

Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 07:54 am BST

PDB ID	:	1JST
Title	:	PHOSPHORYLATED CYCLIN-DEPENDENT KINASE-2 BOUND TO CY-
		CLIN A
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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 A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11
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1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Motria	Whole archive	Similar resolution
wietric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455(2.60-2.60)
Sidechain outliers	138945	3455(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 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain				
1	А	298	53%	40%	7%		
1	С	298	48%	44%	7% •		
2	В	258	60%	34%	5%		
2	D	258	53%	43%	·		



2 Entry composition (i)

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	А	298	Total	C 1EFO	N 409	0	P 1	S	0	0	0
			2402	1559	408	420	1 	8			
1	С	298	10tal 2402	C 1559	N 408	0 426	Р 1	S 8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	160	TPO	THR	MODIFIED RESIDUE	UNP P24941
С	160	TPO	THR	MODIFIED RESIDUE	UNP P24941

• Molecule 2 is a protein called CYCLIN A.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	258	Total 2084	$ m C \\ 1350$	N 339	O 384	S 11	0	0	0
2	D	258	Total 2084	$ m C \\ 1350$	N 339	O 384	S 11	0	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Mn 1 1	0	0
3	С	1	Total Mn 1 1	0	0

• Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
4	Δ	1	Total	С	Ν	Ο	Р	0	0
4	A	L	31	10	5	13	3	0	0
4	C	1	Total	С	Ν	Ο	Р	0	0
4		L	31	10	5	13	3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	38	Total O 38 38	0	0
5	В	24	TotalO2424	0	0
5	С	20	Total O 20 20	0	0
5	D	16	Total O 16 16	0	0



3 Residue-property plots (i)

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. Residues are colorcoded 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. 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





1372 7278 1176 1376 1281 1176 1384 1281 1176 1384 1281 1176 1391 1282 1182 1391 1286 1181 1391 1286 1181 1391 1286 1182 1391 1286 1182 1391 1287 1182 1391 1286 1182 1396 1287 1182 1399 1287 1182 1396 1287 1182 1399 1287 1183 1396 1292 1182 1396 1292 1182 1396 1292 1182 1396 1296 1196 1396 1296 1296 141 1296 1296 141 1296 1296 141 1296 1296 1431 12316 1216 1432 1316 1216 1431 1316 1216 1432 1316 1216 1431 1316 1216 1432 1316 1216 1432 1316

• Molecule 2: CYCLIN A





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	139.60Å 149.10 Å 74.20 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 - 2.60	Depositor
% Data completeness	98.9 (7.00-2.60)	Depositor
(in resolution range)	56.5 (1.00 2.00)	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 (i)

5.1 Standard geometry (i)

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).

Mal	Chain	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.70	0/2452	0.87	1/3325~(0.0%)	
1	С	0.61	0/2452	0.86	2/3325~(0.1%)	
2	В	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	$Observed(^{o})$	$Ideal(^{o})$
1	С	76	LEU	CA-CB-CG	8.68	135.26	115.30
2	В	345	ASP	N-CA-C	-6.05	94.67	111.00
1	А	217	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	С	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:



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-	9	\sim	-

Mol	Chain	Res	Type	Group
2	D	347	TYR	Sidechain

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	А	2402	0	2449	132	0
1	С	2402	0	2449	141	0
2	В	2084	0	2107	78	0
2	D	2084	0	2107	108	0
3	А	1	0	0	0	0
3	С	1	0	0	0	0
4	А	31	0	12	8	0
4	С	31	0	12	4	0
5	А	38	0	0	1	0
5	В	24	0	0	1	0
5	С	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



	Interstomic Clash						
Atom-1	Atom-2	distance (\mathbf{A})	overlap(Å)				
1.C.88.LVS.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.LVS.HZ2	1.C.131.GLN.H	1 23	0.83				
2.D.196.LVS.HD3	$2 \cdot D \cdot 244 \cdot SEB \cdot HB3$	1.20	0.83				
2.D.346.PRO.0	2:D:349:LVS:HG3	1.80	0.89				
2.D.197.VAL.HG11	2:D:349:LVS:HB3	1.50	0.02				
1.C.202.LEU.HD13	1.C.203.PHE.CE2	2 16	0.81				
$\frac{1.0.202.\text{EE}0.\text{IID}15}{2.\text{B}\cdot407.\text{CLN}\cdot0}$	2.B.411.CLU.HC2	1.80	0.81				
1.C.156.VAL.:HG22	2.D.411.GE0.HG2	1.00	0.80				
1.0.100.VRD.H022	1.0.199.1 F.HC13	1.47	0.80				
1.A.1.MET.IIEI	1.C.280.VAL.HC22	1.05	0.30				
1.0.200.1 HE.0 $1.1.155.DD.0.HD2$	1.0.209.VAL.IIG23	1.61	0.79				
1.A.155.F NO.11D2	2.D.310.1111.11G23	2.03	0.79				
1.A.177.015.5G	1.A.255.ME1.5D	2.01	0.76				
1.0.00.1115.11D2	1.0.02.A5N.N	1.01	0.77				
1:A:00:HI5:HD2	1:A:02:A5N:N	1.01	0.77				
1: C: 172: GLU: HB3	$1: \bigcirc 1 \land 1 \land 2 \land 2 \land 3 \land 5 \land 5$	2.25					
1:U:83:LEU:HDII	1:U:142:LY S:HD2	1.00	0.76				
2:B:289:LY S: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				



	A L	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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	$1:C:1\overline{42:LYS:CD}$	2.31	0.60



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	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



		Interatomic Clash			
Atom-1	Atom-2	distance $(Å)$	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		



		Interatomic	Clash	
Atom-1	Atom-2	distance $(Å)$	overlan (Å)	
2.D.219.VAL.HG22	2.D.232.LEU.HD11	1.89	$\frac{0.52}{0.52}$	
1:C:38:ASP:HB2	1:C:43:GLY:N	2.24	0.52	
1:A:15:TYB: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	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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



Interatomic Clash				
Atom-1	Atom-2	distance $(Å)$	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	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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



	A +	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	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



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	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 (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	Perce	ntiles
1	А	295/298~(99%)	264 (90%)	21 (7%)	10 (3%)	3	5
1	С	295/298~(99%)	258~(88%)	24 (8%)	13~(4%)	2	3
2	В	256/258~(99%)	241 (94%)	12~(5%)	3~(1%)	13	27
2	D	256/258~(99%)	241 (94%)	13~(5%)	2(1%)	19	39
All	All	1102/1112~(99%)	1004 (91%)	70~(6%)	28 (2%)	5	9

All (28) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
1	С	18	VAL
1	С	162	GLU
1	С	164	VAL
1	С	287	GLN
2	D	176	PRO
1	А	10	ILE
1	А	14	THR
1	А	97	THR
1	А	164	VAL
2	В	177	ASP
2	В	283	ASP
1	С	11	GLY
2	D	420	GLY
1	А	8	GLU
1	А	162	GLU
1	С	96	LEU
1	А	37	LEU
1	А	39	THR
2	В	319	PHE
1	С	10	ILE
1	С	14	THR
1	С	275	ILE
1	С	283	HIS
1	С	285	PHE
1	А	96	LEU
1	С	145	ASP
1	А	228	PRO
1	С	251	VAL

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	А	262/262~(100%)	230~(88%)	32~(12%)	5 9
1	С	262/262~(100%)	225~(86%)	37~(14%)	3 6
2	В	232/232~(100%)	209~(90%)	23~(10%)	8 15



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	232/232~(100%)	219~(94%)	13~(6%)	21 42
All	All	988/988~(100%)	883 (89%)	105(11%)	6 12

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

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



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



Mol	Chain	Res	Type
1	С	158	THR
1	С	161	HIS
1	С	162	GLU
1	С	172	GLU
1	С	199	ARG
1	С	202	LEU
1	С	230	VAL
1	С	232	SER
1	С	248	PHE
1	С	250	LYS
1	С	255	LEU
1	С	276	SER
1	С	287	GLN
1	С	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	А	59	ASN
1	А	60	HIS
1	А	71	HIS
1	А	119	HIS
1	А	246	GLN
1	А	265	GLN
1	А	272	ASN
2	В	183	HIS
2	В	296	HIS
2	В	313	GLN
2	В	317	GLN



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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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 Typ	True	Chain	Dec	s Link	Bond lengths			Bond angles		
	Moi Type Chain	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	А	160	1	8,10,11	1.09	0	10, 14, 16	1.19	0
1	TPO	С	160	1	8,10,11	1.62	1 (12%)	10, 14, 16	1.41	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	А	160	1	-	1/9/11/13	-
1	TPO	С	160	1	-	1/9/11/13	-

All (1) bond length outliers are listed below:



Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	С	160	TPO	P-OG1	-3.90	1.51	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	160	TPO	OG1-P-O1P	-2.29	100.56	109.39
1	С	160	TPO	O3P-P-O2P	2.01	115.34	107.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
1	А	160	TPO	CB-OG1-P-O3P
1	С	160	TPO	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	С	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	True	Chain	Chain	Chain	Chain	Chain	Chain	Chain	Dec	Timle	Bo	ond leng	\mathbf{ths}	E	Bond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2						
4	ATP	С	300	3	26,33,33	1.31	4 (15%)	31,52,52	2.01	10 (32%)						
4	ATP	А	300	3	26,33,33	1.34	2 (7%)	31,52,52	1.45	4 (12%)						



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	С	300	3	-	5/18/38/38	0/3/3/3
4	ATP	А	300	3	-	7/18/38/38	0/3/3/3

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	А	300	ATP	C2'-C1'	3.45	1.59	1.53
4	С	300	ATP	O4'-C1'	3.29	1.45	1.41
4	А	300	ATP	PA-05'	2.84	1.70	1.59
4	С	300	ATP	C2'-C1'	2.81	1.58	1.53
4	С	300	ATP	C8-N7	-2.58	1.30	1.34
4	С	300	ATP	PA-O2A	-2.09	1.45	1.55

All (6) bond length outliers are listed below:

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	С	300	ATP	O5'-C5'-C4'	6.16	130.21	108.99
4	С	300	ATP	PA-O3A-PB	3.80	145.88	132.83
4	А	300	ATP	C3'-C2'-C1'	3.63	106.44	100.98
4	С	300	ATP	O4'-C4'-C3'	3.58	112.19	105.11
4	А	300	ATP	PA-O5'-C5'	3.27	140.84	121.68
4	А	300	ATP	O2A-PA-O5'	-3.00	93.80	107.75
4	С	300	ATP	O4'-C1'-C2'	2.79	111.01	106.93
4	С	300	ATP	C4-C5-N7	2.78	112.29	109.40
4	С	300	ATP	O2B-PB-O1B	2.73	125.76	112.24
4	С	300	ATP	PA-O5'-C5'	-2.60	106.44	121.68
4	А	300	ATP	C5-C6-N6	2.18	123.66	120.35
4	C	300	ATP	C1'-N9-C4	-2.06	123.02	126.64
4	C	300	ATP	O3G-PG-O2G	2.06	115.51	107.64
4	C	300	ATP	C5'-C4'-C3'	-2.04	107.54	115.18

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
4	С	300	ATP	PB-O3B-PG-O2G
4	А	300	ATP	C5'-O5'-PA-O1A



Mol	Chain	\mathbf{Res}	Type	Atoms
4	А	300	ATP	C5'-O5'-PA-O2A
4	А	300	ATP	C5'-O5'-PA-O3A
4	С	300	ATP	C4'-C5'-O5'-PA
4	А	300	ATP	PB-O3A-PA-O5'
4	А	300	ATP	O4'-C4'-C5'-O5'
4	А	300	ATP	C3'-C4'-C5'-O5'
4	С	300	ATP	O4'-C4'-C5'-O5'
4	С	300	ATP	PB-O3B-PG-O1G
4	С	300	ATP	PB-O3B-PG-O3G
4	А	300	ATP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	С	300	ATP	4	0
4	А	300	ATP	8	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.









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)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

