



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:08 pm GMT

PDB ID : 1JST  
Title : PHOSPHORYLATED CYCLIN-DEPENDENT KINASE-2 BOUND TO CYCLIN A  
Authors : Russo, A.A.; Jeffrey, P.D.; Pavletich, N.P.  
Deposited on : 1996-07-03  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

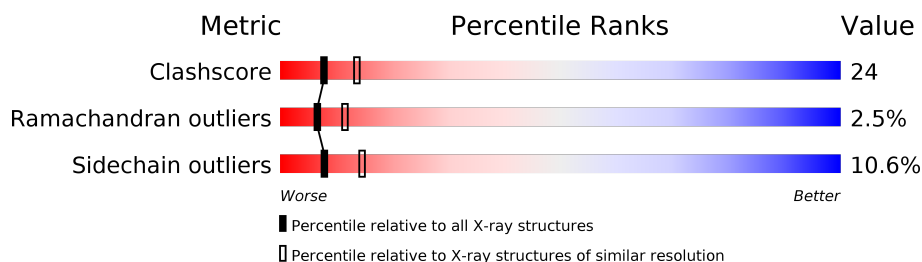
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	298	
1	C	298	
2	B	258	
2	D	258	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9134 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 CYCLIN-DEPENDENT KINASE-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	P	S	0	0	0
			2402	1559	408	426	1	8			
1	C	298	Total	C	N	O	P	S	0	0	0
			2402	1559	408	426	1	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	TPO	THR	MODIFIED RESIDUE	UNP P24941
C	160	TPO	THR	MODIFIED RESIDUE	UNP P24941

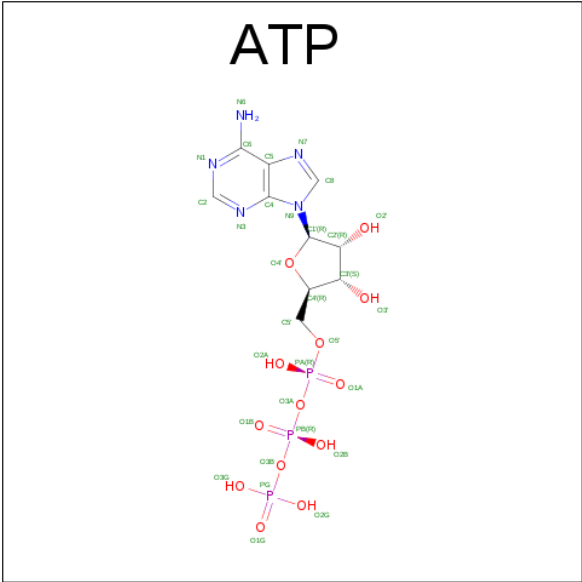
- Molecule 2 is a protein called CYCLIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			
2	D	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).

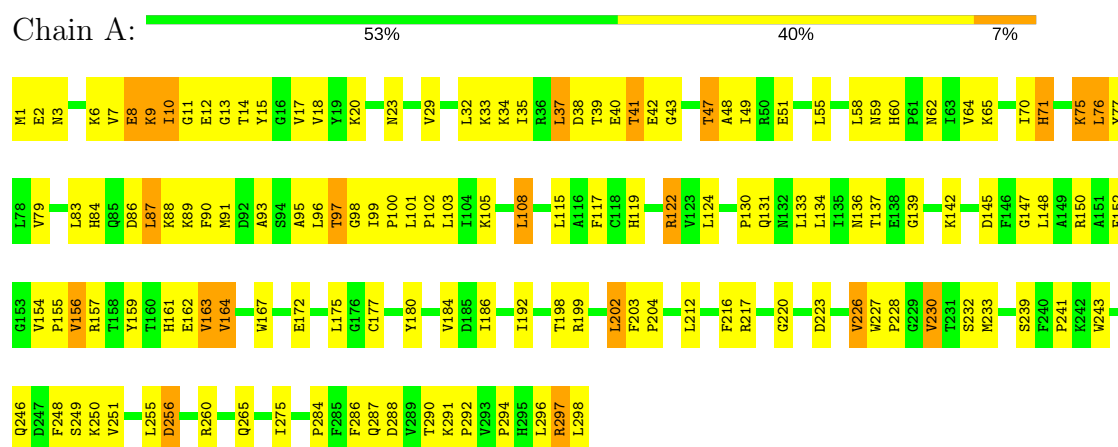


### 3 Residue-property plots

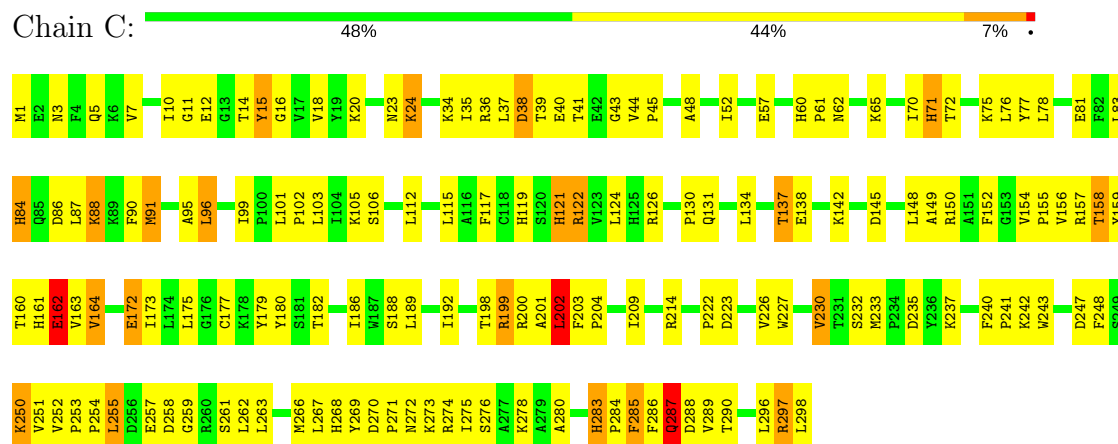
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

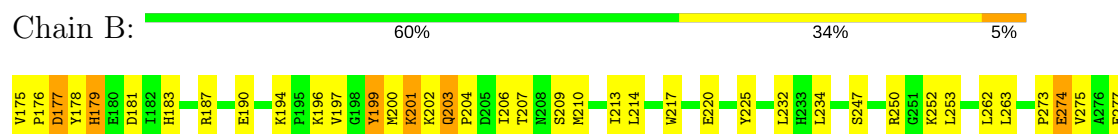
#### • Molecule 1: CYCLIN-DEPENDENT KINASE-2

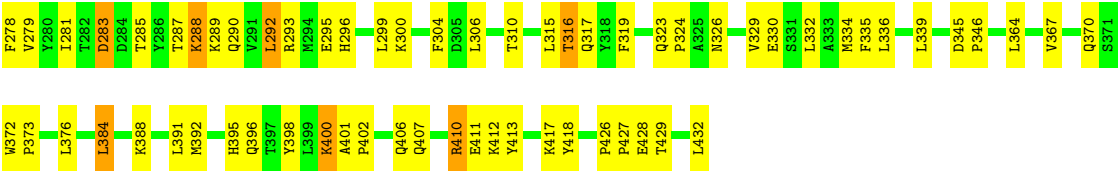


#### • Molecule 1: CYCLIN-DEPENDENT KINASE-2

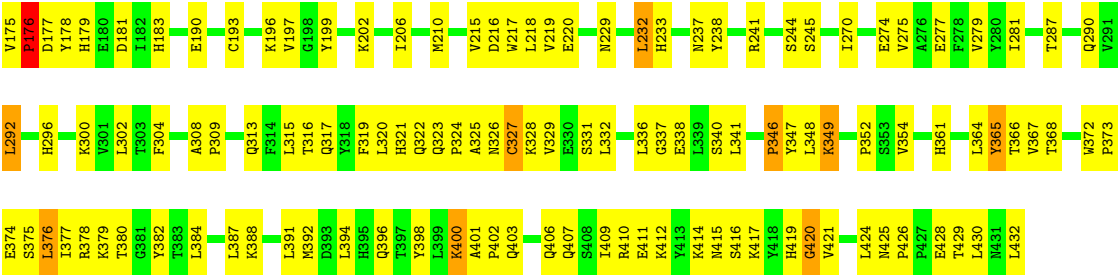


#### • Molecule 2: CYCLIN A





● Molecule 2: CYCLIN A



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.60Å 149.10Å 74.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.9 (7.00-2.60)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9134	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MN, ATP

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	0.70	0/2452	0.87	1/3325 (0.0%)
1	C	0.61	0/2452	0.86	2/3325 (0.1%)
2	B	0.69	0/2134	0.81	1/2897 (0.0%)
2	D	0.60	0/2134	0.79	2/2897 (0.1%)
All	All	0.65	0/9172	0.84	6/12444 (0.0%)

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
2	D	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	LEU	CA-CB-CG	8.68	135.26	115.30
2	B	345	ASP	N-CA-C	-6.05	94.67	111.00
1	A	217	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	202	LEU	CA-CB-CG	5.64	128.27	115.30
2	D	241	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	D	176	PRO	N-CA-C	5.25	125.75	112.10

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
2	D	347	TYR	Sidechain

## 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	2402	0	2449	132	0
1	C	2402	0	2449	141	0
2	B	2084	0	2107	78	0
2	D	2084	0	2107	108	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	31	0	12	8	0
4	C	31	0	12	4	0
5	A	38	0	0	1	0
5	B	24	0	0	1	0
5	C	20	0	0	0	0
5	D	16	0	0	2	0
All	All	9134	0	9136	438	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (438) 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:15:TYR:HB3	1:A:35:ILE:HG12	1.41	0.99
1:C:60:HIS:HD2	1:C:62:ASN:H	1.06	0.98
1:A:156:VAL:HG22	1:A:159:TYR:CE2	2.04	0.93
1:A:1:MET:CE	1:A:70:ILE:HG13	1.99	0.92
1:A:88:LYS:HD2	1:A:131:GLN:HG2	1.52	0.91
1:A:60:HIS:HD2	1:A:62:ASN:H	1.07	0.91
1:C:154:VAL:O	2:D:316:THR:HG22	1.73	0.87
2:D:373:PRO:HG2	2:D:376:LEU:HB2	1.57	0.87
1:A:60:HIS:CD2	1:A:62:ASN:H	1.93	0.85
1:A:38:ASP:HB3	1:A:43:GLY:H	1.43	0.83
1:C:157:ARG:HG2	1:C:158:THR:H	1.44	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:LYS:HD2	1:C:131:GLN:HB3	1.59	0.83
1:C:156:VAL:HG22	1:C:159:TYR:CE2	2.14	0.83
1:C:88:LYS:HZ2	1:C:131:GLN:H	1.23	0.83
2:D:196:LYS:HD3	2:D:244:SER:HB3	1.60	0.83
2:D:346:PRO:O	2:D:349:LYS:HG3	1.80	0.82
2:D:197:VAL:HG11	2:D:349:LYS:HB3	1.59	0.82
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.16	0.81
2:B:407:GLN:O	2:B:411:GLU:HG2	1.80	0.80
1:C:156:VAL:HG22	1:C:159:TYR:HE2	1.47	0.80
1:A:1:MET:HE1	1:A:70:ILE:HG13	1.63	0.80
1:C:286:PHE:O	1:C:289:VAL:HG23	1.81	0.79
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.63	0.79
1:A:177:CYS:SG	1:A:233:MET:SD	2.81	0.78
1:C:60:HIS:HD2	1:C:62:ASN:N	1.81	0.77
1:A:60:HIS:HD2	1:A:62:ASN:N	1.81	0.77
1:C:172:GLU:HB3	1:C:177:CYS:SG	2.25	0.77
1:C:83:LEU:HD11	1:C:142:LYS:HD2	1.66	0.76
2:B:289:LYS:O	2:B:293:ARG:HG3	1.86	0.76
1:C:84:HIS:CE1	1:C:298:LEU:HB3	2.20	0.76
1:C:84:HIS:HB3	1:C:298:LEU:HG	1.68	0.75
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.50	0.75
2:D:396:GLN:NE2	2:D:400:LYS:HE3	2.02	0.75
1:C:119:HIS:CD2	1:C:182:THR:HB	2.21	0.75
1:C:200:ARG:HD2	1:C:201:ALA:H	1.50	0.75
1:A:51:GLU:O	1:A:55:LEU:HB2	1.86	0.74
2:D:216:ASP:HB2	2:D:406:GLN:HG3	1.70	0.73
1:A:88:LYS:CD	1:A:131:GLN:HG2	2.17	0.73
1:C:201:ALA:HB3	1:C:204:PRO:HG3	1.71	0.73
1:A:156:VAL:HG22	1:A:159:TYR:HE2	1.53	0.73
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.23	0.73
2:B:336:LEU:HD23	2:B:339:LEU:HD12	1.71	0.73
1:C:162:GLU:HG3	1:C:173:ILE:HG22	1.71	0.73
1:A:10:ILE:HG22	4:A:300:ATP:H1'	1.73	0.71
1:C:160:TPO:O1P	2:D:270:ILE:HA	1.90	0.71
1:C:60:HIS:CD2	1:C:62:ASN:H	1.99	0.71
2:B:209:SER:O	2:B:213:ILE:HG12	1.91	0.70
1:C:268:HIS:HD2	1:C:270:ASP:N	1.87	0.70
1:C:227:TRP:HB3	1:C:230:VAL:HG22	1.72	0.70
2:B:288:LYS:HD3	2:B:292:LEU:HD22	1.73	0.70
2:D:287:THR:OG1	2:D:290:GLN:HG3	1.92	0.70
1:A:35:ILE:HG22	1:A:37:LEU:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:HD13	1:A:286:PHE:HZ	1.58	0.69
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.28	0.69
1:A:227:TRP:O	1:A:230:VAL:HG22	1.92	0.69
1:C:115:LEU:HD22	1:C:189:LEU:HD22	1.75	0.69
1:C:240:PHE:HB2	1:C:242:LYS:HZ2	1.58	0.68
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.75	0.68
1:C:296:LEU:HD13	1:C:298:LEU:HD23	1.76	0.68
2:B:274:GLU:HG3	2:B:277:GLU:HG2	1.75	0.67
1:C:1:MET:HE1	1:C:70:ILE:HG13	1.76	0.67
1:C:1:MET:HE3	1:C:70:ILE:HG21	1.78	0.66
2:D:417:LYS:HB3	2:D:417:LYS:NZ	2.10	0.66
2:B:213:ILE:HD13	2:B:406:GLN:NE2	2.12	0.65
2:D:274:GLU:HG2	2:D:277:GLU:HG2	1.79	0.65
1:A:7:VAL:O	1:A:8:GLU:HB2	1.95	0.65
1:A:87:LEU:HB3	1:A:130:PRO:HB3	1.79	0.65
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.78	0.65
1:C:38:ASP:HB2	1:C:43:GLY:H	1.62	0.65
2:D:372:TRP:CD1	2:D:377:ILE:HG12	2.32	0.64
2:B:206:ILE:HG22	2:B:210:MET:HE1	1.80	0.64
1:C:283:HIS:CE1	1:C:284:PRO:HG2	2.33	0.64
1:C:15:TYR:HD1	1:C:15:TYR:H	1.44	0.64
1:C:84:HIS:ND1	1:C:137:THR:HG23	2.13	0.63
2:D:175:VAL:HB	2:D:176:PRO:CD	2.29	0.63
1:A:88:LYS:HE3	1:A:131:GLN:N	2.14	0.63
1:A:47:THR:HG22	1:A:147:GLY:O	1.98	0.63
1:A:175:LEU:HD12	1:A:233:MET:HE1	1.79	0.63
2:D:388:LYS:HG3	2:D:432:LEU:HD12	1.81	0.62
2:D:366:THR:HG21	2:D:398:TYR:OH	1.99	0.62
2:B:202:LYS:HD2	2:B:202:LYS:H	1.63	0.62
2:B:263:LEU:HD21	2:B:295:GLU:HG3	1.81	0.62
2:D:216:ASP:CB	2:D:406:GLN:HG3	2.29	0.62
1:A:230:VAL:HA	1:A:233:MET:CE	2.29	0.62
1:A:88:LYS:CE	1:A:131:GLN:HG2	2.30	0.62
1:C:81:GLU:O	1:C:81:GLU:HG3	1.98	0.62
1:C:230:VAL:HA	1:C:233:MET:HE2	1.80	0.61
1:A:38:ASP:CG	1:A:41:THR:HB	2.20	0.61
1:A:99:ILE:HG23	1:A:103:LEU:HD23	1.82	0.61
2:B:202:LYS:HD2	2:B:202:LYS:N	2.15	0.61
1:C:88:LYS:HZ2	1:C:131:GLN:N	1.98	0.61
2:D:396:GLN:HE21	2:D:400:LYS:HE3	1.66	0.61
1:C:83:LEU:HD11	1:C:142:LYS:CD	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:202:LYS:O	2:B:204:PRO:HD3	2.02	0.60
1:A:58:LEU:HA	1:A:117:PHE:HE2	1.66	0.60
1:A:64:VAL:HG22	1:A:83:LEU:CD1	2.31	0.60
1:C:84:HIS:ND1	1:C:298:LEU:HB3	2.16	0.60
1:A:71:HIS:HB3	2:B:300:LYS:HE3	1.84	0.59
1:C:160:TPO:HA	2:D:270:ILE:HD13	1.84	0.59
1:C:38:ASP:HB3	1:C:41:THR:OG1	2.02	0.59
2:B:203:GLN:HG2	2:B:206:ILE:HG12	1.83	0.59
2:B:373:PRO:CG	2:B:376:LEU:HD12	2.32	0.59
2:D:377:ILE:HG23	2:D:382:TYR:O	2.02	0.59
2:B:207:THR:OG1	2:B:210:MET:HG3	2.03	0.59
2:D:396:GLN:O	2:D:400:LYS:HD3	2.02	0.59
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.68	0.59
1:C:240:PHE:HB2	1:C:242:LYS:NZ	2.17	0.59
1:C:160:TPO:OG1	2:D:270:ILE:HG23	2.02	0.59
1:C:1:MET:CE	1:C:70:ILE:HG13	2.32	0.58
1:C:198:THR:O	1:C:199:ARG:HG2	2.04	0.58
1:C:296:LEU:HD13	1:C:298:LEU:CD2	2.34	0.58
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.85	0.58
1:A:145:ASP:HB2	4:A:300:ATP:O2A	2.04	0.58
2:B:288:LYS:HD3	2:B:292:LEU:CD2	2.32	0.58
1:A:265:GLN:NE2	1:A:275:ILE:HD12	2.19	0.58
2:D:217:TRP:CE3	2:D:218:LEU:HD23	2.39	0.58
1:A:83:LEU:CD2	1:A:136:ASN:HB3	2.34	0.58
2:B:388:LYS:O	2:B:392:MET:HG2	2.03	0.58
1:C:247:ASP:HB3	1:C:250:LYS:HG2	1.85	0.57
1:A:93:ALA:HB3	1:A:297:ARG:NH2	2.18	0.57
2:B:176:PRO:HA	2:B:179:HIS:CE1	2.39	0.57
1:A:297:ARG:HH11	1:A:297:ARG:N	2.02	0.57
2:B:275:VAL:O	2:B:279:VAL:HG23	2.04	0.57
2:D:402:PRO:HG3	2:D:410:ARG:HH12	1.69	0.57
2:B:417:LYS:HE2	2:B:418:TYR:CZ	2.39	0.57
2:B:203:GLN:OE1	2:B:247:SER:HA	2.04	0.57
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.34	0.57
2:B:201:LYS:HD3	2:B:202:LYS:HE3	1.87	0.56
2:D:322:GLN:HG3	2:D:325:ALA:HA	1.86	0.56
1:A:32:LEU:HD23	1:A:79:VAL:HG22	1.87	0.56
1:A:297:ARG:HH11	1:A:297:ARG:H	1.54	0.56
1:A:88:LYS:HD2	1:A:131:GLN:CG	2.31	0.56
1:C:237:LYS:HB2	1:C:240:PHE:CE1	2.41	0.56
1:A:11:GLY:HA3	4:A:300:ATP:O4'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:MET:HE1	1:C:130:PRO:HG2	1.88	0.56
2:D:190:GLU:OE1	2:D:352:PRO:HD2	2.06	0.56
1:A:122:ARG:HD2	1:A:122:ARG:O	2.06	0.56
1:C:200:ARG:HD2	1:C:201:ALA:N	2.19	0.56
1:A:10:ILE:HB	1:A:18:VAL:HG12	1.87	0.55
1:A:230:VAL:HA	1:A:233:MET:HE2	1.87	0.55
1:C:255:LEU:HG	1:C:259:GLY:HA3	1.88	0.55
1:A:296:LEU:C	1:A:297:ARG:HD3	2.27	0.55
2:B:225:TYR:CE2	2:B:277:GLU:HB3	2.41	0.55
1:C:105:LYS:HG3	1:C:285:PHE:CZ	2.41	0.55
1:A:8:GLU:HG2	1:A:9:LYS:H	1.72	0.55
2:B:175:VAL:HG12	2:B:175:VAL:O	2.07	0.55
2:D:206:ILE:HG22	2:D:210:MET:HE1	1.88	0.55
2:B:278:PHE:O	2:B:281:ILE:HG13	2.06	0.55
1:C:101:LEU:N	1:C:102:PRO:HD2	2.22	0.55
1:A:71:HIS:CD2	2:B:300:LYS:HG3	2.42	0.54
1:C:222:PRO:HD3	1:C:269:TYR:CZ	2.42	0.54
1:C:223:ASP:H	1:C:226:VAL:HG12	1.72	0.54
1:A:98:GLY:O	1:A:100:PRO:HD3	2.06	0.54
1:A:9:LYS:NZ	1:A:17:VAL:HB	2.23	0.54
2:D:332:LEU:O	2:D:336:LEU:HG	2.07	0.54
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.43	0.54
1:C:296:LEU:HD13	1:C:298:LEU:CG	2.37	0.54
1:A:90:PHE:HA	1:A:297:ARG:HH22	1.72	0.54
1:C:91:MET:HE1	1:C:130:PRO:CG	2.38	0.54
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.88	0.54
1:A:297:ARG:HD3	1:A:297:ARG:N	2.22	0.54
1:C:90:PHE:HD1	1:C:297:ARG:NH2	2.06	0.54
2:D:199:TYR:HE2	2:D:348:LEU:HD21	1.72	0.54
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.72	0.54
2:D:277:GLU:O	2:D:281:ILE:HG12	2.08	0.54
2:D:275:VAL:O	2:D:279:VAL:HG23	2.07	0.54
2:B:373:PRO:HG2	2:B:376:LEU:HD12	1.88	0.53
2:B:364:LEU:HG	2:B:370:GLN:HB2	1.89	0.53
1:C:268:HIS:CD2	1:C:270:ASP:H	2.26	0.53
1:A:15:TYR:OH	1:A:47:THR:HB	2.08	0.53
1:A:13:GLY:HA3	4:A:300:ATP:PB	2.48	0.53
1:A:256:ASP:O	1:A:260:ARG:HG3	2.08	0.53
1:A:249:SER:HA	1:A:260:ARG:HD3	1.90	0.53
1:C:296:LEU:HD13	1:C:298:LEU:HG	1.91	0.53
2:D:327:CYS:SG	2:D:419:HIS:CE1	3.02	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.89	0.52
1:C:38:ASP:HB2	1:C:43:GLY:N	2.24	0.52
1:A:15:TYR:CE1	1:A:48:ALA:HB2	2.45	0.52
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.40	0.52
1:C:91:MET:HE2	1:C:130:PRO:HB3	1.90	0.52
2:D:367:VAL:HG12	2:D:368:THR:HG23	1.91	0.52
1:C:296:LEU:HD22	1:C:298:LEU:HD23	1.92	0.52
1:A:12:GLU:HG2	1:A:17:VAL:HA	1.92	0.52
2:B:395:HIS:HE1	2:B:427:PRO:O	1.93	0.51
1:C:86:ASP:HA	1:C:134:LEU:HA	1.93	0.51
2:D:175:VAL:N	2:D:176:PRO:HD2	2.25	0.51
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.45	0.51
1:A:9:LYS:HZ2	1:A:18:VAL:H	1.58	0.51
2:D:196:LYS:HD3	2:D:196:LYS:H	1.74	0.51
2:D:319:PHE:O	2:D:322:GLN:HG2	2.11	0.51
2:D:372:TRP:HB3	2:D:384:LEU:HD22	1.92	0.51
1:A:154:VAL:O	2:B:316:THR:HG22	2.10	0.51
1:C:162:GLU:HA	1:C:173:ILE:CG2	2.41	0.51
1:C:227:TRP:O	1:C:230:VAL:HG23	2.10	0.51
1:A:1:MET:HG3	1:A:1:MET:O	2.12	0.50
2:D:321:HIS:CE1	2:D:379:LYS:HD2	2.45	0.50
2:D:417:LYS:O	2:D:417:LYS:HG2	2.12	0.50
2:B:388:LYS:HG2	2:B:432:LEU:HD13	1.93	0.50
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.47	0.50
2:B:395:HIS:CE1	2:B:427:PRO:O	2.65	0.50
1:C:105:LYS:HG3	1:C:285:PHE:CE2	2.46	0.50
1:A:241:PRO:HB2	1:A:243:TRP:CZ3	2.47	0.50
1:C:15:TYR:HE1	4:C:300:ATP:O3B	1.95	0.50
1:C:268:HIS:HD2	1:C:270:ASP:H	1.54	0.50
1:C:16:GLY:HA3	4:C:300:ATP:O2B	2.11	0.49
2:D:354:VAL:HG13	2:D:387:LEU:HD23	1.92	0.49
1:A:296:LEU:HA	1:A:297:ARG:HH11	1.77	0.49
1:C:214:ARG:HG2	1:C:214:ARG:NH1	2.27	0.49
1:C:262:LEU:O	1:C:266:MET:HG3	2.12	0.49
1:A:15:TYR:CD1	1:A:48:ALA:HB2	2.47	0.49
1:A:10:ILE:CG2	4:A:300:ATP:H1'	2.41	0.49
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.92	0.49
1:A:93:ALA:HB3	1:A:297:ARG:HH21	1.77	0.49
1:A:64:VAL:HG22	1:A:83:LEU:HD12	1.93	0.49
2:D:196:LYS:HB2	2:D:199:TYR:HB3	1.94	0.49
2:D:337:GLY:O	2:D:340:SER:OG	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:LYS:H	2:D:196:LYS:CD	2.26	0.49
2:D:365:TYR:HE2	2:D:430:LEU:HA	1.77	0.49
1:A:119:HIS:HD2	5:A:326:HOH:O	1.94	0.49
1:A:246:GLN:NE2	1:A:251:VAL:HG22	2.28	0.49
1:A:290:THR:OG1	1:A:292:PRO:HD3	2.13	0.49
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.95	0.49
2:D:326:ASN:OD1	2:D:328:LYS:HB2	2.13	0.49
1:A:157:ARG:HB3	1:A:159:TYR:CE1	2.48	0.48
1:A:6:LYS:HE2	1:A:32:LEU:HD13	1.95	0.48
1:A:223:ASP:H	1:A:226:VAL:HG13	1.78	0.48
2:D:199:TYR:HA	2:D:202:LYS:HE2	1.96	0.48
1:C:198:THR:C	1:C:199:ARG:HG2	2.33	0.48
1:C:112:LEU:HD22	1:C:280:ALA:HB3	1.95	0.48
1:C:95:ALA:O	1:C:96:LEU:HB2	2.13	0.48
1:C:37:LEU:HD22	1:C:44:VAL:HG22	1.96	0.48
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.78	0.48
2:B:332:LEU:O	2:B:335:PHE:HB3	2.14	0.48
1:A:75:LYS:HD2	1:A:77:TYR:OH	2.14	0.48
2:D:428:GLU:HG3	2:D:429:THR:HG23	1.96	0.48
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.48	0.48
2:B:187:ARG:O	2:B:190:GLU:HG2	2.14	0.47
1:A:1:MET:HE3	1:A:70:ILE:HG21	1.96	0.47
1:A:11:GLY:HA3	4:A:300:ATP:C4'	2.43	0.47
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.96	0.47
2:B:274:GLU:HG3	2:B:277:GLU:CG	2.41	0.47
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.96	0.47
2:D:373:PRO:O	2:D:377:ILE:HG13	2.15	0.47
2:B:210:MET:HE1	2:B:250:ARG:CB	2.45	0.47
1:C:35:ILE:HD13	1:C:48:ALA:HB2	1.97	0.47
2:D:331:SER:HB2	2:D:421:VAL:HG11	1.97	0.47
1:A:108:LEU:HD13	1:A:286:PHE:CZ	2.43	0.47
1:A:156:VAL:CG2	1:A:159:TYR:HE2	2.26	0.47
1:A:38:ASP:OD2	1:A:42:GLU:HB3	2.14	0.47
1:C:119:HIS:NE2	1:C:182:THR:HB	2.30	0.47
2:D:407:GLN:O	2:D:411:GLU:HG2	2.15	0.47
1:C:263:LEU:HG	1:C:267:LEU:HD12	1.97	0.47
1:C:163:VAL:HG23	1:C:164:VAL:HG23	1.97	0.46
2:D:388:LYS:O	2:D:392:MET:HG2	2.16	0.46
1:A:71:HIS:ND1	2:B:296:HIS:HE1	2.13	0.46
1:C:257:GLU:HG3	1:C:258:ASP:N	2.31	0.46
2:B:323:GLN:HA	2:B:324:PRO:HA	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HA	1:A:1:MET:HE2	1.96	0.46
1:A:70:ILE:HB	1:A:77:TYR:HB2	1.98	0.46
2:D:202:LYS:HB2	2:D:202:LYS:HE3	1.71	0.46
1:A:35:ILE:HD12	1:A:76:LEU:HD13	1.97	0.46
2:B:373:PRO:HG2	2:B:376:LEU:HB2	1.96	0.46
2:B:396:GLN:HE21	2:B:400:LYS:HE3	1.80	0.46
1:C:71:HIS:CE1	2:D:296:HIS:NE2	2.84	0.46
2:D:238:TYR:HB3	2:D:302:LEU:HD11	1.98	0.46
2:D:387:LEU:O	2:D:391:LEU:HB2	2.16	0.46
2:D:417:LYS:HB3	2:D:417:LYS:HZ3	1.77	0.46
1:A:83:LEU:HD11	1:A:142:LYS:HD2	1.98	0.46
1:C:88:LYS:NZ	1:C:131:GLN:H	2.04	0.46
1:C:101:LEU:O	1:C:101:LEU:HG	2.15	0.46
1:C:84:HIS:CB	1:C:298:LEU:HG	2.42	0.46
1:C:71:HIS:NE2	2:D:304:PHE:HE2	2.13	0.46
2:D:329:VAL:HG22	2:D:367:VAL:HB	1.98	0.46
1:C:284:PRO:O	1:C:285:PHE:C	2.53	0.46
1:A:34:LYS:NZ	1:A:75:LYS:HD3	2.31	0.45
1:A:83:LEU:O	4:A:300:ATP:H2	1.98	0.45
1:C:278:LYS:CD	2:D:177:ASP:HB3	2.46	0.45
2:D:216:ASP:HB2	2:D:406:GLN:CG	2.44	0.45
1:A:89:LYS:HA	1:A:89:LYS:HD3	1.72	0.45
1:C:156:VAL:CG2	1:C:159:TYR:HE2	2.25	0.45
1:C:288:ASP:N	1:C:288:ASP:OD1	2.50	0.45
2:D:412:LYS:O	2:D:415:ASN:HB3	2.16	0.45
2:B:203:GLN:HG2	2:B:206:ILE:CG1	2.46	0.45
1:A:284:PRO:O	1:A:287:GLN:HG2	2.17	0.45
2:D:233:HIS:CD2	2:D:341:LEU:HD21	2.51	0.45
2:D:321:HIS:CD2	2:D:321:HIS:N	2.84	0.45
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.99	0.45
1:C:91:MET:CE	1:C:130:PRO:HB3	2.46	0.45
1:C:272:ASN:HD22	1:C:273:LYS:NZ	2.14	0.45
1:A:291:LYS:N	1:A:292:PRO:HD3	2.32	0.45
2:B:412:LYS:HE2	2:B:413:TYR:CE1	2.51	0.45
1:C:157:ARG:HG2	1:C:158:THR:N	2.23	0.45
1:C:15:TYR:HE1	4:C:300:ATP:PG	2.40	0.45
1:C:86:ASP:OD2	1:C:88:LYS:HB3	2.17	0.45
1:C:270:ASP:HA	1:C:271:PRO:HD2	1.84	0.45
2:D:327:CYS:SG	2:D:419:HIS:NE2	2.89	0.45
1:C:157:ARG:O	1:C:179:TYR:CD1	2.70	0.45
1:C:241:PRO:HB2	1:C:243:TRP:CZ2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLY:HA3	4:A:300:ATP:O1B	2.17	0.44
2:D:315:LEU:HA	2:D:315:LEU:HD23	1.72	0.44
1:C:272:ASN:ND2	1:C:273:LYS:HZ2	2.16	0.44
1:C:124:LEU:O	1:C:149:ALA:HA	2.18	0.44
2:B:199:TYR:CD1	2:B:199:TYR:C	2.91	0.44
1:A:3:ASN:O	1:A:23:ASN:HA	2.17	0.44
1:C:287:GLN:HG2	1:C:288:ASP:OD1	2.17	0.44
2:D:229:ASN:ND2	2:D:338:GLU:OE1	2.50	0.44
2:D:414:LYS:HA	2:D:420:GLY:HA2	1.99	0.44
2:B:217:TRP:O	2:B:220:GLU:HB2	2.18	0.44
2:B:384:LEU:HA	2:B:384:LEU:HD12	1.76	0.44
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.99	0.44
2:B:201:LYS:HD3	2:B:202:LYS:CE	2.47	0.44
1:C:172:GLU:CB	1:C:177:CYS:SG	3.03	0.44
1:C:175:LEU:HA	1:C:235:ASP:HB2	2.00	0.44
1:C:278:LYS:HD3	2:D:177:ASP:HB3	2.00	0.44
1:A:89:LYS:NZ	1:A:131:GLN:OE1	2.51	0.44
1:C:95:ALA:O	1:C:96:LEU:CB	2.66	0.44
2:D:199:TYR:CE2	2:D:348:LEU:HD21	2.50	0.44
2:B:293:ARG:HD2	1:C:24:LYS:NZ	2.33	0.44
1:C:268:HIS:CD2	1:C:270:ASP:N	2.75	0.44
2:D:419:HIS:O	2:D:421:VAL:N	2.50	0.44
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.76	0.43
2:B:329:VAL:HG22	2:B:367:VAL:HB	2.00	0.43
2:B:372:TRP:HB3	2:B:384:LEU:HD13	2.00	0.43
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.82	0.43
1:A:20:LYS:HE3	1:A:29:VAL:HG11	2.00	0.43
1:A:84:HIS:ND1	1:A:84:HIS:N	2.66	0.43
2:D:237:ASN:ND2	2:D:308:ALA:HB1	2.34	0.43
1:A:8:GLU:HG2	1:A:9:LYS:N	2.33	0.43
1:C:126:ARG:NH1	1:C:180:TYR:OH	2.50	0.43
2:B:262:LEU:HD13	2:B:278:PHE:CD2	2.53	0.43
2:D:365:TYR:CD1	2:D:365:TYR:C	2.91	0.43
1:A:97:THR:HG22	1:A:98:GLY:O	2.19	0.43
1:C:60:HIS:CD2	1:C:61:PRO:N	2.87	0.43
1:A:38:ASP:HB3	1:A:43:GLY:N	2.22	0.43
1:A:9:LYS:NZ	1:A:12:GLU:HB2	2.33	0.43
1:A:241:PRO:HB2	1:A:243:TRP:CH2	2.54	0.43
2:B:183:HIS:CE1	5:B:28:HOH:O	2.71	0.43
2:B:372:TRP:CB	2:B:384:LEU:HD13	2.48	0.43
1:A:64:VAL:HG21	1:A:134:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HB3	1:A:65:LYS:HE2	1.91	0.43
2:B:417:LYS:HE2	2:B:418:TYR:CE2	2.54	0.43
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.83	0.43
1:C:198:THR:HG23	1:C:252:VAL:HG13	2.00	0.43
1:A:139:GLY:HA2	1:A:294:PRO:HD2	2.00	0.43
1:A:34:LYS:HZ2	1:A:75:LYS:HD3	1.83	0.43
2:B:315:LEU:HD23	2:B:315:LEU:HA	1.75	0.43
1:A:105:LYS:HE3	1:A:105:LYS:HB2	1.86	0.42
1:A:186:ILE:HG23	1:A:186:ILE:HD12	1.73	0.42
1:A:216:PHE:O	1:A:220:GLY:N	2.51	0.42
2:B:410:ARG:HH11	2:B:410:ARG:HG2	1.84	0.42
1:C:155:PRO:HD3	2:D:320:LEU:HD21	2.00	0.42
1:A:42:GLU:HG2	1:A:42:GLU:O	2.18	0.42
1:C:48:ALA:O	1:C:52:ILE:HG13	2.19	0.42
2:D:375:SER:HA	2:D:378:ARG:NH2	2.35	0.42
1:A:18:VAL:HG22	1:A:33:LYS:HG3	2.01	0.42
1:C:186:ILE:HD13	1:C:186:ILE:HA	1.95	0.42
2:D:309:PRO:HA	2:D:313:GLN:NE2	2.34	0.42
1:A:95:ALA:O	1:A:97:THR:N	2.52	0.42
1:C:34:LYS:HZ1	1:C:36:ARG:HH21	1.67	0.42
2:D:402:PRO:HB2	2:D:403:GLN:OE1	2.20	0.42
1:A:163:VAL:O	1:A:164:VAL:HB	2.19	0.42
2:B:417:LYS:HE2	2:B:418:TYR:OH	2.19	0.42
1:C:126:ARG:HD2	1:C:163:VAL:HG21	2.01	0.42
1:C:209:ILE:HA	1:C:209:ILE:HD12	1.86	0.42
1:A:133:LEU:HD11	1:A:192:ILE:HD13	2.00	0.42
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.53	0.42
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.48	0.42
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.54	0.42
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.82	0.42
1:C:121:HIS:C	1:C:122:ARG:HG3	2.40	0.42
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.86	0.42
1:C:154:VAL:C	2:D:316:THR:HG22	2.38	0.42
2:D:402:PRO:HA	2:D:410:ARG:CZ	2.50	0.42
1:A:297:ARG:NH1	1:A:297:ARG:H	2.17	0.42
2:B:194:LYS:HE3	2:B:197:VAL:CG2	2.49	0.42
1:C:3:ASN:O	1:C:23:ASN:HA	2.20	0.42
1:C:289:VAL:HG12	1:C:290:THR:N	2.35	0.42
1:C:227:TRP:O	1:C:230:VAL:CG2	2.68	0.42
1:C:188:SER:O	1:C:192:ILE:HG13	2.20	0.41
2:D:424:LEU:HB2	5:D:99:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HG22	1:A:11:GLY:N	2.34	0.41
2:B:176:PRO:O	2:B:178:TYR:N	2.53	0.41
2:B:426:PRO:HA	2:B:427:PRO:HD3	1.89	0.41
2:D:215:VAL:O	2:D:219:VAL:HG23	2.19	0.41
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.55	0.41
2:B:252:LYS:HD3	2:B:252:LYS:HA	1.66	0.41
2:B:287:THR:OG1	2:B:290:GLN:HB2	2.21	0.41
2:B:326:ASN:O	2:B:330:GLU:HG3	2.20	0.41
1:C:7:VAL:HB	1:C:20:LYS:O	2.21	0.41
2:D:196:LYS:O	2:D:199:TYR:HD2	2.04	0.41
2:D:327:CYS:HG	2:D:419:HIS:CE1	2.38	0.41
2:D:338:GLU:HG2	2:D:409:ILE:HD13	2.01	0.41
1:C:90:PHE:CE2	1:C:99:ILE:HG12	2.55	0.41
2:D:328:LYS:HB2	2:D:328:LYS:HE3	1.89	0.41
2:D:332:LEU:HD22	2:D:424:LEU:HD12	2.02	0.41
2:B:197:VAL:HG12	2:B:197:VAL:O	2.21	0.41
1:A:71:HIS:CE1	2:B:296:HIS:CE1	3.08	0.41
1:C:84:HIS:CG	1:C:298:LEU:HG	2.55	0.41
2:D:178:TYR:HA	2:D:181:ASP:OD1	2.20	0.41
2:D:380:THR:HB	2:D:382:TYR:CD2	2.55	0.41
1:A:7:VAL:O	1:A:7:VAL:HG12	2.21	0.41
2:B:234:LEU:HD23	2:B:310:THR:CG2	2.50	0.41
2:B:292:LEU:HD12	2:B:292:LEU:HA	1.79	0.41
2:D:364:LEU:HD12	2:D:368:THR:OG1	2.20	0.41
2:D:394:LEU:HD12	2:D:394:LEU:HA	1.63	0.41
1:A:71:HIS:CE1	2:B:296:HIS:HE1	2.39	0.41
1:C:103:LEU:O	1:C:106:SER:HB3	2.21	0.41
1:C:57:GLU:OE1	1:C:122:ARG:NH2	2.54	0.41
2:D:217:TRP:O	2:D:220:GLU:HB3	2.20	0.41
2:D:425:ASN:HA	2:D:426:PRO:HD2	1.91	0.41
1:A:230:VAL:HA	1:A:233:MET:HE3	2.01	0.41
1:C:286:PHE:O	1:C:288:ASP:N	2.54	0.41
2:D:206:ILE:HA	2:D:210:MET:CE	2.50	0.41
1:A:1:MET:HE3	1:A:70:ILE:HG13	1.96	0.40
2:B:299:LEU:HD13	2:B:304:PHE:CZ	2.56	0.40
2:B:376:LEU:HA	2:B:376:LEU:HD23	1.73	0.40
1:C:15:TYR:CD1	1:C:15:TYR:N	2.87	0.40
1:C:258:ASP:O	1:C:261:SER:HB3	2.21	0.40
2:D:407:GLN:HA	5:D:98:HOH:O	2.20	0.40
1:A:180:TYR:HB2	1:A:184:VAL:HG11	2.03	0.40
1:C:117:PHE:CZ	1:C:121:HIS:NE2	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:ILE:HG21	1:C:274:ARG:HG2	2.03	0.40
2:D:323:GLN:HA	2:D:324:PRO:HA	1.87	0.40
2:D:365:TYR:CE2	2:D:430:LEU:HA	2.55	0.40
1:A:101:LEU:N	1:A:102:PRO:CD	2.83	0.40
1:C:119:HIS:CG	1:C:182:THR:HB	2.57	0.40
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.56	0.40
2:D:372:TRP:HA	2:D:373:PRO:HD2	1.82	0.40
2:D:374:GLU:O	2:D:378:ARG:HG3	2.21	0.40
1:C:287:GLN:HG2	1:C:288:ASP:N	2.35	0.40
2:D:175:VAL:CB	2:D:176:PRO:CD	2.96	0.40
1:A:198:THR:O	1:A:199:ARG:HB2	2.21	0.40
1:A:86:ASP:OD1	1:A:88:LYS:HB3	2.21	0.40
2:B:214:LEU:HD22	2:B:253:LEU:HG	2.02	0.40
1:C:15:TYR:HE1	4:C:300:ATP:O1G	2.05	0.40
2:D:232:LEU:HD13	2:D:341:LEU:CD1	2.51	0.40
2:D:375:SER:HA	2:D:378:ARG:HH21	1.87	0.40
2:D:402:PRO:HA	2:D:410:ARG:NH1	2.37	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	295/298 (99%)	264 (90%)	21 (7%)	10 (3%)	4	6
1	C	295/298 (99%)	258 (88%)	24 (8%)	13 (4%)	3	3
2	B	256/258 (99%)	241 (94%)	12 (5%)	3 (1%)	15	32
2	D	256/258 (99%)	241 (94%)	13 (5%)	2 (1%)	22	44
All	All	1102/1112 (99%)	1004 (91%)	70 (6%)	28 (2%)	6	11

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	18	VAL
1	C	162	GLU
1	C	164	VAL
1	C	287	GLN
2	D	176	PRO
1	A	10	ILE
1	A	14	THR
1	A	97	THR
1	A	164	VAL
2	B	177	ASP
2	B	283	ASP
1	C	11	GLY
2	D	420	GLY
1	A	8	GLU
1	A	162	GLU
1	C	96	LEU
1	A	37	LEU
1	A	39	THR
2	B	319	PHE
1	C	10	ILE
1	C	14	THR
1	C	275	ILE
1	C	283	HIS
1	C	285	PHE
1	A	96	LEU
1	C	145	ASP
1	A	228	PRO
1	C	251	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	262/262 (100%)	230 (88%)	32 (12%)	6 10
1	C	262/262 (100%)	225 (86%)	37 (14%)	4 7
2	B	232/232 (100%)	209 (90%)	23 (10%)	9 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	232/232 (100%)	219 (94%)	13 (6%)	25	48
All	All	988/988 (100%)	883 (89%)	105 (11%)	8	14

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	9	LYS
1	A	40	GLU
1	A	41	THR
1	A	47	THR
1	A	59	ASN
1	A	71	HIS
1	A	75	LYS
1	A	76	LEU
1	A	87	LEU
1	A	108	LEU
1	A	115	LEU
1	A	122	ARG
1	A	137	THR
1	A	148	LEU
1	A	150	ARG
1	A	156	VAL
1	A	161	HIS
1	A	163	VAL
1	A	172	GLU
1	A	202	LEU
1	A	226	VAL
1	A	230	VAL
1	A	232	SER
1	A	239	SER
1	A	248	PHE
1	A	250	LYS
1	A	255	LEU
1	A	256	ASP
1	A	288	ASP
1	A	297	ARG
1	A	298	LEU
2	B	177	ASP
2	B	179	HIS
2	B	181	ASP
2	B	196	LYS

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Mol	Chain	Res	Type
2	B	199	TYR
2	B	200	MET
2	B	201	LYS
2	B	203	GLN
2	B	232	LEU
2	B	274	GLU
2	B	283	ASP
2	B	285	THR
2	B	288	LYS
2	B	292	LEU
2	B	316	THR
2	B	334	MET
2	B	346	PRO
2	B	384	LEU
2	B	391	LEU
2	B	400	LYS
2	B	410	ARG
2	B	428	GLU
2	B	429	THR
1	C	5	GLN
1	C	12	GLU
1	C	15	TYR
1	C	24	LYS
1	C	38	ASP
1	C	39	THR
1	C	40	GLU
1	C	65	LYS
1	C	71	HIS
1	C	72	THR
1	C	75	LYS
1	C	77	TYR
1	C	78	LEU
1	C	84	HIS
1	C	87	LEU
1	C	88	LYS
1	C	91	MET
1	C	121	HIS
1	C	122	ARG
1	C	137	THR
1	C	138	GLU
1	C	148	LEU
1	C	150	ARG

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Mol	Chain	Res	Type
1	C	158	THR
1	C	161	HIS
1	C	162	GLU
1	C	172	GLU
1	C	199	ARG
1	C	202	LEU
1	C	230	VAL
1	C	232	SER
1	C	248	PHE
1	C	250	LYS
1	C	255	LEU
1	C	276	SER
1	C	287	GLN
1	C	297	ARG
2	D	179	HIS
2	D	193	CYS
2	D	232	LEU
2	D	245	SER
2	D	292	LEU
2	D	300	LYS
2	D	327	CYS
2	D	346	PRO
2	D	349	LYS
2	D	365	TYR
2	D	376	LEU
2	D	400	LYS
2	D	416	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	71	HIS
1	A	119	HIS
1	A	246	GLN
1	A	265	GLN
1	A	272	ASN
2	B	183	HIS
2	B	296	HIS
2	B	313	GLN
2	B	317	GLN

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Mol	Chain	Res	Type
2	B	370	GLN
2	B	395	HIS
2	B	396	GLN
1	C	59	ASN
1	C	268	HIS
1	C	272	ASN
2	D	313	GLN
2	D	317	GLN
2	D	321	HIS
2	D	361	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	TPO	A	160	1	9,10,11	1.07	0	10,14,16	1.25	1 (10%)
1	TPO	C	160	1	9,10,11	1.83	2 (22%)	10,14,16	1.94	2 (20%)

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
1	TPO	A	160	1	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	-4.37	1.51	1.59
1	C	160	TPO	CA-C	2.40	1.53	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O-C-CA	-2.26	119.89	125.15
1	C	160	TPO	OG1-P-O1P	-2.22	100.56	109.26
1	C	160	TPO	C-CA-N	4.38	118.69	109.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	160	TPO	3	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	ATP	A	300	3	27,33,33	1.67	3 (11%)	25,52,52	1.25	1 (4%)
4	ATP	C	300	3	27,33,33	1.29	3 (11%)	25,52,52	2.47	7 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	A	300	3	-	0/18/38/38	0/3/3/3
4	ATP	C	300	3	-	0/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	300	ATP	C8-N7	-2.45	1.30	1.34
4	A	300	ATP	PA-O5'	2.73	1.70	1.59
4	C	300	ATP	C2'-C1'	2.76	1.58	1.53
4	C	300	ATP	O4'-C1'	3.19	1.45	1.41
4	A	300	ATP	C2'-C1'	3.37	1.59	1.53
4	A	300	ATP	PG-O3B	5.60	1.69	1.60

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	300	ATP	C4'-O4'-C1'	-8.03	101.22	109.77
4	A	300	ATP	O2A-PA-O5'	-3.04	93.80	108.14
4	C	300	ATP	C1'-N9-C4	-2.09	123.02	126.64
4	C	300	ATP	C5'-C4'-C3'	-2.03	107.54	115.29
4	C	300	ATP	O2B-PB-O1B	2.60	125.76	112.28
4	C	300	ATP	C4-C5-N7	2.98	112.29	109.41
4	C	300	ATP	O4'-C4'-C3'	3.53	112.19	105.17
4	C	300	ATP	O5'-C5'-C4'	5.98	130.21	109.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	300	ATP	8	0
4	C	300	ATP	4	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.