Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 10:04 pm GMT

PDB ID	:	4CJ7
Title	:	Structure of Crenactin, an archeal actin-like protein
Authors	:	Izore, T.; Duman, R.E.; Kureisaite-Ciziene, D.; Lowe, J.
Deposited on	:	2013-12-19
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

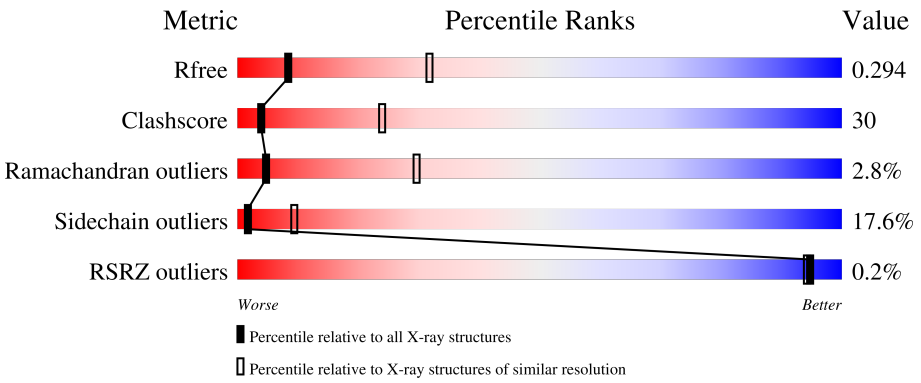
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	432	44% 43% 11% ••
1	B	432	43% 47% 9% •

2 Entry composition (i)

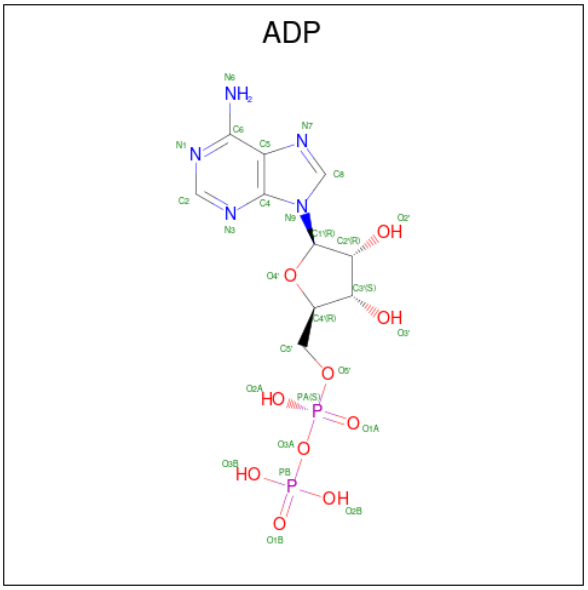
There are 2 unique types of molecules in this entry. The entry contains 6782 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACTIN/ACTIN FAMILY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	426	3362	2155	576	625	6	0	0	0
1	B	426	3366	2158	577	625	6	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



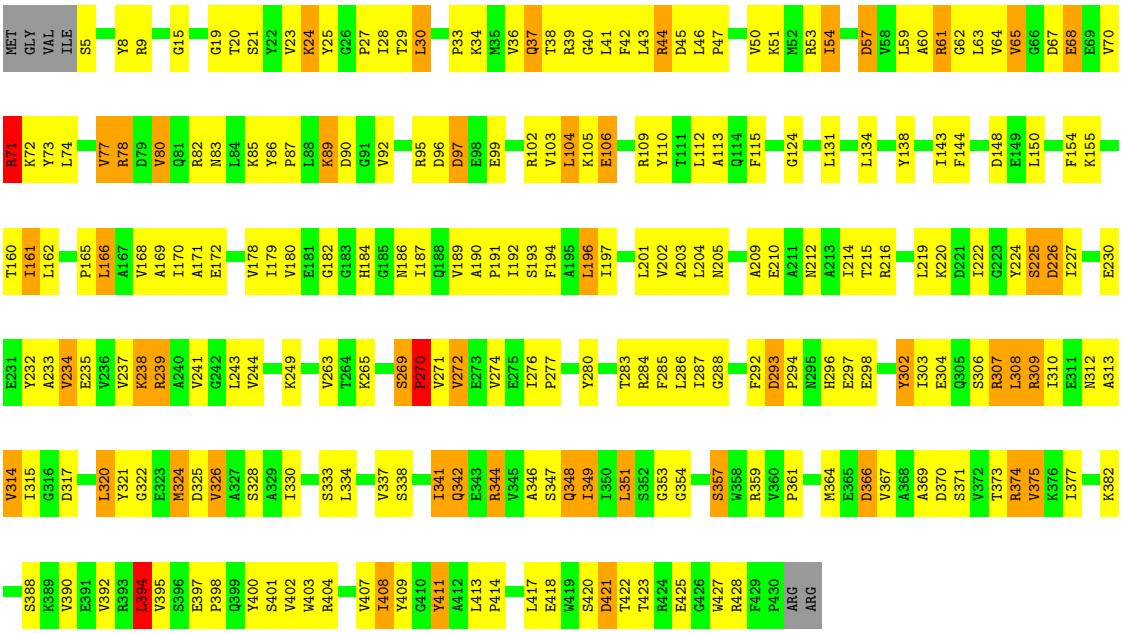
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
2	B	1	27	10	5	10	2	0	0

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.

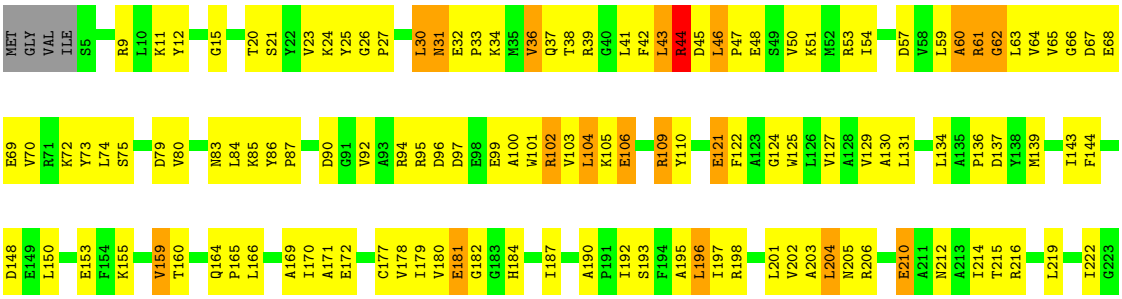
• Molecule 1: ACTIN/ACTIN FAMILY PROTEIN

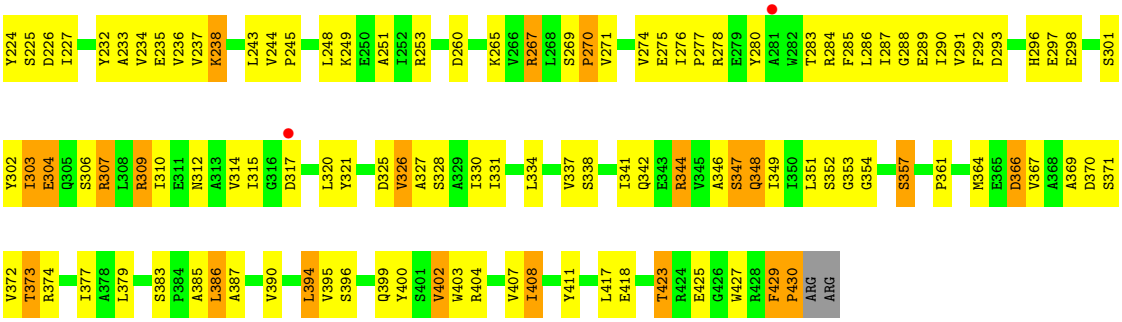
Chain A: 44% 43% 11%



• Molecule 1: ACTIN/ACTIN FAMILY PROTEIN

Chain B: 43% 47% 9%




Y224 S225 D226 I227
Y232 A233 V234 E235 V236 V237 K238
L243 V244 P245
L248 K249 E250 A251 I252 R253
D260
K265 V266 R267 L268 S269 P270 V271
V274 E275 I276 P277 R278 E279 Y280 A281 W282 T283 R284 F285 L286 I287 G288 E289 I290 V291 F292 D293
H296 E297 E298
S301
Y302 I303 E304 Q305 S306 R307 L308 R309 I310 E311 N312 A313 V314 I315 G316 D317
L320 Y321
D325 V326 A327 S328 A329 I330 I331
L334
V337 S338
I341 Q342 E343 R344 V345 A346 S347 Q348 I349 I350 L351 S352 G353 G354
S357
P361
M364 E365 D366 V367 A368 A369 D370 S371
V372 T373 R374
I377 A378 L379
S383 P384 A385 L386 A387
V390
L394 V395 S396
Q399 Y400 S401 V402 W403 R404
V407 I408
Y411
L417 E418
T423 R424 E425 G426 W427 R428 F429 P430 ARG ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	78.13Å 78.13Å 418.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 3.20 48.86 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.86-3.20) 100.0 (48.86-3.20)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.235 , 0.295 0.234 , 0.294	Depositor DCC
R_{free} test set	1129 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	89.2	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 65.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6782	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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: ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.65	1/3432 (0.0%)	1.00	12/4667 (0.3%)
1	B	0.61	1/3436 (0.0%)	0.91	8/4671 (0.2%)
All	All	0.63	2/6868 (0.0%)	0.96	20/9338 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	ARG	CZ-NH2	-6.98	1.24	1.33
1	B	344	ARG	NE-CZ	-5.39	1.26	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	SER	C-N-CD	-14.45	88.82	120.60
1	A	71	ARG	NE-CZ-NH2	10.70	125.65	120.30
1	A	293	ASP	C-N-CD	-9.02	100.75	120.60
1	B	344	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	B	94	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	344	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	A	71	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	A	270	PRO	CA-C-N	-6.19	103.58	117.20
1	A	269	SER	C-N-CA	6.03	147.31	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	430	PRO	N-CA-C	5.89	127.42	112.10
1	A	394	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	344	ARG	NH1-CZ-NH2	5.79	125.77	119.40
1	B	267	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	272	VAL	CG1-CB-CG2	-5.75	101.70	110.90
1	A	309	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	B	394	LEU	CA-CB-CG	5.67	128.34	115.30
1	B	344	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	44	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	B	44	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	308	LEU	CA-CB-CG	5.14	127.12	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	GLY	Peptide

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	3362	0	3398	207	2
1	B	3366	0	3409	219	1
2	A	27	0	12	5	0
2	B	27	0	12	6	0
All	All	6782	0	6831	415	2

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 30.

All (415) 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:B:265:LYS:HD3	1:B:275:GLU:OE1	1.31	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HD11	1:A:73:TYR:HE2	1.06	1.10
1:A:197:ILE:HG21	1:A:337:VAL:HG12	1.38	1.04
1:B:45:ASP:HB2	1:B:83:ASN:HD21	0.92	1.04
1:B:265:LYS:HG2	1:B:275:GLU:CG	1.87	1.04
1:B:265:LYS:HG2	1:B:275:GLU:CB	1.87	1.03
1:B:265:LYS:CD	1:B:275:GLU:OE1	2.05	1.03
1:A:54:ILE:HD11	1:A:73:TYR:CE2	1.93	1.03
1:B:45:ASP:HB2	1:B:83:ASN:ND2	1.74	1.02
1:B:45:ASP:CB	1:B:83:ASN:HD21	1.73	1.01
1:B:265:LYS:HG2	1:B:275:GLU:HG3	1.43	1.00
1:B:265:LYS:CG	1:B:275:GLU:HG3	1.93	0.99
1:B:41:LEU:HD12	1:B:83:ASN:O	1.70	0.91
1:B:134:LEU:HD21	1:B:320:LEU:HD11	1.53	0.90
1:B:180:VAL:HG13	1:B:351:LEU:HD23	1.50	0.90
1:B:54:ILE:HD11	1:B:73:TYR:CE2	2.07	0.90
1:A:134:LEU:HD21	1:A:320:LEU:HD11	1.52	0.89
1:B:20:THR:H	2:B:1431:ADP:PB	1.96	0.89
1:B:197:ILE:HG21	1:B:337:VAL:HG12	1.53	0.88
1:B:265:LYS:CG	1:B:275:GLU:CG	2.51	0.88
1:A:344:ARG:HH12	1:B:72:LYS:HB3	1.40	0.86
1:A:38:THR:HG22	1:A:38:THR:O	1.74	0.85
1:B:178:VAL:CG1	1:B:349:ILE:HD13	2.08	0.83
1:B:178:VAL:HG12	1:B:349:ILE:HD13	1.59	0.83
1:A:312:ASN:OD1	1:A:321:TYR:HA	1.79	0.83
1:B:54:ILE:HD11	1:B:73:TYR:HE2	1.41	0.81
1:B:203:ALA:HB3	1:B:320:LEU:CD1	2.11	0.80
1:B:212:ASN:OD1	1:B:238:LYS:HE2	1.81	0.80
1:A:23:VAL:HG23	1:A:38:THR:OG1	1.78	0.80
1:A:193:SER:HB3	1:B:75:SER:HB2	1.62	0.80
1:B:39:ARG:HB3	1:B:86:TYR:CE1	2.17	0.79
1:A:197:ILE:HG21	1:A:337:VAL:CG1	2.13	0.79
1:A:326:VAL:O	1:A:330:ILE:HG13	1.82	0.78
1:B:265:LYS:HG2	1:B:275:GLU:HB2	1.65	0.78
1:A:409:TYR:CE1	1:A:413:LEU:HD13	2.19	0.78
1:B:47:PRO:HB2	1:B:50:VAL:HG13	1.66	0.78
1:A:361:PRO:HG2	1:A:364:MET:SD	2.24	0.77
1:B:66:GLY:HA3	1:B:69:GLU:OE1	1.83	0.77
1:B:203:ALA:CB	1:B:320:LEU:HD12	2.13	0.77
1:A:172:GLU:OE2	1:A:395:VAL:HG13	1.85	0.77
1:A:186:ASN:HB2	1:A:204:LEU:O	1.86	0.76
1:B:222:ILE:HD13	1:B:277:PRO:HD2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ILE:HG12	1:B:320:LEU:HD21	1.67	0.75
1:B:222:ILE:HG12	1:B:280:TYR:HD2	1.51	0.75
1:B:31:ASN:H	1:B:31:ASN:ND2	1.85	0.75
1:A:193:SER:HB3	1:B:75:SER:CB	2.17	0.74
1:A:337:VAL:HG23	1:A:342:GLN:HG2	1.69	0.74
1:B:192:ILE:HD13	1:B:196:LEU:HA	1.69	0.74
1:B:265:LYS:HG3	1:B:275:GLU:HG3	1.70	0.73
1:A:302:TYR:O	1:A:306:SER:HB2	1.88	0.73
1:A:166:LEU:O	1:A:166:LEU:HD12	1.89	0.73
1:B:21:SER:N	2:B:1431:ADP:O3B	2.20	0.72
1:A:373:THR:HG22	1:A:377:ILE:HD11	1.73	0.71
1:B:41:LEU:CD1	1:B:83:ASN:O	2.38	0.71
1:B:312:ASN:OD1	1:B:321:TYR:HA	1.90	0.71
1:A:269:SER:O	1:A:272:VAL:N	2.23	0.70
1:A:341:ILE:HD11	1:A:344:ARG:HD2	1.72	0.70
1:A:203:ALA:HB3	1:A:320:LEU:HD12	1.73	0.70
1:B:361:PRO:HG2	1:B:364:MET:SD	2.31	0.70
1:A:203:ALA:CB	1:A:320:LEU:HD12	2.22	0.69
1:B:101:TRP:HH2	1:B:139:MET:HG3	1.57	0.69
1:A:216:ARG:HH12	1:A:307:ARG:HB2	1.57	0.69
1:B:39:ARG:HB3	1:B:86:TYR:CD1	2.28	0.68
1:B:181:GLU:HG3	1:B:352:SER:HB3	1.74	0.68
1:A:95:ARG:HA	1:A:138:TYR:CE1	2.29	0.67
1:A:230:GLU:O	1:A:233:ALA:HB3	1.94	0.67
1:A:21:SER:N	2:A:1431:ADP:O3B	2.27	0.67
1:A:39:ARG:HB3	1:A:86:TYR:CE1	2.30	0.67
1:B:232:TYR:O	1:B:236:VAL:HG23	1.94	0.67
1:A:334:LEU:CD1	1:A:346:ALA:HB2	2.24	0.67
1:A:341:ILE:CD1	1:A:344:ARG:HD2	2.26	0.66
1:A:344:ARG:O	1:A:347:SER:HB3	1.96	0.66
1:A:42:PHE:HA	1:A:62:GLY:O	1.95	0.66
1:B:251:ALA:HA	1:B:367:VAL:HG21	1.78	0.66
1:B:44:ARG:HH22	1:B:102:ARG:HH21	1.44	0.66
1:B:203:ALA:HB1	1:B:320:LEU:HD12	1.77	0.66
1:A:45:ASP:HB3	1:A:78:ARG:HB2	1.79	0.65
1:B:216:ARG:NH1	1:B:307:ARG:HD3	2.12	0.65
1:B:386:LEU:HD12	1:B:390:VAL:HG23	1.78	0.65
1:B:46:LEU:CD2	1:B:50:VAL:HG22	2.27	0.65
1:B:302:TYR:O	1:B:306:SER:HB2	1.96	0.65
1:A:106:GLU:HG2	1:A:109:ARG:HH21	1.61	0.65
1:A:110:TYR:O	1:A:113:ALA:HB3	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ALA:HA	1:A:408:ILE:HD11	1.79	0.65
1:B:47:PRO:HB2	1:B:50:VAL:CG1	2.25	0.65
1:B:309:ARG:CD	1:B:309:ARG:H	2.10	0.64
1:B:23:VAL:HG23	1:B:38:THR:OG1	1.97	0.64
1:B:203:ALA:HB3	1:B:320:LEU:HD13	1.78	0.64
1:B:222:ILE:HG12	1:B:280:TYR:CD2	2.31	0.64
1:B:57:ASP:O	1:B:60:ALA:HB3	1.97	0.63
1:A:27:PRO:HD2	1:A:30:LEU:HD21	1.79	0.63
1:A:193:SER:CB	1:B:75:SER:HB2	2.27	0.63
1:B:105:LYS:HE2	1:B:150:LEU:HD21	1.79	0.62
1:A:36:VAL:HG21	1:A:110:TYR:CE1	2.35	0.62
1:B:346:ALA:O	1:B:390:VAL:HG22	1.99	0.62
1:A:265:LYS:HA	1:A:274:VAL:O	1.98	0.62
1:B:249:LYS:HE2	1:B:296:HIS:HD2	1.65	0.62
1:B:160:THR:HG22	1:B:427:TRP:CZ3	2.35	0.62
1:B:354:GLY:O	1:B:357:SER:HB2	1.98	0.62
1:A:344:ARG:NH1	1:B:72:LYS:HB3	2.11	0.62
1:A:99:GLU:O	1:A:103:VAL:HG23	1.98	0.62
1:A:169:ALA:HB2	1:A:179:ILE:CD1	2.30	0.62
1:B:41:LEU:HB3	1:B:64:VAL:HG12	1.81	0.62
1:B:265:LYS:HD3	1:B:275:GLU:CD	2.19	0.62
1:A:238:LYS:NZ	2:A:1431:ADP:O2'	2.30	0.62
1:B:72:LYS:HZ2	1:B:73:TYR:HE1	1.47	0.62
1:A:89:LYS:HG2	1:A:90:ASP:N	2.15	0.61
1:B:203:ALA:CB	1:B:320:LEU:CD1	2.76	0.61
1:B:92:VAL:HG21	1:B:315:ILE:HG21	1.82	0.61
1:A:72:LYS:C	1:A:73:TYR:HD1	2.03	0.61
1:A:216:ARG:HB2	1:A:234:VAL:HG11	1.81	0.61
1:B:72:LYS:NZ	1:B:73:TYR:HE1	1.98	0.61
1:A:184:HIS:CD2	1:A:209:ALA:HB2	2.36	0.60
1:A:194:PHE:HE2	1:B:53:ARG:HD2	1.66	0.60
1:A:216:ARG:NH1	1:A:307:ARG:HD3	2.16	0.60
1:B:31:ASN:H	1:B:31:ASN:HD22	1.48	0.60
1:B:206:ARG:NH2	1:B:291:VAL:O	2.35	0.60
1:A:325:ASP:HB3	1:A:328:SER:H	1.67	0.59
1:A:24:LYS:N	1:A:24:LYS:HD3	2.18	0.59
1:A:170:ILE:HG22	1:A:408:ILE:HG13	1.84	0.59
1:B:180:VAL:CG1	1:B:351:LEU:HD23	2.27	0.59
1:B:129:VAL:HG12	1:B:131:LEU:CD2	2.32	0.59
1:A:227:ILE:HG22	1:A:233:ALA:HB1	1.84	0.59
1:B:206:ARG:HB2	1:B:210:GLU:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LEU:O	1:B:337:VAL:HG22	2.03	0.59
1:B:54:ILE:CD1	1:B:73:TYR:HE2	2.15	0.59
1:B:337:VAL:HG23	1:B:342:GLN:HG2	1.83	0.59
1:A:73:TYR:HD1	1:A:73:TYR:N	2.01	0.59
1:A:334:LEU:O	1:A:337:VAL:HG22	2.03	0.59
1:B:243:LEU:O	1:B:288:GLY:HA3	2.04	0.58
1:B:127:VAL:HB	1:B:159:VAL:HG13	1.85	0.58
1:A:73:TYR:N	1:A:73:TYR:CD1	2.69	0.58
1:A:269:SER:C	1:A:272:VAL:H	2.06	0.58
1:A:341:ILE:HD11	1:A:344:ARG:CD	2.33	0.58
1:B:210:GLU:HB3	1:B:290:ILE:HD13	1.84	0.58
1:A:205:ASN:HB2	1:A:320:LEU:HB2	1.85	0.58
1:A:361:PRO:CG	1:A:364:MET:SD	2.91	0.58
1:A:61:ARG:C	1:A:63:LEU:H	2.06	0.58
1:A:269:SER:O	1:A:271:VAL:N	2.35	0.58
1:B:33:PRO:HD2	1:B:400:TYR:CD1	2.38	0.58
1:B:265:LYS:HG2	1:B:275:GLU:CA	2.34	0.58
1:A:215:THR:OG1	1:A:238:LYS:HB2	2.04	0.57
1:B:105:LYS:HE2	1:B:150:LEU:CD2	2.33	0.57
1:B:344:ARG:HA	1:B:347:SER:HB3	1.86	0.57
1:A:212:ASN:OD1	1:A:238:LYS:HE2	2.04	0.57
1:A:212:ASN:OD1	1:A:238:LYS:CE	2.52	0.57
1:B:383:SER:OG	1:B:385:ALA:HB3	2.04	0.57
1:B:46:LEU:CD2	1:B:50:VAL:CG2	2.82	0.57
1:A:310:ILE:HD12	1:A:310:ILE:O	2.05	0.57
1:B:41:LEU:HD13	1:B:84:LEU:HD13	1.87	0.57
1:A:39:ARG:HB3	1:A:86:TYR:CD1	2.40	0.57
1:A:36:VAL:HG21	1:A:110:TYR:HE1	1.69	0.57
1:A:160:THR:HG22	1:A:427:TRP:CZ3	2.40	0.56
1:B:214:ILE:HG21	1:B:287:ILE:HA	1.87	0.56
1:A:334:LEU:HD11	1:A:346:ALA:HB2	1.87	0.56
1:A:216:ARG:HD2	1:A:307:ARG:NH1	2.20	0.56
1:B:166:LEU:O	1:B:170:ILE:HG13	2.05	0.56
1:A:38:THR:O	1:A:38:THR:CG2	2.49	0.56
1:A:162:LEU:HD23	1:A:162:LEU:H	1.70	0.56
1:A:292:PHE:HZ	1:A:371:SER:HB3	1.70	0.56
1:A:284:ARG:HA	1:A:287:ILE:HD12	1.87	0.56
1:B:373:THR:HG22	1:B:377:ILE:HD11	1.88	0.56
1:B:27:PRO:O	1:B:30:LEU:HG	2.06	0.55
1:B:265:LYS:CG	1:B:275:GLU:HB2	2.35	0.55
1:A:263:VAL:HG13	1:A:276:ILE:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLY:CA	1:B:69:GLU:OE1	2.53	0.55
1:A:87:PRO:CG	1:A:104:LEU:HD13	2.36	0.55
1:A:334:LEU:HD13	1:A:346:ALA:HB2	1.88	0.55
1:B:46:LEU:HB3	1:B:51:LYS:HE2	1.89	0.55
1:B:265:LYS:CG	1:B:275:GLU:CB	2.75	0.55
1:A:184:HIS:ND1	2:A:1431:ADP:O3'	2.32	0.55
1:A:70:VAL:O	1:A:74:LEU:HG	2.07	0.55
1:A:269:SER:C	1:A:271:VAL:H	2.07	0.55
1:A:414:PRO:HD2	1:B:48:GLU:HG2	1.89	0.55
1:A:46:LEU:CD2	1:A:50:VAL:HG23	2.36	0.54
1:B:326:VAL:O	1:B:330:ILE:HG13	2.07	0.54
1:A:241:VAL:HG23	1:A:287:ILE:HD13	1.88	0.54
1:A:354:GLY:O	1:A:357:SER:HB2	2.07	0.54
1:B:61:ARG:C	1:B:63:LEU:H	2.11	0.53
1:B:72:LYS:C	1:B:73:TYR:HD1	2.11	0.53
1:A:68:GLU:O	1:A:71:ARG:HB3	2.08	0.53
1:A:420:SER:O	1:A:422:THR:N	2.40	0.53
1:A:45:ASP:H	1:A:83:ASN:HD21	1.56	0.53
1:A:33:PRO:HG2	1:A:400:TYR:CD1	2.43	0.53
1:A:420:SER:OG	1:A:423:THR:HB	2.08	0.53
1:B:283:THR:HA	1:B:286:LEU:HD13	1.90	0.53
1:A:178:VAL:HG13	1:A:349:ILE:HG23	1.90	0.53
1:A:57:ASP:O	1:A:60:ALA:HB3	2.09	0.53
1:B:179:ILE:HD12	1:B:192:ILE:HG13	1.91	0.53
1:A:394:LEU:HD12	1:A:395:VAL:N	2.24	0.52
1:B:286:LEU:N	1:B:286:LEU:HD12	2.23	0.52
1:A:413:LEU:O	1:A:427:TRP:NE1	2.42	0.52
1:B:212:ASN:O	1:B:215:THR:HB	2.08	0.52
1:A:46:LEU:HD22	1:A:47:PRO:O	2.09	0.52
1:A:249:LYS:HE2	1:A:296:HIS:HD2	1.75	0.52
1:B:106:GLU:HG2	1:B:109:ARG:HH21	1.74	0.52
1:B:87:PRO:HG2	1:B:104:LEU:HD13	1.91	0.52
1:B:129:VAL:HG12	1:B:131:LEU:HD23	1.92	0.52
1:B:178:VAL:HG11	1:B:349:ILE:HD13	1.89	0.52
1:A:269:SER:CB	1:A:270:PRO:HD2	2.36	0.52
1:B:70:VAL:O	1:B:74:LEU:HG	2.09	0.51
1:A:374:ARG:HA	1:A:377:ILE:HD12	1.92	0.51
1:A:227:ILE:CG2	1:A:233:ALA:HB1	2.41	0.51
1:B:205:ASN:HB2	1:B:320:LEU:HB2	1.93	0.51
1:B:386:LEU:HD12	1:B:390:VAL:CG2	2.41	0.51
1:A:328:SER:OG	1:A:382:LYS:HE3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:HD11	1:A:237:VAL:HG21	1.93	0.51
1:A:269:SER:HB2	1:A:270:PRO:HD2	1.92	0.51
1:A:124:GLY:HA2	1:A:155:LYS:O	2.11	0.51
1:A:320:LEU:H	1:A:320:LEU:HD22	1.75	0.51
1:B:27:PRO:HD2	1:B:30:LEU:HD21	1.92	0.50
1:A:39:ARG:HA	1:A:85:LYS:O	2.12	0.50
1:A:313:ALA:HB3	1:A:320:LEU:HD23	1.92	0.50
1:A:190:ALA:HB2	1:A:201:LEU:HD13	1.92	0.50
1:A:235:GLU:HG3	1:A:239:ARG:HD2	1.93	0.50
1:A:192:ILE:HD13	1:A:196:LEU:HA	1.94	0.50
1:B:184:HIS:ND1	2:B:1431:ADP:H3'	2.27	0.50
1:A:277:PRO:HD2	1:A:280:TYR:HB2	1.94	0.49
1:B:327:ALA:O	1:B:331:ILE:HG12	2.12	0.49
1:A:244:VAL:HB	1:A:369:ALA:O	2.11	0.49
1:B:43:LEU:N	1:B:62:GLY:O	2.42	0.49
1:B:244:VAL:HB	1:B:369:ALA:O	2.12	0.49
1:B:303:ILE:HD13	1:B:310:ILE:HD11	1.94	0.49
1:A:64:VAL:HG13	1:A:70:VAL:HG22	1.95	0.49
1:B:205:ASN:HB2	1:B:320:LEU:CB	2.42	0.49
1:B:325:ASP:HB3	1:B:328:SER:H	1.77	0.49
1:A:404:ARG:O	1:A:408:ILE:HG12	2.12	0.49
1:B:36:VAL:HG21	1:B:110:TYR:HE2	1.77	0.49
1:A:162:LEU:HD12	1:A:166:LEU:HG	1.93	0.49
1:A:243:LEU:HB3	1:A:285:PHE:CD1	2.48	0.49
1:B:20:THR:HB	2:B:1431:ADP:O3B	2.12	0.49
1:B:245:PRO:CG	1:B:289:GLU:HB2	2.43	0.49
1:B:57:ASP:O	1:B:60:ALA:CB	2.59	0.49
1:B:130:ALA:C	1:B:131:LEU:HD23	2.33	0.49
1:B:46:LEU:HA	1:B:47:PRO:HD2	1.65	0.49
1:A:162:LEU:HB3	1:A:409:TYR:CE2	2.48	0.48
1:B:219:LEU:HD11	1:B:237:VAL:HG21	1.95	0.48
1:B:39:ARG:O	1:B:65:VAL:HG22	2.12	0.48
1:B:243:LEU:HB3	1:B:285:PHE:CD1	2.48	0.48
1:A:216:ARG:NH1	1:A:307:ARG:HB2	2.27	0.48
1:A:224:TYR:CE2	1:A:274:VAL:HG13	2.47	0.48
1:B:172:GLU:OE2	1:B:395:VAL:HG13	2.13	0.48
1:B:265:LYS:HA	1:B:275:GLU:HA	1.95	0.48
1:A:373:THR:HG22	1:A:377:ILE:CD1	2.43	0.48
1:B:129:VAL:HG12	1:B:131:LEU:HD21	1.96	0.48
1:B:386:LEU:CD1	1:B:390:VAL:CG2	2.92	0.48
1:B:33:PRO:HG3	1:B:403:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLN:NE2	1:A:39:ARG:HD3	2.28	0.48
1:A:346:ALA:O	1:A:390:VAL:HG22	2.14	0.48
1:A:87:PRO:HG3	1:A:104:LEU:HD13	1.96	0.48
1:A:192:ILE:CD1	1:A:196:LEU:HA	2.44	0.48
1:B:65:VAL:CG1	1:B:66:GLY:N	2.77	0.48
1:A:243:LEU:HD13	1:A:285:PHE:CE1	2.48	0.48
1:A:302:TYR:N	1:A:302:TYR:CD1	2.82	0.48
1:B:42:PHE:CZ	1:B:99:GLU:HB2	2.49	0.48
1:A:243:LEU:CD1	1:A:285:PHE:CE1	2.97	0.48
1:A:193:SER:O	1:A:194:PHE:HB2	2.13	0.47
1:A:197:ILE:HG22	1:A:197:ILE:O	2.14	0.47
1:A:312:ASN:OD1	1:A:322:GLY:N	2.43	0.47
1:A:41:LEU:HD12	1:A:83:ASN:O	2.14	0.47
1:A:203:ALA:O	1:A:320:LEU:HA	2.14	0.47
1:B:224:TYR:CE2	1:B:274:VAL:HG13	2.49	0.47
1:A:144:PHE:CE1	1:A:428:ARG:HB2	2.50	0.47
1:A:367:VAL:HG22	1:A:367:VAL:O	2.14	0.47
1:B:265:LYS:CG	1:B:275:GLU:OE1	2.60	0.47
1:B:370:ASP:OD2	1:B:372:VAL:HG23	2.15	0.47
1:B:69:GLU:H	1:B:69:GLU:CD	2.18	0.47
1:B:187:ILE:HB	1:B:204:LEU:HD23	1.97	0.47
1:B:423:THR:HG23	1:B:425:GLU:HG2	1.97	0.47
1:A:39:ARG:O	1:A:65:VAL:HG22	2.15	0.47
1:A:214:ILE:HG21	1:A:287:ILE:HA	1.98	0.46
1:A:216:ARG:HH11	1:A:307:ARG:HD3	1.81	0.46
1:A:191:PRO:HG3	1:A:333:SER:OG	2.16	0.46
1:A:9:ARG:NE	1:A:411:TYR:O	2.48	0.46
1:A:62:GLY:H	1:A:102:ARG:HH12	1.63	0.46
1:B:301:SER:O	1:B:304:GLU:HB3	2.16	0.46
1:A:220:LYS:NZ	1:A:307:ARG:HD2	2.30	0.46
1:B:265:LYS:CD	1:B:275:GLU:HB2	2.45	0.46
1:A:77:VAL:HB	1:A:80:VAL:HG22	1.97	0.46
1:A:348:GLN:HA	1:A:348:GLN:NE2	2.29	0.46
1:B:192:ILE:HD11	1:B:196:LEU:HD12	1.97	0.46
1:B:265:LYS:HG2	1:B:275:GLU:HA	1.96	0.46
1:A:238:LYS:HD2	1:A:239:ARG:N	2.30	0.46
1:A:414:PRO:CD	1:B:48:GLU:HG2	2.46	0.46
1:A:269:SER:O	1:A:271:VAL:HB	2.16	0.46
1:A:269:SER:C	1:A:271:VAL:N	2.69	0.46
1:A:411:TYR:CD1	1:A:411:TYR:C	2.88	0.46
1:B:310:ILE:HD12	1:B:310:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:THR:HA	1:A:286:LEU:HD13	1.98	0.46
1:B:41:LEU:HD12	1:B:41:LEU:HA	1.73	0.46
1:B:184:HIS:ND1	2:B:1431:ADP:C3'	2.79	0.46
1:B:429:PHE:CD1	1:B:429:PHE:N	2.84	0.46
1:B:20:THR:N	2:B:1431:ADP:PB	2.78	0.45
1:B:177:CYS:HB3	1:B:348:GLN:HB3	1.98	0.45
1:A:404:ARG:HA	1:A:407:VAL:HG22	1.99	0.45
1:B:39:ARG:HB3	1:B:86:TYR:HE1	1.78	0.45
1:A:212:ASN:OD1	1:A:238:LYS:HE3	2.16	0.45
1:B:245:PRO:HG3	1:B:289:GLU:HB2	1.99	0.45
1:B:284:ARG:HA	1:B:287:ILE:HD12	1.99	0.45
1:A:15:GLY:O	1:A:25:TYR:HA	2.16	0.45
1:A:314:VAL:C	1:A:315:ILE:HD13	2.36	0.45
1:B:38:THR:HG22	1:B:38:THR:O	2.17	0.45
1:B:292:PHE:HZ	1:B:371:SER:HB3	1.80	0.45
1:A:203:ALA:HB1	1:A:320:LEU:HD12	1.96	0.45
1:A:224:TYR:O	1:A:226:ASP:N	2.50	0.45
1:B:429:PHE:HA	1:B:430:PRO:HD3	1.78	0.45
1:B:87:PRO:HG3	1:B:103:VAL:HB	1.98	0.45
1:A:165:PRO:HA	1:A:168:VAL:HG23	1.98	0.45
1:A:182:GLY:O	1:A:353:GLY:HA3	2.17	0.45
1:A:375:VAL:HG11	1:A:392:VAL:HG21	1.99	0.45
1:B:99:GLU:O	1:B:103:VAL:HG23	2.17	0.45
1:B:309:ARG:H	1:B:309:ARG:HD2	1.79	0.45
1:A:20:THR:H	2:A:1431:ADP:PB	2.40	0.45
1:B:180:VAL:CG1	1:B:351:LEU:CD2	2.95	0.45
1:B:289:GLU:OE2	1:B:293:ASP:HB3	2.17	0.45
1:A:178:VAL:CG1	1:A:349:ILE:HD13	2.47	0.44
1:A:238:LYS:HG2	1:A:287:ILE:CG2	2.48	0.44
1:B:235:GLU:OE2	1:B:238:LYS:HE3	2.17	0.44
1:A:397:GLU:N	1:A:398:PRO:CD	2.80	0.44
1:A:187:ILE:HB	1:A:204:LEU:HD23	1.98	0.44
1:B:65:VAL:HG12	1:B:66:GLY:N	2.32	0.44
1:B:109:ARG:NH1	1:B:153:GLU:OE2	2.51	0.44
1:A:33:PRO:HG2	1:A:400:TYR:HD1	1.82	0.44
1:A:214:ILE:CG2	1:A:287:ILE:HA	2.47	0.44
1:A:341:ILE:CD1	1:A:344:ARG:CD	2.92	0.44
1:B:25:TYR:CZ	1:B:34:LYS:HB2	2.53	0.44
1:B:26:GLY:HA3	1:B:30:LEU:HD11	1.99	0.44
1:B:233:ALA:O	1:B:237:VAL:HG23	2.17	0.44
1:A:397:GLU:N	1:A:398:PRO:HD3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LEU:HB2	1:B:394:LEU:HA	2.00	0.44
1:A:232:TYR:O	1:A:232:TYR:CD1	2.71	0.43
1:B:169:ALA:HB2	1:B:179:ILE:HD11	2.00	0.43
1:B:171:ALA:HA	1:B:408:ILE:HD11	1.99	0.43
1:B:269:SER:HB2	1:B:270:PRO:HD2	2.00	0.43
1:A:190:ALA:HA	1:A:191:PRO:HD3	1.92	0.43
1:B:41:LEU:HD13	1:B:84:LEU:CD1	2.47	0.43
1:B:31:ASN:ND2	1:B:31:ASN:N	2.61	0.43
1:B:170:ILE:HG22	1:B:408:ILE:HG13	2.00	0.43
1:B:269:SER:O	1:B:271:VAL:N	2.51	0.43
1:A:40:GLY:HA2	1:A:65:VAL:HG23	2.00	0.43
1:B:404:ARG:HA	1:B:407:VAL:HG22	2.00	0.43
1:A:162:LEU:HD22	1:A:409:TYR:HD2	1.83	0.43
1:A:344:ARG:HH12	1:B:72:LYS:CB	2.21	0.43
1:A:351:LEU:O	1:A:395:VAL:HG23	2.18	0.43
1:A:131:LEU:HD11	1:A:143:ILE:HG13	2.01	0.43
1:B:276:ILE:HA	1:B:277:PRO:HD2	1.71	0.43
1:B:165:PRO:O	1:B:179:ILE:HD13	2.19	0.43
1:A:409:TYR:HE1	1:A:413:LEU:HD13	1.76	0.43
1:B:386:LEU:CD1	1:B:390:VAL:HG23	2.48	0.43
1:A:8:TYR:OH	1:A:124:GLY:N	2.52	0.42
1:A:33:PRO:HD2	1:A:400:TYR:CD1	2.54	0.42
1:A:184:HIS:ND1	2:A:1431:ADP:C3'	2.82	0.42
1:A:193:SER:CB	1:B:75:SER:CB	2.89	0.42
1:A:214:ILE:HD12	1:A:214:ILE:HA	1.79	0.42
1:B:164:GLN:N	1:B:165:PRO:CD	2.82	0.42
1:A:46:LEU:HB3	1:A:51:LYS:HE2	2.01	0.42
1:B:11:LYS:HD2	1:B:12:TYR:CE2	2.54	0.42
1:B:39:ARG:HA	1:B:85:LYS:O	2.20	0.42
1:B:243:LEU:HA	1:B:243:LEU:HD23	1.70	0.42
1:B:373:THR:O	1:B:374:ARG:C	2.57	0.42
1:B:15:GLY:O	1:B:25:TYR:HA	2.19	0.42
1:B:222:ILE:HD13	1:B:277:PRO:CD	2.43	0.42
1:B:364:MET:C	1:B:366:ASP:N	2.72	0.42
1:A:61:ARG:O	1:A:63:LEU:N	2.52	0.42
1:B:129:VAL:CG1	1:B:131:LEU:HD21	2.50	0.42
1:A:61:ARG:C	1:A:63:LEU:N	2.73	0.42
1:A:420:SER:O	1:A:421:ASP:C	2.58	0.42
1:B:190:ALA:HB2	1:B:201:LEU:CD1	2.49	0.42
1:A:191:PRO:O	1:A:192:ILE:HD13	2.20	0.42
1:A:243:LEU:O	1:A:288:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:PRO:HB3	1:B:100:ALA:HB1	2.01	0.42
1:A:194:PHE:HD2	1:B:50:VAL:HB	1.85	0.42
1:A:324:MET:O	1:A:325:ASP:HB2	2.19	0.42
1:B:121:GLU:H	1:B:121:GLU:HG2	1.72	0.42
1:B:124:GLY:HA2	1:B:155:LYS:O	2.20	0.42
1:B:182:GLY:O	1:B:353:GLY:HA3	2.19	0.42
1:A:222:ILE:HG12	1:A:280:TYR:HD2	1.85	0.41
1:B:243:LEU:HB3	1:B:285:PHE:CE1	2.55	0.41
1:A:27:PRO:C	1:A:29:THR:H	2.24	0.41
1:A:232:TYR:CD1	1:A:232:TYR:C	2.94	0.41
1:B:21:SER:OG	1:B:184:HIS:HB2	2.20	0.41
1:B:193:SER:HB3	1:B:197:ILE:HD11	2.03	0.41
1:B:379:LEU:O	1:B:383:SER:N	2.54	0.41
1:A:113:ALA:HA	1:A:154:PHE:HE2	1.85	0.41
1:B:320:LEU:N	1:B:320:LEU:HD22	2.36	0.41
1:A:90:ASP:C	1:A:92:VAL:H	2.24	0.41
1:A:105:LYS:HE3	1:A:150:LEU:HD21	2.02	0.41
1:A:160:THR:OG1	1:A:161:ILE:N	2.53	0.41
1:A:400:TYR:O	1:A:404:ARG:HG3	2.20	0.41
1:B:337:VAL:CG2	1:B:342:GLN:HG2	2.49	0.41
1:B:395:VAL:HG12	1:B:396:SER:O	2.21	0.41
1:A:34:LYS:HG3	1:A:115:PHE:HZ	1.85	0.41
1:A:170:ILE:CG2	1:A:408:ILE:HG13	2.49	0.41
1:A:180:VAL:HA	1:A:189:VAL:HA	2.02	0.41
1:A:216:ARG:HH11	1:A:216:ARG:HG2	1.85	0.41
1:B:121:GLU:O	1:B:122:PHE:C	2.58	0.41
1:B:122:PHE:HE2	1:B:155:LYS:HB2	1.85	0.41
1:B:193:SER:C	1:B:195:ALA:H	2.24	0.41
1:A:47:PRO:HG2	1:A:50:VAL:CG2	2.50	0.41
1:B:39:ARG:HD3	1:B:86:TYR:HE1	1.85	0.41
1:B:43:LEU:HD12	1:B:43:LEU:HA	1.87	0.40
1:B:54:ILE:CD1	1:B:73:TYR:CE2	2.92	0.40
1:B:72:LYS:HG3	1:B:73:TYR:CE1	2.56	0.40
1:B:134:LEU:O	1:B:136:PRO:HD3	2.21	0.40
1:B:210:GLU:CB	1:B:290:ILE:HD13	2.48	0.40
1:B:227:ILE:HG22	1:B:233:ALA:HB1	2.03	0.40
1:A:97:ASP:OD1	1:A:97:ASP:C	2.59	0.40
1:B:310:ILE:H	1:B:310:ILE:HG13	1.77	0.40
1:A:215:THR:HG22	1:A:234:VAL:HG12	2.03	0.40
1:A:220:LYS:HG2	1:A:225:SER:HB3	2.03	0.40
1:A:222:ILE:HD13	1:A:277:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PHE:HD1	1:A:62:GLY:O	2.04	0.40
1:B:73:TYR:N	1:B:73:TYR:CD1	2.88	0.40
1:B:361:PRO:CG	1:B:364:MET:SD	3.06	0.40
1:B:12:TYR:HA	1:B:125:TRP:CZ3	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:SER:OG	1:B:342:GLN:OE1[3_445]	1.67	0.53
1:A:304:GLU:OE2	1:A:304:GLU:OE2[7_645]	1.74	0.46

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	424/432 (98%)	358 (84%)	51 (12%)	15 (4%)	3 24
1	B	424/432 (98%)	356 (84%)	59 (14%)	9 (2%)	7 37
All	All	848/864 (98%)	714 (84%)	110 (13%)	24 (3%)	5 29

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	PRO
1	A	294	PRO
1	A	307	ARG
1	A	324	MET
1	A	388	SER
1	A	421	ASP
1	B	307	ARG
1	B	402	VAL

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Mol	Chain	Res	Type
1	A	293	ASP
1	A	366	ASP
1	A	97	ASP
1	B	97	ASP
1	A	239	ARG
1	A	342	GLN
1	B	60	ALA
1	B	62	GLY
1	B	304	GLU
1	A	403	TRP
1	A	411	TYR
1	B	387	ALA
1	B	411	TYR
1	B	270	PRO
1	A	161	ILE
1	A	28	ILE

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	357/363 (98%)	297 (83%)	60 (17%)	2 10
1	B	358/363 (99%)	292 (82%)	66 (18%)	1 8
All	All	715/726 (98%)	589 (82%)	126 (18%)	2 9

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	24	LYS
1	A	30	LEU
1	A	37	GLN
1	A	43	LEU
1	A	44	ARG
1	A	53	ARG

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Mol	Chain	Res	Type
1	A	54	ILE
1	A	57	ASP
1	A	59	LEU
1	A	61	ARG
1	A	65	VAL
1	A	67	ASP
1	A	68	GLU
1	A	71	ARG
1	A	77	VAL
1	A	78	ARG
1	A	80	VAL
1	A	82	ARG
1	A	89	LYS
1	A	96	ASP
1	A	104	LEU
1	A	106	GLU
1	A	112	LEU
1	A	148	ASP
1	A	166	LEU
1	A	196	LEU
1	A	202	VAL
1	A	210	GLU
1	A	225	SER
1	A	226	ASP
1	A	234	VAL
1	A	238	LYS
1	A	297	GLU
1	A	298	GLU
1	A	302	TYR
1	A	303	ILE
1	A	308	LEU
1	A	309	ARG
1	A	314	VAL
1	A	317	ASP
1	A	320	LEU
1	A	326	VAL
1	A	338	SER
1	A	341	ILE
1	A	348	GLN
1	A	349	ILE
1	A	351	LEU
1	A	357	SER

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Mol	Chain	Res	Type
1	A	366	ASP
1	A	370	ASP
1	A	374	ARG
1	A	375	VAL
1	A	394	LEU
1	A	401	SER
1	A	402	VAL
1	A	408	ILE
1	A	417	LEU
1	A	418	GLU
1	A	425	GLU
1	B	9	ARG
1	B	24	LYS
1	B	30	LEU
1	B	31	ASN
1	B	32	GLU
1	B	36	VAL
1	B	37	GLN
1	B	43	LEU
1	B	44	ARG
1	B	46	LEU
1	B	59	LEU
1	B	61	ARG
1	B	67	ASP
1	B	68	GLU
1	B	79	ASP
1	B	80	VAL
1	B	90	ASP
1	B	95	ARG
1	B	96	ASP
1	B	102	ARG
1	B	104	LEU
1	B	106	GLU
1	B	109	ARG
1	B	121	GLU
1	B	137	ASP
1	B	143	ILE
1	B	144	PHE
1	B	148	ASP
1	B	159	VAL
1	B	181	GLU
1	B	196	LEU

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Mol	Chain	Res	Type
1	B	198	ARG
1	B	202	VAL
1	B	204	LEU
1	B	210	GLU
1	B	225	SER
1	B	226	ASP
1	B	234	VAL
1	B	238	LYS
1	B	248	LEU
1	B	253	ARG
1	B	260	ASP
1	B	267	ARG
1	B	278	ARG
1	B	297	GLU
1	B	298	GLU
1	B	303	ILE
1	B	309	ARG
1	B	314	VAL
1	B	317	ASP
1	B	326	VAL
1	B	338	SER
1	B	341	ILE
1	B	347	SER
1	B	348	GLN
1	B	357	SER
1	B	366	ASP
1	B	373	THR
1	B	386	LEU
1	B	399	GLN
1	B	402	VAL
1	B	408	ILE
1	B	417	LEU
1	B	418	GLU
1	B	423	THR
1	B	429	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	83	ASN
1	A	296	HIS

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Mol	Chain	Res	Type
1	A	348	GLN
1	B	31	ASN
1	B	83	ASN
1	B	296	HIS
1	B	348	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)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	1431	-	24,29,29	1.25	3 (12%)	29,45,45	1.72	6 (20%)
2	ADP	B	1431	-	24,29,29	1.22	3 (12%)	29,45,45	1.94	7 (24%)

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	ADP	A	1431	-	-	2/12/32/32	0/3/3/3
2	ADP	B	1431	-	-	1/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1431	ADP	C5-C4	3.15	1.49	1.40
2	B	1431	ADP	C5-C4	2.79	1.48	1.40
2	B	1431	ADP	C6-C5	2.46	1.52	1.43
2	A	1431	ADP	C2-N3	2.43	1.36	1.32
2	B	1431	ADP	C2-N3	2.35	1.35	1.32
2	A	1431	ADP	C6-C5	2.24	1.51	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1431	ADP	PA-O3A-PB	-4.75	116.53	132.83
2	B	1431	ADP	C4-C5-N7	-4.23	105.00	109.40
2	B	1431	ADP	N3-C2-N1	-4.15	122.19	128.68
2	A	1431	ADP	O3'-C3'-C2'	-3.86	99.32	111.82
2	A	1431	ADP	O4'-C1'-C2'	-3.86	101.29	106.93
2	A	1431	ADP	C4-C5-N7	-3.62	105.63	109.40
2	A	1431	ADP	PA-O3A-PB	-3.31	121.46	132.83
2	B	1431	ADP	C1'-N9-C4	-2.87	121.60	126.64
2	A	1431	ADP	O2'-C2'-C3'	-2.86	102.56	111.82
2	B	1431	ADP	O4'-C1'-C2'	-2.78	102.87	106.93
2	B	1431	ADP	O3'-C3'-C2'	-2.71	103.05	111.82
2	A	1431	ADP	N3-C2-N1	-2.63	124.57	128.68
2	B	1431	ADP	O2'-C2'-C3'	-2.01	105.32	111.82

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1431	ADP	PB-O3A-PA-O1A
2	A	1431	ADP	PB-O3A-PA-O2A
2	B	1431	ADP	PB-O3A-PA-O2A

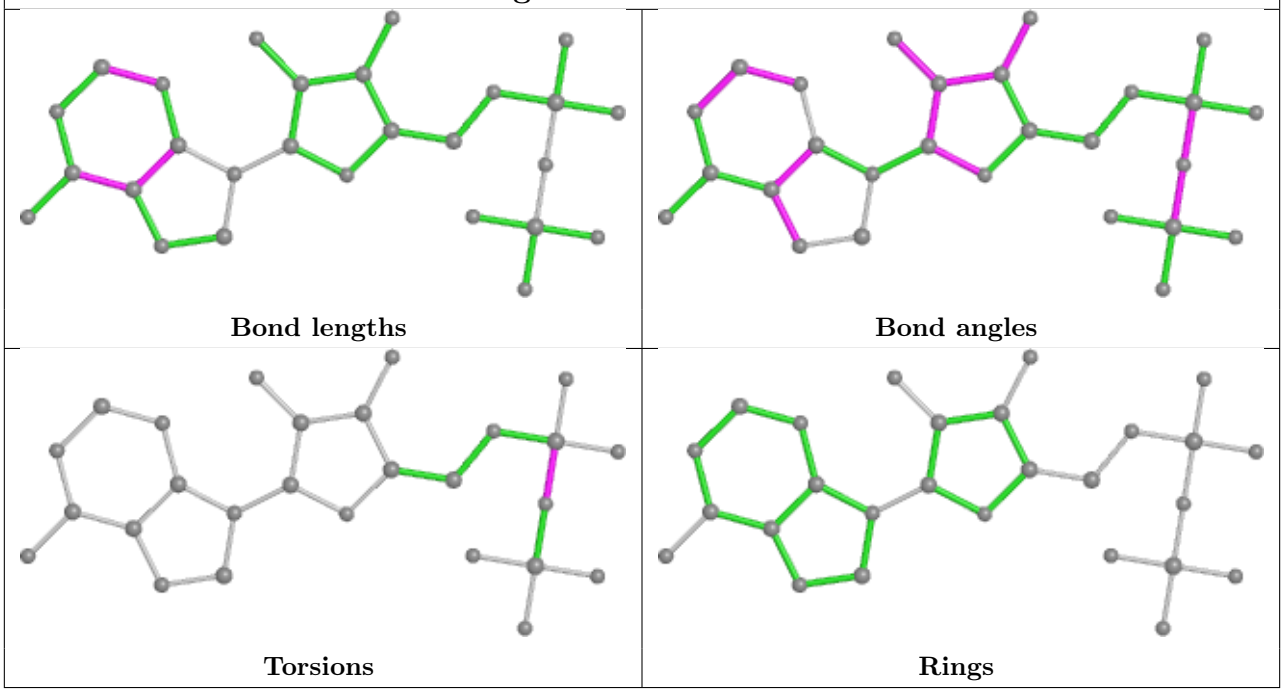
There are no ring outliers.

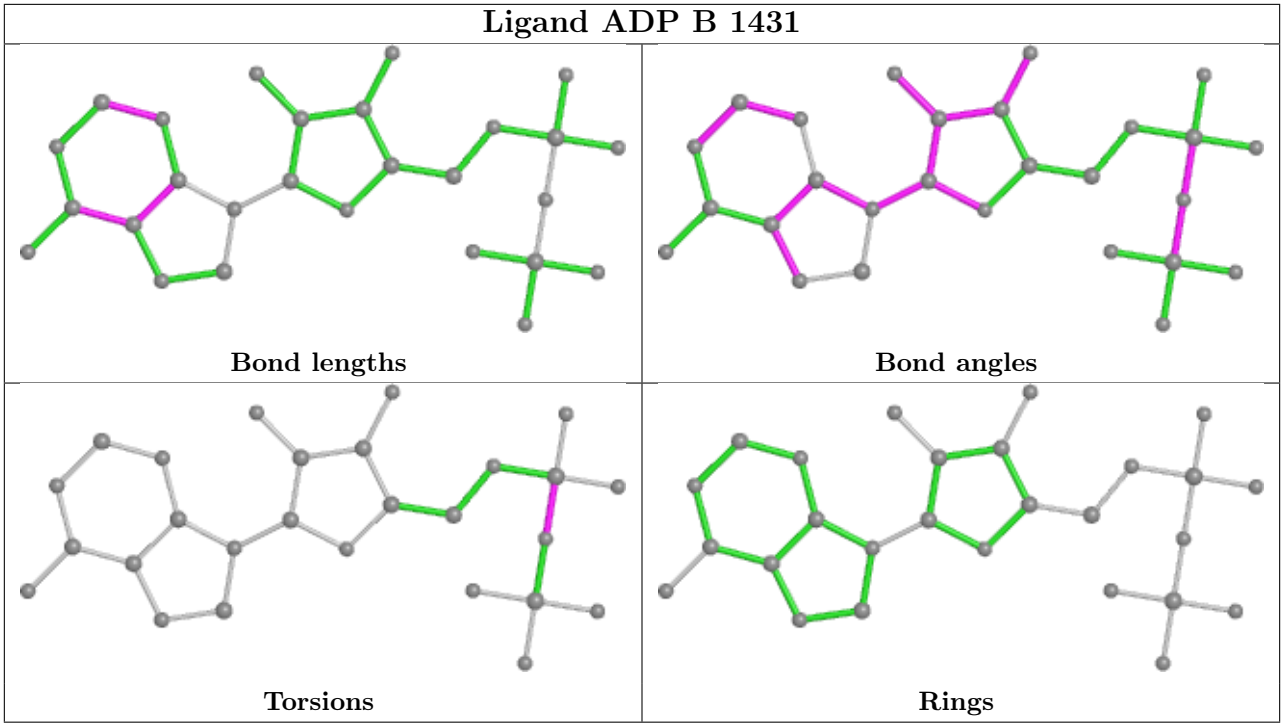
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1431	ADP	5	0
2	B	1431	ADP	6	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 ADP A 1431





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	426/432 (98%)	-0.13	0 100 100	48, 86, 133, 189	0
1	B	426/432 (98%)	-0.08	2 (0%) 91 86	47, 89, 136, 194	0
All	All	852/864 (98%)	-0.11	2 (0%) 95 94	47, 88, 135, 194	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	ALA	2.4
1	B	317	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

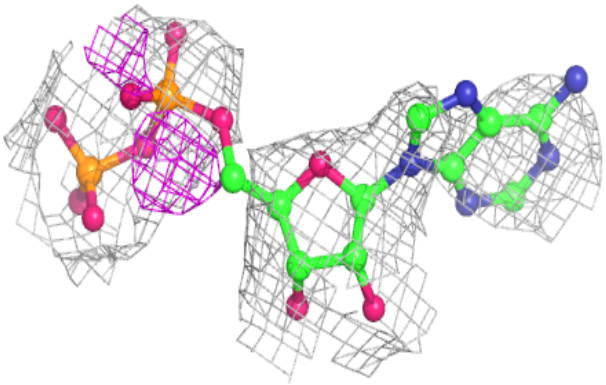
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

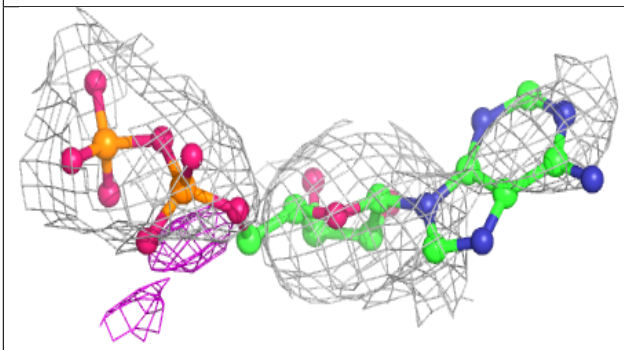
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	A	1431	27/27	0.87	0.26	94,139,168,173	0
2	ADP	B	1431	27/27	0.88	0.28	90,139,152,156	0

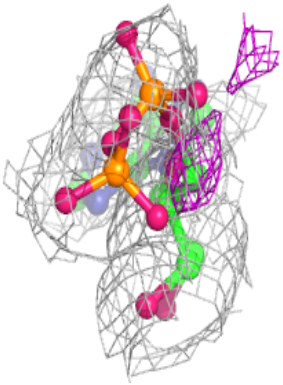
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 1431:

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

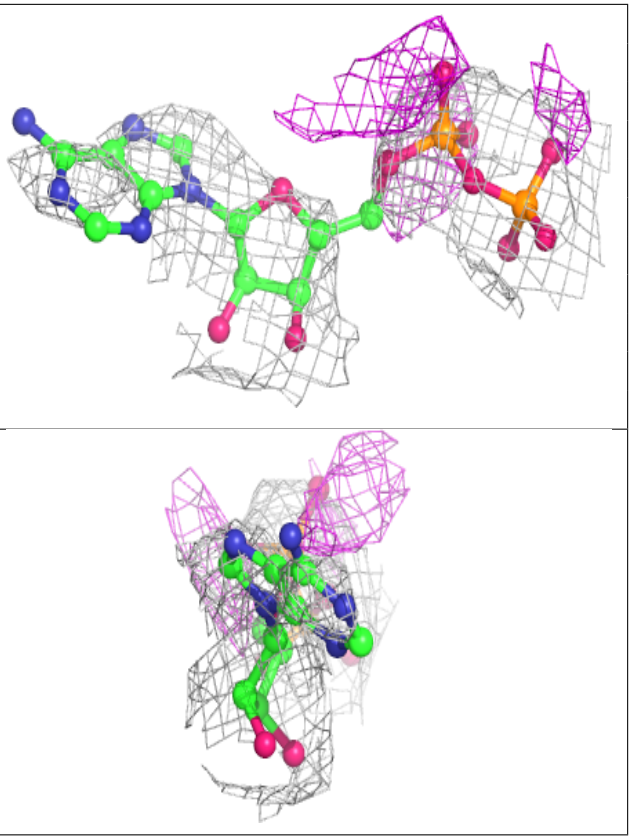


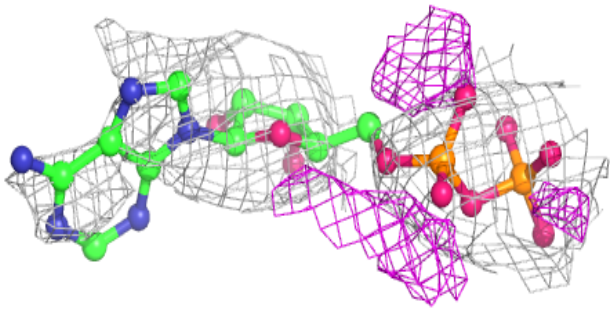




Electron density around ADP B 1431:

$2mF_o$-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.