Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 03:55 PM EST

PDB ID	:	1II9
Title	:	CRYSTAL STRUCTURE OF THE ESCHERICHIA COLI ARSENITE-TRANSLOCATING ATPASE IN COMPLEX WITH AMP-PNP
Authors	:	Zhou, T.; Radaev, S.; Gatti, D.L.; Rosen, B.P.
Deposited on	:	2001-04-21
Resolution	:	2.60 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 (i) 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 (i)) were used in the production of this report:

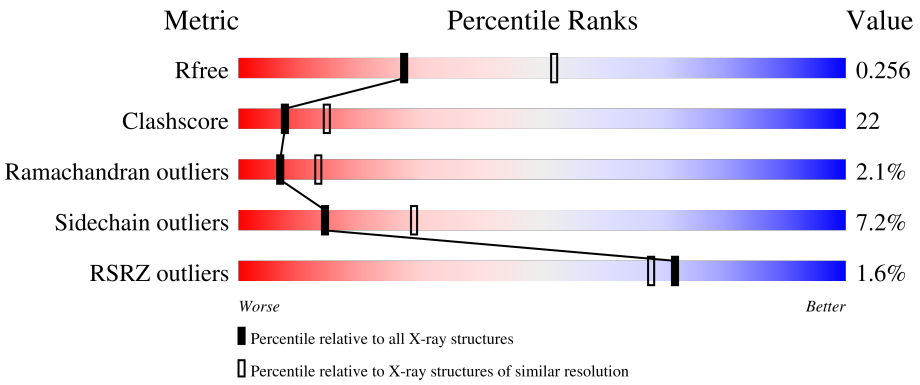
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	589	56% 32% • 8%
1	B	589	3% 55% 34% • 7%

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
7	TAS	A	701	-	-	X	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8786 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 ARSENICAL PUMP-DRIVING ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	544	4163	2620	738	790	15	0	0	0
1	B	550	4202	2641	744	802	15	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASN	ILE	SEE REMARK 999	UNP P08690
A	584	HIS	-	expression tag	UNP P08690
A	585	HIS	-	expression tag	UNP P08690
A	586	HIS	-	expression tag	UNP P08690
A	587	HIS	-	expression tag	UNP P08690
A	588	HIS	-	expression tag	UNP P08690
A	589	HIS	-	expression tag	UNP P08690
B	1060	ASN	ILE	SEE REMARK 999	UNP P08690
B	1584	HIS	-	expression tag	UNP P08690
B	1585	HIS	-	expression tag	UNP P08690
B	1586	HIS	-	expression tag	UNP P08690
B	1587	HIS	-	expression tag	UNP P08690
B	1588	HIS	-	expression tag	UNP P08690
B	1589	HIS	-	expression tag	UNP P08690

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	2	2	2	0	0
2	B	2	2	2	0	0

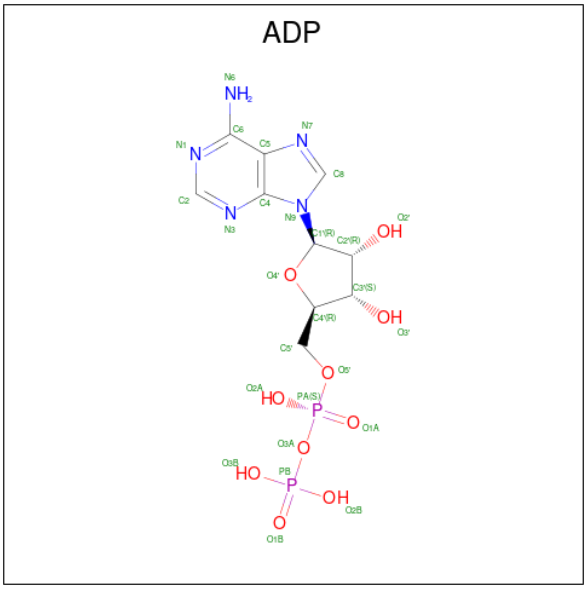
- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
3	A	9	9	9	0	0
			Total	Cd		
3	B	9	9	9	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

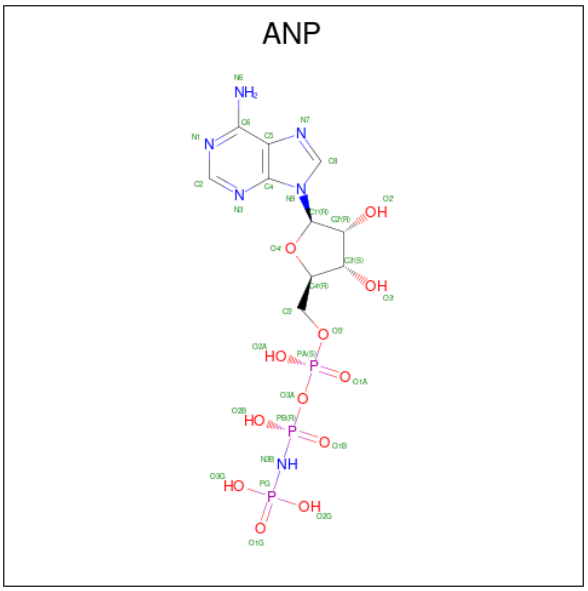
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	4	4	4	0	0
			Total	Cl		
4	B	3	3	3	0	0

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



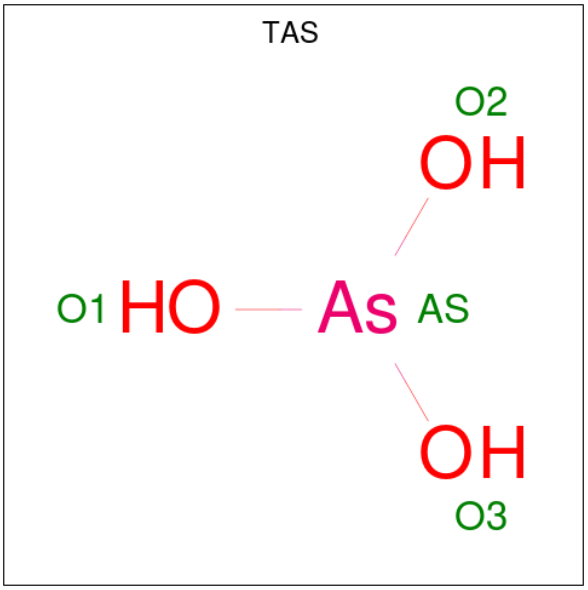
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
5	B	1	27	10	5	10	2	0	0

- Molecule 6 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
			Total	C	N	O	P		
6	A	1	31	10	6	12	3	0	0
			Total	C	N	O	P		
6	B	1	31	10	6	12	3	0	0

- Molecule 7 is TRIHYDROXYARSENITE(III) (three-letter code: TAS) (formula: AsH_3O_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	As	O		
7	A	1	4	1	3	0	0
			Total	As	O		
7	B	1	4	1	3	0	0

- Molecule 8 is water.

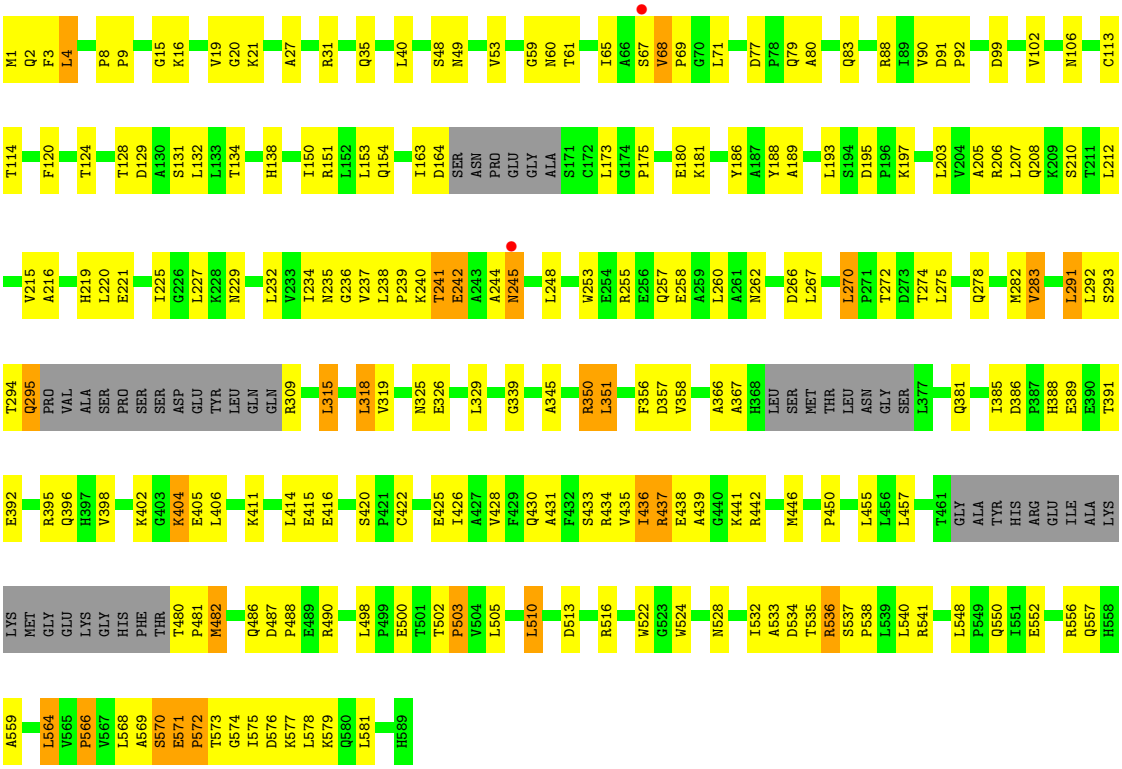
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	143	143	143	0	0
			Total	O		
8	B	125	125	125	0	0

3 Residue-property plots (i)

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.

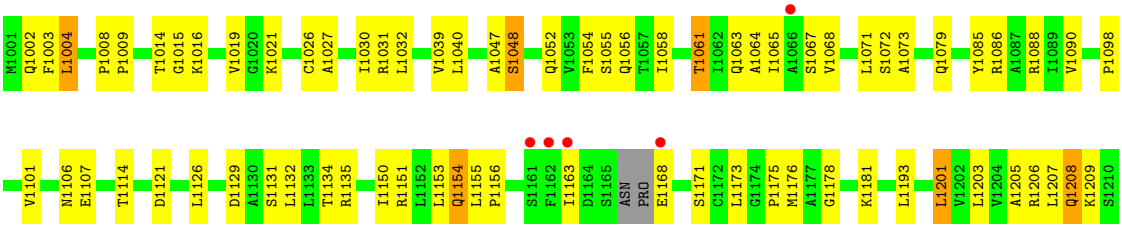
• Molecule 1: ARSENICAL PUMP-DRIVING ATPASE

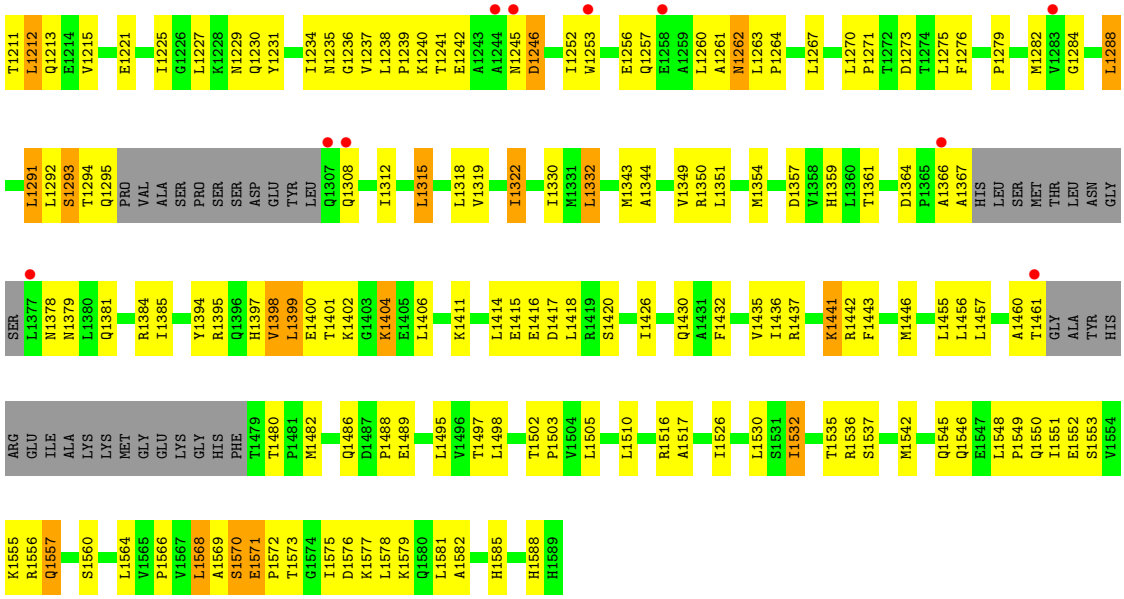
Chain A: 56% 32% • 8%



• Molecule 1: ARSENICAL PUMP-DRIVING ATPASE

Chain B: 3% 55% 34% • 7%




T1211 L1212 Q1213 E1214 V1215 E1221 I1225 G1226 L1227 K1228 N1229 Q1230 Y1231 I1234 N1235 G1236 V1237 L1238 P1239 K1240 T1241 E1242 A1243 A1244 N1245 D1246 I1252 W1253 E1256 Q1257 E1258 A1259 L1260 A1261 N1262 L1263 P1264 L1267 L1270 P1271 T1272 D1273 T1274 L1275 F1276 P1279 M1282 V1283 G1284 L1288
L1291 L1292 S1293 T1294 Q1295 PRO VAL ALA SER PRO SER SER ASP GLU TYR LEU Q1307 Q1308 I1312 L1315 L1318 V1319 I1322 I1330 M1331 L1332 M1343 A1344 V1349 R1350 L1351 M1354 D1357 V1358 H1359 L1360 T1361 D1364 P1365 A1366 A1367 HIS LEU SER MET THR LEU ASN GLY
SER L1377 N1378 N1379 L1380 Q1381 R1384 I1385 Y1394 R1395 Q1396 H1397 V1398 L1399 E1400 T1401 K1402 G1403 K1404 E1405 L1406 K1411 L1414 E1415 E1416 D1417 L1418 R1419 S1420 I1426 Q1430 A1431 F1432 V1435 I1436 R1437 K1441 R1442 F1443 M1446 L1455 L1456 L1457 A1460 T1461 GLY ALA TYR HIS
ARG GLU ILE ALA LYS LYS MET GLY GLU LYS GLY HIS PHE T1479 T1480 P1481 M1482 Q1486 D1487 P1488 E1489 L1495 V1496 T1497 L1498 T1502 P1503 V1504 L1505 L1510 R1516 A1517 I1526 L1530 S1531 I1532 T1535 R1536 S1537 M1542 Q1545 Q1546 E1547 L1548 P1549 Q1550 I1551 E1552 S1553 V1554
K1555 R1556 Q1557 S1560 L1564 V1565 P1566 V1567 L1568 A1569 S1570 E1571 P1572 T1573 G1574 I1575 D1576 K1577 L1578 K1579 Q1580 L1581 A1582 H1585 H1588 H1589

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	76.62Å 222.53Å 74.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.52 – 2.60 37.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.5 (36.52-2.60) 93.4 (37.02-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.191 , 0.265 0.184 , 0.256	Depositor DCC
R_{free} test set	3730 reflections (9.71%)	wwPDB-VP
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8786	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, CD, MG, ANP, ADP, TAS

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	0.41	0/4233	0.69	0/5752
1	B	0.42	0/4271	0.66	1/5803 (0.0%)
All	All	0.41	0/8504	0.68	1/11555 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1406	LEU	N-CA-C	-5.56	95.98	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	4163	0	4226	200	0
1	B	4202	0	4259	175	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	0	0	0
3	B	9	0	0	0	0
4	A	4	0	0	1	0
4	B	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	27	0	12	5	0
5	B	27	0	12	2	0
6	A	31	0	13	2	0
6	B	31	0	13	0	0
7	A	4	0	0	2	0
7	B	4	0	0	0	0
8	A	143	0	0	3	0
8	B	125	0	0	6	0
All	All	8786	0	8535	375	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 22.

All (375) 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:27:ALA:HB1	1:A:292:LEU:HD21	1.27	1.10
1:A:248:LEU:HD23	1:A:535:THR:HB	1.38	1.02
1:B:1322:ILE:HD13	1:B:1330:ILE:HD11	1.42	1.01
1:B:1209:LYS:HG2	1:B:1213:GLN:HE21	1.26	0.99
1:A:235:ASN:HD21	5:A:590:ADP:HN61	1.02	0.95
1:A:381:GLN:HE21	1:A:442:ARG:HH12	1.10	0.93
1:B:1114:THR:OG1	1:B:1175:PRO:HG3	1.69	0.93
1:B:1235:ASN:ND2	1:B:1236:GLY:H	1.66	0.93
1:A:235:ASN:ND2	1:A:236:GLY:H	1.69	0.90
1:A:294:THR:O	1:A:295:GLN:HB2	1.73	0.87
1:B:1090:VAL:HG21	1:B:1106:ASN:HD22	1.37	0.87
1:B:1209:LYS:HG2	1:B:1213:GLN:NE2	1.90	0.85
1:A:532:ILE:HG23	1:A:566:PRO:HB3	1.57	0.84
1:B:1404:LYS:HE3	1:B:1404:LYS:HA	1.58	0.84
1:A:576:ASP:HB2	1:A:577:LYS:NZ	1.91	0.84
1:A:205:ALA:HB2	1:A:215:VAL:HG21	1.60	0.83
1:A:235:ASN:ND2	5:A:590:ADP:HN61	1.76	0.83
1:A:568:LEU:HD22	1:A:570:SER:HB3	1.61	0.82
1:A:255:ARG:HH12	1:A:570:SER:H	1.29	0.80
1:A:381:GLN:HE21	1:A:442:ARG:NH1	1.79	0.79
1:A:381:GLN:NE2	1:A:442:ARG:HH22	1.81	0.79
1:B:1205:ALA:HB2	1:B:1215:VAL:HG21	1.63	0.79
1:A:131:SER:O	1:A:134:THR:HB	1.85	0.77
1:A:244:ALA:O	1:A:245:ASN:HB3	1.84	0.77
1:A:1:MET:HB2	1:A:4:LEU:HD22	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:HA	1:A:541:ARG:NH2	2.00	0.76
1:A:275:LEU:HD13	1:A:291:LEU:HD22	1.67	0.75
1:B:1163:ILE:HD12	1:B:1173:LEU:HD12	1.68	0.75
1:A:537:SER:OG	1:A:540:LEU:HD23	1.88	0.74
1:B:1357:ASP:OD2	1:B:1442:ARG:HD3	1.88	0.73
1:A:433:SER:HA	1:A:436:ILE:HG13	1.71	0.73
1:B:1058:ILE:HD12	1:B:1073:ALA:HB3	1.70	0.72
1:A:391:THR:HG22	1:A:395:ARG:HD2	1.70	0.72
1:A:220:LEU:HD11	1:A:266:ASP:OD1	1.90	0.72
1:B:1395:ARG:HG2	1:B:1418:LEU:HB3	1.72	0.72
1:A:239:PRO:HB3	1:A:295:GLN:HE21	1.55	0.72
1:A:513:ASP:OD1	1:A:516:ARG:NH1	2.23	0.71
1:B:1441:LYS:HD2	1:B:1441:LYS:N	2.06	0.71
1:A:385:ILE:HD11	1:A:428:VAL:HG13	1.73	0.70
1:A:536:ARG:HA	1:A:541:ARG:CZ	2.22	0.70
1:A:255:ARG:NH1	1:A:570:SER:H	1.89	0.70
1:B:1532:ILE:HG12	1:B:1566:PRO:HB3	1.74	0.69
1:A:235:ASN:ND2	1:A:236:GLY:N	2.38	0.69
1:A:68:VAL:HG22	1:A:68:VAL:O	1.93	0.69
1:A:386:ASP:HB3	1:A:389:GLU:HG2	1.74	0.69
1:A:431:ALA:O	1:A:434:ARG:HB2	1.93	0.69
1:B:1349:VAL:HG21	1:B:1575:ILE:HD11	1.75	0.69
1:B:1235:ASN:ND2	1:B:1236:GLY:N	2.39	0.68
1:A:319:VAL:HG13	1:A:351:LEU:HD13	1.76	0.68
1:B:1003:PHE:CE1	1:B:1004:LEU:HD13	2.29	0.68
1:B:1275:LEU:HD13	1:B:1291:LEU:HD22	1.75	0.68
1:A:90:VAL:HG21	1:A:106:ASN:HD22	1.59	0.68
1:A:1:MET:HB2	1:A:4:LEU:CD2	2.25	0.67
1:A:16:LYS:HG2	1:A:19:VAL:CG1	2.24	0.67
1:A:128:THR:HG22	1:A:188:TYR:HD2	1.59	0.67
1:A:206:ARG:HH22	7:A:701:TAS:AS	2.38	0.67
1:B:1312:ILE:HD11	1:B:1555:LYS:HD3	1.76	0.66
1:A:16:LYS:HG2	1:A:19:VAL:HG13	1.76	0.66
1:B:1207:LEU:HG	1:B:1234:ILE:HG21	1.75	0.66
1:A:568:LEU:HD13	1:A:572:PRO:HG3	1.78	0.65
1:B:1107:GLU:OE1	1:B:1516:ARG:NH2	2.30	0.65
1:A:163:ILE:HD12	1:A:173:LEU:CD1	2.26	0.65
1:B:1308:GLN:HB3	8:B:2243:HOH:O	1.95	0.65
1:A:381:GLN:HE22	1:A:442:ARG:HH22	1.44	0.65
1:A:292:LEU:N	1:A:292:LEU:HD22	2.10	0.65
1:B:1436:ILE:HG12	1:B:1446:MET:CE	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASN:O	1:A:53:VAL:HG13	1.97	0.64
1:A:207:LEU:HG	1:A:234:ILE:HG21	1.79	0.64
1:B:1016:LYS:O	1:B:1019:VAL:HG13	1.97	0.64
1:A:283:VAL:HG22	1:A:283:VAL:O	1.98	0.63
1:A:275:LEU:HD13	1:A:291:LEU:CD2	2.28	0.63
1:A:255:ARG:NH2	1:A:569:ALA:HA	2.13	0.63
1:B:1404:LYS:HE3	1:B:1404:LYS:CA	2.28	0.63
1:B:1235:ASN:HD21	5:B:1590:ADP:HN61	1.45	0.63
1:A:88:ARG:HD3	1:A:180:GLU:CD	2.20	0.62
1:A:552:GLU:OE1	1:A:556:ARG:HG3	1.98	0.62
1:A:568:LEU:O	1:A:569:ALA:HB3	2.00	0.62
1:B:1417:ASP:O	1:B:1420:SER:HB2	1.99	0.62
1:B:1426:ILE:O	1:B:1430:GLN:HG3	2.00	0.62
1:A:395:ARG:HB3	1:A:395:ARG:NH1	2.15	0.62
1:A:576:ASP:HB2	1:A:577:LYS:HZ3	1.61	0.62
1:B:1322:ILE:HD13	1:B:1330:ILE:CD1	2.25	0.62
1:B:1086:ARG:HG2	1:B:1106:ASN:HD21	1.65	0.62
1:A:576:ASP:HB2	1:A:577:LYS:HZ2	1.63	0.61
1:B:1315:LEU:O	1:B:1319:VAL:HG23	2.00	0.61
1:B:1400:GLU:HG3	1:B:1401:THR:N	2.15	0.61
1:A:260:LEU:HD13	1:A:260:LEU:C	2.20	0.61
1:B:1071:LEU:HD12	1:B:1072:SER:H	1.65	0.61
1:B:1361:THR:HG21	1:B:1435:VAL:HG21	1.83	0.61
1:A:114:THR:OG1	1:A:175:PRO:HG3	2.02	0.60
1:A:532:ILE:HD11	8:A:2116:HOH:O	2.02	0.60
1:A:235:ASN:HD22	1:A:236:GLY:H	1.45	0.60
1:B:1436:ILE:HG12	1:B:1446:MET:HE3	1.83	0.59
1:A:195:ASP:OD1	1:A:197:LYS:HB2	2.03	0.59
1:B:1151:ARG:NH2	1:B:1221:GLU:OE1	2.34	0.59
1:A:441:LYS:H	1:A:441:LYS:HD2	1.68	0.59
1:B:1502:THR:HB	1:B:1503:PRO:HD3	1.85	0.59
1:A:433:SER:HA	1:A:436:ILE:CG1	2.33	0.59
1:B:1245:ASN:O	1:B:1246:ASP:HB2	2.03	0.59
1:B:1008:PRO:HB2	1:B:1009:PRO:HD2	1.85	0.59
1:A:391:THR:O	1:A:395:ARG:HG3	2.03	0.58
1:B:1207:LEU:HD12	1:B:1237:VAL:HG13	1.86	0.58
1:A:422:CYS:HA	1:A:425:GLU:HB3	1.84	0.58
1:B:1235:ASN:ND2	5:B:1590:ADP:HN61	2.02	0.58
1:A:151:ARG:HD2	1:A:416:GLU:OE1	2.03	0.58
1:B:1086:ARG:HG2	1:B:1106:ASN:ND2	2.19	0.58
1:A:498:LEU:CD2	1:A:528:ASN:HD22	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLN:O	1:A:83:GLN:HG3	2.04	0.57
1:B:1151:ARG:O	1:B:1154:GLN:HG2	2.03	0.57
1:B:1349:VAL:CG2	1:B:1575:ILE:HD11	2.35	0.57
1:A:238:LEU:HD12	1:A:253:TRP:HB2	1.85	0.57
1:B:1064:ALA:HA	1:B:1072:SER:HA	1.86	0.57
1:B:1332:LEU:HD13	1:B:1344:ALA:HB2	1.86	0.57
1:A:235:ASN:HD21	5:A:590:ADP:N6	1.87	0.57
1:A:381:GLN:NE2	1:A:442:ARG:NH2	2.51	0.56
1:B:1397:HIS:O	1:B:1401:THR:HG22	2.06	0.56
1:A:151:ARG:HH21	1:A:221:GLU:HG2	1.70	0.56
1:A:439:ALA:C	1:A:490:ARG:HH22	2.08	0.56
1:B:1238:LEU:HD12	1:B:1239:PRO:HD2	1.88	0.56
1:B:1401:THR:HG23	1:B:1402:LYS:H	1.72	0.56
1:B:1552:GLU:OE1	1:B:1556:ARG:HD2	2.06	0.56
1:A:395:ARG:CB	1:A:395:ARG:HH11	2.18	0.55
1:B:1319:VAL:HG11	1:B:1350:ARG:CG	2.35	0.55
1:A:425:GLU:CG	1:A:450:PRO:HA	2.36	0.55
1:A:395:ARG:HB3	1:A:395:ARG:HH11	1.70	0.55
1:B:1201:LEU:HB3	1:B:1230:GLN:HG2	1.87	0.55
1:B:1553:SER:O	1:B:1557:GLN:HB3	2.06	0.55
1:A:404:LYS:HB3	1:A:405:GLU:OE1	2.06	0.55
1:B:1404:LYS:HA	1:B:1404:LYS:CE	2.35	0.55
1:A:239:PRO:O	1:A:242:GLU:HB2	2.07	0.54
1:A:240:LYS:HB2	1:A:253:TRP:NE1	2.23	0.54
1:A:437:ARG:HG2	1:A:438:GLU:N	2.21	0.54
1:A:128:THR:HG22	1:A:188:TYR:CD2	2.42	0.54
1:B:1235:ASN:HD22	1:B:1275:LEU:HB2	1.72	0.54
1:B:1282:MET:HB3	1:B:1288:LEU:HD13	1.88	0.54
1:B:1486:GLN:O	1:B:1488:PRO:HD3	2.07	0.54
1:B:1150:ILE:HG21	1:B:1225:ILE:HG21	1.90	0.54
1:B:1098:PRO:HB2	1:B:1101:VAL:HG23	1.90	0.54
1:B:1570:SER:O	1:B:1571:GLU:HB2	2.07	0.54
1:A:319:VAL:HG13	1:A:351:LEU:CD1	2.37	0.54
1:A:568:LEU:CD1	1:A:572:PRO:HG3	2.38	0.54
1:A:339:GLY:HA2	6:A:591:ANP:PA	2.48	0.53
1:A:248:LEU:CD1	1:A:569:ALA:HB2	2.39	0.53
1:B:1267:LEU:HA	1:B:1270:LEU:HD13	1.90	0.53
1:A:571:GLU:O	1:A:573:THR:N	2.34	0.53
1:B:1068:VAL:HG11	1:B:1071:LEU:HD23	1.91	0.53
1:A:240:LYS:HB2	1:A:253:TRP:HE1	1.72	0.53
1:A:402:LYS:O	1:A:406:LEU:HD13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LEU:CD2	1:A:570:SER:HB3	2.38	0.52
1:B:1235:ASN:HD22	1:B:1236:GLY:H	1.48	0.52
1:B:1151:ARG:NH1	1:B:1416:GLU:OE2	2.42	0.52
1:A:216:ALA:HA	1:A:267:LEU:HD21	1.91	0.52
1:A:439:ALA:O	1:A:490:ARG:NH2	2.43	0.52
1:A:502:THR:HB	1:A:503:PRO:HD3	1.91	0.52
1:B:1168:GLU:OE2	1:B:1461:THR:HA	2.10	0.52
1:B:1568:LEU:HD12	1:B:1581:LEU:HD21	1.92	0.52
1:A:15:GLY:N	1:A:21:LYS:HD3	2.25	0.52
1:A:426:ILE:O	1:A:430:GLN:HG3	2.10	0.52
1:A:240:LYS:HA	1:A:253:TRP:CD1	2.45	0.51
1:B:1173:LEU:O	1:B:1176:MET:HG2	2.10	0.51
1:A:163:ILE:HD12	1:A:173:LEU:HD13	1.92	0.51
1:B:1322:ILE:HD12	1:B:1443:PHE:CE2	2.46	0.51
1:B:1357:ASP:O	1:B:1442:ARG:HB2	2.10	0.51
1:B:1154:GLN:HG2	1:B:1155:LEU:N	2.26	0.51
1:B:1252:ILE:O	1:B:1256:GLU:HG3	2.11	0.51
1:A:357:ASP:O	1:A:442:ARG:HB2	2.10	0.51
1:B:1168:GLU:HG2	1:B:1460:ALA:O	2.11	0.50
1:B:1532:ILE:CG2	1:B:1564:LEU:HD13	2.41	0.50
1:B:1058:ILE:HD12	1:B:1073:ALA:CB	2.40	0.50
1:A:8:PRO:O	1:A:138:HIS:HD2	1.93	0.50
1:A:309:ARG:NH2	1:A:533:ALA:O	2.44	0.50
1:B:1532:ILE:HG22	1:B:1564:LEU:HD13	1.93	0.50
1:A:90:VAL:HG13	1:A:102:VAL:HG13	1.92	0.50
1:B:1086:ARG:CG	1:B:1106:ASN:ND2	2.74	0.50
1:B:1279:PRO:HB3	1:B:1542:MET:HG2	1.92	0.50
1:B:1532:ILE:O	1:B:1532:ILE:CG1	2.60	0.50
1:B:1284:GLY:O	1:B:1288:LEU:HD22	2.12	0.50
1:B:1242:GLU:HG3	1:B:1537:SER:OG	2.12	0.50
1:A:232:LEU:HD23	1:A:272:THR:CG2	2.42	0.49
1:A:319:VAL:HG11	1:A:350:ARG:HG3	1.94	0.49
1:B:1151:ARG:HH11	1:B:1416:GLU:CD	2.15	0.49
1:B:1437:ARG:HG2	8:B:2242:HOH:O	2.12	0.49
1:A:234:ILE:O	1:A:274:THR:HA	2.12	0.49
1:B:1019:VAL:HG11	8:B:2114:HOH:O	2.12	0.49
1:A:3:PHE:CD1	1:A:4:LEU:HD13	2.47	0.49
1:A:318:LEU:HD22	1:A:522:TRP:CZ3	2.47	0.49
1:B:1312:ILE:CD1	1:B:1555:LYS:HD3	2.42	0.49
1:B:1378:ASN:O	1:B:1379:ASN:CB	2.60	0.49
1:B:1456:LEU:HD21	1:B:1517:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1027:ALA:HB1	1:B:1292:LEU:HD21	1.94	0.49
1:B:1322:ILE:CD1	1:B:1330:ILE:HD11	2.29	0.49
1:B:1332:LEU:HD22	1:B:1343:MET:HB2	1.94	0.49
1:B:1061:THR:CG2	1:B:1063:GLN:HG3	2.43	0.49
1:B:1394:TYR:O	1:B:1398:VAL:HG12	2.13	0.49
1:A:3:PHE:CE1	1:A:4:LEU:HD13	2.47	0.49
1:B:1207:LEU:HG	1:B:1234:ILE:CG2	2.43	0.49
1:A:8:PRO:HB2	1:A:9:PRO:HD2	1.94	0.49
1:A:129:ASP:OD2	1:A:132:LEU:HD13	2.13	0.49
1:A:232:LEU:HD23	1:A:272:THR:HG23	1.94	0.49
1:A:294:THR:O	1:A:295:GLN:CB	2.51	0.48
1:A:385:ILE:CD1	1:A:428:VAL:HG13	2.40	0.48
1:B:1240:LYS:O	1:B:1242:GLU:N	2.46	0.48
1:A:386:ASP:OD2	1:A:388:HIS:HB2	2.13	0.48
1:A:480:THR:N	1:A:481:PRO:CD	2.76	0.48
1:A:240:LYS:O	1:A:242:GLU:N	2.39	0.48
1:A:557:GLN:O	1:A:557:GLN:HG2	2.14	0.48
1:B:1261:ALA:O	1:B:1262:ASN:HB2	2.13	0.48
1:B:1308:GLN:OE1	1:B:1545:GLN:HG3	2.14	0.48
1:B:1052:GLN:O	1:B:1054:PHE:O	2.31	0.48
1:B:1276:PHE:CD2	1:B:1295:GLN:HG3	2.49	0.48
1:B:1332:LEU:HD13	1:B:1344:ALA:CB	2.44	0.48
1:B:1526:ILE:HB	1:B:1564:LEU:HD23	1.95	0.48
1:A:366:ALA:O	1:A:367:ALA:HB2	2.13	0.48
1:A:59:GLY:C	1:A:61:THR:H	2.17	0.47
1:A:411:LYS:O	1:A:415:GLU:HG3	2.15	0.47
1:B:1576:ASP:OD2	1:B:1577:LYS:HE3	2.14	0.47
1:B:1568:LEU:HD12	1:B:1581:LEU:CD2	2.45	0.47
1:B:1270:LEU:HD12	1:B:1270:LEU:H	1.80	0.47
1:B:1319:VAL:HG11	1:B:1350:ARG:HG2	1.96	0.47
1:B:1401:THR:HG23	1:B:1402:LYS:N	2.29	0.47
1:A:88:ARG:HD3	1:A:180:GLU:OE2	2.14	0.47
1:A:203:LEU:HD11	1:A:219:HIS:HB2	1.97	0.47
1:A:532:ILE:CG2	1:A:566:PRO:HB3	2.37	0.47
1:A:568:LEU:HD12	1:A:581:LEU:HD21	1.97	0.47
1:B:1264:PRO:HG2	1:B:1267:LEU:HD12	1.95	0.47
1:B:1225:ILE:HG22	1:B:1225:ILE:O	2.14	0.47
1:B:1411:LYS:O	1:B:1415:GLU:HG3	2.15	0.47
1:B:1246:ASP:OD1	1:B:1535:THR:HA	2.15	0.47
1:A:255:ARG:NH1	1:A:570:SER:N	2.60	0.47
1:B:1056:GLN:OE1	1:B:1065:ILE:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1556:ARG:HD3	8:B:2250:HOH:O	2.15	0.47
1:A:120:PHE:CD1	1:A:153:LEU:HD12	2.50	0.46
1:A:356:PHE:O	1:A:358:VAL:HG23	2.14	0.46
1:A:569:ALA:O	1:A:570:SER:HB2	2.15	0.46
1:B:1240:LYS:C	1:B:1242:GLU:N	2.69	0.46
1:B:1359:HIS:CD2	1:B:1381:GLN:HG3	2.50	0.46
1:B:1480:THR:HG23	1:B:1480:THR:O	2.15	0.46
1:A:1:MET:CB	1:A:4:LEU:HD22	2.43	0.46
1:A:425:GLU:HG3	1:A:450:PRO:HA	1.97	0.46
1:B:1398:VAL:HA	1:B:1401:THR:CG2	2.45	0.46
1:A:113:CYS:HB3	4:A:599:CL:CL	2.53	0.46
1:A:329:LEU:HD11	1:A:446:MET:CE	2.46	0.46
1:A:68:VAL:O	1:A:68:VAL:CG2	2.60	0.46
1:B:1014:THR:CG2	1:B:1203:LEU:HD23	2.45	0.46
1:B:1015:GLY:N	1:B:1021:LYS:HD3	2.31	0.46
1:A:120:PHE:CD1	1:A:153:LEU:CD1	2.99	0.46
1:B:1131:SER:O	1:B:1134:THR:HB	2.16	0.45
1:A:325:ASN:O	1:A:326:GLU:HB2	2.17	0.45
1:B:1026:CYS:O	1:B:1030:ILE:HG13	2.15	0.45
1:B:1129:ASP:OD1	1:B:1132:LEU:HB2	2.17	0.45
1:B:1262:ASN:O	1:B:1263:LEU:C	2.54	0.45
1:B:1367:ALA:HB3	1:B:1384:ARG:HH12	1.81	0.45
1:A:255:ARG:HG2	8:A:2307:HOH:O	2.15	0.45
1:B:1201:LEU:O	1:B:1230:GLN:HA	2.16	0.45
1:A:436:ILE:HG12	1:A:446:MET:CE	2.46	0.45
1:A:575:ILE:O	1:A:579:LYS:HG3	2.17	0.45
1:B:1378:ASN:O	1:B:1379:ASN:HB3	2.15	0.45
1:A:392:GLU:OE2	1:A:395:ARG:HD3	2.16	0.45
1:A:292:LEU:HD22	1:A:292:LEU:H	1.78	0.45
1:B:1052:GLN:O	1:B:1054:PHE:N	2.50	0.45
1:A:239:PRO:HB3	1:A:295:GLN:NE2	2.27	0.45
1:B:1318:LEU:O	1:B:1322:ILE:HG23	2.17	0.45
1:A:240:LYS:C	1:A:242:GLU:H	2.17	0.44
1:A:315:LEU:HD22	1:A:315:LEU:O	2.15	0.44
1:A:540:LEU:N	1:A:540:LEU:HD22	2.32	0.44
1:B:1032:LEU:HB2	1:B:1039:VAL:HG21	1.99	0.44
1:A:278:GLN:HB2	5:A:590:ADP:C2	2.53	0.44
1:B:1441:LYS:N	1:B:1441:LYS:CD	2.76	0.44
1:A:31:ARG:O	1:A:35:GLN:HG3	2.17	0.44
1:A:150:ILE:CG2	1:A:225:ILE:HD13	2.47	0.44
1:A:207:LEU:HD12	1:A:237:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLN:OE1	1:A:210:SER:HB3	2.18	0.44
1:A:433:SER:HA	1:A:436:ILE:CD1	2.48	0.44
1:B:1061:THR:HG23	1:B:1063:GLN:HG3	2.00	0.44
1:A:206:ARG:NH2	7:A:701:TAS:O1	2.49	0.44
1:A:577:LYS:HD3	1:A:577:LYS:N	2.33	0.44
1:B:1088:ARG:NH1	1:B:1178:GLY:O	2.50	0.44
1:B:1546:GLN:O	1:B:1549:PRO:HD2	2.18	0.44
1:A:339:GLY:HA2	6:A:591:ANP:O1A	2.18	0.44
1:A:434:ARG:O	1:A:437:ARG:NH1	2.51	0.44
1:A:524:TRP:CG	1:A:559:ALA:HB2	2.53	0.44
1:A:319:VAL:HG11	1:A:350:ARG:CG	2.48	0.43
1:A:404:LYS:HB3	1:A:404:LYS:HE3	1.85	0.43
1:B:1575:ILE:O	1:B:1578:LEU:HB3	2.17	0.43
1:A:239:PRO:CB	1:A:295:GLN:HE21	2.27	0.43
1:A:258:GLU:OE2	1:A:262:ASN:ND2	2.52	0.43
1:B:1085:TYR:HE2	1:B:1175:PRO:O	2.00	0.43
1:A:77:ASP:HB3	1:A:80:ALA:HB3	2.00	0.43
1:B:1154:GLN:CG	1:B:1155:LEU:N	2.81	0.43
1:A:124:THR:HG23	1:A:189:ALA:HB2	2.01	0.43
1:B:1282:MET:CB	1:B:1288:LEU:HD13	2.48	0.43
1:A:150:ILE:O	1:A:154:GLN:HG2	2.18	0.43
1:A:181:LYS:HB2	1:A:186:TYR:CZ	2.54	0.43
1:B:1135:ARG:HH11	1:B:1135:ARG:HG3	1.83	0.43
1:B:1206:ARG:O	1:B:1212:LEU:HD13	2.19	0.43
1:A:422:CYS:O	1:A:426:ILE:HG13	2.19	0.43
1:A:498:LEU:HD22	1:A:528:ASN:HD22	1.82	0.43
1:B:1231:TYR:CD2	1:B:1271:PRO:HG2	2.54	0.43
1:B:1332:LEU:HD13	1:B:1344:ALA:CA	2.48	0.43
1:A:568:LEU:O	1:A:568:LEU:HD23	2.19	0.43
1:B:1367:ALA:C	1:B:1384:ARG:HH12	2.23	0.43
1:B:1571:GLU:O	1:B:1573:THR:N	2.51	0.43
1:A:235:ASN:HD22	1:A:275:LEU:HB2	1.84	0.43
1:B:1364:ASP:OD1	1:B:1364:ASP:C	2.57	0.43
1:A:65:ILE:HG22	1:A:68:VAL:HG13	2.00	0.42
1:B:1155:LEU:HA	1:B:1156:PRO:HD3	1.74	0.42
1:B:1350:ARG:O	1:B:1354:MET:HG2	2.18	0.42
1:A:193:LEU:O	1:A:227:LEU:HG	2.19	0.42
1:A:435:VAL:O	1:A:437:ARG:N	2.52	0.42
1:A:500:GLU:HB2	1:A:503:PRO:HD2	2.01	0.42
1:B:1240:LYS:HA	1:B:1253:TRP:CD1	2.54	0.42
1:B:1497:THR:OG1	1:B:1498:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:N	1:A:292:LEU:CD2	2.81	0.42
1:A:577:LYS:H	1:A:577:LYS:HE2	1.84	0.42
1:B:1171:SER:HB2	1:B:1417:ASP:OD2	2.19	0.42
1:B:1293:SER:OG	1:B:1294:THR:N	2.52	0.42
1:B:1385:ILE:HD12	1:B:1385:ILE:C	2.39	0.42
1:A:267:LEU:HA	1:A:270:LEU:HD22	2.01	0.42
1:A:385:ILE:HD11	1:A:428:VAL:HG22	2.00	0.42
1:A:480:THR:N	1:A:481:PRO:HD3	2.34	0.42
1:A:537:SER:CB	1:A:540:LEU:HD23	2.49	0.42
1:A:574:GLY:C	1:A:576:ASP:N	2.72	0.42
1:A:579:LYS:HA	8:A:2122:HOH:O	2.19	0.42
1:B:1208:GLN:O	1:B:1212:LEU:HB2	2.19	0.42
1:A:20:GLY:HA2	5:A:590:ADP:O2A	2.20	0.42
1:A:68:VAL:HG22	1:A:71:LEU:HB3	2.00	0.42
1:A:345:ALA:HB1	1:A:578:LEU:HD21	2.02	0.42
1:A:398:VAL:O	1:A:398:VAL:HG12	2.18	0.42
1:B:1332:LEU:HD13	1:B:1344:ALA:HA	2.02	0.42
1:B:1550:GLN:O	1:B:1551:ILE:C	2.58	0.42
1:B:1575:ILE:CG2	1:B:1576:ASP:N	2.83	0.42
1:B:1193:LEU:O	1:B:1227:LEU:HG	2.20	0.42
1:B:1361:THR:OG1	1:B:1446:MET:HG2	2.20	0.42
1:B:1432:PHE:O	1:B:1435:VAL:HG22	2.20	0.42
1:B:1436:ILE:CG1	1:B:1446:MET:CE	2.97	0.42
1:B:1530:LEU:HD23	1:B:1530:LEU:HA	1.85	0.42
1:B:1548:LEU:HB2	1:B:1549:PRO:HD3	2.02	0.42
1:B:1052:GLN:C	1:B:1054:PHE:N	2.73	0.42
1:B:1211:THR:O	1:B:1215:VAL:HG23	2.20	0.42
1:B:1399:LEU:HD22	1:B:1418:LEU:HD12	2.02	0.42
1:B:1240:LYS:C	1:B:1242:GLU:H	2.21	0.41
1:A:329:LEU:HD11	1:A:446:MET:HE3	2.02	0.41
1:B:1315:LEU:HB3	1:B:1582:ALA:HA	2.01	0.41
1:B:1047:ALA:O	1:B:1048:SER:C	2.58	0.41
1:B:1575:ILE:O	1:B:1579:LYS:HG3	2.19	0.41
1:A:548:LEU:O	1:A:552:GLU:HB2	2.21	0.41
1:A:435:VAL:C	1:A:437:ARG:N	2.74	0.41
1:B:1173:LEU:HD23	1:B:1173:LEU:HA	1.91	0.41
1:B:1585:HIS:HA	8:B:2025:HOH:O	2.20	0.41
1:A:3:PHE:CE1	1:A:4:LEU:CD1	3.03	0.41
1:A:238:LEU:HD22	1:A:239:PRO:HD2	2.02	0.41
1:A:487:ASP:HA	1:A:488:PRO:HD3	1.89	0.41
1:B:1482:MET:O	1:B:1486:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:SER:C	1:A:68:VAL:HG12	2.42	0.41
1:A:68:VAL:HA	1:A:69:PRO:HD2	1.95	0.41
1:A:283:VAL:O	1:A:283:VAL:CG2	2.69	0.41
1:A:381:GLN:HE21	1:A:442:ARG:CZ	2.33	0.41
1:A:532:ILE:HB	1:A:564:LEU:HD13	2.03	0.41
1:A:568:LEU:HD11	1:A:577:LYS:HB3	2.03	0.41
1:B:1068:VAL:CG1	1:B:1071:LEU:HD23	2.51	0.41
1:B:1568:LEU:HD23	1:B:1569:ALA:H	1.86	0.41
1:B:1588:HIS:HB2	8:B:2101:HOH:O	2.20	0.41
1:A:91:ASP:HB2	1:A:92:PRO:HD3	2.02	0.41
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.87	0.41
1:A:510:LEU:HA	1:A:510:LEU:HD12	1.89	0.41
1:B:1495:LEU:HD12	1:B:1495:LEU:HA	1.90	0.41
1:B:1575:ILE:HD12	1:B:1575:ILE:HA	1.90	0.41
1:A:392:GLU:O	1:A:396:GLN:HB2	2.21	0.40
1:A:482:MET:O	1:A:486:GLN:HG3	2.21	0.40
1:B:1002:GLN:HG3	1:B:1273:ASP:OD1	2.21	0.40
1:B:1121:ASP:O	1:B:1181:LYS:NZ	2.53	0.40
1:A:2:GLN:NE2	1:A:272:THR:O	2.54	0.40
1:A:537:SER:HA	1:A:538:PRO:HD2	1.94	0.40
1:A:241:THR:O	1:A:242:GLU:HG2	2.22	0.40
1:A:240:LYS:C	1:A:242:GLU:N	2.74	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	534/589 (91%)	488 (91%)	35 (7%)	11 (2%)	7 13
1	B	540/589 (92%)	495 (92%)	33 (6%)	12 (2%)	6 12
All	All	1074/1178 (91%)	983 (92%)	68 (6%)	23 (2%)	7 13

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	VAL
1	A	570	SER
1	B	1262	ASN
1	B	1293	SER
1	A	404	LYS
1	B	1067	SER
1	B	1246	ASP
1	B	1557	GLN
1	B	1572	PRO
1	A	48	SER
1	A	245	ASN
1	B	1241	THR
1	B	1366	ALA
1	B	1570	SER
1	A	60	ASN
1	A	282	MET
1	A	242	GLU
1	B	1055	SER
1	B	1571	GLU
1	A	241	THR
1	B	1048	SER
1	A	436	ILE
1	A	572	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	451/487 (93%)	420 (93%)	31 (7%)	15 31
1	B	455/487 (93%)	421 (92%)	34 (8%)	13 27
All	All	906/974 (93%)	841 (93%)	65 (7%)	14 29

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	40	LEU
1	A	68	VAL
1	A	99	ASP
1	A	164	ASP
1	A	212	LEU
1	A	229	ASN
1	A	257	GLN
1	A	270	LEU
1	A	291	LEU
1	A	293	SER
1	A	295	GLN
1	A	315	LEU
1	A	318	LEU
1	A	350	ARG
1	A	351	LEU
1	A	414	LEU
1	A	420	SER
1	A	437	ARG
1	A	455	LEU
1	A	457	LEU
1	A	482	MET
1	A	503	PRO
1	A	505	LEU
1	A	510	LEU
1	A	534	ASP
1	A	536	ARG
1	A	550	GLN
1	A	564	LEU
1	A	566	PRO
1	A	571	GLU
1	B	1004	LEU
1	B	1031	ARG
1	B	1040	LEU
1	B	1061	THR
1	B	1079	GLN
1	B	1126	LEU
1	B	1153	LEU
1	B	1154	GLN
1	B	1201	LEU
1	B	1208	GLN
1	B	1212	LEU
1	B	1229	ASN

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Mol	Chain	Res	Type
1	B	1257	GLN
1	B	1260	LEU
1	B	1288	LEU
1	B	1291	LEU
1	B	1315	LEU
1	B	1322	ILE
1	B	1332	LEU
1	B	1351	LEU
1	B	1398	VAL
1	B	1399	LEU
1	B	1404	LYS
1	B	1414	LEU
1	B	1441	LYS
1	B	1455	LEU
1	B	1457	LEU
1	B	1489	GLU
1	B	1505	LEU
1	B	1510	LEU
1	B	1532	ILE
1	B	1536	ARG
1	B	1560	SER
1	B	1568	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	52	GLN
1	A	83	GLN
1	A	106	ASN
1	A	154	GLN
1	A	229	ASN
1	A	235	ASN
1	A	295	GLN
1	A	325	ASN
1	A	381	GLN
1	A	486	GLN
1	A	509	ASN
1	A	528	ASN
1	B	1035	GLN
1	B	1052	GLN
1	B	1079	GLN

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Mol	Chain	Res	Type
1	B	1106	ASN
1	B	1138	HIS
1	B	1154	GLN
1	B	1213	GLN
1	B	1229	ASN
1	B	1235	ASN
1	B	1262	ASN
1	B	1307	GLN
1	B	1325	ASN
1	B	1486	GLN
1	B	1509	ASN
1	B	1557	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 29 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
6	ANP	B	1591	2	29,33,33	1.28	7 (24%)	31,52,52	3.90	13 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	ANP	A	591	2	29,33,33	1.36	5 (17%)	31,52,52	3.62	11 (35%)
7	TAS	B	1701	-	0,3,3	-	-	0,3,3	-	-
7	TAS	A	701	-	0,3,3	-	-	0,3,3	-	-
5	ADP	A	590	2	24,29,29	1.24	2 (8%)	29,45,45	4.55	17 (58%)
5	ADP	B	1590	2	24,29,29	1.22	1 (4%)	29,45,45	3.61	17 (58%)

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
5	ADP	A	590	2	-	6/12/32/32	0/3/3/3
5	ADP	B	1590	2	-	1/12/32/32	0/3/3/3
6	ANP	B	1591	2	-	5/14/38/38	0/3/3/3
6	ANP	A	591	2	-	9/14/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	590	ADP	C8-N7	-3.59	1.28	1.34
5	B	1590	ADP	C8-N7	-3.47	1.28	1.34
6	A	591	ANP	PG-O1G	3.33	1.51	1.46
6	A	591	ANP	PB-O1B	2.95	1.50	1.46
6	A	591	ANP	PB-O2B	-2.81	1.49	1.56
6	B	1591	ANP	PG-O2G	-2.80	1.49	1.56
6	B	1591	ANP	PG-O1G	2.68	1.50	1.46
6	A	591	ANP	PG-O2G	-2.53	1.49	1.56
6	B	1591	ANP	PB-O2B	-2.48	1.50	1.56
6	B	1591	ANP	C2-N3	2.38	1.35	1.32
6	A	591	ANP	PG-O3G	-2.35	1.50	1.56
6	B	1591	ANP	PB-O1B	2.22	1.49	1.46
5	A	590	ADP	C2'-C3'	2.19	1.59	1.53
6	B	1591	ANP	C8-N7	-2.16	1.30	1.34
6	B	1591	ANP	PG-O3G	-2.14	1.51	1.56

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	590	ADP	O4'-C1'-C2'	-12.10	89.25	106.93
6	A	591	ANP	O2B-PB-O1B	11.94	134.95	109.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1591	ANP	O2B-PB-O1B	11.64	134.33	109.92
6	B	1591	ANP	O1B-PB-N3B	-11.29	95.15	111.77
5	A	590	ADP	PA-O3A-PB	10.24	167.98	132.83
5	A	590	ADP	O4'-C4'-C3'	-8.20	88.89	105.11
5	B	1590	ADP	O4'-C1'-C2'	-8.20	94.95	106.93
6	A	591	ANP	O1B-PB-N3B	-7.85	100.21	111.77
6	B	1591	ANP	O1G-PG-N3B	-7.68	100.47	111.77
5	B	1590	ADP	N3-C2-N1	-7.52	116.93	128.68
6	A	591	ANP	O1G-PG-N3B	-7.09	101.33	111.77
6	A	591	ANP	N3-C2-N1	-6.72	118.17	128.68
6	B	1591	ANP	N3-C2-N1	-6.41	118.67	128.68
5	B	1590	ADP	C1'-N9-C4	-6.37	115.45	126.64
5	A	590	ADP	C5'-C4'-C3'	6.18	138.33	115.18
5	B	1590	ADP	C5'-C4'-C3'	6.15	138.24	115.18
5	B	1590	ADP	O4'-C4'-C3'	-6.01	93.23	105.11
5	A	590	ADP	C5-C6-N6	5.99	129.45	120.35
5	A	590	ADP	N3-C2-N1	-5.78	119.65	128.68
5	A	590	ADP	O2A-PA-O5'	5.34	132.55	107.75
5	A	590	ADP	PA-O5'-C5'	5.33	152.92	121.68
6	B	1591	ANP	O2B-PB-O3A	-4.88	88.35	104.64
6	A	591	ANP	O2'-C2'-C3'	4.80	127.35	111.82
6	A	591	ANP	O3A-PB-N3B	-4.66	93.67	106.59
5	B	1590	ADP	O4'-C4'-C5'	-4.62	94.17	109.37
5	A	590	ADP	C3'-C2'-C1'	4.52	107.79	100.98
5	A	590	ADP	O4'-C4'-C5'	-4.41	94.85	109.37
5	B	1590	ADP	O2'-C2'-C1'	4.14	126.15	110.85
6	B	1591	ANP	O4'-C1'-C2'	-3.81	101.36	106.93
5	A	590	ADP	O5'-PA-O1A	-3.80	94.23	109.07
5	B	1590	ADP	C2-N1-C6	3.70	125.08	118.75
5	B	1590	ADP	O3'-C3'-C2'	-3.53	100.42	111.82
6	A	591	ANP	C2'-C3'-C4'	3.47	109.39	102.64
5	B	1590	ADP	O2A-PA-O1A	3.44	129.26	112.24
5	A	590	ADP	N6-C6-N1	-3.32	111.69	118.57
5	B	1590	ADP	O3'-C3'-C4'	3.25	120.45	111.05
6	B	1591	ANP	O2'-C2'-C1'	3.22	122.76	110.85
5	B	1590	ADP	PA-O5'-C5'	3.16	140.22	121.68
5	A	590	ADP	O5'-C5'-C4'	-3.12	98.24	108.99
5	B	1590	ADP	O5'-PA-O1A	-3.00	97.33	109.07
5	A	590	ADP	C2-N1-C6	3.00	123.88	118.75
5	A	590	ADP	O2'-C2'-C1'	2.98	121.87	110.85
6	A	591	ANP	O2G-PG-O3G	2.95	115.49	107.64
5	A	590	ADP	C2'-C3'-C4'	2.84	108.15	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	591	ANP	C1'-N9-C4	-2.67	121.96	126.64
6	B	1591	ANP	C2-N1-C6	2.65	123.29	118.75
5	B	1590	ADP	C2'-C3'-C4'	2.64	107.77	102.64
6	B	1591	ANP	C5-C6-N6	2.63	124.35	120.35
6	B	1591	ANP	O5'-C5'-C4'	2.62	118.02	108.99
6	B	1591	ANP	O2G-PG-O3G	2.61	114.59	107.64
5	B	1590	ADP	C3'-C2'-C1'	2.46	104.68	100.98
5	A	590	ADP	C4-C5-N7	-2.24	107.06	109.40
6	A	591	ANP	C5'-C4'-C3'	2.23	123.55	115.18
5	B	1590	ADP	C5-C6-N6	2.15	123.61	120.35
6	A	591	ANP	PB-O3A-PA	2.12	140.08	132.62
5	B	1590	ADP	O5'-C5'-C4'	-2.08	101.82	108.99
6	B	1591	ANP	O2A-PA-O5'	2.08	117.40	107.75
6	B	1591	ANP	O4'-C4'-C3'	-2.02	101.11	105.11

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	590	ADP	O4'-C4'-C5'-O5'
6	A	591	ANP	PB-N3B-PG-O1G
6	A	591	ANP	PG-N3B-PB-O1B
6	A	591	ANP	PG-N3B-PB-O3A
6	A	591	ANP	PA-O3A-PB-O1B
6	A	591	ANP	PA-O3A-PB-O2B
6	A	591	ANP	C5'-O5'-PA-O2A
6	B	1591	ANP	PB-N3B-PG-O1G
6	B	1591	ANP	PG-N3B-PB-O1B
6	B	1591	ANP	PG-N3B-PB-O3A
6	B	1591	ANP	PA-O3A-PB-O1B
5	B	1590	ADP	O4'-C4'-C5'-O5'
5	A	590	ADP	PB-O3A-PA-O5'
6	A	591	ANP	C4'-C5'-O5'-PA
6	A	591	ANP	C5'-O5'-PA-O1A
5	A	590	ADP	C3'-C4'-C5'-O5'
5	A	590	ADP	PA-O3A-PB-O1B
5	A	590	ADP	PA-O3A-PB-O2B
5	A	590	ADP	PA-O3A-PB-O3B
6	A	591	ANP	C5'-O5'-PA-O3A
6	B	1591	ANP	C4'-C5'-O5'-PA

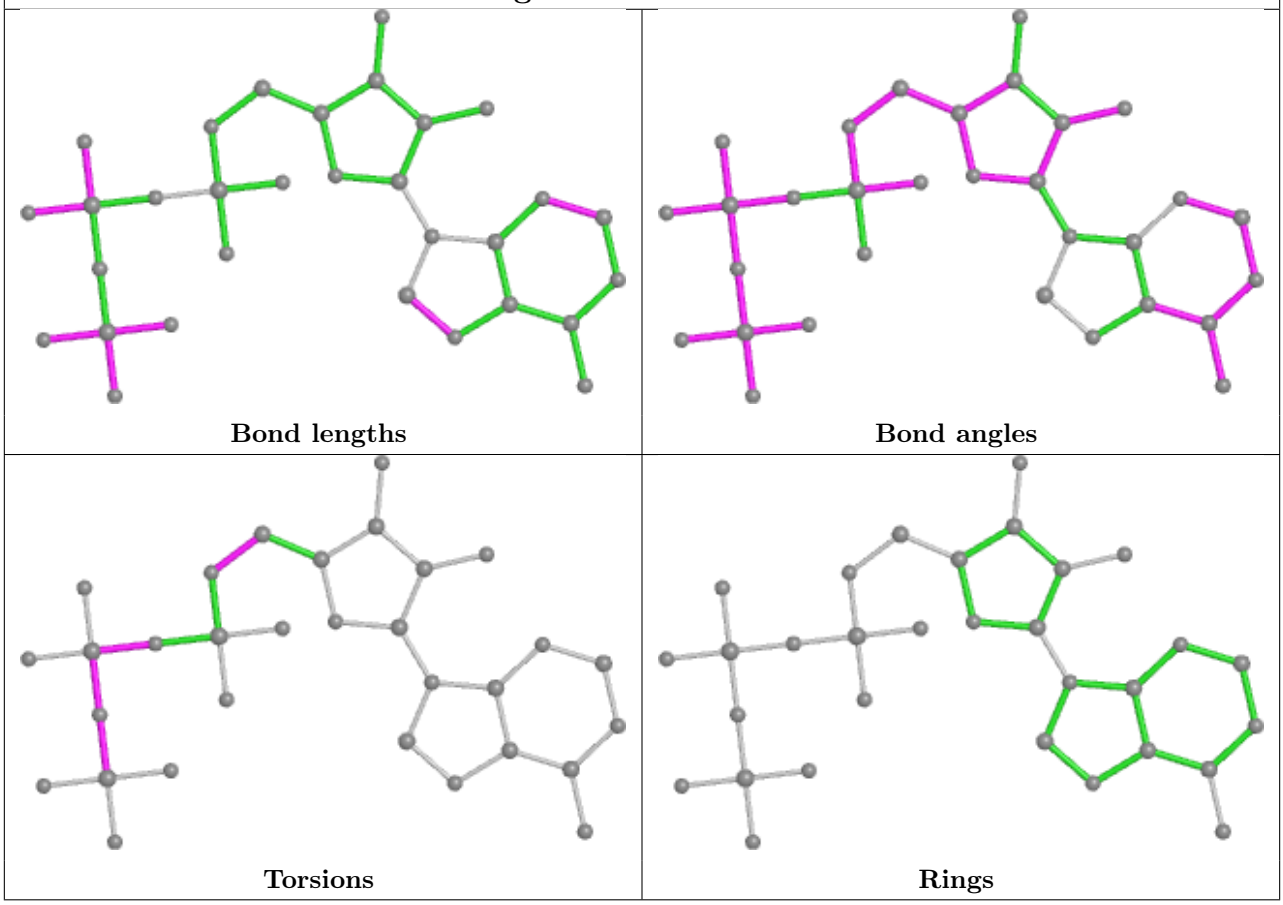
There are no ring outliers.

4 monomers are involved in 11 short contacts:

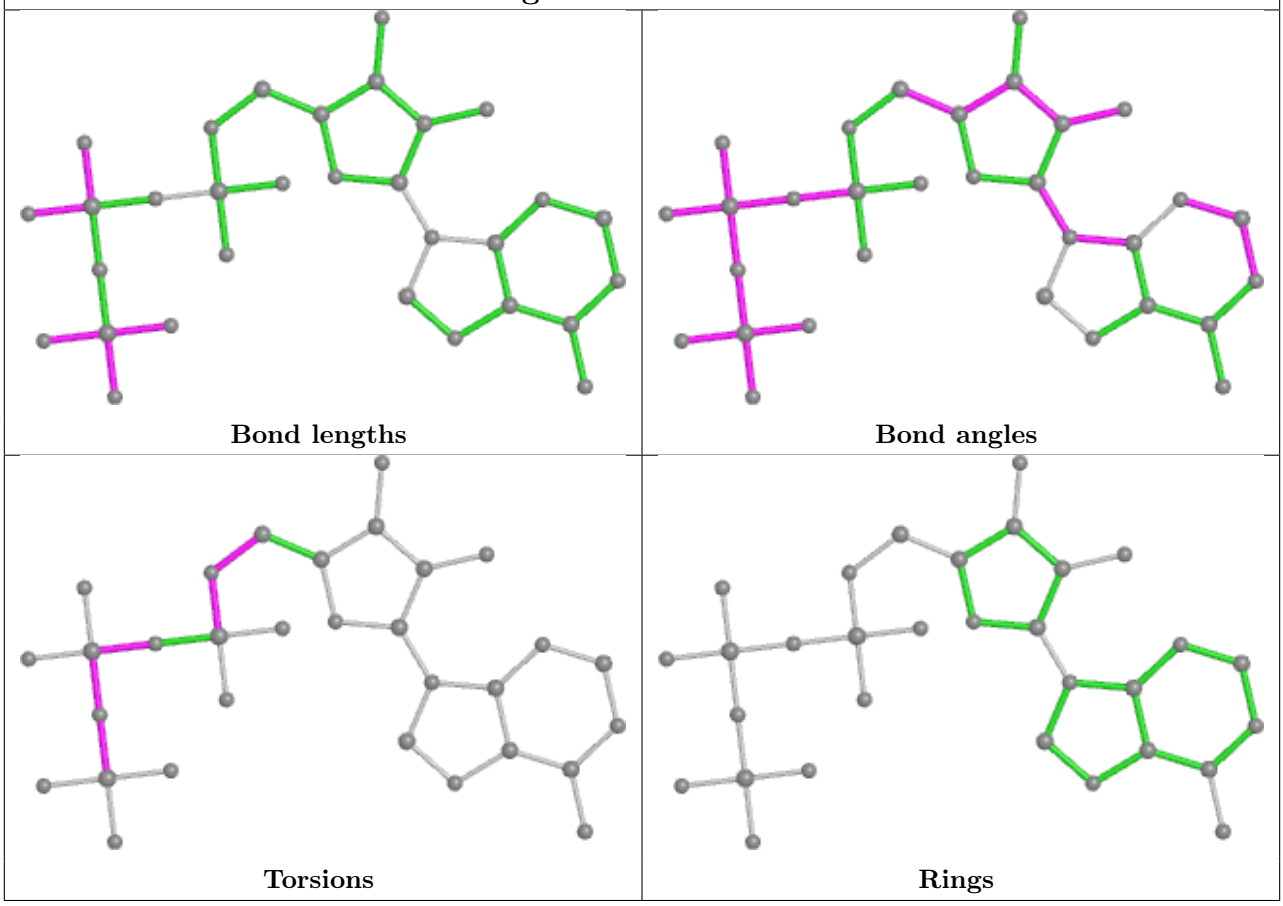
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	591	ANP	2	0
7	A	701	TAS	2	0
5	A	590	ADP	5	0
5	B	1590	ADP	2	0

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

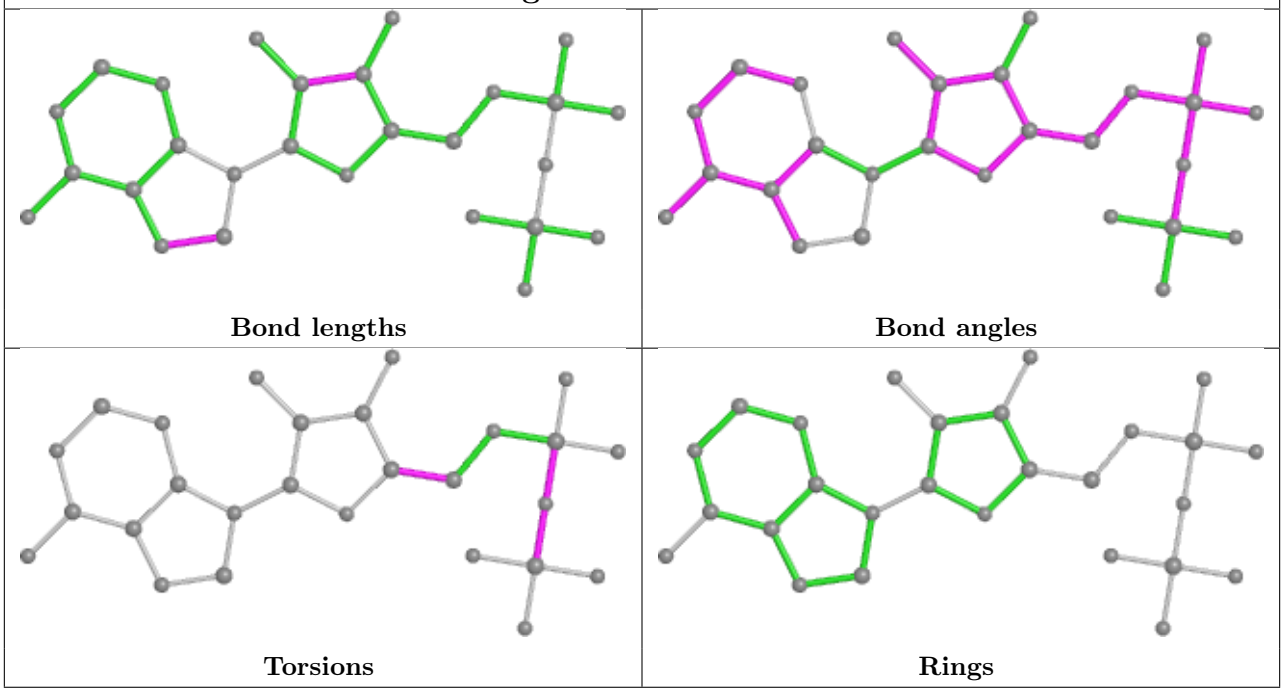
Ligand ANP B 1591



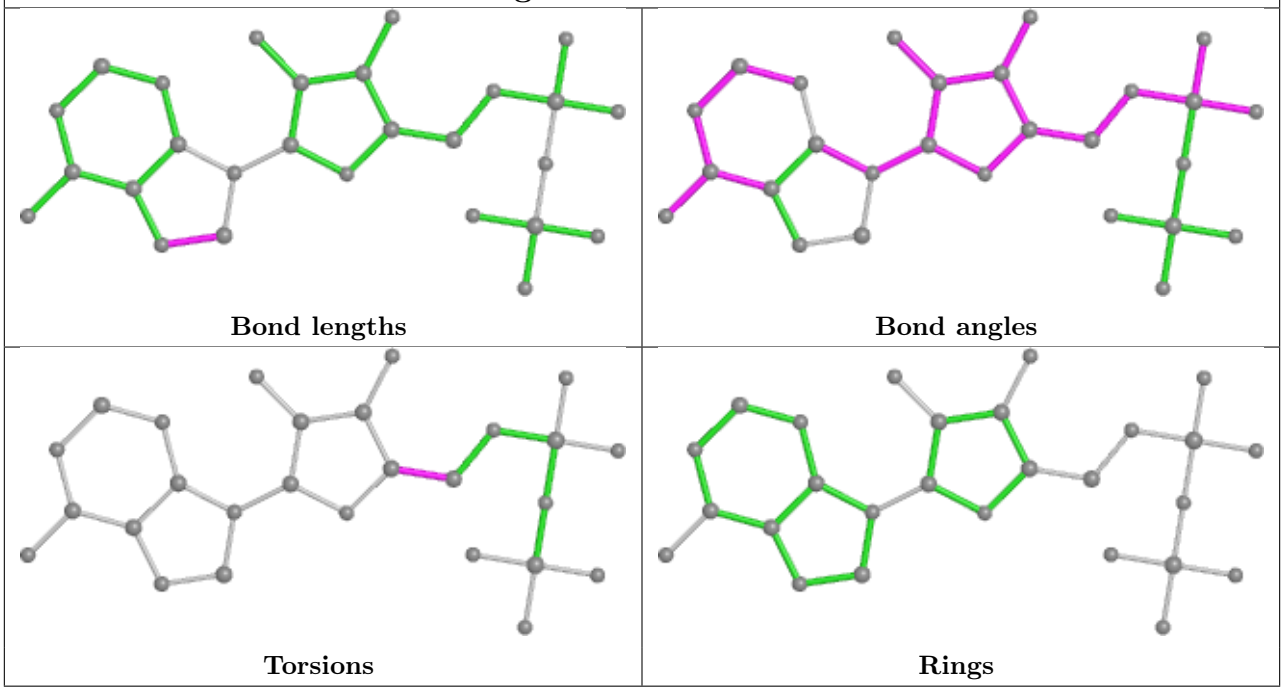
Ligand ANP A 591



Ligand ADP A 590



Ligand ADP B 1590



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	544/589 (92%)	-0.21	2 (0%)	92	91	21, 42, 76, 94	0
1	B	550/589 (93%)	-0.16	15 (2%)	54	48	20, 42, 77, 100	0
All	All	1094/1178 (92%)	-0.18	17 (1%)	72	68	20, 42, 76, 100	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1307	GLN	4.7
1	B	1308	GLN	4.3
1	B	1162	PHE	4.0
1	B	1168	GLU	3.4
1	A	245	ASN	3.2
1	B	1244	ALA	2.7
1	B	1253	TRP	2.5
1	B	1066	ALA	2.5
1	B	1366	ALA	2.5
1	A	67	SER	2.4
1	B	1161	SER	2.4
1	B	1245	ASN	2.2
1	B	1377	LEU	2.2
1	B	1163	ILE	2.2
1	B	1461	THR	2.1
1	B	1283	VAL	2.1
1	B	1258	GLU	2.1

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(Å^2)	Q<0.9
7	TAS	A	701	4/4	0.78	0.51	80,81,83,90	4
3	CD	B	1606	1/1	0.80	0.08	118,118,118,118	1
7	TAS	B	1701	4/4	0.81	0.51	72,74,74,85	4
3	CD	B	1605	1/1	0.91	0.17	89,89,89,89	1
3	CD	A	605	1/1	0.94	0.09	60,60,60,60	1
4	CL	B	1599	1/1	0.95	0.21	75,75,75,75	0
5	ADP	B	1590	27/27	0.96	0.17	35,44,51,52	0
3	CD	B	1603	1/1	0.96	0.08	78,78,78,78	0
3	CD	A	603	1/1	0.96	0.07	98,98,98,98	0
5	ADP	A	590	27/27	0.97	0.18	37,45,56,59	0
2	MG	A	592	1/1	0.97	0.19	17,17,17,17	0
2	MG	B	1593	1/1	0.98	0.12	14,14,14,14	0
6	ANP	A	591	31/31	0.98	0.14	27,41,52,54	0
6	ANP	B	1591	31/31	0.98	0.12	23,35,48,50	0
2	MG	A	593	1/1	0.98	0.14	21,21,21,21	0
3	CD	A	604	1/1	0.98	0.08	46,46,46,46	0
2	MG	B	1592	1/1	0.99	0.15	24,24,24,24	0
3	CD	B	1607	1/1	0.99	0.03	84,84,84,84	0
4	CL	A	2000	1/1	0.99	0.08	27,27,27,27	0
4	CL	B	1597	1/1	0.99	0.10	28,28,28,28	0
4	CL	B	1598	1/1	0.99	0.09	32,32,32,32	0
3	CD	B	1602	1/1	0.99	0.09	38,38,38,38	0
4	CL	A	597	1/1	1.00	0.06	28,28,28,28	0
4	CL	A	598	1/1	1.00	0.10	35,35,35,35	0
4	CL	A	599	1/1	1.00	0.11	69,69,69,69	0
3	CD	A	596	1/1	1.00	0.10	34,34,34,34	0
3	CD	B	1594	1/1	1.00	0.10	35,35,35,35	0
3	CD	B	1595	1/1	1.00	0.10	30,30,30,30	0
3	CD	B	1596	1/1	1.00	0.11	36,36,36,36	0
3	CD	B	1601	1/1	1.00	0.09	32,32,32,32	0
3	CD	A	600	1/1	1.00	0.10	29,29,29,29	0
3	CD	A	601	1/1	1.00	0.12	31,31,31,31	0

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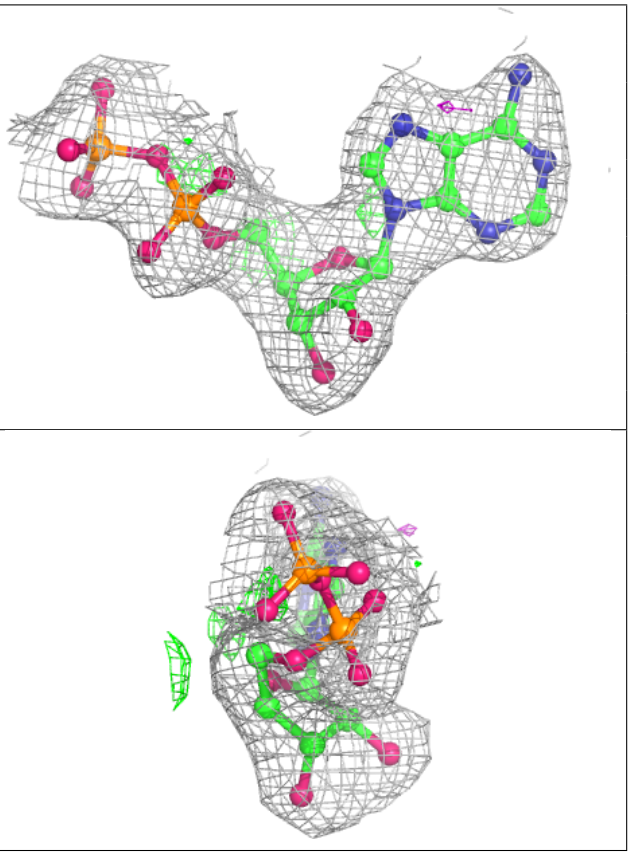
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CD	A	602	1/1	1.00	0.09	39,39,39,39	0
3	CD	A	594	1/1	1.00	0.11	40,40,40,40	0
3	CD	A	595	1/1	1.00	0.12	34,34,34,34	0

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.

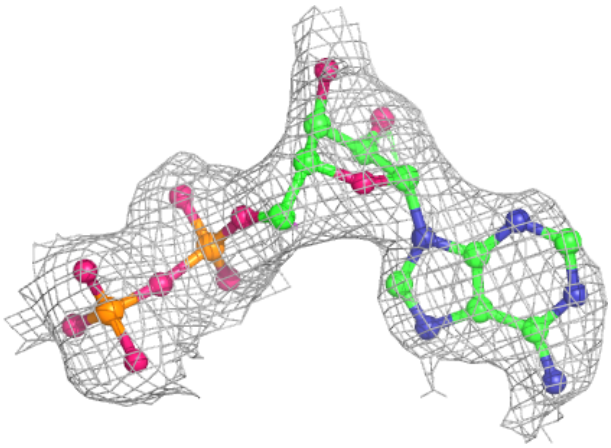
Electron density around ADP B 1590:

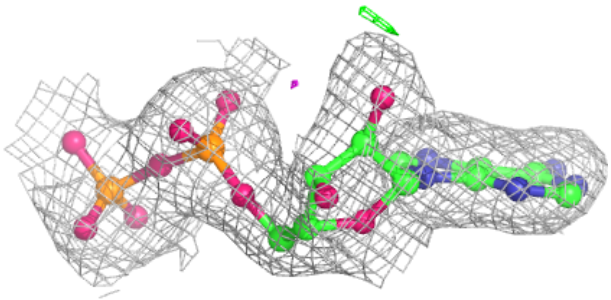
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

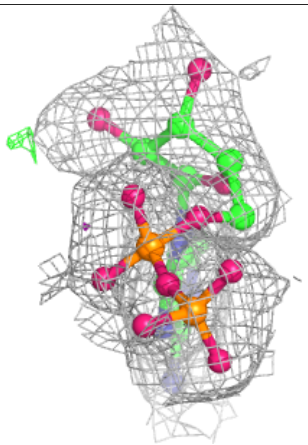


Electron density around ADP A 590:

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

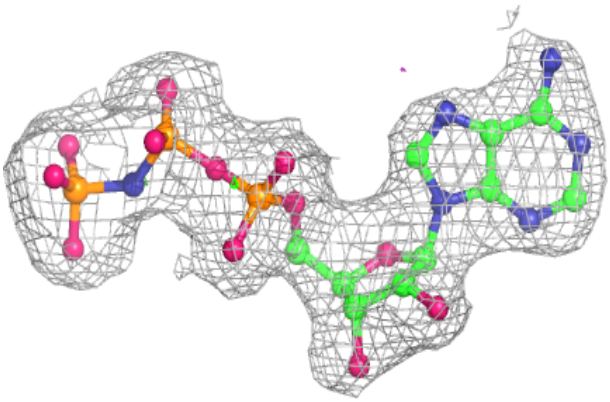


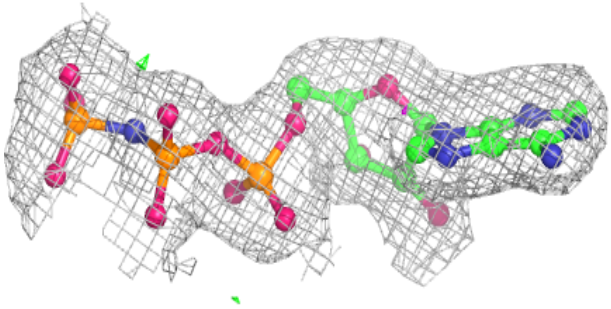


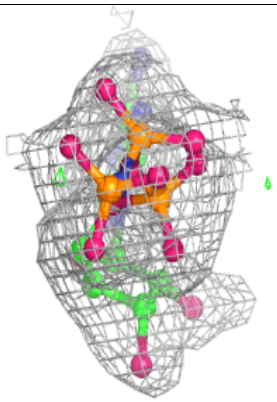


Electron density around ANP A 591:

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

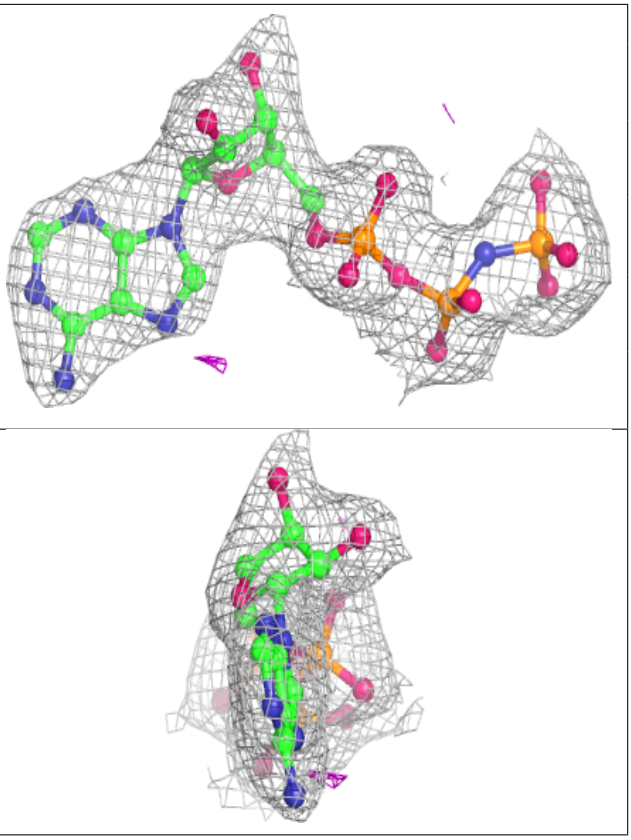


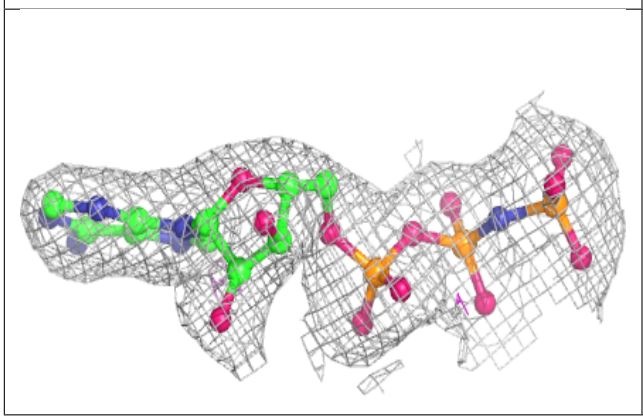




Electron density around ANP B 1591:

$2mF_o$-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.