



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:40 AM 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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

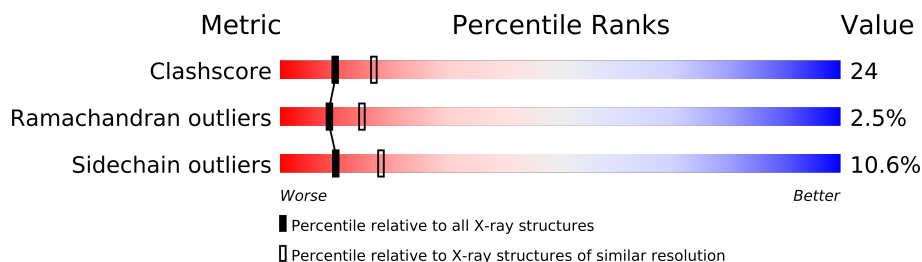
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	24	Total	O	0	0
			24	24		
5	C	20	Total	O	0	0
			20	20		
5	D	16	Total	O	0	0
			16	16		

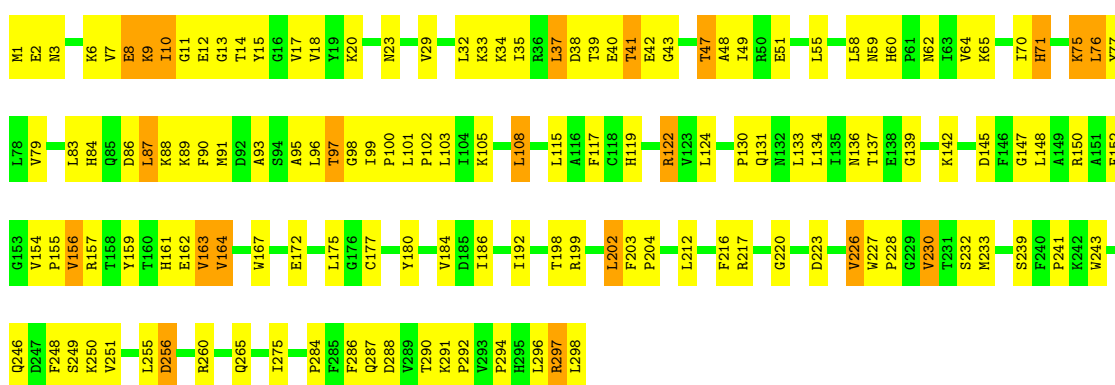
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

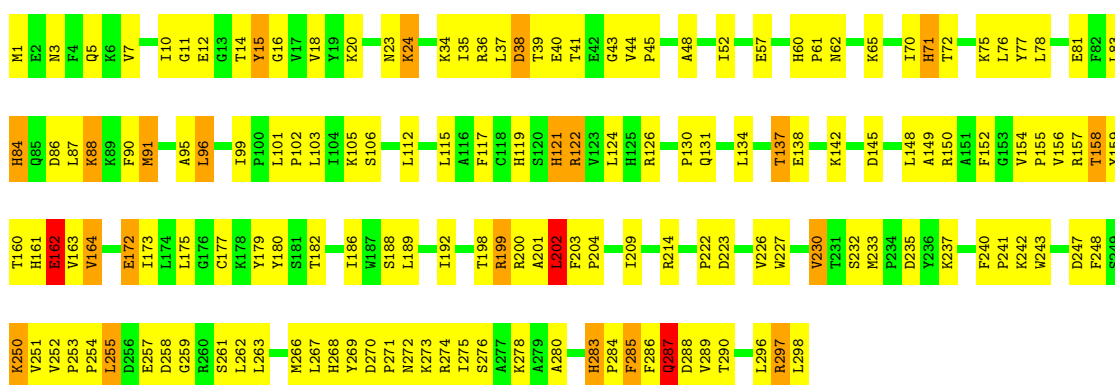
• Molecule 1: CYCLIN-DEPENDENT KINASE-2

Chain A:



• Molecule 1: CYCLIN-DEPENDENT KINASE-2

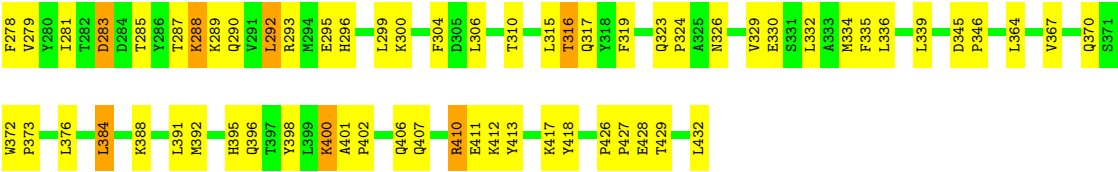
Chain C:



• Molecule 2: CYCLIN A

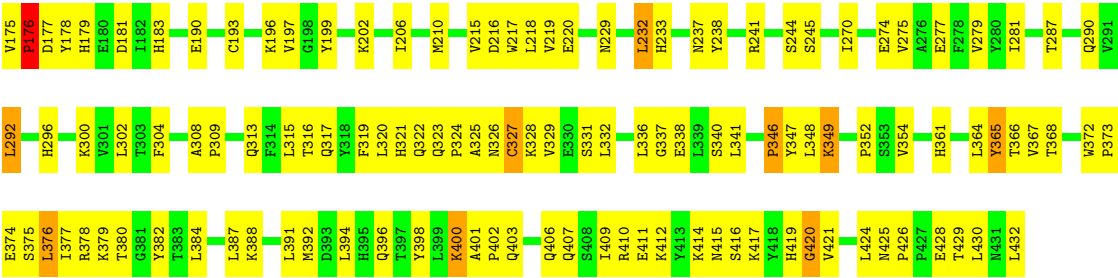
Chain B:





• Molecule 2: CYCLIN A

Chain D:



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (438) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:C:156:VAL:HG22	1:C:159:TYR:HE2	1.47	0.80
2:B:407:GLN:O	2:B:411:GLU:HG2	1.80	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
1:A:108:LEU:HD13	1:A:286:PHE:HZ	1.58	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:38:ASP:HB2	1:C:43:GLY:H	1.62	0.65
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.78	0.65
1:A:87:LEU:HB3	1:A:130:PRO:HB3	1.79	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:263:LEU:HD21	2:B:295:GLU:HG3	1.81	0.62
2:B:202:LYS:HD2	2:B:202:LYS:H	1.63	0.62
2:D:216:ASP:CB	2:D:406:GLN:HG3	2.29	0.62
1:A:88:LYS:CE	1:A:131:GLN:HG2	2.30	0.62
1:A:230:VAL:HA	1:A:233:MET:CE	2.29	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
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
2:B:202:LYS:HD2	2:B:202:LYS:N	2.15	0.61
1:C:83:LEU:HD11	1:C:142:LYS:CD	2.31	0.60
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:160:TPO:HA	2:D:270:ILE:HD13	1.84	0.59
1:A:71:HIS:HB3	2:B:300:LYS:HE3	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:D:396:GLN:O	2:D:400:LYS:HD3	2.02	0.59
2:B:207:THR:OG1	2:B:210:MET:HG3	2.03	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
2:B:176:PRO:HA	2:B:179:HIS:CE1	2.39	0.57
1:A:93:ALA:HB3	1:A:297:ARG:NH2	2.18	0.57
1:A:297:ARG:HH11	1:A:297:ARG:N	2.02	0.57
2:D:402:PRO:HG3	2:D:410:ARG:HH12	1.69	0.57
2:B:275:VAL:O	2:B:279:VAL:HG23	2.04	0.57
2:B:417:LYS:HE2	2:B:418:TYR:CZ	2.39	0.57
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.34	0.57
2:B:203:GLN:OE1	2:B:247:SER:HA	2.04	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:88:LYS:HD2	1:A:131:GLN:CG	2.31	0.56
1:A:297:ARG:HH11	1:A:297:ARG:H	1.54	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
2:D:190:GLU:OE1	2:D:352:PRO:HD2	2.06	0.56
1:C:91:MET:HE1	1:C:130:PRO:HG2	1.88	0.56
1:C:200:ARG:HD2	1:C:201:ALA:N	2.19	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:122:ARG:HD2	1:A:122:ARG:O	2.06	0.56
1:A:230:VAL:HA	1:A:233:MET:HE2	1.87	0.55
1:A:10:ILE:HB	1:A:18:VAL:HG12	1.87	0.55
1:C:255:LEU:HG	1:C:259:GLY:HA3	1.88	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:296:LEU:C	1:A:297:ARG:HD3	2.27	0.55
1:A:8:GLU:HG2	1:A:9:LYS:H	1.72	0.55
2:B:175:VAL:O	2:B:175:VAL:HG12	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:9:LYS:NZ	1:A:17:VAL:HB	2.23	0.54
1:A:98:GLY:O	1:A:100:PRO:HD3	2.06	0.54
2:D:332:LEU:O	2:D:336:LEU:HG	2.07	0.54
1:C:296:LEU:HD13	1:C:298:LEU:CG	2.37	0.54
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.43	0.54
1:A:90:PHE:HA	1:A:297:ARG:HH22	1.72	0.54
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.88	0.54
1:C:91:MET:HE1	1:C:130:PRO:CG	2.38	0.54
1:A:297:ARG:HD3	1:A:297:ARG:N	2.22	0.54
2:D:199:TYR:HE2	2:D:348:LEU:HD21	1.72	0.54
1:C:90:PHE:HD1	1:C:297:ARG:NH2	2.06	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
1:C:268:HIS:CD2	1:C:270:ASP:H	2.26	0.53
2:B:364:LEU:HG	2:B:370:GLN:HB2	1.89	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:C:296:LEU:HD13	1:C:298:LEU:HG	1.91	0.53
1:A:249:SER:HA	1:A:260:ARG:HD3	1.90	0.53
1:A:256:ASP:O	1:A:260:ARG:HG3	2.08	0.53
2:D:327:CYS:SG	2:D:419:HIS:CE1	3.02	0.53
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:C:86:ASP:HA	1:C:134:LEU:HA	1.93	0.51
2:B:395:HIS:HE1	2:B:427:PRO:O	1.93	0.51
2:D:175:VAL:N	2:D:176:PRO:HD2	2.25	0.51
1:A:9:LYS:HZ2	1:A:18:VAL:H	1.58	0.51
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.45	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:395:HIS:CE1	2:B:427:PRO:O	2.65	0.50
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.47	0.50
1:C:105:LYS:HG3	1:C:285:PHE:CE2	2.46	0.50
1:C:268:HIS:HD2	1:C:270:ASP:H	1.54	0.50
1:C:15:TYR:HE1	4:C:300:ATP:O3B	1.95	0.50
1:A:241:PRO:HB2	1:A:243:TRP:CZ3	2.47	0.50
2:D:354:VAL:HG13	2:D:387:LEU:HD23	1.92	0.49
1:C:16:GLY:HA3	4:C:300:ATP:O2B	2.11	0.49
1:A:296:LEU:HA	1:A:297:ARG:HH11	1.77	0.49
1:C:262:LEU:O	1:C:266:MET:HG3	2.12	0.49
1:C:214:ARG:HG2	1:C:214:ARG:NH1	2.27	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
2:D:196:LYS:HB2	2:D:199:TYR:HB3	1.94	0.49
1:A:64:VAL:HG22	1:A:83:LEU:HD12	1.93	0.49
2:D:337:GLY:O	2:D:340:SER:OG	2.29	0.49
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: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:290:THR:OG1	1:A:292:PRO:HD3	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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
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:252:VAL:HG11	1:C:255:LEU:HD22	1.96	0.47
2:D:331:SER:HB2	2:D:421:VAL:HG11	1.97	0.47
1:C:35:ILE:HD13	1:C:48:ALA:HB2	1.97	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:A:108:LEU:HD13	1:A:286:PHE:CZ	2.43	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
2:D:388:LYS:O	2:D:392:MET:HG2	2.16	0.46
1:C:163:VAL:HG23	1:C:164:VAL:HG23	1.97	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
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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:C:88:LYS:NZ	1:C:131:GLN:H	2.04	0.46
1:A:83:LEU:HD11	1:A:142:LYS:HD2	1.98	0.46
1:C:84:HIS:CB	1:C:298:LEU:HG	2.42	0.46
1:C:101:LEU:O	1:C:101:LEU:HG	2.15	0.46
2:D:329:VAL:HG22	2:D:367:VAL:HB	1.98	0.46
1:C:71:HIS:NE2	2:D:304:PHE:HE2	2.13	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
2:D:216:ASP:HB2	2:D:406:GLN:CG	2.44	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
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
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:284:PRO:O	1:A:287:GLN:HG2	2.17	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:C:157:ARG:HG2	1:C:158:THR:N	2.23	0.45
1:C:86:ASP:OD2	1:C:88:LYS:HB3	2.17	0.45
1:C:15:TYR:HE1	4:C:300:ATP:PG	2.40	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: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
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:C:287:GLN:HG2	1:C:288:ASP:OD1	2.17	0.44
2:D:414:LYS:HA	2:D:420:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:3:ASN:O	1:A:23:ASN:HA	2.17	0.44
2:D:229:ASN:ND2	2:D:338:GLU:OE1	2.50	0.44
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.99	0.44
2:B:384:LEU:HA	2:B:384:LEU:HD12	1.76	0.44
2:B:217:TRP:O	2:B:220:GLU:HB2	2.18	0.44
1:C:172:GLU:CB	1:C:177:CYS:SG	3.03	0.44
2:B:201:LYS:HD3	2:B:202:LYS:CE	2.47	0.44
1:C:278:LYS:HD3	2:D:177:ASP:HB3	2.00	0.44
1:C:175:LEU:HA	1:C:235:ASP:HB2	2.00	0.44
1:A:89:LYS:NZ	1:A:131:GLN:OE1	2.51	0.44
2:D:199:TYR:CE2	2:D:348:LEU:HD21	2.50	0.44
1:C:95:ALA:O	1:C:96:LEU:CB	2.66	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:372:TRP:HB3	2:B:384:LEU:HD13	2.00	0.43
2:B:329:VAL:HG22	2:B:367:VAL:HB	2.00	0.43
2:D:237:ASN:ND2	2:D:308:ALA:HB1	2.34	0.43
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.82	0.43
1:A:84:HIS:ND1	1:A:84:HIS:N	2.66	0.43
1:A:20:LYS:HE3	1:A:29:VAL:HG11	2.00	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:C	2:D:365:TYR:CD1	2.91	0.43
1:C:60:HIS:CD2	1:C:61:PRO:N	2.87	0.43
1:A:97:THR:HG22	1:A:98:GLY:O	2.19	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
2:B:183:HIS:CE1	5:B:28:HOH:O	2.71	0.43
1:A:241:PRO:HB2	1:A:243:TRP:CH2	2.54	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
1:C:198:THR:HG23	1:C:252:VAL:HG13	2.00	0.43
2:B:417:LYS:HE2	2:B:418:TYR:CE2	2.54	0.43
1:C:214:ARG:HH11	1:C:214:ARG:HG2	1.83	0.43
1:A:65:LYS:HB3	1:A:65:LYS:HE2	1.91	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:139:GLY:HA2	1:A:294:PRO:HD2	2.00	0.43
1:C:155:PRO:HD3	2:D:320:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:410:ARG:HH11	2:B:410:ARG:HG2	1.84	0.42
1:A:186:ILE:HG23	1:A:186:ILE:HD12	1.73	0.42
1:A:105:LYS:HE3	1:A:105:LYS:HB2	1.86	0.42
1:A:216:PHE:O	1:A:220:GLY:N	2.51	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
2:D:402:PRO:HB2	2:D:403:GLN:OE1	2.20	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: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:163:VAL:O	1:A:164:VAL:HB	2.19	0.42
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.53	0.42
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.54	0.42
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.48	0.42
1:A:133:LEU:HD11	1:A:192:ILE:HD13	2.00	0.42
1:C:154:VAL:C	2:D:316:THR:HG22	2.38	0.42
1:A:175:LEU:HA	1:A:175:LEU:HD23	1.82	0.42
2:D:402:PRO:HA	2:D:410:ARG:CZ	2.50	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:289:VAL:HG12	1:C:290:THR:N	2.35	0.42
1:A:297:ARG:NH1	1:A:297:ARG:H	2.17	0.42
1:C:3:ASN:O	1:C:23:ASN:HA	2.20	0.42
2:B:194:LYS:HE3	2:B:197:VAL:CG2	2.49	0.42
1:C:227:TRP:O	1:C:230:VAL:CG2	2.68	0.42
2:D:424:LEU:HB2	5:D:99:HOH:O	2.20	0.41
1:C:188:SER:O	1:C:192:ILE:HG13	2.20	0.41
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:D:215:VAL:O	2:D:219:VAL:HG23	2.19	0.41
2:B:426:PRO:HA	2:B:427:PRO:HD3	1.89	0.41
2:D:196:LYS:O	2:D:199:TYR:HD2	2.04	0.41
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.55	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
2:B:287:THR:OG1	2:B:290:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:252:LYS:HD3	2:B:252:LYS:HA	1.66	0.41
1:C:7:VAL:HB	1:C:20:LYS:O	2.21	0.41
2:B:326:ASN:O	2:B:330:GLU:HG3	2.20	0.41
2:D:332:LEU:HD22	2:D:424:LEU:HD12	2.02	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
1:C:84:HIS:CG	1:C:298:LEU:HG	2.55	0.41
1:A:71:HIS:CE1	2:B:296:HIS:CE1	3.08	0.41
2:B:197:VAL:HG12	2:B:197:VAL:O	2.21	0.41
2:D:380:THR:HB	2:D:382:TYR:CD2	2.55	0.41
2:D:178:TYR:HA	2:D:181:ASP:OD1	2.20	0.41
1:A:7:VAL:O	1:A:7:VAL:HG12	2.21	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
2:B:234:LEU:HD23	2:B:310:THR:CG2	2.50	0.41
1:A:71:HIS:CE1	2:B:296:HIS:HE1	2.39	0.41
2:D:217:TRP:O	2:D:220:GLU:HB3	2.20	0.41
1:C:57:GLU:OE1	1:C:122:ARG:NH2	2.54	0.41
2:D:425:ASN:HA	2:D:426:PRO:HD2	1.91	0.41
1:C:103:LEU:O	1:C:106:SER:HB3	2.21	0.41
1:C:286:PHE:O	1:C:288:ASP:N	2.54	0.41
1:A:230:VAL:HA	1:A:233:MET:HE3	2.01	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
1:C:15:TYR:CD1	1:C:15:TYR:N	2.87	0.40
2:B:376:LEU:HA	2:B:376:LEU:HD23	1.73	0.40
2:D:407:GLN:HA	5:D:98:HOH:O	2.20	0.40
1:C:258:ASP:O	1:C:261:SER:HB3	2.21	0.40
2:B:299:LEU:HD13	2:B:304:PHE:CZ	2.56	0.40
1:C:117:PHE:CZ	1:C:121:HIS:NE2	2.89	0.40
2:D:365:TYR:CE2	2:D:430:LEU:HA	2.55	0.40
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
1:A:180:TYR:HB2	1:A:184:VAL:HG11	2.03	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
1:C:119:HIS:CG	1:C:182:THR:HB	2.57	0.40
2:D:374:GLU:O	2:D:378:ARG:HG3	2.21	0.40
1:A:101:LEU:N	1:A:102:PRO:CD	2.83	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:86:ASP:OD1	1:A:88:LYS:HB3	2.21	0.40
1:C:15:TYR:HE1	4:C:300:ATP:O1G	2.05	0.40
2:D:402:PRO:HA	2:D:410:ARG:NH1	2.37	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
1:A:198:THR:O	1:A:199:ARG:HB2	2.21	0.40
2:B:214:LEU:HD22	2:B:253:LEU:HG	2.02	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%)	6 8
1	C	295/298 (99%)	258 (88%)	24 (8%)	13 (4%)	4 5
2	B	256/258 (99%)	241 (94%)	12 (5%)	3 (1%)	19 39
2	D	256/258 (99%)	241 (94%)	13 (5%)	2 (1%)	27 53
All	All	1102/1112 (99%)	1004 (91%)	70 (6%)	28 (2%)	9 14

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

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Mol	Chain	Res	Type
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%)	7	13
1	C	262/262 (100%)	225 (86%)	37 (14%)	5	9
2	B	232/232 (100%)	209 (90%)	23 (10%)	11	21
2	D	232/232 (100%)	219 (94%)	13 (6%)	30	55
All	All	988/988 (100%)	883 (89%)	105 (11%)	10	18

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 chains 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	10,10,11	5.24	2 (20%)	12,14,16	1.16	0
1	TPO	C	160	1	10,10,11	6.22	3 (30%)	12,14,16	1.88	4 (33%)

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	-	0/9/11/13	0/0/0/0
1	TPO	C	160	1	-	0/9/11/13	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	O-C	19.15	1.24	1.11
1	A	160	TPO	O-C	16.25	1.22	1.11
1	C	160	TPO	CA-C	2.73	1.53	1.48
1	C	160	TPO	P-OG1	-2.57	1.51	1.59
1	A	160	TPO	P-O3P	-2.07	1.47	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	C-CA-N	4.16	118.69	111.94
1	C	160	TPO	O3P-P-OG1	-2.73	99.23	107.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	OG1-P-O1P	-2.23	100.56	106.79
1	C	160	TPO	O2P-P-O1P	2.05	117.14	110.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	33,33,33	2.19	7 (21%)	52,52,52	1.82	6 (11%)
4	ATP	C	300	3	33,33,33	1.51	6 (18%)	52,52,52	2.72	16 (30%)

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	-	0/22/38/38	0/1/3/3
4	ATP	C	300	3	-	0/22/38/38	0/1/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	300	ATP	PB-O3B	5.85	1.70	1.59
4	A	300	ATP	PB-O3A	5.62	1.70	1.59
4	A	300	ATP	PG-O3B	5.13	1.69	1.60
4	C	300	ATP	PB-O3A	4.16	1.67	1.59
4	A	300	ATP	C2'-C1'	3.91	1.59	1.53
4	C	300	ATP	C2'-C1'	3.22	1.58	1.53
4	A	300	ATP	PA-O3A	3.05	1.65	1.59
4	A	300	ATP	C4-N9	3.05	1.42	1.37
4	C	300	ATP	O4'-C1'	2.82	1.45	1.41
4	A	300	ATP	PA-O5'	2.57	1.70	1.59
4	C	300	ATP	PB-O3B	-2.45	1.55	1.59
4	C	300	ATP	C8-N7	-2.29	1.30	1.34
4	C	300	ATP	PA-O2A	-2.14	1.45	1.55

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	300	ATP	O4'-C1'-N9	10.14	117.87	108.44
4	A	300	ATP	O4'-C1'-N9	8.68	116.52	108.44
4	C	300	ATP	C4'-O4'-C1'	-7.85	101.22	109.75
4	C	300	ATP	O5'-C5'-C4'	5.80	130.21	108.94
4	C	300	ATP	O3A-PB-O3B	-5.73	90.00	101.66
4	C	300	ATP	C2'-C1'-N9	-5.22	99.87	113.27
4	C	300	ATP	PA-O3A-PB	4.84	145.88	131.68
4	A	300	ATP	C2'-C1'-N9	-3.66	103.88	113.27
4	A	300	ATP	C3'-C2'-C1'	3.54	106.44	100.91
4	C	300	ATP	O4'-C4'-C3'	3.46	112.19	105.17
4	C	300	ATP	C8-N9-C4	-3.26	104.41	106.90
4	C	300	ATP	C4-C5-N7	3.24	112.29	109.52
4	C	300	ATP	C8-N9-C1'	3.13	132.55	126.38
4	A	300	ATP	O2A-PA-O5'	-2.92	93.80	108.51
4	A	300	ATP	C8-N9-C4	-2.80	104.76	106.90
4	C	300	ATP	O4'-C1'-C2'	2.76	111.01	106.77
4	A	300	ATP	PA-O5'-C5'	2.62	140.84	122.03
4	C	300	ATP	O2B-PB-O3A	2.59	117.44	105.14
4	C	300	ATP	O2B-PB-O1B	2.42	125.76	112.21
4	C	300	ATP	PA-O5'-C5'	-2.17	106.44	122.03
4	C	300	ATP	C1'-N9-C4	-2.09	123.02	126.64
4	C	300	ATP	O3G-PG-O2G	2.03	115.51	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.