSION TAG	UNP P45985
B	79	MET	-	INITIATING METHIONINE	UNP P45985
B	400	HIS	-	EXPRESSION TAG	UNP P45985
B	401	HIS	-	EXPRESSION TAG	UNP P45985
B	402	HIS	-	EXPRESSION TAG	UNP P45985
B	403	HIS	-	EXPRESSION TAG	UNP P45985
B	404	HIS	-	EXPRESSION TAG	UNP P45985
B	405	HIS	-	EXPRESSION TAG	UNP P45985
C	79	MET	-	INITIATING METHIONINE	UNP P45985
C	400	HIS	-	EXPRESSION TAG	UNP P45985
C	401	HIS	-	EXPRESSION TAG	UNP P45985
C	402	HIS	-	EXPRESSION TAG	UNP P45985
C	403	HIS	-	EXPRESSION TAG	UNP P45985
C	404	HIS	-	EXPRESSION TAG	UNP P45985
C	405	HIS	-	EXPRESSION TAG	UNP P45985

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter

code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



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

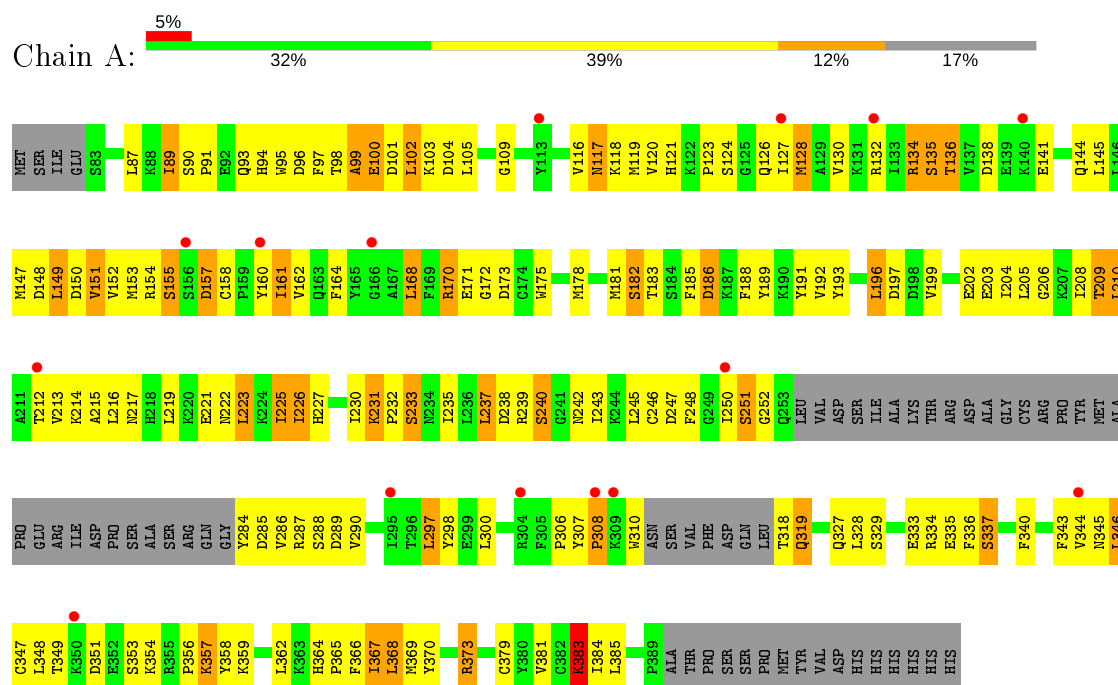
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

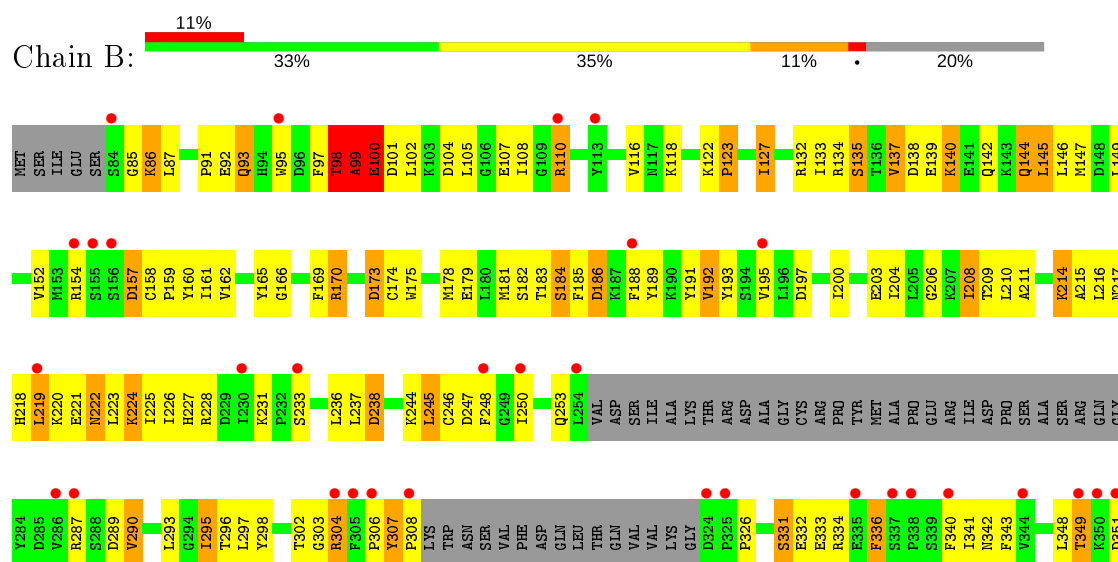
3 Residue-property plots

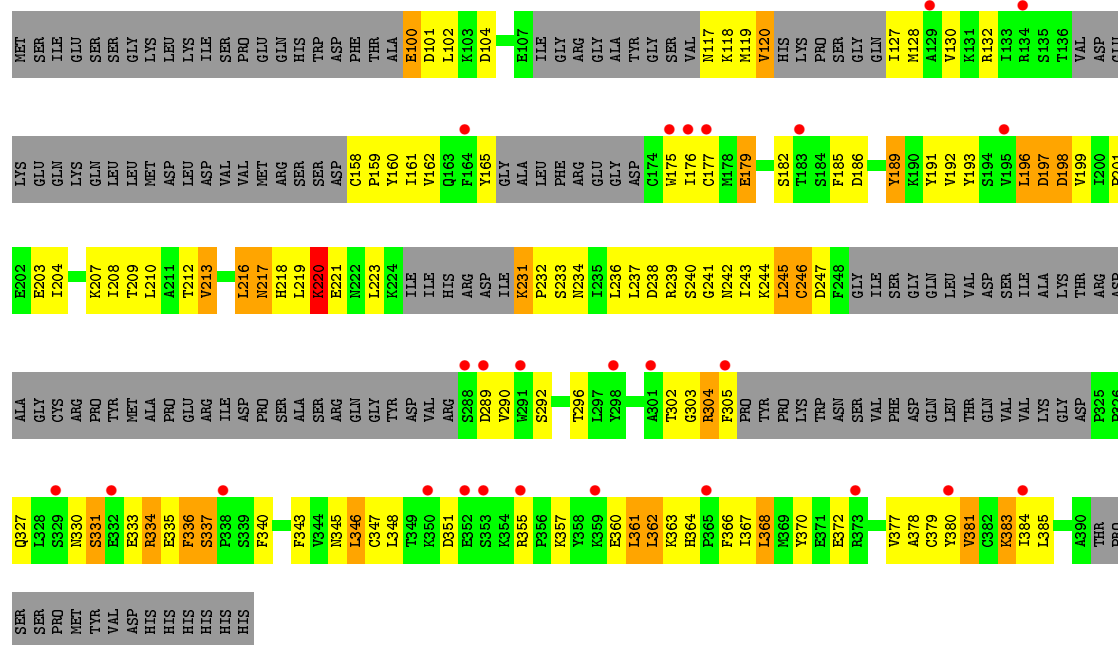
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Dual specificity mitogen-activated protein kinase kinase 4



- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.51Å 76.12Å 173.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.00 – 2.30 45.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.7 (46.00-2.30) 96.7 (45.99-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.6.0081	Depositor
R, R_{free}	0.284 , 0.378 0.284 , 0.380	Depositor DCC
R_{free} test set	1943 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	47.2	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5773	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.77% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	0.76	1/2177 (0.0%)	0.91	2/2939 (0.1%)
1	B	0.68	0/2133	0.85	2/2877 (0.1%)
1	C	0.56	0/1479	0.77	1/1987 (0.1%)
All	All	0.69	1/5789 (0.0%)	0.85	5/7803 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	CYS	CB-SG	-6.70	1.70	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	THR	N-CA-C	-6.45	93.59	111.00
1	C	368	LEU	CA-CB-CG	6.44	130.12	115.30
1	A	308	PRO	N-CA-CB	6.11	110.63	103.30
1	A	210	LEU	CB-CG-CD1	-5.83	101.09	111.00
1	B	99	ALA	N-CA-C	-5.04	97.40	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	GLU	Peptide
1	B	100	GLU	Peptide
1	B	98	THR	Peptide

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	2133	0	2100	181	0
1	B	2090	0	2067	165	0
1	C	1455	0	1448	120	0
2	A	31	0	13	2	0
2	B	31	0	13	4	0
2	C	31	0	13	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	5773	0	5654	453	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 40.

All (453) 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:196:LEU:H	1:A:196:LEU:HD12	1.04	1.18
1:A:287:ARG:HG2	1:A:357:LYS:HZ3	1.09	1.13
1:A:287:ARG:HG2	1:A:357:LYS:NZ	1.65	1.11
1:A:357:LYS:HE3	1:A:357:LYS:HA	1.31	1.11
1:B:287:ARG:HG2	1:B:357:LYS:NZ	1.65	1.10
1:C:236:LEU:HG	1:C:246:CYS:SG	1.97	1.04
1:B:306:PRO:O	1:B:308:PRO:HD3	1.59	1.03
1:A:287:ARG:HG2	1:A:357:LYS:CE	1.89	1.02
1:C:232:PRO:HD3	1:C:296:THR:HG22	1.38	1.02
1:C:304:ARG:HH11	1:C:304:ARG:HG2	1.22	1.01
1:B:92:GLU:HA	1:B:93:GLN:CB	1.91	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:PHE:CZ	1:A:168:LEU:HD23	1.98	0.99
1:A:93:GLN:NE2	1:A:95:TRP:HE1	1.59	0.99
1:B:98:THR:CG2	1:B:99:ALA:HB3	1.93	0.98
1:B:92:GLU:HA	1:B:93:GLN:HB3	1.43	0.98
1:C:186:ASP:OD2	1:C:233:SER:HA	1.64	0.96
1:A:196:LEU:N	1:A:196:LEU:HD12	1.77	0.96
1:A:287:ARG:CG	1:A:357:LYS:HZ3	1.81	0.93
1:C:367:ILE:H	1:C:367:ILE:HD12	1.31	0.93
1:B:287:ARG:HG2	1:B:357:LYS:HZ3	1.29	0.93
1:A:196:LEU:H	1:A:196:LEU:CD1	1.81	0.93
1:C:203:GLU:HA	1:C:370:TYR:OH	1.69	0.93
1:B:98:THR:HG22	1:B:99:ALA:HB3	1.50	0.91
1:A:149:LEU:HD13	1:A:153:MET:CE	2.00	0.91
1:A:216:LEU:HD11	1:A:230:ILE:HD11	1.52	0.89
1:B:98:THR:O	1:B:101:ASP:HB2	1.73	0.88
1:C:128:MET:HE1	1:C:165:TYR:HD2	1.40	0.87
1:A:298:TYR:CD2	1:A:306:PRO:HG3	2.11	0.85
1:A:94:HIS:HA	1:B:87:LEU:O	1.76	0.85
1:A:93:GLN:HE21	1:A:95:TRP:HE1	0.89	0.85
1:A:118:LYS:HG2	1:A:127:ILE:HD11	1.60	0.84
1:C:236:LEU:CG	1:C:246:CYS:SG	2.66	0.84
1:A:158:CYS:O	1:A:161:ILE:HD11	1.78	0.83
1:C:100:GLU:CA	1:C:101:ASP:HB2	2.08	0.83
1:C:330:ASN:ND2	1:C:335:GLU:HA	1.94	0.83
1:A:287:ARG:HG2	1:A:357:LYS:HE2	1.59	0.83
1:B:222:ASN:HD22	1:B:222:ASN:H	1.27	0.83
1:B:210:LEU:HD21	1:B:214:LYS:NZ	1.95	0.82
1:A:100:GLU:H	1:A:101:ASP:HB2	1.45	0.82
1:A:226:ILE:HD13	1:A:226:ILE:H	1.45	0.82
1:C:100:GLU:HA	1:C:101:ASP:HB2	1.60	0.81
1:B:287:ARG:HG2	1:B:357:LYS:HZ1	1.43	0.81
1:C:381:VAL:HG13	1:C:385:LEU:HD12	1.63	0.81
1:B:160:TYR:CE1	1:B:211:ALA:HA	2.17	0.80
1:B:145:LEU:HG	1:B:250:ILE:HG23	1.64	0.79
1:B:349:THR:OG1	1:B:355:ARG:HG2	1.82	0.79
1:A:100:GLU:HA	1:A:102:LEU:H	1.48	0.79
1:B:340:PHE:HB2	1:B:366:PHE:CD1	2.17	0.79
1:B:104:ASP:O	1:B:105:LEU:HD23	1.82	0.78
1:A:126:GLN:HB2	1:B:91:PRO:HG3	1.65	0.78
1:A:248:PHE:O	1:A:248:PHE:CD1	2.36	0.78
1:C:292:SER:O	1:C:296:THR:HG23	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:THR:O	1:C:213:VAL:HG22	1.84	0.77
1:C:304:ARG:NH1	1:C:304:ARG:HG2	1.93	0.77
1:A:238:ASP:O	1:A:240:SER:N	2.17	0.77
1:C:381:VAL:O	1:C:385:LEU:HB2	1.85	0.77
1:B:135:SER:HB2	1:B:137:VAL:HG22	1.66	0.77
1:A:100:GLU:CG	1:A:100:GLU:O	2.28	0.76
1:C:158:CYS:N	1:C:159:PRO:HD2	2.00	0.76
1:A:215:ALA:O	1:A:219:LEU:HD12	1.84	0.76
1:B:165:TYR:HE2	1:B:179:GLU:HA	1.51	0.76
1:B:351:ASP:C	1:B:353:SER:H	1.89	0.76
1:A:95:TRP:O	1:B:86:LYS:HA	1.86	0.76
1:C:236:LEU:CD1	1:C:246:CYS:SG	2.74	0.75
1:A:286:VAL:HG12	1:A:357:LYS:HE2	1.68	0.75
1:C:381:VAL:CG1	1:C:385:LEU:HD12	2.16	0.75
1:A:357:LYS:CA	1:A:357:LYS:HE3	2.15	0.75
1:A:168:LEU:HD21	1:B:85:GLY:CA	2.17	0.74
1:A:170:ARG:HD3	1:A:173:ASP:HB3	1.69	0.74
1:A:204:ILE:HG22	1:A:208:ILE:HD11	1.69	0.74
1:A:149:LEU:HD13	1:A:153:MET:HE1	1.68	0.74
1:A:149:LEU:HD13	1:A:153:MET:HE3	1.69	0.74
2:C:1:ANP:H5'2	2:C:1:ANP:H8	1.69	0.74
1:C:204:ILE:HG13	1:C:380:TYR:CD2	2.22	0.74
1:B:200:ILE:O	1:B:334:ARG:NH2	2.19	0.74
1:C:340:PHE:HD1	1:C:366:PHE:CZ	2.05	0.74
1:C:367:ILE:N	1:C:367:ILE:HD12	2.03	0.74
1:B:170:ARG:O	1:B:170:ARG:HG3	1.84	0.73
1:A:121:HIS:HD2	1:A:124:SER:OG	1.71	0.73
1:B:102:LEU:HD12	1:B:175:TRP:CZ3	2.24	0.73
1:A:357:LYS:CE	1:A:357:LYS:HA	2.17	0.72
1:A:89:ILE:HG22	1:B:165:TYR:CD1	2.23	0.72
1:A:340:PHE:O	1:A:344:VAL:HG23	1.89	0.72
1:C:128:MET:CE	1:C:165:TYR:HD2	2.02	0.72
1:A:154:ARG:O	1:A:155:SER:HB3	1.88	0.71
1:B:289:ASP:HB2	1:B:358:TYR:OH	1.91	0.70
1:B:385:LEU:O	1:B:388:MET:HG3	1.91	0.70
1:C:232:PRO:HD3	1:C:296:THR:CG2	2.19	0.70
1:B:306:PRO:C	1:B:308:PRO:HD3	2.11	0.70
1:B:343:PHE:CE1	1:B:367:ILE:HD12	2.26	0.70
1:A:100:GLU:HG3	1:A:100:GLU:O	1.91	0.70
1:B:210:LEU:HD21	1:B:214:LYS:HZ2	1.57	0.69
1:C:340:PHE:CD1	1:C:366:PHE:CZ	2.79	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLU:CA	1:B:93:GLN:CB	2.68	0.69
1:A:168:LEU:CD2	1:B:85:GLY:HA2	2.22	0.69
1:A:158:CYS:O	1:A:161:ILE:CD1	2.39	0.69
1:A:290:VAL:O	1:A:347:CYS:HB3	1.92	0.69
1:A:148:ASP:HA	1:A:151:VAL:CG1	2.23	0.68
1:A:287:ARG:C	1:A:289:ASP:H	1.95	0.68
1:B:144:GLN:HG3	1:B:145:LEU:N	2.07	0.68
1:B:145:LEU:HD12	1:B:250:ILE:HD12	1.76	0.68
1:B:98:THR:HG23	1:B:99:ALA:HB3	1.75	0.68
1:B:220:LYS:O	1:B:224:LYS:NZ	2.24	0.68
1:A:192:VAL:HA	1:A:196:LEU:HD13	1.74	0.68
1:A:318:THR:HG23	1:A:318:THR:O	1.94	0.68
1:C:379:CYS:O	1:C:383:LYS:HB2	1.94	0.68
1:B:371:GLU:HG3	1:B:371:GLU:O	1.94	0.67
1:A:232:PRO:HB3	1:A:300:LEU:HD21	1.75	0.67
1:B:102:LEU:HD12	1:B:175:TRP:CE3	2.30	0.67
1:C:334:ARG:NH1	1:C:335:GLU:O	2.28	0.67
1:B:181:MET:O	2:B:1:ANP:H2	1.94	0.67
1:C:209:THR:O	1:C:213:VAL:CG2	2.41	0.67
1:A:148:ASP:HA	1:A:151:VAL:HG12	1.77	0.66
1:C:334:ARG:HG2	1:C:334:ARG:HH11	1.60	0.66
1:A:185:PHE:CZ	1:A:237:LEU:HD13	2.30	0.66
1:B:161:ILE:HD12	1:B:161:ILE:O	1.95	0.66
1:A:97:PHE:CE2	1:A:168:LEU:HD23	2.31	0.66
1:B:92:GLU:HA	1:B:93:GLN:HB2	1.79	0.65
1:B:160:TYR:CD1	1:B:211:ALA:HA	2.31	0.65
1:A:100:GLU:N	1:A:101:ASP:HB2	2.12	0.65
1:C:343:PHE:CE1	1:C:367:ILE:HD11	2.31	0.65
1:C:100:GLU:N	1:C:101:ASP:HB2	2.12	0.65
1:B:144:GLN:HG3	1:B:145:LEU:H	1.63	0.64
1:A:319:GLN:OE1	1:A:319:GLN:HA	1.96	0.64
1:C:100:GLU:HA	1:C:101:ASP:CB	2.22	0.64
1:A:119:MET:O	1:A:127:ILE:HD12	1.97	0.64
1:A:89:ILE:HD11	1:B:95:TRP:CD1	2.33	0.64
1:C:367:ILE:H	1:C:367:ILE:CD1	2.04	0.63
1:B:134:ARG:HA	1:B:173:ASP:HA	1.80	0.63
1:C:330:ASN:HD21	1:C:336:PHE:H	1.45	0.63
1:A:186:ASP:HA	1:A:189:TYR:HD2	1.62	0.63
1:A:104:ASP:C	1:A:105:LEU:HD23	2.18	0.63
1:A:173:ASP:CG	1:A:175:TRP:HE1	2.01	0.63
1:C:217:ASN:ND2	1:C:218:HIS:N	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:HH22	1:A:136:THR:HG23	1.63	0.63
1:C:346:LEU:C	1:C:348:LEU:H	2.03	0.62
1:A:157:ASP:N	1:A:157:ASP:OD1	2.31	0.62
1:A:168:LEU:HD21	1:B:85:GLY:HA2	1.80	0.62
1:C:204:ILE:O	1:C:207:LYS:N	2.33	0.62
1:C:219:LEU:O	1:C:220:LYS:HG3	1.99	0.62
1:C:199:VAL:HG21	1:C:334:ARG:HE	1.64	0.62
1:A:116:VAL:C	1:A:117:ASN:HD22	2.03	0.62
1:B:160:TYR:HB3	1:B:215:ALA:HB2	1.81	0.62
1:A:104:ASP:O	1:A:105:LEU:HD23	1.99	0.61
1:B:377:VAL:O	1:B:381:VAL:HB	1.99	0.61
1:A:298:TYR:CE2	1:A:306:PRO:HG3	2.36	0.61
1:B:287:ARG:CG	1:B:357:LYS:NZ	2.54	0.61
1:B:351:ASP:C	1:B:353:SER:N	2.54	0.61
1:B:149:LEU:H	1:B:250:ILE:HD11	1.65	0.60
1:C:213:VAL:O	1:C:217:ASN:HB3	2.01	0.60
1:A:149:LEU:CD1	1:A:153:MET:HE1	2.31	0.60
1:B:287:ARG:CG	1:B:357:LYS:HZ1	2.14	0.60
1:C:100:GLU:N	1:C:100:GLU:CD	2.53	0.60
1:C:120:VAL:O	1:C:120:VAL:HG23	2.02	0.60
1:B:182:SER:O	1:B:183:THR:HB	2.02	0.60
1:B:165:TYR:HE2	1:B:179:GLU:CA	2.14	0.60
1:A:99:ALA:O	1:A:100:GLU:HB3	2.00	0.60
1:C:380:TYR:O	1:C:383:LYS:HB3	2.01	0.60
1:A:186:ASP:HA	1:A:189:TYR:CD2	2.37	0.60
1:A:93:GLN:HG3	1:A:95:TRP:HE1	1.67	0.59
1:A:128:MET:HG3	1:A:130:VAL:CG2	2.32	0.59
1:C:304:ARG:HH11	1:C:304:ARG:CG	2.07	0.59
1:B:98:THR:O	1:B:101:ASP:CB	2.48	0.59
1:B:219:LEU:HD23	1:B:227:HIS:HB2	1.84	0.59
1:A:144:GLN:O	1:A:148:ASP:N	2.34	0.59
1:A:168:LEU:CD2	1:B:85:GLY:CA	2.80	0.59
1:A:340:PHE:HB2	1:A:366:PHE:CE1	2.38	0.59
1:A:182:SER:OG	1:A:238:ASP:HA	2.03	0.59
1:C:240:SER:HB2	1:C:242:ASN:HD22	1.68	0.59
1:A:227:HIS:CD2	1:A:248:PHE:HB3	2.38	0.58
1:A:328:LEU:N	1:A:345:ASN:HD21	2.01	0.58
1:C:362:LEU:CD2	1:C:362:LEU:H	2.15	0.58
1:C:189:TYR:CE1	1:C:303:GLY:HA2	2.38	0.58
1:B:290:VAL:HG11	1:B:355:ARG:HB3	1.85	0.58
1:C:119:MET:SD	1:C:130:VAL:HB	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LEU:O	1:A:347:CYS:C	2.40	0.58
1:A:89:ILE:HD11	1:B:95:TRP:HD1	1.68	0.58
1:A:334:ARG:HG2	1:A:336:PHE:CZ	2.38	0.58
1:B:139:GLU:HA	1:B:142:GLN:HG2	1.85	0.57
1:C:337:SER:HB2	1:C:340:PHE:HB2	1.85	0.57
1:A:286:VAL:HG22	1:A:358:TYR:CE2	2.39	0.57
1:A:89:ILE:O	1:B:93:GLN:HB3	2.04	0.57
1:B:158:CYS:HB2	1:B:218:HIS:CE1	2.40	0.57
1:B:290:VAL:CG1	1:B:355:ARG:HD2	2.35	0.57
1:B:218:HIS:CD2	1:B:218:HIS:O	2.58	0.57
1:A:287:ARG:O	1:A:289:ASP:N	2.38	0.56
1:B:351:ASP:O	1:B:353:SER:N	2.38	0.56
1:B:160:TYR:HE1	1:B:211:ALA:HA	1.70	0.56
1:B:222:ASN:HD22	1:B:222:ASN:N	2.00	0.56
1:B:290:VAL:HG12	1:B:355:ARG:HH11	1.70	0.56
1:C:236:LEU:HD12	1:C:246:CYS:SG	2.44	0.56
1:A:250:ILE:O	1:A:251:SER:C	2.42	0.56
1:B:326:PRO:O	1:B:348:LEU:HD13	2.06	0.56
1:C:343:PHE:CZ	1:C:361:LEU:HD23	2.41	0.56
1:C:119:MET:SD	1:C:130:VAL:HG21	2.45	0.56
1:A:226:ILE:HG22	1:A:286:VAL:HG23	1.88	0.56
1:C:100:GLU:CA	1:C:102:LEU:H	2.19	0.56
1:A:351:ASP:OD2	1:A:354:LYS:HB2	2.07	0.55
1:C:201:PRO:HD2	1:C:380:TYR:CZ	2.41	0.55
1:B:227:HIS:CD2	1:B:248:PHE:HB3	2.41	0.55
1:A:231:LYS:O	1:A:235:ILE:HG13	2.06	0.55
1:A:162:VAL:HG22	1:A:245:LEU:O	2.05	0.55
2:C:1:ANP:C5'	2:C:1:ANP:H8	2.35	0.55
1:C:199:VAL:CG2	1:C:334:ARG:HE	2.20	0.55
1:B:231:LYS:CE	2:B:1:ANP:O3G	2.54	0.55
1:C:237:LEU:HA	1:C:242:ASN:O	2.06	0.55
1:B:370:TYR:O	1:B:372:GLU:N	2.40	0.55
1:B:98:THR:C	1:B:100:GLU:H	2.08	0.55
1:B:98:THR:HA	1:B:99:ALA:HB2	1.89	0.55
1:B:222:ASN:ND2	1:B:222:ASN:H	2.01	0.54
1:C:343:PHE:HB2	1:C:364:HIS:CE1	2.42	0.54
1:C:231:LYS:HE3	1:C:234:ASN:ND2	2.22	0.54
1:B:189:TYR:O	1:B:193:TYR:HD2	1.89	0.54
1:A:183:THR:O	1:A:237:LEU:HD23	2.08	0.54
1:A:287:ARG:C	1:A:289:ASP:N	2.61	0.54
1:A:238:ASP:C	1:A:240:SER:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:HD12	1:B:223:LEU:HD12	1.90	0.54
1:A:193:TYR:O	1:A:197:ASP:HA	2.08	0.54
1:A:364:HIS:ND1	1:A:365:PRO:HD2	2.23	0.54
1:A:222:ASN:O	1:A:223:LEU:HD23	2.08	0.53
1:A:340:PHE:CD1	1:A:366:PHE:CZ	2.96	0.53
1:C:343:PHE:HZ	1:C:361:LEU:HD23	1.73	0.53
1:C:203:GLU:HA	1:C:370:TYR:HH	1.70	0.53
1:C:337:SER:HB3	1:C:340:PHE:H	1.73	0.53
1:C:185:PHE:CZ	1:C:208:ILE:HD11	2.42	0.53
1:B:179:GLU:OE1	1:B:244:LYS:NZ	2.36	0.53
1:C:245:LEU:C	1:C:245:LEU:HD12	2.29	0.53
1:A:192:VAL:CA	1:A:196:LEU:HD13	2.38	0.53
1:A:93:GLN:HG3	1:A:95:TRP:NE1	2.24	0.53
1:C:330:ASN:CG	1:C:335:GLU:HA	2.28	0.53
1:C:130:VAL:HG13	1:C:177:CYS:SG	2.49	0.53
1:C:334:ARG:HH11	1:C:334:ARG:CG	2.21	0.52
1:A:204:ILE:O	1:A:208:ILE:HG13	2.10	0.52
1:B:216:LEU:HB3	1:B:358:TYR:CE2	2.45	0.52
1:A:212:THR:O	1:A:216:LEU:HB2	2.10	0.52
1:B:157:ASP:O	1:B:159:PRO:HD3	2.09	0.52
1:C:212:THR:O	1:C:216:LEU:HB2	2.09	0.52
2:C:1:ANP:H5'2	2:C:1:ANP:C8	2.38	0.52
1:C:128:MET:HE1	1:C:165:TYR:CD2	2.32	0.52
1:C:333:GLU:O	1:C:334:ARG:HB2	2.09	0.51
1:A:356:PRO:O	1:A:357:LYS:NZ	2.38	0.51
1:B:118:LYS:HE3	1:B:127:ILE:HG21	1.91	0.51
1:B:231:LYS:HE3	2:B:1:ANP:O3G	2.10	0.51
1:A:221:GLU:C	1:A:222:ASN:HD22	2.13	0.51
1:C:327:GLN:HA	1:C:345:ASN:HD21	1.76	0.51
1:A:148:ASP:CA	1:A:151:VAL:HG12	2.40	0.51
1:A:237:LEU:HD12	1:A:381:VAL:HG11	1.91	0.51
1:C:217:ASN:HD22	1:C:218:HIS:N	2.08	0.51
1:B:161:ILE:HG21	1:B:219:LEU:HD13	1.93	0.51
1:A:149:LEU:CD1	1:A:153:MET:CE	2.81	0.51
1:A:286:VAL:HG22	1:A:358:TYR:HE2	1.75	0.51
1:C:104:ASP:HA	1:C:119:MET:HG2	1.93	0.50
1:B:204:ILE:HD13	1:B:377:VAL:HG22	1.93	0.50
1:A:168:LEU:HD21	1:B:85:GLY:HA3	1.91	0.50
1:A:109:GLY:HA3	2:A:1:ANP:H3'	1.92	0.50
1:A:87:LEU:HD23	1:A:89:ILE:HD12	1.92	0.50
1:B:384:ILE:HD12	1:B:384:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:THR:HA	1:B:99:ALA:CB	2.42	0.50
1:B:342:ASN:OD1	1:B:364:HIS:NE2	2.44	0.50
1:A:210:LEU:C	1:A:210:LEU:HD12	2.32	0.50
1:C:100:GLU:HA	1:C:102:LEU:H	1.76	0.50
1:B:132:ARG:HA	1:B:174:CYS:O	2.12	0.50
1:C:238:ASP:O	1:C:381:VAL:HG11	2.12	0.50
1:A:383:LYS:O	1:A:384:ILE:C	2.48	0.50
1:A:93:GLN:NE2	1:A:95:TRP:NE1	2.34	0.50
1:A:102:LEU:HA	1:A:120:VAL:O	2.12	0.49
1:B:343:PHE:HE1	1:B:367:ILE:HD12	1.71	0.49
1:B:92:GLU:CA	1:B:93:GLN:HB2	2.39	0.49
1:C:346:LEU:C	1:C:348:LEU:N	2.65	0.49
1:A:135:SER:OG	1:A:136:THR:N	2.42	0.49
1:A:286:VAL:HG12	1:A:357:LYS:CE	2.40	0.49
1:B:132:ARG:HD2	1:B:175:TRP:CE2	2.47	0.49
1:C:102:LEU:HD12	1:C:175:TRP:HZ3	1.77	0.49
1:B:293:LEU:HG	1:B:297:LEU:CD1	2.43	0.49
1:B:336:PHE:HD2	1:B:341:ILE:HD11	1.76	0.49
1:B:287:ARG:NH2	1:B:353:SER:HA	2.27	0.49
1:B:206:GLY:HA2	1:B:366:PHE:CZ	2.48	0.49
1:C:198:ASP:OD2	1:C:198:ASP:N	2.46	0.49
1:B:336:PHE:CD2	1:B:341:ILE:HD11	2.48	0.49
1:B:222:ASN:N	1:B:222:ASN:ND2	2.60	0.49
1:C:182:SER:OG	1:C:238:ASP:HA	2.13	0.49
1:A:213:VAL:HG12	1:A:362:LEU:HD22	1.95	0.48
1:B:118:LYS:CE	1:B:127:ILE:HG21	2.43	0.48
1:B:302:THR:HG21	1:B:304:ARG:NH2	2.27	0.48
1:B:246:CYS:O	1:B:247:ASP:HB2	2.13	0.48
1:B:287:ARG:O	1:B:355:ARG:NH1	2.47	0.48
1:A:203:GLU:HA	1:A:370:TYR:CE1	2.49	0.48
1:C:119:MET:SD	1:C:130:VAL:CG2	3.01	0.48
1:C:196:LEU:O	1:C:197:ASP:HB2	2.13	0.48
1:A:203:GLU:OE2	1:A:373:ARG:NH2	2.46	0.48
1:B:221:GLU:HB2	1:B:222:ASN:HD22	1.78	0.48
1:B:297:LEU:O	1:B:298:TYR:C	2.52	0.48
1:A:170:ARG:CD	1:A:173:ASP:HB3	2.43	0.48
1:A:287:ARG:CG	1:A:357:LYS:HE2	2.37	0.48
1:A:364:HIS:ND1	1:A:365:PRO:CD	2.77	0.48
1:B:149:LEU:HB2	1:B:250:ILE:HG12	1.94	0.48
1:B:295:ILE:O	1:B:296:THR:C	2.52	0.48
1:C:199:VAL:HG21	1:C:334:ARG:NE	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:LYS:HE2	1:C:127:ILE:HD12	1.95	0.47
1:A:121:HIS:CD2	1:A:124:SER:OG	2.61	0.47
1:B:225:ILE:HG22	1:B:226:ILE:O	2.13	0.47
1:C:357:LYS:H	1:C:360:GLU:HG3	1.79	0.47
1:A:245:LEU:HD12	1:A:245:LEU:N	2.30	0.47
1:B:144:GLN:HA	1:B:147:MET:HE2	1.95	0.47
1:A:209:THR:OG1	1:A:297:LEU:HD21	2.14	0.47
1:A:233:SER:HG	2:A:1:ANP:PB	2.38	0.47
1:B:364:HIS:HA	1:B:365:PRO:HD2	1.75	0.47
1:B:98:THR:CA	1:B:99:ALA:CB	2.92	0.47
1:A:148:ASP:HA	1:A:151:VAL:HG11	1.96	0.47
1:B:185:PHE:CE1	1:B:208:ILE:HD11	2.49	0.47
1:C:346:LEU:O	1:C:346:LEU:HD12	2.15	0.47
1:B:223:LEU:HB3	1:B:225:ILE:HG13	1.96	0.47
1:B:293:LEU:HG	1:B:297:LEU:HD11	1.97	0.47
1:A:103:LYS:O	1:A:119:MET:HA	2.14	0.47
1:A:148:ASP:CA	1:A:151:VAL:CG1	2.92	0.47
1:A:346:LEU:HG	1:A:356:PRO:HG3	1.96	0.47
1:B:385:LEU:O	1:B:387:GLN:N	2.48	0.47
1:C:158:CYS:SG	1:C:218:HIS:CE1	3.08	0.47
1:A:346:LEU:O	1:A:348:LEU:N	2.48	0.46
1:B:343:PHE:CE1	1:B:367:ILE:CD1	2.98	0.46
1:C:160:TYR:HA	1:C:244:LYS:HG2	1.98	0.46
1:C:208:ILE:HG13	1:C:243:ILE:HG21	1.97	0.46
1:A:205:LEU:HA	1:A:208:ILE:HD12	1.98	0.46
1:B:158:CYS:HB2	1:B:218:HIS:ND1	2.31	0.46
1:C:104:ASP:OD1	1:C:117:ASN:HB3	2.15	0.46
1:C:290:VAL:HG12	1:C:355:ARG:HD2	1.97	0.46
1:B:191:TYR:O	1:B:192:VAL:C	2.53	0.46
1:A:154:ARG:O	1:A:155:SER:CB	2.60	0.46
1:A:191:TYR:CD2	1:A:196:LEU:HD11	2.50	0.46
1:C:191:TYR:HD2	1:C:384:ILE:HG23	1.80	0.46
1:C:192:VAL:HG12	1:C:198:ASP:HB2	1.98	0.46
1:C:119:MET:SD	1:C:130:VAL:CB	3.03	0.46
1:A:93:GLN:CG	1:A:95:TRP:HE1	2.29	0.45
1:B:185:PHE:CE2	1:B:237:LEU:HB3	2.51	0.45
1:B:193:TYR:O	1:B:197:ASP:HA	2.16	0.45
1:A:193:TYR:CE1	1:A:199:VAL:HG12	2.51	0.45
1:C:245:LEU:HD12	1:C:246:CYS:N	2.30	0.45
1:A:246:CYS:SG	1:A:247:ASP:OD2	2.63	0.45
1:B:388:MET:C	1:B:390:ALA:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASP:C	1:A:151:VAL:CG1	2.85	0.45
1:C:238:ASP:OD1	1:C:242:ASN:HB2	2.16	0.45
1:A:212:THR:HG23	1:A:245:LEU:HD21	1.99	0.45
1:B:186:ASP:HA	1:B:189:TYR:HD2	1.82	0.45
1:A:284:TYR:O	1:A:285:ASP:HB2	2.17	0.45
1:B:102:LEU:HD12	1:B:175:TRP:HZ3	1.78	0.45
1:C:377:VAL:O	1:C:378:ALA:C	2.54	0.45
1:B:104:ASP:C	1:B:105:LEU:HD23	2.37	0.45
1:B:138:ASP:OD2	1:B:140:LYS:HB3	2.16	0.45
1:C:217:ASN:HD22	1:C:218:HIS:H	1.63	0.45
1:A:357:LYS:O	1:A:358:TYR:C	2.54	0.44
1:C:158:CYS:HG	1:C:218:HIS:CE1	2.35	0.44
1:A:170:ARG:CD	1:A:173:ASP:O	2.66	0.44
1:B:186:ASP:HA	1:B:189:TYR:CD2	2.52	0.44
1:A:87:LEU:HD12	1:B:166:GLY:HA3	1.99	0.44
1:C:158:CYS:N	1:C:159:PRO:CD	2.73	0.44
1:C:159:PRO:O	1:C:244:LYS:HE2	2.17	0.44
1:A:100:GLU:HG2	1:A:100:GLU:O	2.16	0.44
1:A:232:PRO:HD2	1:A:310:TRP:CH2	2.52	0.44
1:A:162:VAL:HG23	1:A:164:PHE:CE2	2.53	0.44
1:B:203:GLU:HA	1:B:370:TYR:CE1	2.52	0.44
1:C:196:LEU:O	1:C:197:ASP:CB	2.64	0.44
1:B:208:ILE:HG22	1:B:209:THR:N	2.33	0.44
1:B:228:ARG:HA	1:B:289:ASP:OD1	2.18	0.44
1:C:239:ARG:C	1:C:241:GLY:H	2.21	0.44
1:A:365:PRO:HA	1:A:368:LEU:HB2	1.99	0.44
1:B:189:TYR:CD1	1:B:303:GLY:HA2	2.53	0.44
1:C:161:ILE:HD11	1:C:219:LEU:CD1	2.48	0.44
1:A:185:PHE:HE2	1:A:243:ILE:HG23	1.83	0.44
1:A:89:ILE:HG12	1:B:93:GLN:HG2	1.99	0.44
1:A:101:ASP:O	1:A:121:HIS:HA	2.18	0.43
1:A:327:GLN:HA	1:A:345:ASN:ND2	2.33	0.43
1:B:170:ARG:CG	1:B:170:ARG:O	2.63	0.43
1:B:236:LEU:HA	1:B:236:LEU:HD23	1.81	0.43
1:A:105:LEU:HB2	1:A:118:LYS:HB3	2.00	0.43
1:B:107:GLU:OE1	1:B:110:ARG:HD3	2.18	0.43
1:B:210:LEU:HD21	1:B:214:LYS:HZ3	1.78	0.43
1:C:128:MET:CE	1:C:165:TYR:CD2	2.93	0.43
1:A:346:LEU:O	1:A:349:THR:OG1	2.30	0.43
1:B:238:ASP:OD1	1:B:238:ASP:C	2.57	0.43
1:C:231:LYS:N	1:C:232:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:MET:HE3	1:A:238:ASP:HB3	2.00	0.43
1:A:318:THR:CG2	1:A:318:THR:O	2.64	0.43
1:A:202:GLU:OE1	1:A:337:SER:HB3	2.18	0.43
1:B:359:LYS:HE2	1:B:363:LYS:HE3	2.00	0.43
1:C:102:LEU:HD12	1:C:175:TRP:CZ3	2.54	0.43
1:C:165:TYR:OH	1:C:179:GLU:HB2	2.18	0.43
1:A:171:GLU:HA	1:A:172:GLY:HA2	1.78	0.43
1:B:290:VAL:HG12	1:B:355:ARG:HD2	2.01	0.43
1:B:191:TYR:HE1	1:B:195:VAL:HG11	1.84	0.43
1:A:357:LYS:CE	1:A:357:LYS:CA	2.85	0.43
1:B:221:GLU:O	1:B:224:LYS:HE2	2.18	0.43
1:C:362:LEU:N	1:C:362:LEU:CD2	2.82	0.43
1:A:364:HIS:CE1	1:A:365:PRO:HD2	2.53	0.42
1:B:188:PHE:CZ	1:B:384:ILE:HB	2.54	0.42
1:A:124:SER:HB2	1:B:91:PRO:HG2	2.00	0.42
1:A:151:VAL:HG13	1:A:152:VAL:H	1.84	0.42
1:A:160:TYR:HE2	1:A:214:LYS:HZ3	1.65	0.42
1:B:162:VAL:HG11	1:B:236:LEU:HD12	2.01	0.42
1:C:100:GLU:HA	1:C:102:LEU:N	2.34	0.42
1:A:219:LEU:C	1:A:225:ILE:O	2.57	0.42
1:A:128:MET:HG3	1:A:130:VAL:HG23	2.00	0.42
1:B:116:VAL:HG21	2:B:1:ANP:O4'	2.20	0.42
1:B:253:GLN:CD	1:B:253:GLN:N	2.73	0.42
1:B:191:TYR:CZ	1:B:388:MET:HA	2.55	0.42
1:A:149:LEU:O	1:A:153:MET:HB2	2.19	0.42
1:C:119:MET:O	1:C:128:MET:HG3	2.19	0.42
1:A:343:PHE:HE1	1:A:367:ILE:HG13	1.85	0.42
1:C:192:VAL:HG22	1:C:384:ILE:HD13	2.02	0.42
1:B:191:TYR:CE1	1:B:195:VAL:HG11	2.55	0.41
1:C:219:LEU:C	1:C:221:GLU:H	2.23	0.41
1:A:117:ASN:HD22	1:A:117:ASN:N	2.18	0.41
1:A:226:ILE:H	1:A:226:ILE:CD1	2.20	0.41
1:A:95:TRP:CZ3	1:A:123:PRO:HB2	2.55	0.41
1:A:89:ILE:HD13	1:A:89:ILE:N	2.35	0.41
1:C:330:ASN:O	1:C:331:SER:C	2.58	0.41
1:A:87:LEU:HB2	1:B:97:PHE:CD2	2.56	0.41
1:C:327:GLN:CB	1:C:345:ASN:HD21	2.33	0.41
1:A:237:LEU:HD12	1:A:381:VAL:CG1	2.49	0.41
1:A:90:SER:N	1:A:91:PRO:CD	2.84	0.41
1:C:364:HIS:HB3	1:C:367:ILE:HD13	2.02	0.41
1:A:213:VAL:CG1	1:A:362:LEU:HD22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LEU:CD1	1:B:246:CYS:H	2.33	0.41
1:A:191:TYR:CE2	1:A:196:LEU:HD11	2.56	0.41
1:A:185:PHE:HA	1:A:188:PHE:HB3	2.02	0.41
1:A:186:ASP:HB3	1:A:232:PRO:HB2	2.02	0.41
1:B:342:ASN:OD1	1:B:343:PHE:N	2.54	0.41
1:C:362:LEU:HD23	1:C:362:LEU:H	1.82	0.41
1:B:160:TYR:CD1	1:B:211:ALA:CA	3.02	0.41
1:B:332:GLU:HG2	1:B:332:GLU:H	1.69	0.41
1:B:122:LYS:N	1:B:123:PRO:CD	2.84	0.41
1:B:331:SER:OG	1:B:333:GLU:HB2	2.20	0.41
1:A:206:GLY:HA3	1:A:370:TYR:CD1	2.57	0.40
1:A:346:LEU:O	1:A:349:THR:N	2.53	0.40
1:B:188:PHE:O	1:B:192:VAL:HG23	2.21	0.40
1:B:152:VAL:HG22	1:B:225:ILE:HD11	2.02	0.40
1:B:98:THR:O	1:B:101:ASP:N	2.44	0.40
1:A:287:ARG:CG	1:A:357:LYS:NZ	2.53	0.40
1:B:380:TYR:O	1:B:384:ILE:HD13	2.21	0.40
1:A:237:LEU:HA	1:A:242:ASN:O	2.22	0.40
1:B:343:PHE:CZ	1:B:361:LEU:HD22	2.56	0.40
1:B:92:GLU:O	1:B:92:GLU:HG3	2.21	0.40
1:C:160:TYR:O	1:C:244:LYS:HA	2.22	0.40
1:C:302:THR:OG1	1:C:304:ARG:CB	2.70	0.40
1:C:335:GLU:HG3	1:C:336:PHE:N	2.36	0.40
1:C:362:LEU:HD22	1:C:362:LEU:H	1.85	0.40
1:A:381:VAL:HG12	1:A:385:LEU:HD12	2.04	0.40
1:B:184:SER:OG	1:B:186:ASP:N	2.55	0.40
1:A:103:LYS:HB3	1:A:120:VAL:HG12	2.02	0.40
1:A:168:LEU:HA	1:A:168:LEU:HD22	1.80	0.40
1:A:216:LEU:CD1	1:A:230:ILE:HD11	2.38	0.40
1:B:165:TYR:CE2	1:B:179:GLU:HA	2.42	0.40
1:B:306:PRO:O	1:B:308:PRO:CD	2.50	0.40
1:C:189:TYR:CD1	1:C:189:TYR:C	2.95	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	264/327 (81%)	219 (83%)	33 (12%)	12 (4%)	2	1
1	B	257/327 (79%)	199 (77%)	42 (16%)	16 (6%)	1	0
1	C	167/327 (51%)	124 (74%)	33 (20%)	10 (6%)	1	0
All	All	688/981 (70%)	542 (79%)	108 (16%)	38 (6%)	2	1

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ALA
1	A	100	GLU
1	A	155	SER
1	A	239	ARG
1	A	252	GLY
1	A	308	PRO
1	B	93	GLN
1	B	307	TYR
1	B	357	LYS
1	B	371	GLU
1	C	381	VAL
1	A	288	SER
1	A	346	LEU
1	B	137	VAL
1	B	352	GLU
1	C	223	LEU
1	C	331	SER
1	A	138	ASP
1	A	251	SER
1	B	86	LYS
1	B	233	SER
1	C	210	LEU
1	C	220	LYS
1	C	247	ASP
1	C	351	ASP
1	A	136	THR
1	A	383	LYS
1	B	108	ILE
1	B	386	ASP
1	C	193	TYR

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Mol	Chain	Res	Type
1	C	383	LYS
1	B	99	ALA
1	B	217	ASN
1	B	365	PRO
1	B	373	ARG
1	C	347	CYS
1	B	331	SER
1	B	192	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	233/296 (79%)	187 (80%)	46 (20%)	1	1
1	B	232/296 (78%)	193 (83%)	39 (17%)	2	2
1	C	163/296 (55%)	134 (82%)	29 (18%)	2	1
All	All	628/888 (71%)	514 (82%)	114 (18%)	1	1

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ILE
1	A	96	ASP
1	A	98	THR
1	A	102	LEU
1	A	117	ASN
1	A	128	MET
1	A	132	ARG
1	A	134	ARG
1	A	135	SER
1	A	141	GLU
1	A	145	LEU
1	A	147	MET
1	A	149	LEU
1	A	150	ASP

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Mol	Chain	Res	Type
1	A	151	VAL
1	A	157	ASP
1	A	161	ILE
1	A	168	LEU
1	A	170	ARG
1	A	178	MET
1	A	182	SER
1	A	186	ASP
1	A	196	LEU
1	A	209	THR
1	A	217	ASN
1	A	223	LEU
1	A	225	ILE
1	A	226	ILE
1	A	231	LYS
1	A	233	SER
1	A	237	LEU
1	A	240	SER
1	A	297	LEU
1	A	307	TYR
1	A	319	GLN
1	A	329	SER
1	A	335	GLU
1	A	337	SER
1	A	353	SER
1	A	357	LYS
1	A	359	LYS
1	A	367	ILE
1	A	368	LEU
1	A	369	MET
1	A	373	ARG
1	A	383	LYS
1	B	100	GLU
1	B	110	ARG
1	B	123	PRO
1	B	127	ILE
1	B	133	ILE
1	B	135	SER
1	B	140	LYS
1	B	144	GLN
1	B	145	LEU
1	B	146	LEU

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Mol	Chain	Res	Type
1	B	154	ARG
1	B	157	ASP
1	B	169	PHE
1	B	170	ARG
1	B	173	ASP
1	B	178	MET
1	B	184	SER
1	B	186	ASP
1	B	208	ILE
1	B	214	LYS
1	B	219	LEU
1	B	222	ASN
1	B	224	LYS
1	B	238	ASP
1	B	245	LEU
1	B	290	VAL
1	B	295	ILE
1	B	304	ARG
1	B	307	TYR
1	B	336	PHE
1	B	349	THR
1	B	357	LYS
1	B	367	ILE
1	B	369	MET
1	B	371	GLU
1	B	372	GLU
1	B	376	GLU
1	B	381	VAL
1	B	388	MET
1	C	100	GLU
1	C	120	VAL
1	C	132	ARG
1	C	162	VAL
1	C	176	ILE
1	C	179	GLU
1	C	189	TYR
1	C	196	LEU
1	C	197	ASP
1	C	198	ASP
1	C	213	VAL
1	C	216	LEU
1	C	217	ASN

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Mol	Chain	Res	Type
1	C	220	LYS
1	C	231	LYS
1	C	245	LEU
1	C	246	CYS
1	C	289	ASP
1	C	304	ARG
1	C	305	PHE
1	C	334	ARG
1	C	336	PHE
1	C	337	SER
1	C	346	LEU
1	C	361	LEU
1	C	362	LEU
1	C	363	LYS
1	C	368	LEU
1	C	372	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	117	ASN
1	A	121	HIS
1	A	142	GLN
1	A	222	ASN
1	A	345	ASN
1	B	117	ASN
1	B	121	HIS
1	B	218	HIS
1	B	222	ASN
1	B	234	ASN
1	C	217	ASN
1	C	234	ASN
1	C	242	ASN
1	C	330	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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$
2	ANP	C	1	-	29,33,33	2.02	9 (31%)	31,52,52	1.84	8 (25%)
2	ANP	A	1	3	29,33,33	1.84	7 (24%)	31,52,52	2.12	9 (29%)
2	ANP	B	1	3	29,33,33	1.82	8 (27%)	31,52,52	2.66	7 (22%)

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	1	-	4/4/7/8	6/14/38/38	0/3/3/3
2	ANP	A	1	3	4/4/7/8	7/14/38/38	0/3/3/3
2	ANP	B	1	3	4/4/7/8	6/14/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1	ANP	PB-N3B	4.61	1.75	1.63
2	C	1	ANP	PG-N3B	4.60	1.75	1.63
2	A	1	ANP	PG-N3B	4.16	1.74	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	ANP	PB-N3B	4.08	1.74	1.63
2	B	1	ANP	PG-N3B	3.89	1.73	1.63
2	A	1	ANP	PB-N3B	3.65	1.72	1.63
2	A	1	ANP	PG-O1G	3.55	1.51	1.46
2	C	1	ANP	PG-O1G	3.47	1.51	1.46
2	B	1	ANP	PB-O1B	3.43	1.51	1.46
2	C	1	ANP	PB-O1B	3.22	1.51	1.46
2	A	1	ANP	C2'-C1'	-3.13	1.49	1.53
2	B	1	ANP	C2-N3	3.09	1.37	1.32
2	C	1	ANP	C5-C4	3.02	1.48	1.40
2	C	1	ANP	O4'-C1'	3.01	1.45	1.41
2	B	1	ANP	PG-O1G	2.98	1.50	1.46
2	A	1	ANP	PB-O1B	2.94	1.50	1.46
2	A	1	ANP	C2-N3	2.75	1.36	1.32
2	B	1	ANP	C5-C4	2.64	1.47	1.40
2	A	1	ANP	O4'-C1'	2.50	1.44	1.41
2	C	1	ANP	PB-O3A	2.47	1.62	1.59
2	C	1	ANP	PB-O2B	-2.23	1.50	1.56
2	B	1	ANP	C5-N7	-2.16	1.31	1.39
2	B	1	ANP	PB-O2B	-2.13	1.51	1.56
2	C	1	ANP	PG-O3G	-2.10	1.51	1.56

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	ANP	O1G-PG-N3B	-8.61	99.09	111.77
2	A	1	ANP	O1G-PG-N3B	-6.27	102.53	111.77
2	B	1	ANP	O2B-PB-O1B	5.81	122.10	109.92
2	B	1	ANP	O1B-PB-N3B	-5.71	103.36	111.77
2	B	1	ANP	C4-C5-N7	-4.71	104.49	109.40
2	A	1	ANP	O1B-PB-N3B	-4.47	105.19	111.77
2	B	1	ANP	PA-O3A-PB	-4.32	117.39	132.62
2	C	1	ANP	PA-O3A-PB	-4.05	118.35	132.62
2	C	1	ANP	O1G-PG-N3B	-3.92	106.00	111.77
2	C	1	ANP	O2B-PB-O1B	3.81	117.91	109.92
2	A	1	ANP	O2B-PB-O1B	3.42	117.09	109.92
2	A	1	ANP	N3-C2-N1	-3.40	123.36	128.68
2	A	1	ANP	O3G-PG-O2G	3.20	116.16	107.64
2	C	1	ANP	N3-C2-N1	-3.16	123.74	128.68
2	B	1	ANP	C1'-N9-C4	3.12	132.12	126.64
2	C	1	ANP	O1B-PB-N3B	-2.99	107.36	111.77
2	B	1	ANP	O3G-PG-O2G	2.50	114.29	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	ANP	C4-C5-N7	-2.50	106.80	109.40
2	C	1	ANP	O3G-PG-O2G	2.48	114.25	107.64
2	C	1	ANP	C2-N1-C6	2.48	123.00	118.75
2	A	1	ANP	C5-C6-N6	-2.38	116.73	120.35
2	C	1	ANP	C4-C5-N7	-2.36	106.94	109.40
2	A	1	ANP	N6-C6-N1	2.24	123.23	118.57
2	A	1	ANP	C2'-C3'-C4'	2.16	106.84	102.64

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	ANP	C4'
2	C	1	ANP	C2'
2	C	1	ANP	C3'
2	C	1	ANP	C1'
2	A	1	ANP	C4'
2	A	1	ANP	C2'
2	A	1	ANP	C3'
2	A	1	ANP	C1'
2	B	1	ANP	C4'
2	B	1	ANP	C2'
2	B	1	ANP	C3'
2	B	1	ANP	C1'

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1	ANP	PB-N3B-PG-O1G
2	C	1	ANP	C5'-O5'-PA-O3A
2	C	1	ANP	O4'-C4'-C5'-O5'
2	A	1	ANP	PB-N3B-PG-O1G
2	A	1	ANP	PG-N3B-PB-O1B
2	A	1	ANP	C5'-O5'-PA-O1A
2	A	1	ANP	C4'-C5'-O5'-PA
2	A	1	ANP	C3'-C4'-C5'-O5'
2	B	1	ANP	PG-N3B-PB-O1B
2	B	1	ANP	C5'-O5'-PA-O1A
2	B	1	ANP	C4'-C5'-O5'-PA
2	A	1	ANP	O4'-C4'-C5'-O5'
2	A	1	ANP	C5'-O5'-PA-O3A
2	B	1	ANP	C5'-O5'-PA-O3A
2	C	1	ANP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	C	1	ANP	C3'-C4'-C5'-O5'
2	C	1	ANP	PB-O3A-PA-O2A
2	B	1	ANP	C5'-O5'-PA-O2A
2	B	1	ANP	PB-N3B-PG-O1G

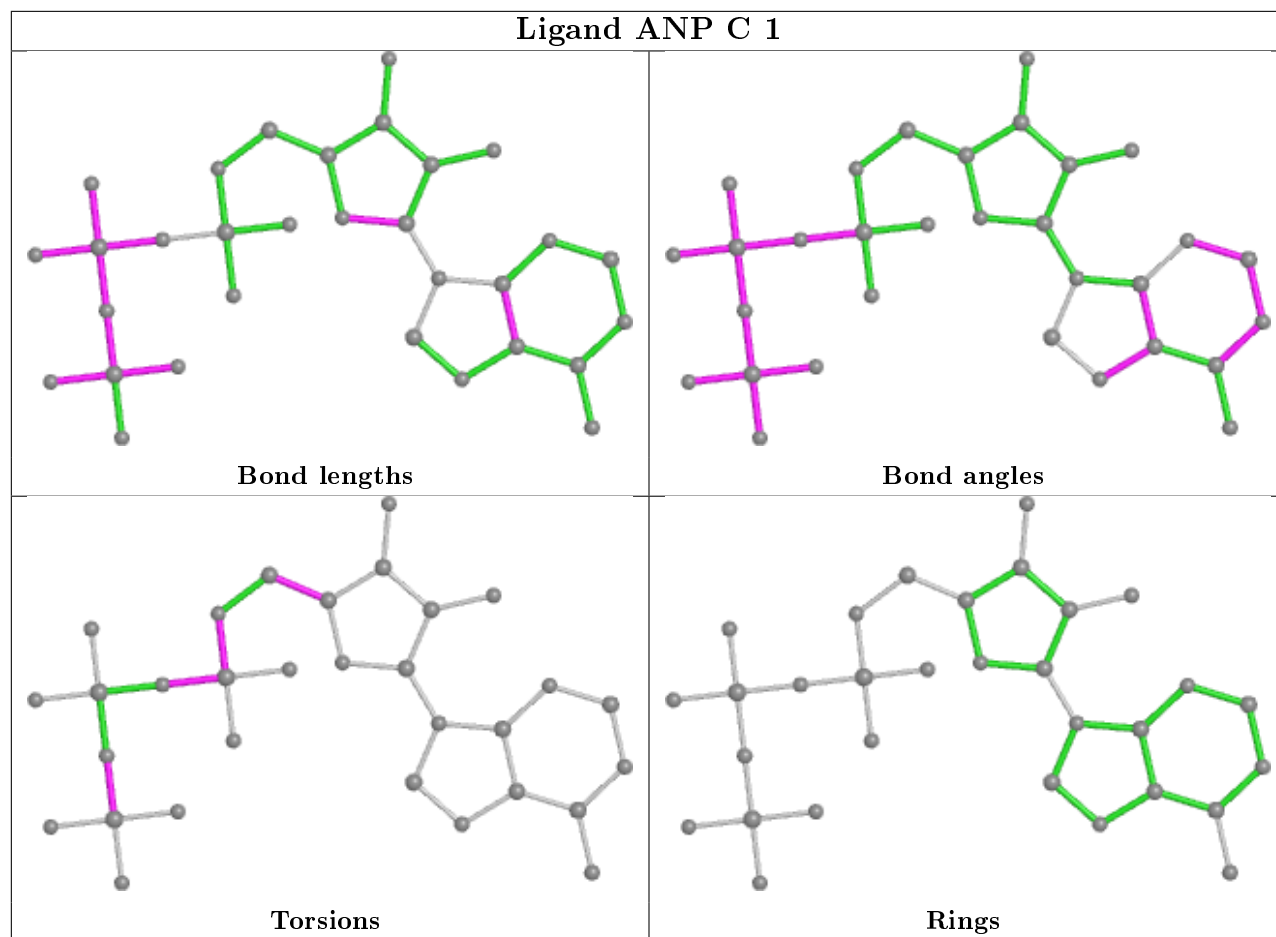
There are no ring outliers.

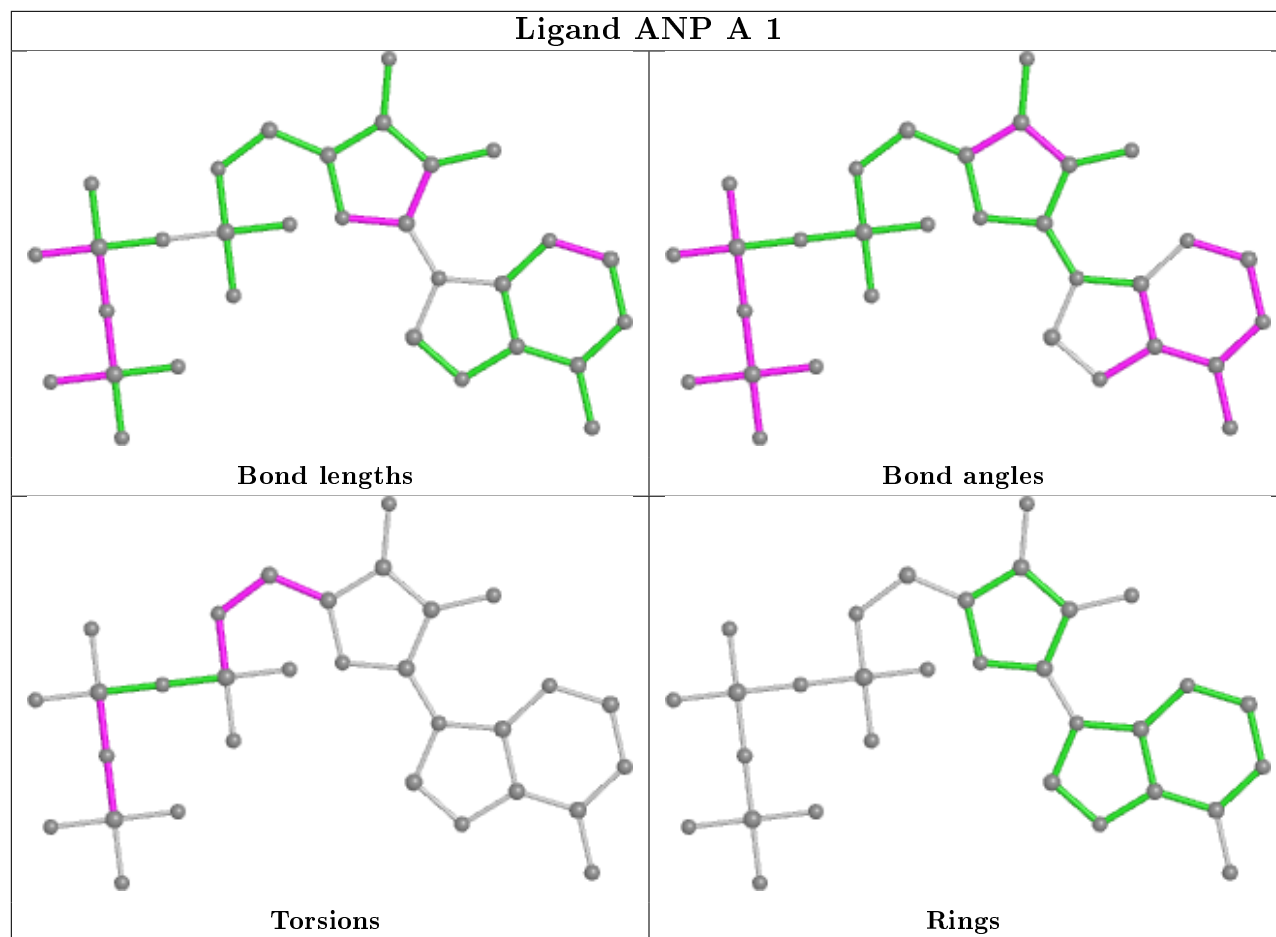
3 monomers are involved in 9 short contacts:

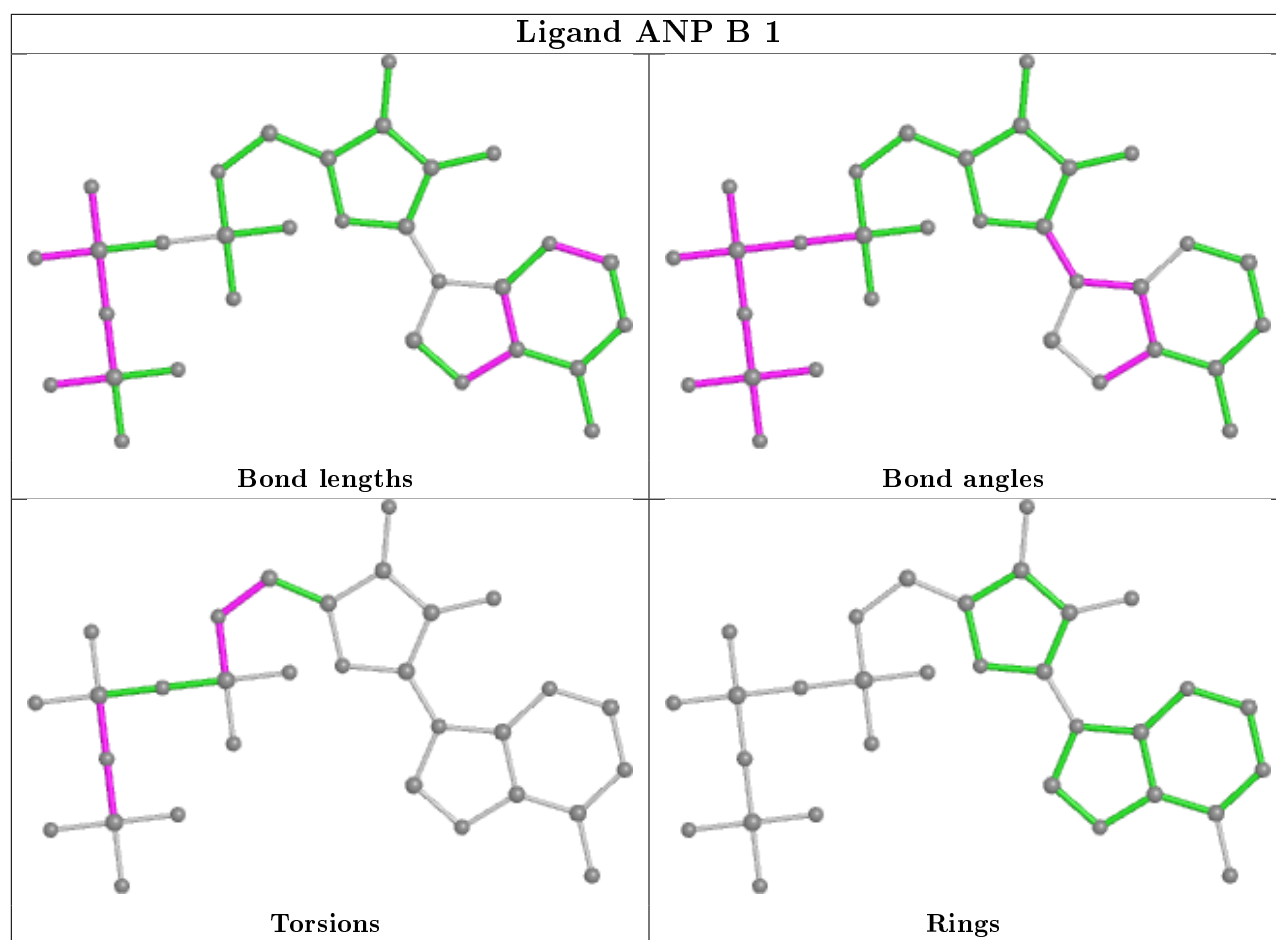
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	ANP	3	0
2	A	1	ANP	2	0
2	B	1	ANP	4	0

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

Ligand ANP C 1







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, 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	270/327 (82%)	0.53	15 (5%) 24 30	27, 47, 78, 118	0
1	B	263/327 (80%)	0.76	35 (13%) 3 4	27, 54, 83, 109	0
1	C	183/327 (55%)	0.87	26 (14%) 2 3	44, 67, 93, 108	0
All	All	716/981 (72%)	0.70	76 (10%) 6 8	27, 56, 86, 118	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	PRO	14.9
1	B	304	ARG	5.6
1	B	325	PRO	5.6
1	C	365	PRO	5.2
1	B	155	SER	5.1
1	B	360	GLU	5.1
1	B	305	PHE	4.6
1	B	110	ARG	4.5
1	B	335	GLU	4.4
1	B	219	LEU	4.3
1	C	298	TYR	4.3
1	C	338	PRO	4.2
1	A	113	TYR	4.2
1	B	350	LYS	4.2
1	C	329	SER	4.2
1	C	177	CYS	4.0
1	B	366	PHE	3.8
1	C	384	ILE	3.8
1	C	289	ASP	3.7
1	B	361	LEU	3.6
1	C	175	TRP	3.6
1	B	344	VAL	3.6
1	A	309	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	113	TYR	3.5
1	B	156	SER	3.5
1	C	332	GLU	3.4
1	A	350	LYS	3.3
1	C	164	PHE	3.3
1	C	288	SER	3.2
1	C	291	TRP	3.2
1	A	250	ILE	3.1
1	C	350	LYS	3.1
1	C	359	LYS	3.1
1	B	248	PHE	3.1
1	B	230	ILE	3.0
1	B	250	ILE	3.0
1	B	84	SER	3.0
1	B	349	THR	3.0
1	C	380	TYR	2.9
1	B	351	ASP	2.7
1	C	305	PHE	2.7
1	C	355	ARG	2.7
1	C	183	THR	2.6
1	A	344	VAL	2.6
1	B	254	LEU	2.6
1	C	373	ARG	2.5
1	B	337	SER	2.5
1	A	132	ARG	2.5
1	A	140	LYS	2.5
1	B	340	PHE	2.5
1	C	134	ARG	2.5
1	C	301	ALA	2.4
1	B	338	PRO	2.4
1	C	195	VAL	2.4
1	A	127	ILE	2.4
1	A	295	ILE	2.4
1	C	129	ALA	2.3
1	C	353	SER	2.3
1	C	352	GLU	2.3
1	B	324	ASP	2.3
1	B	287	ARG	2.3
1	A	212	THR	2.2
1	B	188	PHE	2.2
1	B	233	SER	2.2
1	B	390	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	286	VAL	2.2
1	B	95	TRP	2.2
1	B	154	ARG	2.1
1	A	156	SER	2.1
1	A	166	GLY	2.1
1	C	176	ILE	2.1
1	B	195	VAL	2.1
1	A	304	ARG	2.1
1	B	306	PRO	2.1
1	B	308	PRO	2.1
1	A	160	TYR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

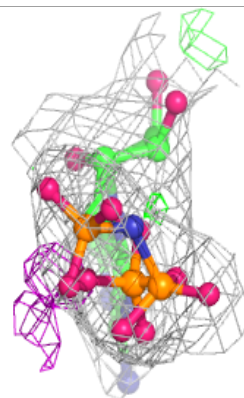
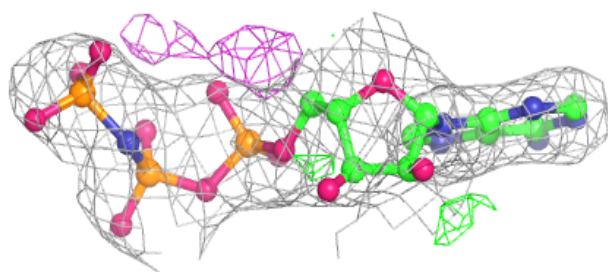
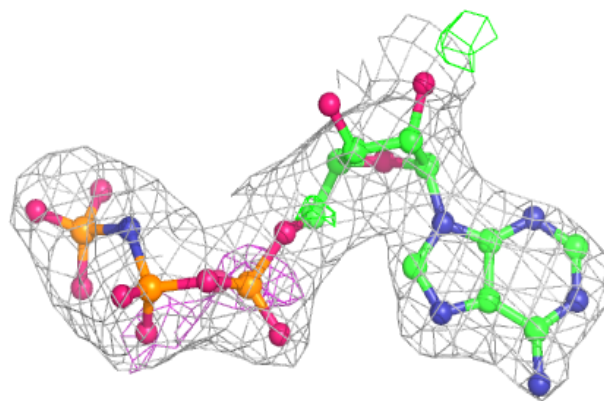
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ANP	C	1	31/31	0.90	0.14	46,56,87,94	0
3	MG	B	406	1/1	0.90	0.17	63,63,63,63	0
2	ANP	B	1	31/31	0.93	0.13	27,52,81,99	0
2	ANP	A	1	31/31	0.96	0.14	26,43,61,72	0
3	MG	A	406	1/1	0.96	0.13	53,53,53,53	0

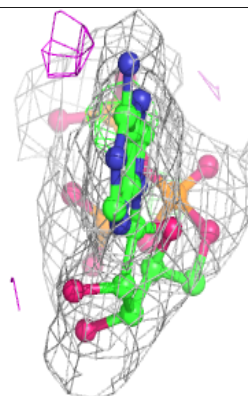
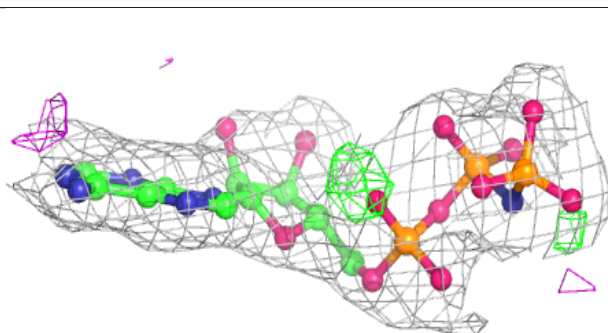
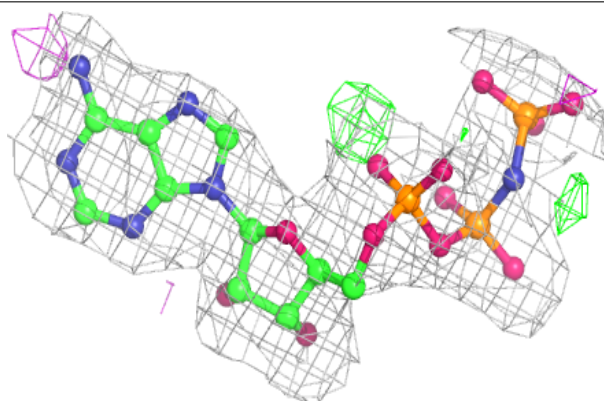
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

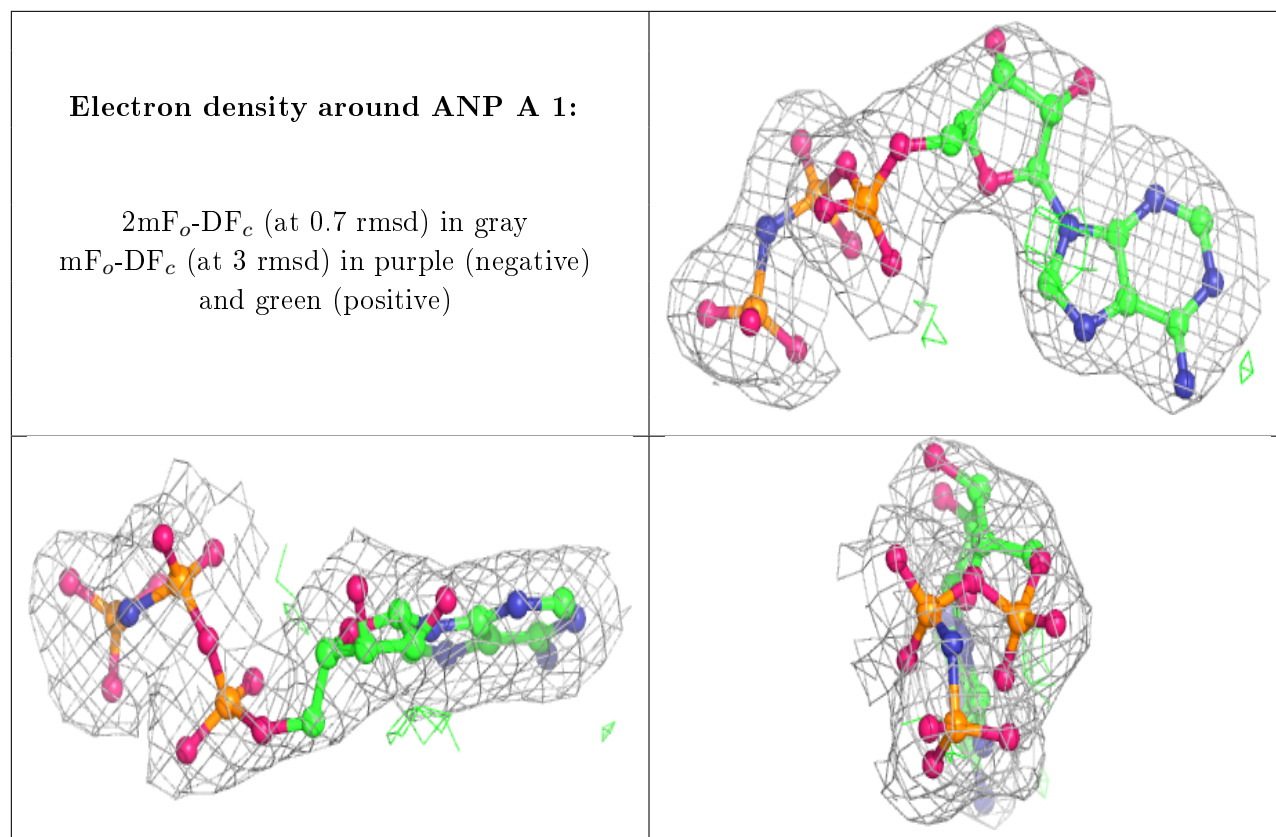
Electron density around ANP C 1:

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

**Electron density around ANP B 1:**

$2mF_o-DF_c$ (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.