

# Full wwPDB X-ray Structure Validation Report (i)

Dec 6, 2023 - 05:52 pm GMT

PDB ID	:	2C5O
Title	:	Differential Binding Of Inhibitors To Active And Inactive Cdk2 Provides In-
		sights For Drug Design
Authors	:	Kontopidis, G.; McInnes, C.; Pandalaneni, S.R.; McNae, I.; Gibson, D.;
		Mezna, M.; Thomas, M.; Wood, G.; Wang, S.; Walkinshaw, M.D.; Fischer,
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Deposited on	:	2005-10-30
Resolution	:	2.10 Å(reported)

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

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

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.10 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
	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1	А	298	6%	26%	8% ••
1	С	298	61%	28%	10% •
2	В	260	3% 70%	22%	6% ••
2	D	260	<sup>2%</sup> <b>7</b> 0%	21%	7% ••



The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CK2	С	1298[A]	-	-	Х	-



#### 2C5O

## 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9709 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Δ	206	Total	С	Ν	Ο	$\mathbf{S}$	0	1	0
1	Л	290	2385	1552	404	420	9	0	I	0
1	C	207	Total	С	Ν	0	S	0	0	1
		291	2379	1547	404	420	8	0	0	1

• Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

• Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	В	258	Total 2082	C 1350	N 339	O 382	S 11	0	0	0
2	D	258	Total 2082	C 1350	N 339	O 382	S 11	0	0	0

• Molecule 3 is 4-(2,4-DIMETHYL-1,3-THIAZOL-5-YL)PYRIMIDIN-2-AMINE (three-letter code: CK2) (formula: C<sub>9</sub>H<sub>10</sub>N<sub>4</sub>S).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	А	1	Total 28	C 18	N 8	$\frac{S}{2}$	0	1
3	С	1	Total 28	C 18	N 8	S 2	0	1

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	174	Total O 174 174	0	0
4	В	165	Total O 165 165	0	0
4	С	195	Total O 195 195	0	0
4	D	191	Total O 191 191	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.



• Molecule 1: CELL DIVISION PROTEIN KINASE 2





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	74.48Å 113.51Å 157.08Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution (Å)	22.00 - 2.10	Depositor
Resolution (A)	14.92 - 2.10	EDS
% Data completeness	89.1 (22.00-2.10)	Depositor
(in resolution range)	89.3 (14.92-2.10)	EDS
R <sub>merge</sub>	0.10	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.70 (at 2.10 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
P. P.	0.195 , $0.256$	Depositor
$n, n_{free}$	0.197 , $0.252$	DCC
$R_{free}$ test set	2114 reflections $(3.02\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	27.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.35 , $50.2$	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9709	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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:  $\rm CK2$ 

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	0.59	0/2447	1.22	18/3322~(0.5%)	
1	С	0.57	0/2441	1.20	14/3315~(0.4%)	
2	В	0.57	0/2132	1.13	13/2896~(0.4%)	
2	D	0.55	0/2132	1.17	15/2896~(0.5%)	
All	All	0.57	0/9152	1.18	60/12429~(0.5%)	

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	А	0	3
1	С	0	3
2	В	0	3
2	D	0	3
All	All	0	12

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}(^{o})$
1	С	150	ARG	NE-CZ-NH1	14.14	127.37	120.30
2	D	345	ASP	CB-CG-OD2	9.65	126.98	118.30
2	В	205	ASP	CB-CG-OD2	9.32	126.69	118.30
2	D	393	ASP	CB-CG-OD2	9.29	126.66	118.30
1	А	235	ASP	CB-CG-OD2	8.87	126.28	118.30
2	В	345	ASP	CB-CG-OD2	8.84	126.26	118.30
2	D	241	ARG	NE-CZ-NH2	-8.79	115.90	120.30
2	В	241	ARG	NE-CZ-NH2	-8.67	115.96	120.30



В

В

ASP

ARG

Chain	$\mathbf{Res}$	Type	Atoms		$Observed(^{o})$	$  \text{Ideal}(\overline{^{o}})  $
D	241	ARG	NE-CZ-NH1	8.22	124.41	120.30
D	343	ASP	CB-CG-OD2	8.12	125.61	118.30
С	126	ARG	NE-CZ-NH2	-8.10	116.25	120.30
С	235	ASP	CB-CG-OD2	7.97	125.48	118.30
А	124	LEU	CB-CG-CD2	-7.51	98.24	111.00
В	240	ASP	CB-CG-OD2	7.14	124.72	118.30
С	245	ARG	NE-CZ-NH2	-7.03	116.78	120.30
А	258	ASP	CB-CG-OD1	6.77	124.39	118.30
С	210	ASP	CB-CG-OD2	6.75	124.38	118.30
С	270	ASP	CB-CG-OD1	6.73	124.36	118.30
А	270	ASP	CB-CG-OD2	6.60	124.24	118.30
В	284	ASP	CB-CG-OD2	6.54	124.18	118.30
А	145	ASP	CB-CG-OD2	6.48	124.14	118.30
А	76	LEU	CB-CG-CD2	6.47	122.00	111.00
А	230	VAL	CB-CA-C	-6.44	99.17	111.40
А	86	ASP	CB-CG-OD2	6.41	124.07	118.30
D	283	ASP	CB-CG-OD2	6.37	124.03	118.30
В	316	THR	OG1-CB-CG2	-6.23	95.67	110.00
А	68	ASP	CB-CG-OD2	6.22	123.90	118.30
А	202	LEU	CB-CG-CD2	6.17	121.48	111.00
D	187	ARG	NE-CZ-NH2	-6.15	117.22	120.30
D	284	ASP	CB-CG-OD2	6.14	123.83	118.30
D	205	ASP	CB-CG-OD2	6.11	123.80	118.30
D	285	THR	OG1-CB-CG2	-6.08	96.01	110.00
А	150	ARG	NE-CZ-NH1	5.99	123.30	120.30
А	38	ASP	CB-CG-OD2	5.93	123.64	118.30
D	232	LEU	CB-CG-CD2	5.92	121.06	111.00
D	249	LEU	CB-CG-CD1	5.90	121.02	111.00
D	334	MET	CG-SD-CE	-5.89	90.78	100.20
А	206	ASP	CB-CG-OD2	5.85	123.56	118.30
С	256	ASP	CB-CG-OD2	5.84	123.55	118.30
С	56	LYS	CA-CB-CG	5.74	126.03	113.40
В	283	ASP	CB-CG-OD2	5.63	123.36	118.30
А	124	LEU	CB-CG-CD1	-5.61	101.47	111.00
С	87	LEU	CB-CG-CD2	5.58	120.48	111.00
С	191	CYS	CA-CB-SG	-5.44	104.21	114.00
С	150	ARG	NH1-CZ-NH2	-5.43	113.42	119.40
А	257	GLU	OE1-CD-OE2	-5.42	116.79	123.30
С	206	ASP	CB-CG-OD2	5.36	123.12	118.30
А	247	ASP	CB-CG-OD1	5.35	123.12	118.30

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118.30

120.30

123.08

122.96



5.32

5.31

CB-CG-OD2

NE-CZ-NH1

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	262	LEU	CB-CG-CD1	5.27	119.96	111.00
2	В	216	ASP	CB-CG-OD2	5.22	123.00	118.30
2	В	263	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	А	87	LEU	CB-CG-CD2	5.16	119.77	111.00
1	С	145	ASP	CB-CG-OD2	5.16	122.94	118.30
1	А	245	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	D	240	ASP	CB-CG-OD2	5.10	122.89	118.30
2	В	285	THR	OG1-CB-CG2	-5.05	98.39	110.00
1	C	78	LEU	CB-CG-CD2	5.04	119.57	111.00
2	D	345	ASP	OD1-CG-OD2	-5.03	113.73	123.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	15	TYR	Peptide
1	А	16	GLY	Peptide
1	А	70	ILE	Peptide
2	В	175	VAL	Peptide
2	В	344	ALA	Peptide
2	В	345	ASP	Peptide
1	С	15	TYR	Peptide
1	С	16	GLY	Peptide
1	С	70	ILE	Peptide
2	D	175	VAL	Peptide
2	D	344	ALA	Peptide
2	D	345	ASP	Peptide

### 5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2385	0	2436	126	1
1	С	2379	0	2426	157	3
2	В	2082	0	2107	93	2
2	D	2082	0	2107	88	0
3	А	28	0	20	8	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	С	28	0	20	10	0
4	А	174	0	0	30	1
4	В	165	0	0	41	1
4	С	195	0	0	41	0
4	D	191	0	0	37	0
All	All	9709	0	9116	453	4

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 25.

All (453) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:C:247:ASP:HB3	4:C:2156:HOH:O	1.26	1.34
2:B:178:TYR:HE2	4:B:2029:HOH:O	1.03	1.33
1:C:1:MET:CE	1:C:70:ILE:HD13	1.58	1.32
2:D:300:LYS:HB2	4:D:2112:HOH:O	1.15	1.27
1:C:162:GLU:OE2	1:C:164:VAL:HG23	1.19	1.24
1:C:162:GLU:HA	4:C:2111:HOH:O	1.31	1.22
1:C:36:ARG:HB2	4:C:2036:HOH:O	1.35	1.21
1:A:177:CYS:HB2	4:A:2113:HOH:O	1.40	1.20
2:D:178:TYR:HE2	4:D:2036:HOH:O	1.21	1.18
2:B:288:LYS:HE3	4:B:2083:HOH:O	1.37	1.17
1:A:162:GLU:OE2	1:A:164:VAL:HG23	1.46	1.16
1:C:1:MET:CE	1:C:70:ILE:CD1	2.24	1.13
1:C:162:GLU:OE2	1:C:164:VAL:CG2	1.95	1.13
1:C:38:ASP:OD1	1:C:41:THR:HB	1.49	1.11
1:C:177:CYS:HB2	4:C:2121:HOH:O	1.51	1.11
2:B:317:GLN:NE2	4:B:2103:HOH:O	1.85	1.09
4:A:2085:HOH:O	2:B:178:TYR:CD2	2.05	1.09
1:A:1[A]:MET:HE3	1:A:3:ASN:H	1.09	1.09
1:C:15:TYR:CE2	1:C:33:LYS:HD3	1.88	1.08
1:C:95:ALA:O	1:C:96:LEU:HB3	1.28	1.08
1:A:162:GLU:OE1	4:A:2104:HOH:O	1.69	1.08
1:C:165:THR:HG22	4:C:2116:HOH:O	0.92	1.08
2:D:304:PHE:HD1	4:D:2115:HOH:O	1.36	1.08
2:D:385:GLU:HA	4:D:2159:HOH:O	1.54	1.06
4:B:2047:HOH:O	1:C:65:LYS:HE2	1.53	1.05
1:C:15:TYR:CB	4:C:2015:HOH:O	2.03	1.05
1:A:1[A]:MET:CE	1:A:3:ASN:H	1.70	1.04
2:B:207:THR:HG22	2:B:210:MET:H	1.22	1.04



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		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:91:MET:CE	1:A:196:MET:HG2	1.89	1.03
4:A:2085:HOH:O	2:B:178:TYR:CE2	2.11	1.02
3:A:1297[A]:CK2:H6A1	3:A:1297[A]:CK2:H5	1.41	1.02
2:D:404:HIS:CD2	2:D:406:GLN:H	1.77	1.02
2:B:247:SER:HB3	4:B:2065:HOH:O	1.60	1.01
2:D:193:CYS:SG	4:D:2116:HOH:O	2.17	1.01
2:B:325:ALA:HB1	4:B:2105:HOH:O	1.57	1.01
1:A:95:ALA:O	1:A:96:LEU:HB3	1.24	1.00
2:D:421:VAL:O	4:D:2185:HOH:O	1.79	1.00
1:A:15:TYR:HD1	1:A:47:THR:OG1	1.43	1.00
1:A:91:MET:HE2	1:A:196:MET:HG2	1.39	1.00
2:D:178:TYR:CE2	4:D:2036:HOH:O	2.01	1.00
1:A:38:ASP:OD1	1:A:41:THR:HB	1.63	0.99
1:C:1:MET:HE3	1:C:70:ILE:CD1	1.90	0.99
1:C:1:MET:HE1	1:C:70:ILE:HD13	1.41	0.99
1:C:15:TYR:HD1	1:C:47:THR:OG1	1.46	0.99
1:C:1:MET:N	4:C:2001:HOH:O	1.83	0.98
1:C:60:HIS:HD2	1:C:62:ASN:H	1.11	0.97
2:B:178:TYR:CE2	4:B:2029:HOH:O	1.88	0.96
1:C:145:ASP:HA	3:C:1298[A]:CK2:H7A3	1.45	0.96
2:B:325:ALA:CB	4:B:2105:HOH:O	2.10	0.95
1:A:33:LYS:HE3	3:A:1297[B]:CK2:H7A2	1.47	0.94
1:C:95:ALA:O	1:C:96:LEU:CB	2.13	0.94
1:C:60:HIS:CD2	1:C:62:ASN:H	1.85	0.94
2:D:207:THR:HG22	2:D:210:MET:H	1.31	0.94
2:B:404:HIS:HD2	2:B:406:GLN:H	1.08	0.94
1:C:15:TYR:HB3	4:C:2015:HOH:O	1.61	0.94
3:C:1298[B]:CK2:H6A1	3:C:1298[B]:CK2:H5	1.47	0.93
1:A:60:HIS:CD2	1:A:62:ASN:H	1.85	0.93
1:A:60:HIS:HD2	1:A:62:ASN:H	1.12	0.93
2:D:379:LYS:NZ	4:D:2154:HOH:O	2.03	0.92
1:C:38:ASP:OD1	1:C:41:THR:CB	2.17	0.92
1:C:15:TYR:HE2	1:C:33:LYS:HD3	1.30	0.91
2:B:250:ARG:CD	4:B:2069:HOH:O	2.19	0.91
1:C:6:LYS:NZ	4:C:2007:HOH:O	1.79	0.91
1:A:162:GLU:OE2	1:A:164:VAL:CG2	2.17	0.91
1:A:131:GLN:H	1:A:131:GLN:HE21	1.11	0.90
1:A:95:ALA:O	1:A:96:LEU:CB	2.10	0.88
1:C:165:THR:OG1	4:C:2115:HOH:O	1.91	0.88
2:D:345:ASP:OD2	4:D:2138:HOH:O	1.91	0.88
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.36	0.88



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:1:MET:HE3	1:C:70:ILE:HD12	1.55	0.88
1:C:131:GLN:HE21	1:C:131:GLN:H	1.17	0.88
2:B:282:THR:O	2:B:285:THR:HG22	1.74	0.87
2:B:282:THR:O	2:B:285:THR:CG2	2.23	0.87
2:D:404:HIS:HD2	2:D:406:GLN:N	1.72	0.87
2:D:396:GLN:HG3	4:D:2165:HOH:O	1.73	0.86
1:A:1[A]:MET:HG2	1:A:2:GLU:N	1.86	0.86
2:B:372:TRP:HB3	4:B:2124:HOH:O	1.76	0.85
1:A:91:MET:CE	1:A:196:MET:CG	2.54	0.85
2:D:289:LYS:HE2	4:D:2105:HOH:O	1.76	0.84
1:C:15:TYR:CD1	1:C:47:THR:OG1	2.25	0.83
2:D:404:HIS:HD2	2:D:406:GLN:H	0.89	0.83
1:C:247:ASP:CB	4:C:2156:HOH:O	1.98	0.82
2:D:379:LYS:CE	4:D:2154:HOH:O	2.27	0.82
2:B:323:GLN:CB	4:B:2106:HOH:O	2.26	0.82
1:A:1[A]:MET:HE3	1:A:3:ASN:N	1.92	0.82
2:D:207:THR:HG21	4:D:2057:HOH:O	1.80	0.82
1:A:15:TYR:CE2	1:A:33:LYS:HD3	2.15	0.81
1:A:81:GLU:O	3:A:1297[B]:CK2:H6	1.80	0.81
2:D:304:PHE:CD1	4:D:2115:HOH:O	2.17	0.81
1:C:1:MET:HE2	1:C:70:ILE:HD13	1.62	0.81
1:C:250:LYS:HD3	4:C:2158:HOH:O	1.79	0.80
2:B:323:GLN:CA	4:B:2106:HOH:O	2.30	0.80
2:D:179:HIS:CE1	2:D:320:LEU:HD12	2.15	0.80
1:C:1:MET:HE1	1:C:70:ILE:CD1	2.02	0.80
1:C:145:ASP:CA	3:C:1298[A]:CK2:H7A3	2.12	0.80
2:B:250:ARG:HD3	4:B:2069:HOH:O	1.81	0.79
1:C:15:TYR:HB2	4:C:2015:HOH:O	1.75	0.79
2:D:345:ASP:O	4:D:2137:HOH:O	1.99	0.78
2:B:404:HIS:CD2	2:B:406:GLN:H	1.99	0.78
1:A:33:LYS:CE	3:A:1297[B]:CK2:H7A2	2.14	0.77
1:C:91:MET:CE	1:C:196:MET:HG2	2.13	0.77
1:A:38:ASP:OD1	1:A:41:THR:CB	2.31	0.77
1:A:22:ARG:HG3	4:A:2019:HOH:O	1.85	0.76
1:C:91:MET:HE3	1:C:196:MET:HG2	1.68	0.76
1:A:15:TYR:HE2	1:A:33:LYS:HD3	1.51	0.76
3:A:1297[A]:CK2:H6A2	4:A:2093:HOH:O	1.85	0.76
1:A:37:LEU:N	4:A:2036:HOH:O	1.69	0.76
1:C:83:LEU:O	3:C:1298[B]:CK2:N7	2.18	0.75
2:B:304:PHE:HD1	4:B:2095:HOH:O	1.69	0.75
1:C:173:ILE:HD11	1:C:184:VAL:HG11	1.68	0.75



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:207:THR:HG23	2:D:209:SER:H	1.51	0.75
1:A:15:TYR:CD1	1:A:47:THR:OG1	2.26	0.75
1:C:131:GLN:H	1:C:131:GLN:NE2	1.84	0.75
2:D:300:LYS:HD2	4:D:2022:HOH:O	1.87	0.75
1:A:36:ARG:HA	4:A:2036:HOH:O	1.86	0.75
1:A:36:ARG:HD3	4:A:2034:HOH:O	1.86	0.74
1:A:40:GLU:O	2:B:288:LYS:HD3	1.87	0.73
2:B:322:GLN:OE1	4:B:2105:HOH:O	2.06	0.73
1:C:71:HIS:HE1	4:D:2110:HOH:O	1.70	0.73
2:D:334:MET:HE3	4:D:2132:HOH:O	1.87	0.73
1:A:42:GLU:OE2	2:B:275:VAL:HG23	1.89	0.73
2:B:312:ASN:OD1	2:B:334:MET:CE	2.36	0.73
2:D:179:HIS:CD2	2:D:379:LYS:NZ	2.57	0.73
2:D:323:GLN:OE1	2:D:323:GLN:N	2.22	0.73
2:B:207:THR:HG23	2:B:209:SER:H	1.54	0.72
1:A:84:HIS:HB2	4:A:2071:HOH:O	1.90	0.71
1:A:162:GLU:HB2	4:A:2104:HOH:O	1.89	0.71
1:A:159:TYR:HD1	1:A:159:TYR:N	1.89	0.71
1:A:38:ASP:OD1	1:A:38:ASP:O	2.09	0.71
1:C:153:GLY:HA2	4:C:2103:HOH:O	1.88	0.71
2:B:289:LYS:HE3	2:B:293:ARG:HH11	1.56	0.70
1:C:214:ARG:HH11	1:C:214:ARG:CG	2.04	0.70
1:C:5:GLN:HG3	1:C:5:GLN:O	1.92	0.70
1:C:131:GLN:HE21	1:C:131:GLN:N	1.90	0.69
2:B:194:LYS:HG3	4:B:2117:HOH:O	1.91	0.69
2:B:207:THR:HG22	2:B:210:MET:N	2.01	0.69
1:C:7:VAL:O	1:C:8:GLU:HB3	1.92	0.69
1:A:159:TYR:N	1:A:159:TYR:CD1	2.61	0.69
1:A:164:VAL:O	4:A:2106:HOH:O	2.09	0.69
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.75	0.69
1:C:247:ASP:CG	4:C:2156:HOH:O	2.24	0.68
1:C:41:THR:HA	4:C:2042:HOH:O	1.92	0.68
1:A:60:HIS:HD2	1:A:62:ASN:N	1.89	0.68
1:A:164:VAL:HG12	1:A:165:THR:N	2.09	0.68
1:A:131:GLN:H	1:A:131:GLN:NE2	1.91	0.68
2:B:289:LYS:HE3	2:B:293:ARG:NH1	2.09	0.67
1:C:160:THR:OG1	4:C:2109:HOH:O	2.12	0.67
2:B:178:TYR:HA	4:B:2034:HOH:O	1.95	0.67
2:D:176:PRO:HA	4:D:2034:HOH:O	1.94	0.67
1:A:165:THR:HG21	1:A:168:TYR:HD2	1.60	0.67
4:A:2085:HOH:O	2:B:178:TYR:HD2	1.59	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:246:GLN:CG	4:C:2151:HOH:O	2.43	0.66
2:D:207:THR:CG2	2:D:209:SER:H	2.07	0.66
2:B:175:VAL:N	2:B:176:PRO:CD	2.59	0.66
1:C:40:GLU:O	2:D:288:LYS:HD3	1.96	0.66
1:A:51:GLU:O	1:A:55:LEU:HB2	1.95	0.65
1:A:38:ASP:N	4:A:2037:HOH:O	2.00	0.65
1:C:15:TYR:HB3	4:C:2046:HOH:O	1.95	0.65
2:B:323:GLN:HA	4:B:2106:HOH:O	1.95	0.65
2:B:179:HIS:CE1	2:B:320:LEU:HD12	2.31	0.65
1:A:14:THR:O	1:A:15:TYR:CG	2.49	0.65
1:C:15:TYR:HE2	1:C:33:LYS:CD	2.08	0.65
1:C:91:MET:CE	1:C:196:MET:CG	2.74	0.65
2:B:207:THR:CG2	2:B:209:SER:HB3	2.28	0.64
1:C:15:TYR:O	4:C:2016:HOH:O	2.14	0.64
2:B:343:ASP:HB3	2:B:345:ASP:HB2	1.79	0.64
1:A:257:GLU:HG3	1:A:260:ARG:NH2	2.12	0.64
1:A:89:LYS:HE2	4:A:2073:HOH:O	1.97	0.63
2:D:379:LYS:HE2	4:D:2154:HOH:O	1.92	0.63
1:A:1[A]:MET:CE	1:A:3:ASN:N	2.54	0.63
1:A:78:LEU:HD23	1:A:78:LEU:N	2.13	0.63
1:C:165:THR:HG21	1:C:168:TYR:HD2	1.62	0.63
2:D:304:PHE:HB3	4:D:2115:HOH:O	1.98	0.63
1:A:164:VAL:HG12	1:A:165:THR:H	1.63	0.63
2:D:175:VAL:HG22	2:D:175:VAL:O	1.99	0.63
1:A:84:HIS:CB	4:A:2071:HOH:O	2.47	0.62
2:D:343:ASP:HB3	2:D:345:ASP:HB2	1.81	0.62
2:B:289:LYS:HE2	4:B:2087:HOH:O	1.99	0.62
1:C:74:ASN:ND2	4:C:2063:HOH:O	2.31	0.62
2:B:312:ASN:OD1	2:B:334:MET:HE3	1.99	0.62
1:C:198:THR:O	1:C:199:ARG:HB2	1.99	0.62
1:A:91:MET:HE3	1:A:196:MET:CG	2.29	0.62
1:A:38:ASP:CG	1:A:41:THR:OG1	2.37	0.61
2:D:179:HIS:CD2	2:D:379:LYS:HZ2	2.18	0.61
4:C:2126:HOH:O	2:D:176:PRO:HB3	2.00	0.61
1:A:5:GLN:O	1:A:5:GLN:HG3	2.01	0.61
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.36	0.61
1:A:91:MET:HE3	1:A:196:MET:HG2	1.80	0.61
2:D:204:PRO:HG2	4:D:2001:HOH:O	2.01	0.61
1:C:42:GLU:OE2	2:D:275:VAL:HG23	2.01	0.60
1:C:14:THR:O	1:C:15:TYR:CG	2.54	0.60
1:C:60:HIS:HD2	1:C:62:ASN:N	1.89	0.60



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:398:TYR:OH	4:B:2145:HOH:O	2.15	0.60
1:C:159:TYR:HD1	1:C:159:TYR:N	2.00	0.60
1:C:164:VAL:HG12	1:C:165:THR:H	1.67	0.60
2:D:345:ASP:CB	2:D:346:PRO:CD	2.80	0.60
2:B:350:TYR:OH	2:B:393:ASP:OD2	2.12	0.60
2:D:403:GLN:HG2	4:D:2169:HOH:O	2.02	0.60
1:C:1:MET:CE	1:C:70:ILE:HD12	2.16	0.59
2:B:296:HIS:HB2	4:B:2092:HOH:O	2.02	0.59
2:B:179:HIS:NE2	2:B:379:LYS:NZ	2.50	0.59
1:A:101:LEU:HD12	4:A:2078:HOH:O	2.01	0.59
2:D:296:HIS:CD2	4:D:2113:HOH:O	2.56	0.59
2:D:175:VAL:N	2:D:176:PRO:CD	2.66	0.59
2:D:388:LYS:HB2	4:D:2159:HOH:O	2.01	0.59
1:A:91:MET:HE2	1:A:196:MET:CG	2.21	0.59
2:D:371:SER:HB3	4:D:2149:HOH:O	2.03	0.59
1:C:115:LEU:HD11	1:C:185:ASP:HB3	1.84	0.58
1:A:96:LEU:HD23	1:A:97:THR:HG22	1.85	0.58
2:D:345:ASP:HB2	2:D:346:PRO:CD	2.33	0.58
1:C:71:HIS:NE2	2:D:296:HIS:CD2	2.72	0.58
2:D:220:GLU:HB3	4:D:2067:HOH:O	2.04	0.58
1:A:1[A]:MET:HE1	1:A:3:ASN:HB2	1.86	0.58
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.39	0.58
2:B:323:GLN:HB3	4:B:2106:HOH:O	1.93	0.58
1:C:91:MET:HE2	1:C:196:MET:HG2	1.86	0.57
1:C:91:MET:HE3	1:C:196:MET:CG	2.34	0.57
1:C:159:TYR:N	1:C:159:TYR:CD1	2.71	0.57
2:D:207:THR:HG22	2:D:210:MET:N	2.12	0.57
2:D:289:LYS:HE3	2:D:293:ARG:NH1	2.19	0.57
1:A:34:LYS:HE3	1:A:75:LYS:HD3	1.85	0.57
2:B:178:TYR:OH	4:B:2031:HOH:O	2.10	0.57
2:B:378:ARG:NE	4:B:2127:HOH:O	2.36	0.57
2:B:175:VAL:HG22	2:B:175:VAL:O	2.05	0.57
1:C:7:VAL:C	4:C:2011:HOH:O	2.42	0.57
1:A:227:TRP:O	1:A:230:VAL:HG22	2.05	0.56
2:B:217:TRP:CZ2	2:B:281:ILE:HD12	2.40	0.56
2:B:194:LYS:HE3	4:B:2117:HOH:O	2.05	0.56
1:C:158:THR:HG21	4:C:2120:HOH:O	2.05	0.56
1:C:278:LYS:NZ	2:D:177:ASP:O	2.35	0.56
2:D:417:LYS:O	2:D:417:LYS:HG2	2.06	0.56
1:A:131:GLN:HE21	1:A:131:GLN:N	1.91	0.56
2:D:176:PRO:CA	4:D:2034:HOH:O	2.53	0.56



		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:91:MET:CE	1:A:196:MET:HG3	2.36	0.56
1:C:51:GLU:O	1:C:55:LEU:HB2	2.06	0.56
2:D:289:LYS:HE3	2:D:293:ARG:HH11	1.70	0.56
1:C:294:PRO:HB2	1:C:296:LEU:HD13	1.88	0.55
2:B:194:LYS:NZ	4:B:2040:HOH:O	2.36	0.55
1:A:81:GLU:O	3:A:1297[A]:CK2:H6	2.07	0.55
2:B:378:ARG:NH2	4:B:2127:HOH:O	2.39	0.55
1:C:145:ASP:CG	3:C:1298[A]:CK2:H7A1	2.26	0.55
1:C:158:THR:HG23	4:C:2113:HOH:O	2.07	0.55
2:B:345:ASP:CB	2:B:346:PRO:CD	2.85	0.54
1:C:173:ILE:HD11	1:C:184:VAL:CG1	2.35	0.54
2:D:208:ASN:HB3	2:D:345:ASP:OD1	2.07	0.54
1:A:71:HIS:CE1	2:B:296:HIS:CE1	2.95	0.54
1:C:51:GLU:HG3	1:C:55:LEU:HD22	1.88	0.54
2:B:233:HIS:HD2	4:B:2100:HOH:O	1.89	0.54
1:A:38:ASP:CG	4:A:2037:HOH:O	2.45	0.54
1:C:73:GLU:HB2	4:C:2062:HOH:O	2.07	0.54
2:B:207:THR:HG23	2:B:209:SER:N	2.22	0.53
2:B:278:PHE:HA	2:B:281:ILE:HG12	1.90	0.53
1:C:169:ARG:HD3	1:C:173:ILE:CG2	2.37	0.53
1:C:81:GLU:O	3:C:1298[B]:CK2:H6	2.08	0.53
2:D:415:ASN:HB2	4:D:2183:HOH:O	2.09	0.53
1:C:1:MET:HE2	1:C:70:ILE:HG21	1.88	0.53
1:C:59:ASN:ND2	4:C:2055:HOH:O	2.41	0.53
1:C:38:ASP:CG	1:C:41:THR:OG1	2.46	0.53
1:C:164:VAL:HG12	1:C:165:THR:N	2.22	0.53
1:A:1[A]:MET:HE2	1:A:1[A]:MET:C	2.29	0.53
2:B:202:LYS:O	2:B:204:PRO:HD3	2.09	0.53
2:B:404:HIS:HD2	2:B:406:GLN:N	1.91	0.53
1:C:81:GLU:O	3:C:1298[A]:CK2:H6	2.08	0.53
1:C:71:HIS:CE1	2:D:296:HIS:CE1	2.97	0.53
1:C:124:LEU:HD11	1:C:180:TYR:HB3	1.90	0.53
3:A:1297[A]:CK2:C6A	4:A:2093:HOH:O	2.51	0.53
2:B:179:HIS:CD2	2:B:379:LYS:NZ	2.77	0.53
1:A:165:THR:HG21	1:A:168:TYR:CD2	2.43	0.52
2:D:233:HIS:HD2	4:D:2119:HOH:O	1.92	0.52
1:A:101:LEU:HD13	1:A:104:ILE:HD12	1.90	0.52
1:A:72:THR:O	2:B:296:HIS:HE1	1.93	0.52
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.92	0.52
1:A:54:LEU:HD22	1:A:123:VAL:HG22	1.92	0.52
1:C:38:ASP:HA	4:C:2037:HOH:O	2.08	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:D:177:ASP:N	2:D:177:ASP:OD1	2.43	0.52
1:C:135:ILE:HD11	1:C:296:LEU:HD11	1.92	0.52
1:A:126:ARG:HE	1:A:150:ARG:HG2	1.74	0.52
2:D:312:ASN:OD1	2:D:334:MET:CE	2.58	0.52
1:C:227:TRP:O	1:C:230:VAL:HG12	2.10	0.52
1:C:246:GLN:HG2	4:C:2151:HOH:O	2.08	0.52
1:A:38:ASP:CG	1:A:41:THR:CB	2.78	0.52
2:D:323:GLN:N	2:D:323:GLN:CD	2.64	0.51
2:B:176:PRO:CG	4:B:2033:HOH:O	2.57	0.51
2:D:345:ASP:CB	2:D:346:PRO:HD3	2.41	0.51
1:C:169:ARG:HD3	1:C:173:ILE:HG21	1.92	0.51
1:A:84:HIS:HD2	1:A:85:GLN:HB3	1.76	0.51
2:D:327:CYS:SG	4:D:2130:HOH:O	2.59	0.51
1:A:256:ASP:CG	4:A:2147:HOH:O	2.48	0.50
1:A:163:VAL:HG12	4:A:2105:HOH:O	2.11	0.50
1:C:15:TYR:CE2	1:C:33:LYS:CD	2.79	0.50
2:B:217:TRP:CH2	2:B:281:ILE:HD12	2.47	0.50
1:C:154:VAL:HG13	4:C:2104:HOH:O	2.10	0.50
2:D:304:PHE:CB	4:D:2115:HOH:O	2.59	0.50
2:B:208:ASN:HB3	2:B:345:ASP:OD1	2.12	0.50
3:A:1297[B]:CK2:H6A1	3:A:1297[B]:CK2:N3	2.27	0.49
1:A:294:PRO:HB2	1:A:296:LEU:HD13	1.93	0.49
2:B:179:HIS:CD2	2:B:379:LYS:HZ2	2.31	0.49
2:B:196:LYS:NZ	4:B:2041:HOH:O	2.18	0.49
2:B:430:LEU:O	2:B:431:ASN:HB2	2.11	0.49
2:B:270:ILE:HG22	2:B:271:TYR:CD2	2.47	0.49
1:A:101:LEU:HB3	4:A:2078:HOH:O	2.12	0.49
1:A:115:LEU:HD21	1:A:128:LEU:HD11	1.94	0.49
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.94	0.49
1:A:38:ASP:CG	1:A:41:THR:HB	2.32	0.49
1:A:162:GLU:OE1	1:A:180:TYR:OH	2.30	0.49
1:A:73:GLU:OE2	1:C:2:GLU:HG2	2.13	0.48
1:C:97:THR:CG2	4:C:2078:HOH:O	2.60	0.48
2:D:430:LEU:O	2:D:431:ASN:HB2	2.12	0.48
1:C:256:ASP:OD2	4:C:2160:HOH:O	2.20	0.48
1:C:162:GLU:OE1	1:C:180:TYR:OH	2.32	0.48
1:A:73:GLU:CD	1:C:2:GLU:HG2	2.34	0.48
1:A:229:GLY:O	1:A:230:VAL:C	2.49	0.48
1:C:162:GLU:HG2	1:C:169:ARG:CZ	2.43	0.48
2:B:345:ASP:HB2	2:B:346:PRO:CD	2.44	0.48
1:C:250:LYS:NZ	4:C:2157:HOH:O	2.45	0.48



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		Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:D:371:SER:CB	4:D:2149:HOH:O	2.60	0.48
1:C:91:MET:HE2	1:C:196:MET:HA	1.96	0.48
1:A:51:GLU:HG3	1:A:55:LEU:HD22	1.96	0.48
1:C:97:THR:HG22	4:C:2078:HOH:O	2.12	0.48
1:C:38:ASP:CG	1:C:41:THR:CB	2.82	0.47
1:C:278:LYS:HE3	4:C:2184:HOH:O	2.13	0.47
4:A:2085:HOH:O	2:B:178:TYR:HE2	1.74	0.47
1:C:223:ASP:OD1	1:C:226:VAL:HG23	2.15	0.47
1:A:60:HIS:CD2	1:A:61:PRO:HD2	2.49	0.47
2:B:334:MET:HE3	4:B:2111:HOH:O	2.14	0.47
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.96	0.47
1:C:162:GLU:OE2	1:C:164:VAL:HG21	2.04	0.47
2:D:179:HIS:NE2	2:D:379:LYS:NZ	2.62	0.47
1:A:214:ARG:NH1	4:A:2129:HOH:O	2.48	0.47
1:A:56:LYS:HE3	2:B:303:THR:O	2.14	0.46
2:B:378:ARG:CZ	4:B:2128:HOH:O	2.63	0.46
1:C:94:SER:O	1:C:97:THR:HG23	2.15	0.46
1:C:101:LEU:N	1:C:102:PRO:CD	2.78	0.46
1:C:189:LEU:HD12	1:C:189:LEU:HA	1.74	0.46
2:B:202:LYS:HE2	4:B:2045:HOH:O	2.15	0.46
1:C:145:ASP:CB	3:C:1298[A]:CK2:C7A	2.94	0.46
1:C:246:GLN:HG3	4:C:2151:HOH:O	2.09	0.46
2:B:249:LEU:HD12	2:B:249:LEU:HA	1.79	0.46
1:C:165:THR:HG21	1:C:168:TYR:CD2	2.46	0.46
2:D:202:LYS:O	2:D:204:PRO:HD3	2.16	0.46
1:A:159:TYR:O	1:A:160:THR:C	2.54	0.46
2:B:196:LYS:CE	4:B:2041:HOH:O	2.62	0.46
1:C:163:VAL:HG13	1:C:163:VAL:O	2.15	0.46
1:C:165:THR:CG2	1:C:168:TYR:H	2.29	0.46
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.98	0.46
1:C:145:ASP:CB	3:C:1298[A]:CK2:H7A1	2.46	0.46
2:D:384:LEU:HD12	2:D:384:LEU:O	2.16	0.46
1:A:165:THR:CG2	1:A:168:TYR:H	2.28	0.45
2:B:282:THR:O	2:B:285:THR:HG23	2.12	0.45
2:B:378:ARG:CZ	4:B:2127:HOH:O	2.64	0.45
2:D:323:GLN:HA	2:D:324:PRO:HA	1.63	0.45
1:A:125:HIS:O	1:A:126:ARG:CB	2.63	0.45
1:C:126:ARG:HE	1:C:150:ARG:HG2	1.81	0.45
1:A:15:TYR:CE1	1:A:47:THR:HB	2.51	0.45
2:D:400:LYS:O	2:D:401:ALA:C	2.55	0.45
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.98	0.45



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:84:HIS:C	1:A:84:HIS:CD2	2.89	0.45
1:A:121:HIS:O	1:A:122:ARG:HG3	2.16	0.45
2:B:177:ASP:N	2:B:177:ASP:OD1	2.48	0.45
1:C:41:THR:HB	1:C:42:GLU:H	1.53	0.45
2:B:250:ARG:HD2	4:B:2069:HOH:O	2.00	0.45
1:C:231:THR:HG22	1:C:236:TYR:CE1	2.52	0.45
2:D:176:PRO:HG2	2:D:179:HIS:HB2	1.99	0.45
2:D:345:ASP:HB2	2:D:346:PRO:HD2	1.98	0.45
1:C:145:ASP:CA	3:C:1298[A]:CK2:C7A	2.91	0.45
2:B:288:LYS:CE	4:B:2083:HOH:O	2.23	0.45
1:C:165:THR:HG23	1:C:168:TYR:H	1.82	0.44
1:A:15:TYR:HD1	1:A:47:THR:HG1	0.61	0.44
1:A:15:TYR:CD1	1:A:47:THR:CB	3.00	0.44
1:C:91:MET:HE2	1:C:196:MET:CG	2.44	0.44
1:A:65:LYS:HD2	4:A:2057:HOH:O	2.16	0.44
1:A:84:HIS:ND1	1:A:296:LEU:HD23	2.32	0.44
1:A:163:VAL:HG13	1:A:163:VAL:O	2.18	0.44
1:C:61:PRO:HA	4:C:2056:HOH:O	2.16	0.44
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.52	0.44
1:C:73:GLU:CG	2:D:293:ARG:HH21	2.30	0.44
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.53	0.44
2:B:207:THR:HG21	2:B:209:SER:HB3	2.00	0.44
2:B:208:ASN:ND2	2:B:344:ALA:HB3	2.32	0.44
2:B:175:VAL:N	2:B:176:PRO:HD3	2.33	0.44
1:A:164:VAL:CG1	1:A:165:THR:N	2.79	0.44
2:B:404:HIS:CD2	2:B:406:GLN:HB2	2.52	0.44
1:A:38:ASP:HB2	1:A:41:THR:OG1	2.18	0.44
1:C:125:HIS:O	1:C:126:ARG:CB	2.66	0.44
2:B:312:ASN:OD1	2:B:334:MET:HE1	2.17	0.43
1:C:15:TYR:CD2	1:C:33:LYS:HD3	2.47	0.43
1:A:43:GLY:HA2	4:B:2014:HOH:O	2.17	0.43
1:C:162:GLU:HG3	1:C:164:VAL:H	1.84	0.43
2:D:175:VAL:O	2:D:175:VAL:CG2	2.66	0.43
1:C:32:LEU:CD2	1:C:79:VAL:HG22	2.49	0.43
1:A:15:TYR:CE1	1:A:47:THR:CB	3.01	0.43
1:C:5:GLN:HE21	1:C:22:ARG:HH21	1.67	0.43
1:C:22:ARG:HG3	4:C:2021:HOH:O	2.18	0.43
2:D:180:GLU:HB2	4:D:2037:HOH:O	2.17	0.43
1:A:126:ARG:NH2	1:A:159:TYR:OH	2.52	0.43
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.80	0.43
2:D:207:THR:CG2	2:D:209:SER:N	2.78	0.43



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		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap $(\text{\AA})$
1:C:253:PRO:HB2	1:C:254:PRO:HD3	2.00	0.43
2:B:176:PRO:HB2	2:B:178:TYR:CD1	2.54	0.42
1:A:291:LYS:N	1:A:292:PRO:HD3	2.34	0.42
2:B:207:THR:HG23	2:B:209:SER:HB3	1.99	0.42
1:A:35:ILE:HD13	1:A:76:LEU:HD13	2.00	0.42
1:A:40:GLU:CD	4:A:2042:HOH:O	2.58	0.42
1:C:5:GLN:NE2	1:C:22:ARG:HH21	2.16	0.42
2:D:220:GLU:CD	4:D:2066:HOH:O	2.58	0.42
1:C:10:ILE:HD13	1:C:20:LYS:HB2	2.01	0.42
1:C:115:LEU:HD23	1:C:115:LEU:HA	1.88	0.42
2:D:345:ASP:HB3	2:D:346:PRO:HD3	2.02	0.42
1:A:248:PHE:HB3	1:A:260:ARG:HD2	2.02	0.42
2:B:199:TYR:CD1	2:B:199:TYR:C	2.93	0.42
1:C:91:MET:CE	1:C:196:MET:HG3	2.50	0.42
1:A:213:PHE:O	1:A:217:ARG:HG2	2.20	0.42
1:A:36:ARG:HB2	4:A:2034:HOH:O	2.20	0.42
1:A:111:LEU:HD21	1:A:141:ILE:HG12	2.01	0.42
2:B:270:ILE:HD12	4:B:2075:HOH:O	2.19	0.42
2:D:176:PRO:HB2	2:D:178:TYR:H	1.85	0.42
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.82	0.41
1:A:158:THR:HG21	4:A:2112:HOH:O	2.20	0.41
2:B:176:PRO:HG2	4:B:2033:HOH:O	2.19	0.41
2:B:323:GLN:HA	2:B:324:PRO:HA	1.61	0.41
2:B:361:HIS:CD2	2:B:391:LEU:HD21	2.55	0.41
2:D:430:LEU:O	2:D:431:ASN:CB	2.68	0.41
1:A:83:LEU:HD23	1:A:136:ASN:HB3	2.03	0.41
1:C:38:ASP:OD1	1:C:41:THR:OG1	2.38	0.41
1:C:186:ILE:HA	1:C:186:ILE:HD13	1.85	0.41
1:C:217:ARG:HH11	1:C:217:ARG:HD2	1.69	0.41
1:A:77:TYR:C	1:A:78:LEU:HD23	2.40	0.41
2:D:424:LEU:HD12	2:D:424:LEU:HA	1.93	0.41
1:C:15:TYR:CE1	1:C:47:THR:CB	3.04	0.41
1:C:128:LEU:HA	1:C:128:LEU:HD23	1.84	0.41
2:D:179:HIS:CD2	2:D:379:LYS:HZ1	2.38	0.41
1:A:249:SER:HB3	4:A:2142:HOH:O	2.20	0.41
1:C:37:LEU:HD23	1:C:37:LEU:HA	1.93	0.41
1:C:198:THR:O	1:C:199:ARG:CB	2.65	0.41
1:C:73:GLU:HG3	2:D:293:ARG:HH21	1.85	0.41
1:C:278:LYS:CE	4:C:2184:HOH:O	2.67	0.41
1:A:38:ASP:CB	1:A:41:THR:OG1	2.69	0.40
1:C:150:ARG:NH1	4:C:2100:HOH:O	2.46	0.40



200	$\sim$
200	$\mathbf{O}$

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1[B]:MET:HG3	1:A:77:TYR:CE1	2.57	0.40
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.37	0.40
2:B:304:PHE:CD1	4:B:2095:HOH:O	2.57	0.40
1:C:15:TYR:HD1	1:C:47:THR:HG1	0.64	0.40
1:C:73:GLU:OE1	2:D:293:ARG:NH2	2.55	0.40
1:C:257:GLU:HG2	1:C:260:ARG:NH2	2.37	0.40
2:D:422:SER:HA	4:D:2185:HOH:O	2.21	0.40
1:C:33:LYS:HB3	1:C:78:LEU:HB2	2.04	0.40
2:D:421:VAL:HA	2:D:424:LEU:HD22	2.04	0.40
1:A:15:TYR:HE1	1:A:47:THR:HB	1.86	0.40
1:A:177:CYS:CB	4:A:2113:HOH:O	2.24	0.40
1:C:15:TYR:CD1	1:C:47:THR:CB	3.05	0.40
1:C:200:ARG:HG3	4:C:2133:HOH:O	2.22	0.40
2:D:229:ASN:HB3	4:D:2132:HOH:O	2.22	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:ASN:ND2	$1:C:210:ASP:OD1[2_664]$	1.45	0.75
1:A:223:ASP:OD2	1:C:161:HIS:NE2[2_564]	2.00	0.20
2:B:431:ASN:CG	1:C:210:ASP:OD1[2_664]	2.15	0.05
4:A:2012:HOH:O	4:B:2146:HOH:O[4_455]	2.18	0.02

### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	294/298~(99%)	282 (96%)	8 (3%)	4 (1%)	11 6
1	С	295/298~(99%)	283~(96%)	9(3%)	3(1%)	15 11
2	В	256/260~(98%)	247 (96%)	6 (2%)	3 (1%)	13 8



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	D	256/260~(98%)	245~(96%)	9 (4%)	2(1%)	19 15
All	All	1101/1116~(99%)	1057 (96%)	32 (3%)	12 (1%)	14 9

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All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	17	VAL
1	А	96	LEU
2	В	345	ASP
1	С	17	VAL
1	С	96	LEU
2	D	345	ASP
2	В	346	PRO
2	В	424	LEU
1	А	41	THR
1	С	41	THR
2	D	346	PRO
1	А	160	THR

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	А	262/263~(100%)	225~(86%)	37~(14%)	3	1
1	С	261/263~(99%)	228~(87%)	33~(13%)	4	2
2	В	232/234~(99%)	211 (91%)	21 (9%)	9	6
2	D	232/234~(99%)	207~(89%)	25 (11%)	6	3
All	All	987/994 (99%)	871 (88%)	116 (12%)	5	2

All (116) residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	А	1[A]	MET
1	А	1[B]	MET



1       A       2       GLU         1       A       5       GLN         1       A       6       LYS         1       A       17       VAL         1       A       22       ARG         1       A       36       ARG         1       A       40       GLU         1       A       40       GLU         1       A       40       GLU         1       A       40       GLU         1       A       55       LEU         1       A       56       LYS         1       A       76       LEU         1       A       86       ASP         1       A       87       LEU         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       158       THR         1       A       159       TYR         1       A       160       THR         1       A <t< th=""><th>Mol</th><th>Chain</th><th>Res</th><th>Type</th></t<>	Mol	Chain	Res	Type
1       A       5       GLN         1       A       17       VAL         1       A       22       ARG         1       A       36       ARG         1       A       40       GLU         1       A       40       GLU         1       A       41       THR         1       A       41       THR         1       A       55       LEU         1       A       74       ASN         1       A       76       LEU         1       A       86       ASP         1       A       86       ASP         1       A       96       LEU         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       158       THR         1       A       160       THR         1       A       163       VAL         1       A	1	А	2	GLU
1       A       6       LYS         1       A       17       VAL         1       A       22       ARG         1       A       36       ARG         1       A       40       GLU         1       A       41       THR         1       A       55       LEU         1       A       56       LYS         1       A       76       LEU         1       A       76       LEU         1       A       83       LEU         1       A       86       ASP         1       A       86       ASP         1       A       96       LEU         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       131       GLN         1       A       159       TYR         1       A       165       THR         1       A	1	А	5	GLN
1       A       17       VAL         1       A       22       ARG         1       A       36       ARG         1       A       40       GLU         1       A       41       THR         1       A       55       LEU         1       A       56       LYS         1       A       74       ASN         1       A       76       LEU         1       A       83       LEU         1       A       86       ASP         1       A       87       LEU         1       A       87       LEU         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       122       ARG         1       A       122       ARG         1       A       122       ARG         1       A       124       LEU         1       A       125       THR         1       A       165       THR         1       A	1	А	6	LYS
1       A       22       ARG         1       A       36       ARG         1       A       40       GLU         1       A       41       THR         1       A       55       LEU         1       A       56       LYS         1       A       74       ASN         1       A       76       LEU         1       A       83       LEU         1       A       86       ASP         1       A       86       ASP         1       A       96       LEU         1       A       97       THR         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       158       THR         1       A       160       THR         1       A       163       VAL         1       A	1	А	17	VAL
1       A       36       ARG         1       A       40       GLU         1       A       41       THR         1       A       55       LEU         1       A       56       LYS         1       A       74       ASN         1       A       76       LEU         1       A       86       ASP         1       A       87       LEU         1       A       86       ASP         1       A       87       LEU         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       158       THR         1       A       159       TYR         1       A       163       VAL         1       A       202       LEU         1       A       230       VAL         1       A       230       VAL         1       A	1	А	22	ARG
1       A       40       GLU         1       A       41       THR         1       A       55       LEU         1       A       56       LYS         1       A       74       ASN         1       A       76       LEU         1       A       83       LEU         1       A       86       ASP         1       A       87       LEU         1       A       96       LEU         1       A       97       THR         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       158       THR         1       A       159       TYR         1       A       163       VAL         1       A       163       VAL         1       A       202       LEU         1       A       203       VAL         1       A       204       SER         1       A	1	А	36	ARG
1       A       41       THR         1       A       55       LEU         1       A       56       LYS         1       A       74       ASN         1       A       76       LEU         1       A       83       LEU         1       A       86       ASP         1       A       86       ASP         1       A       87       LEU         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       131       GLN         1       A       158       THR         1       A       159       TYR         1       A       160       THR         1       A       163       VAL         1       A       202       LEU         1       A       203       VAL         1       A       204       VAL         1       A       232       SER         1       A	1	А	40	GLU
1       A       55       LEU         1       A       56       LYS         1       A       74       ASN         1       A       76       LEU         1       A       83       LEU         1       A       86       ASP         1       A       86       ASP         1       A       87       LEU         1       A       96       LEU         1       A       97       THR         1       A       97       THR         1       A       122       ARG         1       A       122       ARG         1       A       124       LEU         1       A       131       GLN         1       A       158       THR         1       A       160       THR         1       A       163       VAL         1       A       202       LEU         1       A       202       LEU         1       A       202       LEU         1       A       202       LEU         1       A	1	А	41	THR
1       A       56       LYS         1       A       74       ASN         1       A       76       LEU         1       A       83       LEU         1       A       86       ASP         1       A       86       ASP         1       A       87       LEU         1       A       89       LYS         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       158       THR         1       A       159       TYR         1       A       163       VAL         1       A       163       VAL         1       A       202       LEU         1       A       203       VAL         1       A       204       VAL         1       A       226       VAL         1       A       230       VAL         1       A <th>1</th> <th>А</th> <th>55</th> <th>LEU</th>	1	А	55	LEU
1       A       74       ASN         1       A       76       LEU         1       A       83       LEU         1       A       86       ASP         1       A       86       ASP         1       A       87       LEU         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       131       GLN         1       A       158       THR         1       A       159       TYR         1       A       160       THR         1       A       163       VAL         1       A       202       LEU         1       A       202       LEU         1       A       202       LEU         1       A       202       VAL         1       A       230       VAL         1       A       249       SER         1       A </th <th>1</th> <th>А</th> <th>56</th> <th>LYS</th>	1	А	56	LYS
1       A       76       LEU         1       A       83       LEU         1       A       86       ASP         1       A       87       LEU         1       A       87       LEU         1       A       87       LEU         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       158       THR         1       A       159       TYR         1       A       160       THR         1       A       163       VAL         1       A       202       LEU         1       A       230       VAL         1       A       232       SER         1       A </th <th>1</th> <th>А</th> <th>74</th> <th>ASN</th>	1	А	74	ASN
1       A       83       LEU         1       A       86       ASP         1       A       87       LEU         1       A       89       LYS         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       131       GLN         1       A       158       THR         1       A       159       TYR         1       A       160       THR         1       A       163       VAL         1       A       202       LEU         1       A       230       VAL         1       A       230       VAL         1       A       257       GLU         1       A	1	А	76	LEU
1A86ASP1A87LEU1A99LYS1A96LEU1A97THR1A122ARG1A124LEU1A131GLN1A158THR1A159TYR1A160THR1A165THR1A165THR1A202LEU1A230VAL1A230VAL1A252VAL1A257GLU1A257GLU1A291LYS2B177ASP2B178TYR2B207THR2B207THR2B245SER	1	А	83	LEU
1       A       87       LEU         1       A       89       LYS         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       131       GLN         1       A       158       THR         1       A       159       TYR         1       A       160       THR         1       A       163       VAL         1       A       202       LEU         1       A       202       LEU         1       A       203       VAL         1       A       230       VAL         1       A       232       SER         1       A       249       SER         1       A       257       GLU         1       A       257       GLU         1       A       257       GLU         1 <td< td=""><th>1</th><td>А</td><td>86</td><td>ASP</td></td<>	1	А	86	ASP
1       A       89       LYS         1       A       96       LEU         1       A       97       THR         1       A       122       ARG         1       A       124       LEU         1       A       124       LEU         1       A       131       GLN         1       A       158       THR         1       A       159       TYR         1       A       160       THR         1       A       163       VAL         1       A       202       LEU         1       A       202       LEU         1       A       202       LEU         1       A       202       LEU         1       A       202       VAL         1       A       230       VAL         1       A       230       VAL         1       A       232       SER         1       A       257       GLU         1       A       257       GLU         1       A       291       LYS         2 <t< td=""><th>1</th><td>А</td><td>87</td><td>LEU</td></t<>	1	А	87	LEU
1A96LEU1A97THR1A122ARG1A124LEU1A131GLN1A158THR1A159TYR1A160THR1A163VAL1A165THR1A202LEU1A202LEU1A230VAL1A230VAL1A252VAL1A257GLU1A278LYS2B177ASP2B178TYR2B106LYS2B201LYS2B207THR2B245SER	1	А	89	LYS
1A97THR1A122ARG1A124LEU1A131GLN1A158THR1A159TYR1A160THR1A165THR1A165THR1A202LEU1A230VAL1A230VAL1A232SER1A252VAL1A257GLU1A291LYS2B177ASP2B178TYR2B201LYS2B207THR2B207THR2B245SER	1	А	96	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	97	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	122	ARG
1       A       131       GLN         1       A       158       THR         1       A       159       TYR         1       A       160       THR         1       A       160       THR         1       A       163       VAL         1       A       165       THR         1       A       165       THR         1       A       202       LEU         1       A       202       LEU         1       A       202       LEU         1       A       202       VAL         1       A       230       VAL         1       A       230       VAL         1       A       232       SER         1       A       249       SER         1       A       257       GLU         1       A       257       GLU         1       A       291       LYS         2       B       177       ASP         2       B       178       TYR         2       B       196       LYS         2	1	А	124	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	131	GLN
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	158	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	159	TYR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	160	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	163	VAL
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	165	THR
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	202	LEU
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	1	А	226	VAL
1       A       232       SER         1       A       249       SER         1       A       252       VAL         1       A       257       GLU         1       A       257       GLU         1       A       257       GLU         1       A       278       LYS         1       A       291       LYS         2       B       177       ASP         2       B       178       TYR         2       B       196       LYS         2       B       201       LYS         2       B       201       LYS         2       B       207       THR         2       B       245       SER	1	А	230	VAL
1       A       249       SER         1       A       252       VAL         1       A       257       GLU         1       A       257       GLU         1       A       278       LYS         1       A       291       LYS         2       B       177       ASP         2       B       196       LYS         2       B       201       LYS         2       B       207       THR         2       B       245       SER	1	А	232	SER
1       A       252       VAL         1       A       257       GLU         1       A       257       GLU         1       A       278       LYS         1       A       291       LYS         2       B       177       ASP         2       B       178       TYR         2       B       196       LYS         2       B       201       LYS         2       B       201       LYS         2       B       205       SER         2       B       245       SER	1	А	249	SER
1         A         257         GLU           1         A         278         LYS           1         A         291         LYS           2         B         177         ASP           2         B         178         TYR           2         B         196         LYS           2         B         201         LYS           2         B         201         LYS           2         B         201         LYS           2         B         201         LYS           2         B         207         THR           2         B         245         SER	1	А	252	VAL
1         A         278         LYS           1         A         291         LYS           2         B         177         ASP           2         B         178         TYR           2         B         196         LYS           2         B         201         LYS           2         B         201         LYS           2         B         201         LYS           2         B         201         LYS           2         B         205         THR           2         B         245         SER	1	А	257	GLU
1         A         291         LYS           2         B         177         ASP           2         B         178         TYR           2         B         196         LYS           2         B         201         LYS           2         B         201         LYS           2         B         201         LYS           2         B         207         THR           2         B         245         SER	1	А	278	LYS
2         B         177         ASP           2         B         178         TYR           2         B         196         LYS           2         B         201         LYS           2         B         207         THR           2         B         245         SER	1	А	291	LYS
2         B         178         TYR           2         B         196         LYS           2         B         201         LYS           2         B         207         THR           2         B         245         SER	2	В	177	ASP
2         B         196         LYS           2         B         201         LYS           2         B         207         THR           2         B         245         SER	2	В	178	TYR
2         B         201         LYS           2         B         207         THR           2         B         245         SER	2	В	196	LYS
2         B         207         THR           2         B         245         SER	2	В	201	LYS
2 B 245 SER	2	В	207	THR
	2	В	245	SER
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	2	В	249	LEU



Mol	Chain	Res	Type
2	В	284	ASP
2	В	285	THR
2	В	289	LYS
2	В	292	LEU
2	В	293	ARG
2	В	323	GLN
2	В	348	LEU
2	В	364	LEU
2	В	370	GLN
2	В	378	ARG
2	В	391	LEU
2	В	424	LEU
2	В	429	THR
2	В	432	LEU
1	С	2	GLU
1	С	5	GLN
1	С	17	VAL
1	С	22	ARG
1	С	36	ARG
1	С	40	GLU
1	С	41	THR
1	С	55	LEU
1	С	56	LYS
1	С	74	ASN
1	С	86	ASP
1	С	87	LEU
1	С	89	LYS
1	С	96	LEU
1	C	97	THR
1	C	115	LEU
1	С	122	ARG
1	C	124	LEU
1	C	131	GLN
1	С	154	VAL
1	C	159	TYR
1	С	160	THR
1	C	165	THR
1	С	166	LEU
1	C	214	ARG
1	С	217	ARG
1	C	226	VAL
1	С	232	SER



Mol	Chain	Res	Type
1	С	249	SER
1	С	252	VAL
1	С	255	LEU
1	С	278	LYS
1	С	291	LYS
2	D	177	ASP
2	D	178	TYR
2	D	180	GLU
2	D	196	LYS
2	D	197	VAL
2	D	199	TYR
2	D	201	LYS
2	D	207	THR
2	D	232	LEU
2	D	249	LEU
2	D	289	LYS
2	D	292	LEU
2	D	293	ARG
2	D	323	GLN
2	D	348	LEU
2	D	364	LEU
2	D	371	SER
2	D	378	ARG
2	D	391	LEU
2	D	400	LYS
2	D	424	LEU
2	D	428	GLU
2	D	429	THR
2	D	431	ASN
2	D	432	LEU

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

Mol	Chain	Res	Type
1	А	60	HIS
1	А	71	HIS
1	А	84	HIS
1	А	121	HIS
1	А	131	GLN
1	А	246	GLN
2	В	208	ASN
2	В	233	HIS



Mol	Chain	Res	Type
2	В	296	HIS
2	В	322	GLN
2	В	404	HIS
2	В	419	HIS
2	В	431	ASN
1	С	5	GLN
1	С	60	HIS
1	С	84	HIS
1	С	85	GLN
1	С	131	GLN
1	С	246	GLN
1	С	287	GLN
2	D	179	HIS
2	D	208	ASN
2	D	233	HIS
2	D	296	HIS
2	D	322	GLN
2	D	404	HIS
2	D	419	HIS
2	D	431	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



Mal	Turne	Chain	Dec	Tink	Bond lengths			Bond angles		
MOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	CK2	С	1298[A]	-	$10,\!15,\!15$	1.57	3 (30%)	10,21,21	2.67	4 (40%)
3	CK2	А	1297[A]	-	10,15,15	1.57	2 (20%)	10,21,21	2.77	4 (40%)
3	CK2	С	1298[B]	-	10,15,15	1.61	3 (30%)	10,21,21	2.89	4 (40%)
3	CK2	А	1297[B]	-	10,15,15	1.57	3 (30%)	10,21,21	2.74	4 (40%)

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).

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
3	CK2	С	1298[A]	-	-	0/0/4/4	0/2/2/2
3	CK2	А	1297[A]	-	-	0/0/4/4	0/2/2/2
3	CK2	С	1298[B]	-	-	0/0/4/4	0/2/2/2
3	CK2	А	1297[B]	-	-	0/0/4/4	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
3	С	1298[A]	CK2	C2-N7	3.52	1.41	1.33
3	С	1298[B]	CK2	C2-N7	3.48	1.40	1.33
3	А	1297[B]	CK2	C2-N7	3.47	1.40	1.33
3	А	1297[A]	CK2	C2-N7	3.46	1.40	1.33
3	А	1297[A]	CK2	C5-C6	2.26	1.39	1.36
3	С	1298[B]	CK2	C4-N3	-2.23	1.33	1.37
3	А	1297[B]	CK2	C5-C6	2.21	1.39	1.36
3	С	1298[A]	CK2	C5-C6	2.09	1.39	1.36
3	С	1298[B]	CK2	C5-C6	2.09	1.39	1.36
3	С	1298[A]	CK2	C4-N3	-2.04	1.34	1.37
3	A	1297[B]	CK2	C4-N3	-2.03	1.34	1.37

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	С	1298[B]	CK2	C6-N1-C2	5.01	121.36	116.24
3	А	1297[A]	CK2	C6-N1-C2	4.98	121.34	116.24
3	А	1297[B]	CK2	C6-N1-C2	4.83	121.18	116.24



Mol	Chain	$\operatorname{Res}$	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	А	1297[B]	CK2	C5-C6-N1	-4.77	119.11	123.81
3	А	1297[A]	CK2	C5-C6-N1	-4.75	119.13	123.81
3	С	1298[B]	CK2	C5-C6-N1	-4.69	119.19	123.81
3	С	1298[A]	CK2	C5-C6-N1	-4.58	119.30	123.81
3	С	1298[A]	CK2	C6-N1-C2	4.56	120.91	116.24
3	С	1298[B]	CK2	N1-C2-N3	-3.96	120.89	125.70
3	А	1297[A]	CK2	N1-C2-N3	-3.96	120.90	125.70
3	С	1298[A]	CK2	N1-C2-N3	-3.95	120.91	125.70
3	А	1297[B]	CK2	N1-C2-N3	-3.93	120.93	125.70
3	С	1298[B]	CK2	N7-C2-N1	3.68	121.18	117.44
3	А	1297[B]	CK2	N7-C2-N1	2.35	119.82	117.44
3	A	1297[A]	CK2	N7-C2-N1	2.26	119.73	117.44
3	С	1298[A]	CK2	N7-C2-N1	2.06	119.53	117.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	1298[A]	CK2	7	0
3	А	1297[A]	CK2	4	0
3	С	1298[B]	CK2	3	0
3	А	1297[B]	CK2	4	0

### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	< <b>RSRZ</b> >	#RSRZ>2		$OWAB(Å^2)$	Q<0.9	
1	А	296/298~(99%)	-0.17	18 (6%)	21	26	18, 31, 65, 84	1 (0%)
1	С	297/298~(99%)	-0.09	20 (6%)	17	22	18, 31, 65, 85	0
2	В	258/260~(99%)	-0.23	9(3%)	44	50	18, 34, 54, 82	0
2	D	258/260~(99%)	-0.26	5 (1%)	66	71	17, 34, 54, 81	0
All	All	1109/1116 (99%)	-0.18	52 (4%)	31	37	17, 32, 61, 85	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	175	VAL	8.4
2	В	175	VAL	7.4
1	С	39	THR	6.7
1	С	13	GLY	6.4
1	С	15	TYR	5.8
1	С	40	GLU	5.6
1	С	297	ARG	5.3
1	А	15	TYR	5.0
1	С	163	VAL	5.0
1	С	36	ARG	4.8
1	С	96	LEU	4.8
1	А	163	VAL	4.7
1	С	14	THR	4.5
1	А	36	ARG	4.5
2	В	323	GLN	4.4
2	В	176	PRO	4.3
1	А	37	LEU	4.0
1	С	38	ASP	3.9
1	С	41	THR	3.4
1	А	84	HIS	3.3
2	В	271	TYR	3.3



2C5O
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Mol	Chain	Res	Type	RSRZ	
2	В	345	ASP	3.1	
2	D	178	TYR	2.9	
1	А	96	LEU	2.9	
1	С	164	VAL	2.9	
2	В	378	ARG	2.9	
1	С	295	HIS	2.8	
1	А	73	GLU	2.8	
1	А	38	ASP	2.8	
1	С	296	LEU	2.7	
1	А	39	THR	2.6	
1	С	160	THR	2.6	
1	А	295	HIS	2.5	
1	С	37	LEU	2.5	
2	В	178	TYR	2.5	
1	С	206	ASP	2.5	
2	В	179	HIS	2.4	
2	D	179	HIS	2.4	
1	А	287	GLN	2.4	
2	В	280	TYR	2.4	
2	D	323	GLN	2.3	
1	А	159	TYR	2.3	
1	А	160	THR	2.2	
1	С	71	HIS	2.2	
1	А	14	THR	2.2	
1	А	200	ARG	2.2	
2	D	176	PRO	2.2	
1	С	162	GLU	2.0	
1	С	200	ARG	2.0	
1	А	32	LEU	2.0	
1	A	257	GLU	2.0	
1	А	95	ALA	2.0	

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

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

#### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



### 6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	CK2	А	1297[A]	14/14	0.92	0.13	$17,\!27,\!38,\!42$	14
3	CK2	А	1297[B]	14/14	0.92	0.13	$53,\!64,\!76,\!77$	14
3	CK2	С	1298[A]	14/14	0.95	0.14	83,84,85,85	14
3	CK2	С	1298[B]	14/14	0.95	0.14	12,26,42,44	14

#### 6.5 Other polymers (i)

There are no such residues in this entry.

