



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:10 am BST

PDB ID : 3UYT  
Title : crystal structure of ck1d with PF670462 from P1 crystal form  
Authors : Huang, X.  
Deposited on : 2011-12-06  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

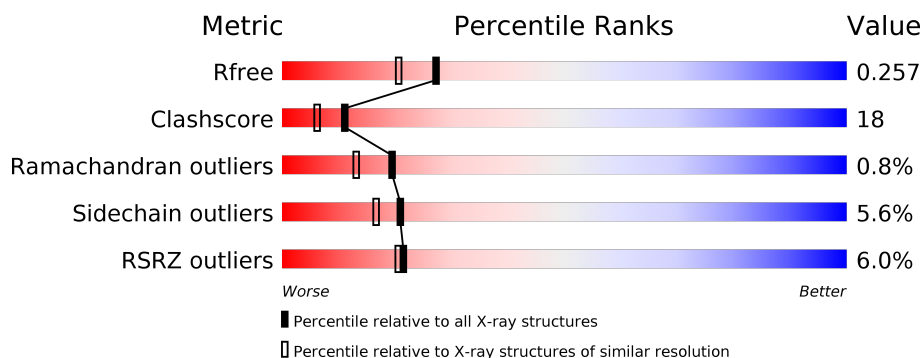
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	296	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>26%</div> <div>• •</div> </div> </div>
1	B	296	<div> <div>8%</div> <div> <div></div> <div>61%</div> <div>30%</div> <div>5%</div> <div>•</div> </div> </div>
1	C	296	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>30%</div> <div>• •</div> </div> </div>
1	D	296	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>24%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10156 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.

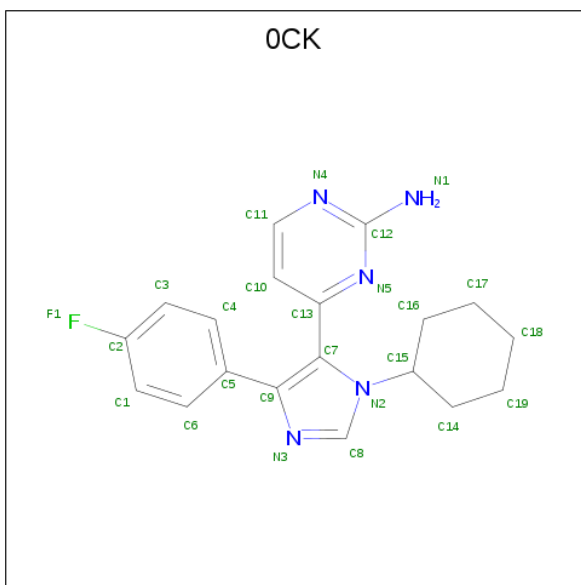
- Molecule 1 is a protein called Casein kinase I isoform delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2315	1485	398	418	14			
1	B	286	Total	C	N	O	S	0	0	0
			2321	1488	403	416	14			
1	C	286	Total	C	N	O	S	0	0	0
			2284	1468	391	411	14			
1	D	268	Total	C	N	O	S	0	0	0
			2161	1393	367	387	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P48730
A	0	SER	-	EXPRESSION TAG	UNP P48730
B	-1	GLY	-	EXPRESSION TAG	UNP P48730
B	0	SER	-	EXPRESSION TAG	UNP P48730
C	-1	GLY	-	EXPRESSION TAG	UNP P48730
C	0	SER	-	EXPRESSION TAG	UNP P48730
D	-1	GLY	-	EXPRESSION TAG	UNP P48730
D	0	SER	-	EXPRESSION TAG	UNP P48730

- Molecule 2 is 4-[1-cyclohexyl-4-(4-fluorophenyl)-1H-imidazol-5-yl]pyrimidin-2-amine (three-letter code: OCK) (formula: C<sub>19</sub>H<sub>20</sub>FN<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	N	0	0
			25	19	1	5		
2	B	1	Total	C	F	N	0	0
			25	19	1	5		
2	C	1	Total	C	F	N	0	0
			25	19	1	5		
2	D	1	Total	C	F	N	0	0
			25	19	1	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

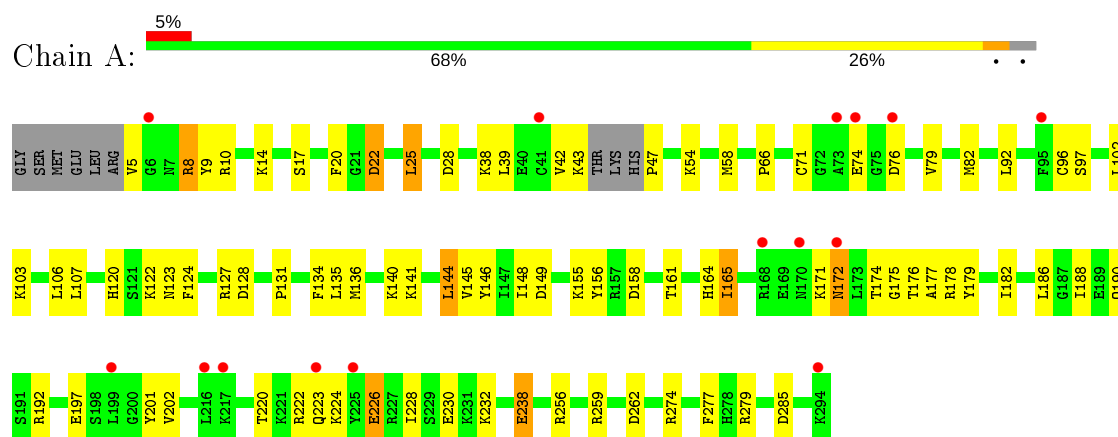
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	251	Total O 251 251	0	0
4	B	225	Total O 225 225	0	0
4	C	236	Total O 236 236	0	0
4	D	228	Total O 228 228	0	0

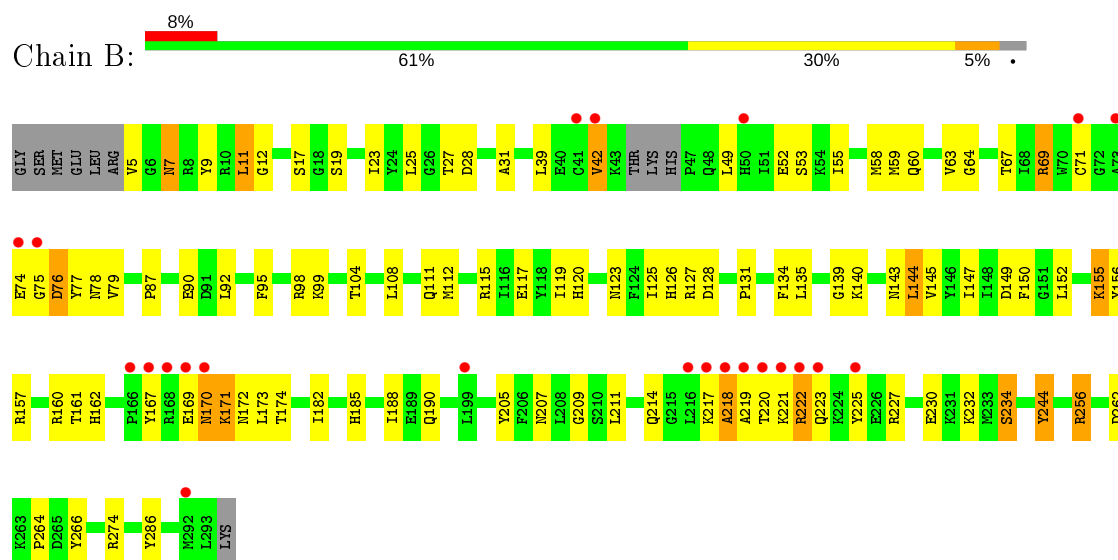
### 3 Residue-property plots

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

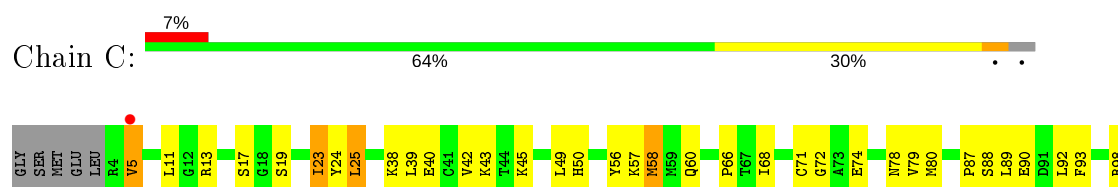
#### • Molecule 1: Casein kinase I isoform delta

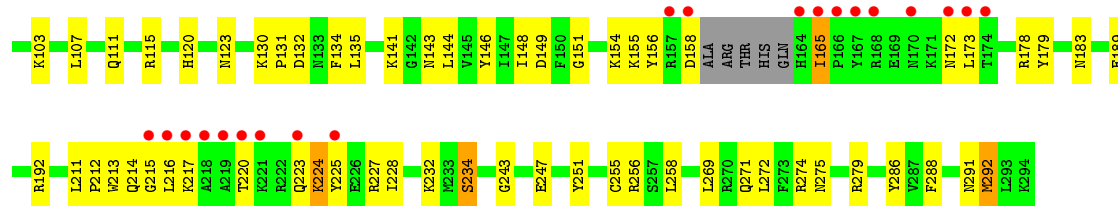


#### • Molecule 1: Casein kinase I isoform delta

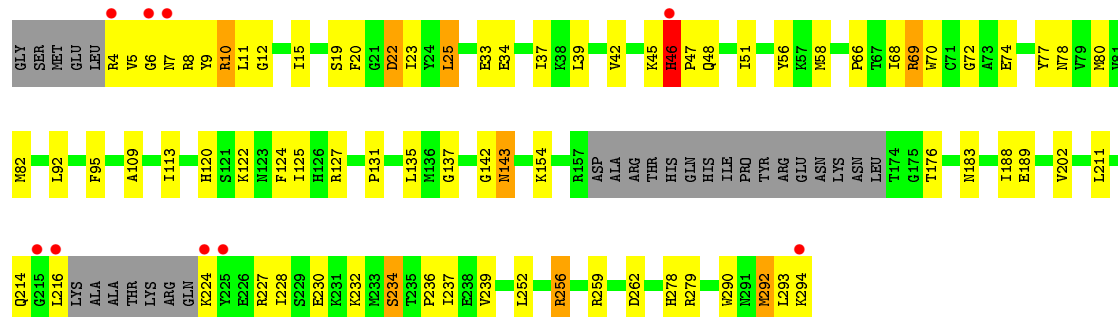


#### • Molecule 1: Casein kinase I isoform delta





● Molecule 1: Casein kinase I isoform delta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.15Å 85.34Å 89.14Å 72.87° 74.36° 87.26°	Depositor
Resolution (Å)	50.00 – 2.00 32.98 – 1.84	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.00) 84.1 (32.98-1.84)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 1.84Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.244 , 0.264 0.239 , 0.257	Depositor DCC
$R_{free}$ test set	4878 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.9	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.074 for h,-k,h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.



## 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: OCK, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.48	0/2368	0.71	0/3186
1	B	0.47	0/2374	0.72	0/3193
1	C	0.46	0/2335	0.70	0/3144
1	D	0.50	1/2210 (0.0%)	0.76	3/2970 (0.1%)
All	All	0.48	1/9287 (0.0%)	0.72	3/12493 (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
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	69	ARG	NE-CZ	-5.47	1.25	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	D	78	ASN	N-CA-C	-6.24	94.16	111.00
1	D	69	ARG	NE-CZ-NH1	5.21	122.90	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	244	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2315	0	2278	75	0
1	B	2321	0	2298	80	0
1	C	2284	0	2242	93	0
1	D	2161	0	2137	80	0
2	A	25	0	20	2	0
2	B	25	0	20	3	0
2	C	25	0	20	0	0
2	D	25	0	20	6	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
3	C	10	0	0	2	0
3	D	10	0	0	0	0
4	A	251	0	0	16	2
4	B	225	0	0	20	0
4	C	236	0	0	23	0
4	D	228	0	0	14	1
All	All	10156	0	9035	328	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (328) 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:D:46:HIS:HB3	1:D:47:PRO:CA	1.78	1.13
1:A:172:ASN:OD1	1:B:170:ASN:HB3	1.56	1.04
1:D:46:HIS:HB3	1:D:47:PRO:HA	1.39	1.04
1:C:156:TYR:HA	1:C:165:ILE:HD13	1.39	1.04
1:D:256:ARG:HD2	4:D:336:HOH:O	1.70	0.92
1:B:170:ASN:HA	4:B:334:HOH:O	1.71	0.89
1:A:140:LYS:HD2	1:A:140:LYS:H	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:HIS:CB	1:D:47:PRO:HA	2.04	0.87
1:B:220:THR:HG23	4:B:1435:HOH:O	1.75	0.85
1:D:46:HIS:HB3	1:D:47:PRO:C	2.00	0.82
1:B:140:LYS:HD2	1:B:140:LYS:H	1.43	0.82
1:A:172:ASN:OD1	1:B:170:ASN:CB	2.28	0.82
1:C:274:ARG:NH2	3:C:296:SO4:O3	2.13	0.81
1:D:46:HIS:CB	1:D:47:PRO:CA	2.59	0.81
1:A:224:LYS:HE2	1:A:228:ILE:HD11	1.63	0.81
1:C:13:ARG:HG3	1:C:13:ARG:HH11	1.46	0.81
1:A:165:ILE:H	1:A:165:ILE:HD13	1.45	0.80
1:A:259:ARG:HD2	4:D:320:HOH:O	1.79	0.80
1:C:68:ILE:HD13	1:C:80:MET:SD	2.23	0.79
1:C:19:SER:HB2	4:C:356:HOH:O	1.84	0.77
1:D:10:ARG:HH11	1:D:10:ARG:HG3	1.50	0.77
1:A:279:ARG:HD3	4:A:479:HOH:O	1.85	0.77
1:B:5:VAL:HG22	1:B:74:GLU:HG3	1.67	0.77
1:C:271:GLN:NE2	1:C:274:ARG:HH11	1.83	0.76
1:D:278:HIS:HB3	4:D:1477:HOH:O	1.85	0.76
1:B:140:LYS:N	1:B:140:LYS:HD2	2.01	0.75
1:B:98:ARG:NH1	1:B:209:GLY:O	2.20	0.74
1:B:119:ILE:HD11	1:B:147:ILE:HD13	1.68	0.74
1:A:161:THR:HG21	4:A:326:HOH:O	1.86	0.74
1:D:279:ARG:HD2	4:D:366:HOH:O	1.87	0.74
1:C:165:ILE:HD12	1:C:189:GLU:OE2	1.87	0.74
1:C:5:VAL:HG13	1:C:74:GLU:HG2	1.69	0.74
1:C:13:ARG:NH1	1:C:13:ARG:HG3	2.02	0.72
1:B:223:GLN:NE2	4:B:1435:HOH:O	2.23	0.71
1:C:272:LEU:HD12	4:C:644:HOH:O	1.90	0.71
1:D:48:GLN:HA	1:D:51:ILE:HD12	1.73	0.70
1:A:20:PHE:O	1:A:38:LYS:HE2	1.92	0.70
1:D:20:PHE:CD2	1:D:48:GLN:HG2	2.26	0.70
1:C:217:LYS:O	1:C:227:ARG:NH1	2.25	0.69
1:B:230:GLU:O	1:B:234:SER:HB2	1.93	0.69
1:C:158:ASP:OD2	4:C:1187:HOH:O	2.11	0.68
1:D:259:ARG:HB2	1:D:262:ASP:OD2	1.93	0.68
1:A:140:LYS:CD	1:A:140:LYS:H	2.07	0.68
1:B:140:LYS:CD	1:B:140:LYS:H	2.07	0.67
1:C:224:LYS:O	1:C:228:ILE:HG13	1.95	0.67
1:D:143:ASN:H	1:D:143:ASN:HD22	1.39	0.67
1:D:11:LEU:HD12	1:D:37:ILE:HD12	1.75	0.67
1:A:174:THR:HA	4:A:583:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:LEU:CD2	1:C:79:VAL:HG22	2.25	0.67
1:B:52:GLU:HG3	1:B:150:PHE:HB2	1.78	0.66
1:D:20:PHE:HD2	1:D:48:GLN:HG2	1.61	0.66
1:B:134:PHE:C	1:B:135:LEU:HD12	2.15	0.66
1:D:22:ASP:OD1	4:D:821:HOH:O	2.14	0.65
1:D:230:GLU:O	1:D:234:SER:HB3	1.94	0.65
1:A:103:LYS:O	1:A:107:LEU:HG	1.96	0.65
1:B:223:GLN:HG2	4:B:1755:HOH:O	1.97	0.65
1:A:178:ARG:HD2	1:A:179:TYR:CZ	2.32	0.64
1:C:141:LYS:HE3	4:C:1176:HOH:O	1.97	0.64
1:B:161:THR:O	1:B:162:HIS:HB2	1.98	0.63
1:C:50:HIS:CB	4:C:851:HOH:O	2.46	0.63
1:D:292:MET:C	1:D:294:LYS:H	2.00	0.63
1:A:165:ILE:N	1:A:165:ILE:HD13	2.13	0.63
1:A:25:LEU:HD23	1:A:25:LEU:O	1.99	0.63
1:B:75:GLY:N	4:B:567:HOH:O	2.31	0.63
1:C:154:LYS:HG2	1:C:155:LYS:N	2.14	0.62
1:A:220:THR:HB	1:A:223:GLN:H	1.62	0.62
1:B:207:ASN:HB3	1:B:244:TYR:CE1	2.34	0.62
1:B:99:LYS:HA	4:B:350:HOH:O	1.98	0.62
1:C:271:GLN:OE1	1:C:275:ASN:ND2	2.32	0.62
1:A:186:LEU:HB2	1:A:188:ILE:HD12	1.82	0.62
1:B:98:ARG:NH2	1:B:205:TYR:OH	2.32	0.62
1:A:165:ILE:H	1:A:165:ILE:CD1	2.12	0.62
1:C:217:LYS:NZ	4:C:1420:HOH:O	2.32	0.62
1:A:8:ARG:NH1	1:A:28:ASP:OD2	2.33	0.61
1:C:214:GLN:HG2	3:C:297:SO4:O1	1.99	0.61
1:C:173:LEU:HD13	1:C:225:TYR:CD2	2.35	0.61
1:D:224:LYS:HA	4:D:498:HOH:O	1.99	0.61
1:B:12:GLY:HA3	4:B:917:HOH:O	2.01	0.60
1:B:90:GLU:HB2	1:B:131:PRO:HB2	1.83	0.60
1:B:71:CYS:SG	4:B:975:HOH:O	2.57	0.60
1:B:219:ALA:HB3	4:B:1435:HOH:O	2.01	0.60
1:D:292:MET:C	1:D:294:LYS:N	2.52	0.60
1:D:256:ARG:HB3	4:D:336:HOH:O	2.01	0.59
1:D:45:LYS:O	1:D:46:HIS:O	2.20	0.59
1:B:119:ILE:CD1	1:B:147:ILE:HD13	2.31	0.59
1:B:171:LYS:HE3	4:B:575:HOH:O	2.03	0.59
1:C:173:LEU:HD23	1:C:173:LEU:C	2.22	0.59
1:A:120:HIS:CG	1:A:192:ARG:HG2	2.38	0.59
1:B:31:ALA:HB1	4:B:562:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:TRP:CZ2	1:D:72:GLY:HA3	2.37	0.58
1:D:33:GLU:OE1	1:D:69:ARG:NH2	2.36	0.58
1:A:42:VAL:O	1:A:43:LYS:CB	2.50	0.58
1:B:5:VAL:HG11	1:B:79:VAL:HG21	1.86	0.58
1:D:23:ILE:HG23	2:D:295:OCK:H20	1.85	0.58
1:B:111:GLN:O	1:B:115:ARG:HG2	2.03	0.57
1:D:68:ILE:HD13	1:D:80:MET:SD	2.43	0.57
1:A:92:LEU:HD11	1:A:136:MET:HG3	1.85	0.57
1:C:5:VAL:HG11	1:C:79:VAL:HG21	1.87	0.57
1:B:220:THR:N	4:B:1435:HOH:O	2.36	0.56
1:D:211:LEU:O	1:D:214:GLN:HB2	2.05	0.56
1:A:141:LYS:HD2	1:A:144:LEU:HD22	1.85	0.56
1:B:49:LEU:HD23	1:B:78:ASN:HB3	1.87	0.56
1:B:117:GLU:HB2	1:B:266:TYR:CD1	2.39	0.56
1:B:222:ARG:HG2	1:B:222:ARG:HH11	1.67	0.56
1:A:134:PHE:HA	1:A:146:TYR:O	2.06	0.56
1:C:292:MET:HG3	4:C:690:HOH:O	2.05	0.56
1:A:279:ARG:CD	4:A:479:HOH:O	2.48	0.55
1:C:111:GLN:O	1:C:115:ARG:HG2	2.06	0.55
1:D:10:ARG:HH11	1:D:10:ARG:CG	2.20	0.55
1:D:4:ARG:CB	1:D:9:TYR:O	2.55	0.55
1:B:217:LYS:O	1:B:218:ALA:HB2	2.06	0.55
1:C:58:MET:CE	4:C:973:HOH:O	2.54	0.55
1:B:211:LEU:O	1:B:214:GLN:HB2	2.07	0.55
1:C:24:TYR:CE1	1:C:39:LEU:HD12	2.41	0.55
1:D:143:ASN:HB3	4:D:517:HOH:O	2.07	0.55
1:C:89:LEU:O	1:C:93:PHE:HB2	2.07	0.55
1:C:292:MET:HE2	4:C:690:HOH:O	2.06	0.54
1:D:15:ILE:HG21	1:D:25:LEU:HD12	1.88	0.54
1:D:109:ALA:O	1:D:113:ILE:HG13	2.07	0.54
1:B:221:LYS:HE3	1:B:225:TYR:OH	2.07	0.54
1:B:120:HIS:ND1	1:B:266:TYR:OH	2.35	0.54
1:B:9:TYR:HA	1:B:27:THR:O	2.08	0.54
1:D:252:LEU:O	1:D:256:ARG:CG	2.55	0.54
1:C:135:LEU:N	1:C:135:LEU:HD12	2.23	0.54
1:A:220:THR:HG22	1:A:222:ARG:H	1.72	0.54
1:D:135:LEU:HD21	2:D:295:OCK:H8	1.89	0.53
1:C:269:LEU:O	1:C:272:LEU:HB2	2.08	0.53
1:D:10:ARG:NH1	1:D:10:ARG:HG3	2.23	0.53
1:D:5:VAL:HG22	1:D:9:TYR:HB2	1.91	0.53
1:D:58:MET:HE1	4:D:521:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ASN:HB2	4:D:384:HOH:O	2.09	0.53
1:A:127:ARG:HA	1:A:190:GLN:HE22	1.73	0.53
1:C:134:PHE:C	1:C:135:LEU:HD12	2.29	0.53
1:A:164:HIS:HD1	1:A:165:ILE:HD13	1.74	0.52
1:A:226:GLU:O	1:A:230:GLU:HG2	2.09	0.52
1:D:120:HIS:HA	1:D:124:PHE:O	2.09	0.52
1:B:262:ASP:O	1:B:264:PRO:HD3	2.09	0.52
1:C:103:LYS:O	1:C:107:LEU:HG	2.09	0.52
1:C:141:LYS:HD2	1:C:144:LEU:HD12	1.91	0.52
1:C:271:GLN:HE21	1:C:274:ARG:HH11	1.56	0.52
1:A:220:THR:OG1	1:A:223:GLN:NE2	2.42	0.52
4:A:345:HOH:O	1:D:188:ILE:HD13	2.09	0.52
1:B:58:MET:CE	4:B:1366:HOH:O	2.57	0.52
1:D:252:LEU:O	1:D:256:ARG:HG3	2.10	0.52
1:A:66:PRO:HG3	1:A:148:ILE:HG22	1.91	0.52
1:C:269:LEU:HD22	4:C:644:HOH:O	2.10	0.52
1:A:10:ARG:NH1	4:A:1055:HOH:O	2.42	0.51
1:A:71:CYS:SG	4:A:354:HOH:O	2.59	0.51
1:D:23:ILE:CG2	2:D:295:OCK:H20	2.40	0.51
1:D:5:VAL:CG2	1:D:9:TYR:HB2	2.40	0.51
1:C:39:LEU:HD23	1:C:79:VAL:HG22	1.89	0.51
1:C:88:SER:HA	1:C:135:LEU:HG	1.92	0.51
1:C:271:GLN:HE21	1:C:274:ARG:NH1	2.07	0.51
1:B:172:ASN:OD1	4:B:702:HOH:O	2.19	0.51
1:B:42:VAL:HG22	1:B:78:ASN:ND2	2.25	0.51
1:B:87:PRO:HB2	1:B:92:LEU:HG	1.92	0.51
1:D:20:PHE:CD1	1:D:20:PHE:N	2.77	0.51
1:B:63:VAL:HG12	1:B:144:LEU:HD21	1.91	0.51
1:C:13:ARG:HH11	1:C:13:ARG:CG	2.18	0.51
1:C:143:ASN:HB2	1:C:286:TYR:HB3	1.93	0.51
1:C:66:PRO:HG3	1:C:148:ILE:HG22	1.91	0.51
1:B:274:ARG:HD2	4:B:941:HOH:O	2.11	0.51
1:C:256:ARG:NH1	4:C:332:HOH:O	2.32	0.50
1:A:96:CYS:O	1:A:97:SER:HB2	2.11	0.50
1:D:228:ILE:O	1:D:232:LYS:HB2	2.10	0.50
1:D:237:ILE:HD11	1:D:256:ARG:CZ	2.41	0.50
1:C:288:PHE:O	1:C:291:ASN:HB2	2.12	0.50
1:D:10:ARG:NH1	1:D:10:ARG:CG	2.75	0.50
1:A:39:LEU:CD2	1:A:79:VAL:HG13	2.42	0.49
1:A:128:ASP:OD2	4:A:303:HOH:O	2.17	0.49
1:D:56:TYR:HE1	1:D:66:PRO:HG2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:GLU:HB2	4:A:374:HOH:O	2.11	0.49
1:C:215:GLY:O	1:C:216:LEU:C	2.50	0.49
1:C:56:TYR:CD2	1:C:68:ILE:HD11	2.47	0.49
1:C:251:TYR:HD2	4:C:644:HOH:O	1.94	0.49
1:D:92:LEU:HD13	1:D:290:TRP:CE2	2.47	0.49
1:A:171:LYS:NZ	3:A:297:SO4:O2	2.42	0.49
1:C:93:PHE:O	1:C:98:ARG:N	2.43	0.49
1:D:19:SER:HA	4:D:1149:HOH:O	2.13	0.49
1:A:14:LYS:CB	4:A:392:HOH:O	2.60	0.49
1:A:39:LEU:HD23	1:A:79:VAL:HG13	1.95	0.49
1:D:68:ILE:CD1	1:D:80:MET:SD	3.00	0.49
1:B:123:ASN:O	1:B:155:LYS:HG3	2.13	0.49
1:B:143:ASN:HB2	1:B:286:TYR:CG	2.48	0.49
1:D:137:GLY:O	1:D:142:GLY:HA2	2.12	0.49
1:D:20:PHE:HD2	1:D:48:GLN:CG	2.24	0.48
1:C:243:GLY:C	4:C:607:HOH:O	2.52	0.48
1:C:247:GLU:OE2	1:C:279:ARG:NH2	2.46	0.48
1:C:151:GLY:HA3	4:C:356:HOH:O	2.14	0.48
1:A:197:GLU:HG2	1:A:201:TYR:CE2	2.48	0.48
1:D:127:ARG:NH1	1:D:154:LYS:HD3	2.29	0.48
1:B:69:ARG:HH11	1:B:69:ARG:HG3	1.78	0.48
1:C:271:GLN:NE2	1:C:274:ARG:NH1	2.55	0.48
1:A:224:LYS:O	1:A:228:ILE:HG13	2.12	0.48
1:A:164:HIS:ND1	1:A:165:ILE:HD13	2.29	0.48
1:A:20:PHE:O	1:A:38:LYS:CE	2.61	0.48
1:C:255:CYS:HA	1:C:258:LEU:HD12	1.96	0.47
1:D:58:MET:CE	4:D:521:HOH:O	2.62	0.47
1:C:255:CYS:HA	1:C:258:LEU:CD1	2.44	0.47
1:B:167:TYR:OH	1:B:188:ILE:HD12	2.15	0.47
1:C:23:ILE:HD12	1:C:38:LYS:HG3	1.96	0.47
1:C:72:GLY:O	1:C:79:VAL:N	2.40	0.47
1:A:238:GLU:HG2	4:A:306:HOH:O	2.15	0.47
1:C:132:ASP:OD1	4:C:350:HOH:O	2.20	0.47
1:A:156:TYR:HA	1:A:165:ILE:HD12	1.95	0.47
1:B:135:LEU:N	1:B:135:LEU:HD12	2.29	0.47
1:D:39:LEU:HB3	1:D:77:TYR:CD2	2.50	0.47
1:B:127:ARG:HG2	1:B:190:GLN:NE2	2.30	0.47
1:D:56:TYR:CE1	1:D:66:PRO:HG2	2.50	0.47
1:C:45:LYS:HA	4:C:1255:HOH:O	2.15	0.47
1:B:125:ILE:HG23	1:B:156:TYR:CD2	2.50	0.46
1:B:112:MET:HG2	1:B:134:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ASN:HB2	1:B:286:TYR:CB	2.44	0.46
1:C:211:LEU:O	1:C:214:GLN:HB2	2.15	0.46
1:A:66:PRO:HB2	1:A:82:MET:SD	2.55	0.46
1:C:224:LYS:HG2	1:C:225:TYR:HD1	1.81	0.46
1:A:285:ASP:HB3	4:A:704:HOH:O	2.15	0.46
1:C:143:ASN:HB3	4:C:716:HOH:O	2.16	0.46
1:C:120:HIS:CG	1:C:192:ARG:HG2	2.50	0.46
1:A:182:ILE:HD12	1:A:256:ARG:HD3	1.97	0.46
1:C:42:VAL:HG12	1:C:43:LYS:N	2.30	0.46
1:B:223:GLN:CD	4:B:1435:HOH:O	2.53	0.46
1:A:158:ASP:HB3	1:A:161:THR:OG1	2.16	0.46
1:A:71:CYS:HA	1:A:79:VAL:O	2.15	0.46
2:B:295:OCK:H19	4:B:320:HOH:O	2.16	0.46
1:C:173:LEU:HD22	1:C:225:TYR:HE2	1.80	0.46
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.52	0.46
1:D:6:GLY:O	1:D:7:ASN:HB3	2.16	0.46
1:A:177:ALA:O	1:A:232:LYS:NZ	2.47	0.45
1:C:213:TRP:CE2	1:C:232:LYS:HE2	2.51	0.45
1:A:82:MET:HG2	2:A:295:OCK:C1	2.46	0.45
1:C:234:SER:OG	4:C:1038:HOH:O	2.20	0.45
1:A:123:ASN:O	1:A:155:LYS:HA	2.17	0.45
1:A:178:ARG:HD2	1:A:179:TYR:CE1	2.51	0.45
1:B:169:GLU:O	1:B:171:LYS:N	2.49	0.45
1:C:155:LYS:CE	4:C:973:HOH:O	2.64	0.45
1:B:104:THR:O	1:B:108:LEU:HG	2.17	0.45
1:B:217:LYS:O	1:B:227:ARG:NH1	2.48	0.45
1:D:252:LEU:O	1:D:256:ARG:HG2	2.15	0.45
1:A:92:LEU:CD1	1:A:136:MET:HG3	2.46	0.45
1:A:92:LEU:HD11	1:A:136:MET:CG	2.46	0.45
1:C:130:LYS:HE3	1:C:132:ASP:HB2	1.98	0.45
1:B:256:ARG:HB3	4:B:1124:HOH:O	2.17	0.45
1:D:12:GLY:N	1:D:25:LEU:O	2.50	0.45
1:D:5:VAL:HG12	1:D:74:GLU:OE1	2.17	0.45
1:A:238:GLU:CG	4:A:306:HOH:O	2.65	0.44
1:B:123:ASN:OD1	1:B:157:ARG:NE	2.46	0.44
1:B:63:VAL:CG1	1:B:144:LEU:HD21	2.47	0.44
1:D:95:PHE:CE2	1:D:293:LEU:HD13	2.51	0.44
1:D:22:ASP:OD1	1:D:22:ASP:N	2.49	0.44
1:B:64:GLY:HA3	1:B:115:ARG:NE	2.32	0.44
1:C:90:GLU:HB2	1:C:131:PRO:HB2	1.98	0.44
1:C:123:ASN:HA	1:C:156:TYR:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LYS:O	1:A:124:PHE:HD1	2.00	0.44
1:B:5:VAL:HG22	1:B:74:GLU:CG	2.43	0.44
1:A:259:ARG:HB2	1:A:262:ASP:CG	2.38	0.44
1:D:10:ARG:HB2	1:D:10:ARG:CZ	2.47	0.44
1:A:175:GLY:N	4:A:583:HOH:O	2.50	0.43
1:A:82:MET:SD	2:A:295:OCK:H2	2.58	0.43
1:B:128:ASP:HB2	1:B:152:LEU:HD12	1.99	0.43
1:C:38:LYS:HD3	1:C:49:LEU:HD11	1.99	0.43
1:D:122:LYS:HA	1:D:122:LYS:HD3	1.86	0.43
1:D:15:ILE:CG2	1:D:25:LEU:HD12	2.49	0.43
1:A:136:MET:SD	1:A:145:VAL:HG22	2.58	0.43
1:C:42:VAL:HG12	1:C:43:LYS:HG3	2.01	0.43
1:A:5:VAL:HG22	1:A:9:TYR:HB2	2.00	0.43
1:A:39:LEU:CD2	1:A:79:VAL:HG22	2.47	0.43
1:C:154:LYS:HE3	4:C:1247:HOH:O	2.18	0.43
1:D:183:ASN:ND2	4:D:384:HOH:O	2.46	0.43
1:B:76:ASP:O	1:B:77:TYR:CG	2.71	0.43
1:C:5:VAL:HG13	1:C:74:GLU:CG	2.43	0.43
1:D:131:PRO:HG3	1:D:202:VAL:HG13	2.01	0.43
1:D:236:PRO:HG2	1:D:239:VAL:HG23	2.01	0.43
1:C:183:ASN:ND2	4:C:332:HOH:O	2.52	0.43
1:B:111:GLN:NE2	1:B:145:VAL:HG23	2.33	0.43
1:B:58:MET:HE1	4:B:1366:HOH:O	2.19	0.43
1:C:71:CYS:HA	1:C:79:VAL:O	2.19	0.43
1:B:28:ASP:OD1	1:B:28:ASP:C	2.58	0.42
1:C:178:ARG:HD2	1:C:179:TYR:CZ	2.54	0.42
1:D:23:ILE:HG13	2:D:295:OCK:C8	2.49	0.42
1:A:54:LYS:HD3	1:A:54:LYS:HA	1.74	0.42
1:B:182:ILE:HD12	1:B:256:ARG:CZ	2.49	0.42
1:C:178:ARG:O	1:C:213:TRP:NE1	2.46	0.42
1:C:58:MET:HE1	4:C:973:HOH:O	2.15	0.42
1:D:227:ARG:HG3	4:D:498:HOH:O	2.19	0.42
1:B:25:LEU:HD23	1:B:25:LEU:C	2.40	0.42
1:C:154:LYS:HE2	1:C:189:GLU:OE2	2.18	0.42
1:D:216:LEU:C	1:D:227:ARG:HH21	2.23	0.42
1:A:156:TYR:O	1:A:165:ILE:HD12	2.19	0.42
1:D:292:MET:O	1:D:294:LYS:N	2.52	0.42
1:A:22:ASP:O	1:A:38:LYS:HA	2.18	0.42
1:C:156:TYR:HA	1:C:165:ILE:CD1	2.28	0.42
1:C:87:PRO:HB2	1:C:92:LEU:HG	2.01	0.42
1:C:40:GLU:HB3	1:C:78:ASN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ILE:HG13	2:D:295:0CK:N3	2.35	0.42
1:A:176:THR:HG22	4:A:612:HOH:O	2.20	0.42
1:B:256:ARG:HD2	4:B:1124:HOH:O	2.19	0.42
1:B:225:TYR:N	1:B:225:TYR:CD1	2.88	0.41
1:B:23:ILE:HG13	2:B:295:0CK:C8	2.49	0.41
1:C:134:PHE:HA	1:C:146:TYR:O	2.20	0.41
1:D:143:ASN:ND2	1:D:143:ASN:H	2.12	0.41
1:A:47:PRO:CD	4:A:580:HOH:O	2.68	0.41
2:B:295:0CK:H8	2:B:295:0CK:N5	2.35	0.41
1:C:68:ILE:CD1	1:C:80:MET:SD	3.02	0.41
1:B:126:HIS:O	1:B:127:ARG:HB2	2.21	0.41
1:B:217:LYS:O	1:B:218:ALA:CB	2.68	0.41
1:C:220:THR:OG1	1:C:223:GLN:N	2.45	0.41
1:C:224:LYS:HE2	1:C:228:ILE:HD11	2.02	0.41
1:B:55:ILE:O	1:B:59:MET:HG2	2.21	0.41
1:C:23:ILE:N	1:C:23:ILE:CD1	2.83	0.41
1:B:5:VAL:CG1	1:B:79:VAL:HG21	2.51	0.41
1:B:185:HIS:CD2	1:B:232:LYS:HD2	2.56	0.41
1:B:39:LEU:HD23	1:B:79:VAL:HB	2.01	0.41
1:B:5:VAL:HG21	1:B:11:LEU:HD13	2.03	0.41
1:D:95:PHE:CD2	1:D:293:LEU:HD13	2.56	0.41
1:A:135:LEU:N	1:A:135:LEU:HD12	2.36	0.40
1:A:131:PRO:HG3	1:A:202:VAL:HG13	2.03	0.40
1:C:223:GLN:O	1:C:227:ARG:HG3	2.22	0.40
1:C:57:LYS:O	1:C:60:GLN:HB2	2.21	0.40
1:D:66:PRO:HB2	1:D:82:MET:CE	2.51	0.40
1:A:274:ARG:O	1:A:277:PHE:HB3	2.21	0.40
1:C:212:PRO:HG2	1:C:213:TRP:CE3	2.57	0.40
1:D:66:PRO:HB2	1:D:82:MET:HE2	2.04	0.40
1:C:183:ASN:ND2	4:C:437:HOH:O	2.26	0.40
1:D:236:PRO:HG2	1:D:239:VAL:CG2	2.51	0.40
1:D:23:ILE:HD12	2:D:295:0CK:C6	2.51	0.40
1:A:102:LEU:O	1:A:106:LEU:HG	2.22	0.40
1:A:54:LYS:O	1:A:58:MET:HG3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:805:HOH:O	4:D:327:HOH:O[1_455]	2.08	0.12
4:A:1015:HOH:O	4:A:1134:HOH:O[1_455]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/296 (96%)	277 (98%)	5 (2%)	1 (0%)	34	30
1	B	282/296 (95%)	264 (94%)	12 (4%)	6 (2%)	7	2
1	C	282/296 (95%)	266 (94%)	15 (5%)	1 (0%)	34	30
1	D	262/296 (88%)	251 (96%)	10 (4%)	1 (0%)	34	30
All	All	1109/1184 (94%)	1058 (95%)	42 (4%)	9 (1%)	19	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	170	ASN
1	B	218	ALA
1	D	46	HIS
1	B	139	GLY
1	B	7	ASN
1	B	149	ASP
1	C	149	ASP
1	A	149	ASP
1	B	42	VAL

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/259 (95%)	235 (96%)	10 (4%)	30	28
1	B	247/259 (95%)	228 (92%)	19 (8%)	13	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	239/259 (92%)	228 (95%)	11 (5%)	27	23
1	D	230/259 (89%)	216 (94%)	14 (6%)	18	14
All	All	961/1036 (93%)	907 (94%)	54 (6%)	21	17

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	17	SER
1	A	22	ASP
1	A	25	LEU
1	A	76	ASP
1	A	144	LEU
1	A	165	ILE
1	A	172	ASN
1	A	226	GLU
1	A	238	GLU
1	B	7	ASN
1	B	11	LEU
1	B	17	SER
1	B	19	SER
1	B	53	SER
1	B	60	GLN
1	B	67	THR
1	B	69	ARG
1	B	76	ASP
1	B	95	PHE
1	B	144	LEU
1	B	155	LYS
1	B	160	ARG
1	B	171	LYS
1	B	173	LEU
1	B	174	THR
1	B	222	ARG
1	B	234	SER
1	B	256	ARG
1	C	5	VAL
1	C	11	LEU
1	C	17	SER
1	C	23	ILE
1	C	25	LEU

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Mol	Chain	Res	Type
1	C	58	MET
1	C	165	ILE
1	C	172	ASN
1	C	224	LYS
1	C	234	SER
1	C	292	MET
1	D	8	ARG
1	D	10	ARG
1	D	22	ASP
1	D	25	LEU
1	D	34	GLU
1	D	42	VAL
1	D	46	HIS
1	D	125	ILE
1	D	143	ASN
1	D	176	THR
1	D	189	GLU
1	D	234	SER
1	D	256	ARG
1	D	292	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	190	GLN
1	A	223	GLN
1	A	271	GLN
1	A	280	GLN
1	B	7	ASN
1	B	78	ASN
1	B	162	HIS
1	B	190	GLN
1	B	223	GLN
1	C	78	ASN
1	C	172	ASN
1	C	190	GLN
1	C	271	GLN
1	C	275	ASN
1	D	46	HIS
1	D	143	ASN
1	D	275	ASN

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Mol	Chain	Res	Type
1	D	280	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	SO4	D	297	-	4,4,4	0.42	0	6,6,6	0.36	0
3	SO4	C	297	-	4,4,4	0.71	0	6,6,6	0.67	0
3	SO4	D	296	-	4,4,4	0.70	0	6,6,6	1.12	1 (16%)
3	SO4	B	296	-	4,4,4	0.54	0	6,6,6	1.30	0
2	OCK	B	295	-	24,28,28	3.11	15 (62%)	29,39,39	3.33	11 (37%)
2	OCK	A	295	-	24,28,28	3.08	14 (58%)	29,39,39	2.24	9 (31%)
2	OCK	D	295	-	24,28,28	2.78	11 (45%)	29,39,39	2.24	12 (41%)
2	OCK	C	295	-	24,28,28	2.69	11 (45%)	29,39,39	2.50	10 (34%)
3	SO4	C	296	-	4,4,4	0.38	0	6,6,6	0.69	0
3	SO4	A	296	-	4,4,4	0.51	0	6,6,6	0.50	0
3	SO4	A	297	-	4,4,4	0.49	0	6,6,6	1.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0CK	B	295	-	-	2/5/20/20	0/4/4/4
2	0CK	A	295	-	-	2/5/20/20	0/4/4/4
2	0CK	D	295	-	-	2/5/20/20	0/4/4/4
2	0CK	C	295	-	-	2/5/20/20	0/4/4/4

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	295	0CK	C3-C2	5.98	1.48	1.37
2	A	295	0CK	C13-N5	5.92	1.43	1.34
2	D	295	0CK	C3-C2	5.59	1.48	1.37
2	C	295	0CK	C3-C2	5.33	1.47	1.37
2	A	295	0CK	C3-C2	5.27	1.47	1.37
2	B	295	0CK	C6-C5	5.03	1.50	1.39
2	B	295	0CK	C1-C2	4.93	1.46	1.37
2	A	295	0CK	C4-C3	4.83	1.47	1.38
2	D	295	0CK	C5-C9	4.71	1.54	1.49
2	A	295	0CK	C1-C2	4.61	1.46	1.37
2	C	295	0CK	C6-C5	4.60	1.49	1.39
2	B	295	0CK	C13-N5	4.58	1.41	1.34
2	B	295	0CK	C6-C1	4.52	1.47	1.38
2	B	295	0CK	C4-C3	4.42	1.46	1.38
2	D	295	0CK	C4-C3	4.37	1.46	1.38
2	A	295	0CK	C6-C1	4.35	1.46	1.38
2	D	295	0CK	C6-C1	4.29	1.46	1.38
2	A	295	0CK	C6-C5	4.23	1.48	1.39
2	B	295	0CK	C7-C13	4.20	1.56	1.49
2	D	295	0CK	C6-C5	4.18	1.48	1.39
2	D	295	0CK	C13-N5	4.13	1.41	1.34
2	C	295	0CK	C12-N4	4.13	1.41	1.35
2	C	295	0CK	C10-C13	4.02	1.48	1.38
2	C	295	0CK	C1-C2	3.99	1.44	1.37
2	D	295	0CK	C1-C2	3.86	1.44	1.37
2	C	295	0CK	C4-C3	3.82	1.45	1.38
2	A	295	0CK	C7-C9	3.72	1.52	1.43
2	A	295	0CK	C4-C5	3.69	1.47	1.39
2	B	295	0CK	C10-C13	3.54	1.47	1.38
2	B	295	0CK	C12-N4	3.50	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	295	0CK	C12-N4	3.38	1.40	1.35
2	C	295	0CK	C6-C1	3.37	1.44	1.38
2	D	295	0CK	C10-C13	3.34	1.46	1.38
2	C	295	0CK	C13-N5	3.33	1.40	1.34
2	D	295	0CK	C7-C9	3.32	1.51	1.43
2	A	295	0CK	C10-C13	3.29	1.46	1.38
2	A	295	0CK	C7-C13	3.09	1.54	1.49
2	B	295	0CK	C7-C9	3.01	1.50	1.43
2	B	295	0CK	C4-C5	2.88	1.45	1.39
2	A	295	0CK	C5-C9	2.85	1.52	1.49
2	B	295	0CK	C10-C11	2.82	1.44	1.38
2	C	295	0CK	C5-C9	2.75	1.52	1.49
2	D	295	0CK	C4-C5	2.70	1.45	1.39
2	C	295	0CK	C10-C11	2.62	1.43	1.38
2	C	295	0CK	C7-C9	2.51	1.49	1.43
2	D	295	0CK	C12-N4	2.50	1.39	1.35
2	B	295	0CK	C12-N5	2.37	1.39	1.35
2	A	295	0CK	C11-N4	2.32	1.39	1.34
2	B	295	0CK	C11-N4	2.28	1.39	1.34
2	A	295	0CK	C10-C11	2.12	1.42	1.38
2	B	295	0CK	C5-C9	2.08	1.51	1.49

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	295	0CK	C13-N5-C12	9.72	121.88	116.34
2	B	295	0CK	C9-C7-N2	-9.58	103.16	108.14
2	C	295	0CK	C9-C7-N2	-6.49	104.76	108.14
2	C	295	0CK	C13-N5-C12	6.45	120.02	116.34
2	A	295	0CK	C13-N5-C12	6.38	119.98	116.34
2	D	295	0CK	C13-N5-C12	5.11	119.25	116.34
2	D	295	0CK	C11-N4-C12	4.99	121.35	116.24
2	B	295	0CK	C16-C15-C14	4.87	119.46	110.16
2	B	295	0CK	C10-C13-N5	-4.78	115.78	121.97
2	A	295	0CK	C9-C7-N2	-4.77	105.66	108.14
2	C	295	0CK	C10-C11-N4	-4.30	118.62	123.96
2	D	295	0CK	C10-C11-N4	-4.13	118.83	123.96
2	C	295	0CK	C11-N4-C12	4.06	120.40	116.24
2	B	295	0CK	C11-C10-C13	4.02	121.01	117.22
2	A	295	0CK	C10-C13-N5	-3.76	117.10	121.97
2	B	295	0CK	C10-C11-N4	-3.40	119.74	123.96
2	B	295	0CK	C7-C13-N5	3.31	121.27	115.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	295	0CK	C11-C10-C13	3.30	120.33	117.22
2	C	295	0CK	C11-C10-C13	3.17	120.22	117.22
2	C	295	0CK	C10-C13-N5	-3.16	117.87	121.97
2	D	295	0CK	C7-C13-N5	3.15	121.00	115.62
2	B	295	0CK	C11-N4-C12	3.10	119.41	116.24
2	A	295	0CK	C11-N4-C12	3.09	119.40	116.24
2	A	295	0CK	C10-C11-N4	-3.06	120.16	123.96
2	D	295	0CK	C10-C13-N5	-3.02	118.06	121.97
2	B	295	0CK	N1-C12-N4	2.96	120.44	117.44
2	B	295	0CK	N4-C12-N5	-2.89	122.17	125.70
2	D	295	0CK	C11-C10-C13	2.83	119.89	117.22
2	A	295	0CK	C7-C13-N5	2.83	120.45	115.62
2	D	295	0CK	C17-C16-C15	2.77	115.67	111.57
2	C	295	0CK	C16-C15-C14	2.70	115.32	110.16
2	A	295	0CK	C7-N2-C15	2.68	132.04	126.72
2	D	295	0CK	N4-C12-N5	-2.53	122.62	125.70
2	C	295	0CK	C7-C13-N5	2.50	119.90	115.62
2	B	295	0CK	C17-C16-C15	2.45	115.20	111.57
2	C	295	0CK	N4-C12-N5	-2.31	122.88	125.70
2	D	295	0CK	C7-N2-C15	2.30	131.28	126.72
2	C	295	0CK	C17-C16-C15	2.29	114.97	111.57
2	D	295	0CK	F1-C2-C3	2.25	122.37	118.54
3	D	296	SO4	O4-S-O3	2.20	118.46	109.06
2	A	295	0CK	N4-C12-N5	-2.19	123.03	125.70
2	D	295	0CK	C6-C1-C2	-2.11	116.18	118.36
2	D	295	0CK	F1-C2-C1	-2.08	115.00	118.54

There are no chirality outliers.

All (8) torsion outliers are listed below:

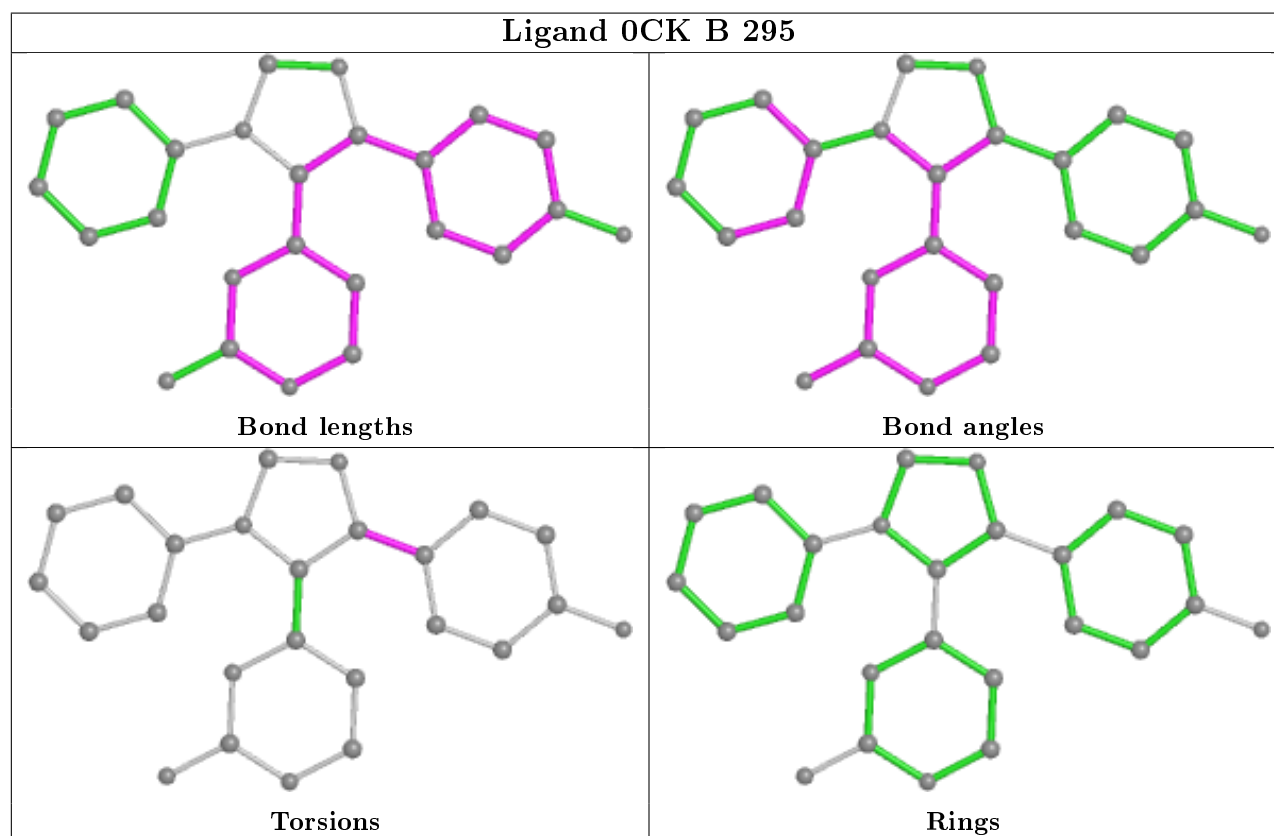
Mol	Chain	Res	Type	Atoms
2	D	295	0CK	C6-C5-C9-N3
2	C	295	0CK	C4-C5-C9-N3
2	C	295	0CK	C6-C5-C9-N3
2	D	295	0CK	C4-C5-C9-N3
2	B	295	0CK	C4-C5-C9-N3
2	A	295	0CK	C4-C5-C9-N3
2	A	295	0CK	C6-C5-C9-N3
2	B	295	0CK	C6-C5-C9-N3

There are no ring outliers.

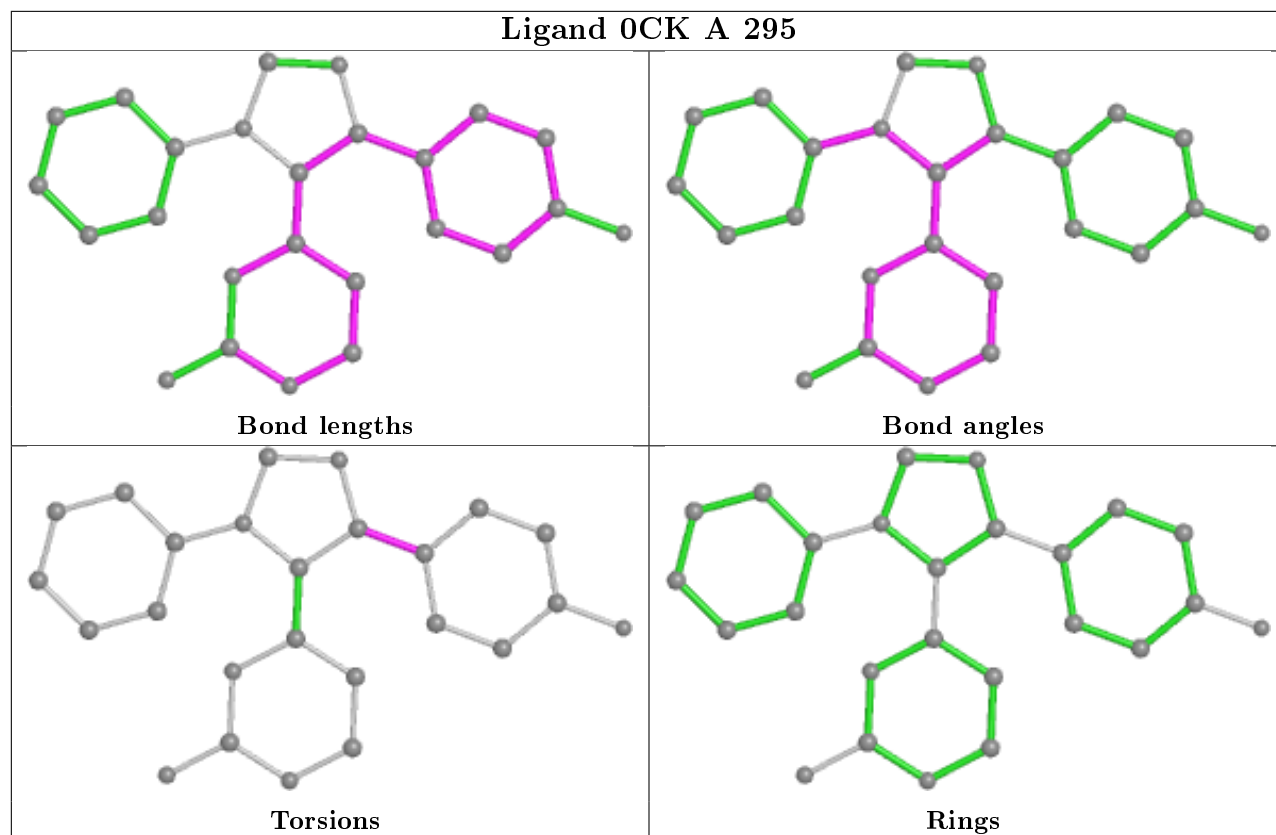
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	297	SO4	1	0
2	B	295	OCK	3	0
2	A	295	OCK	2	0
2	D	295	OCK	6	0
3	C	296	SO4	1	0
3	A	297	SO4	1	0

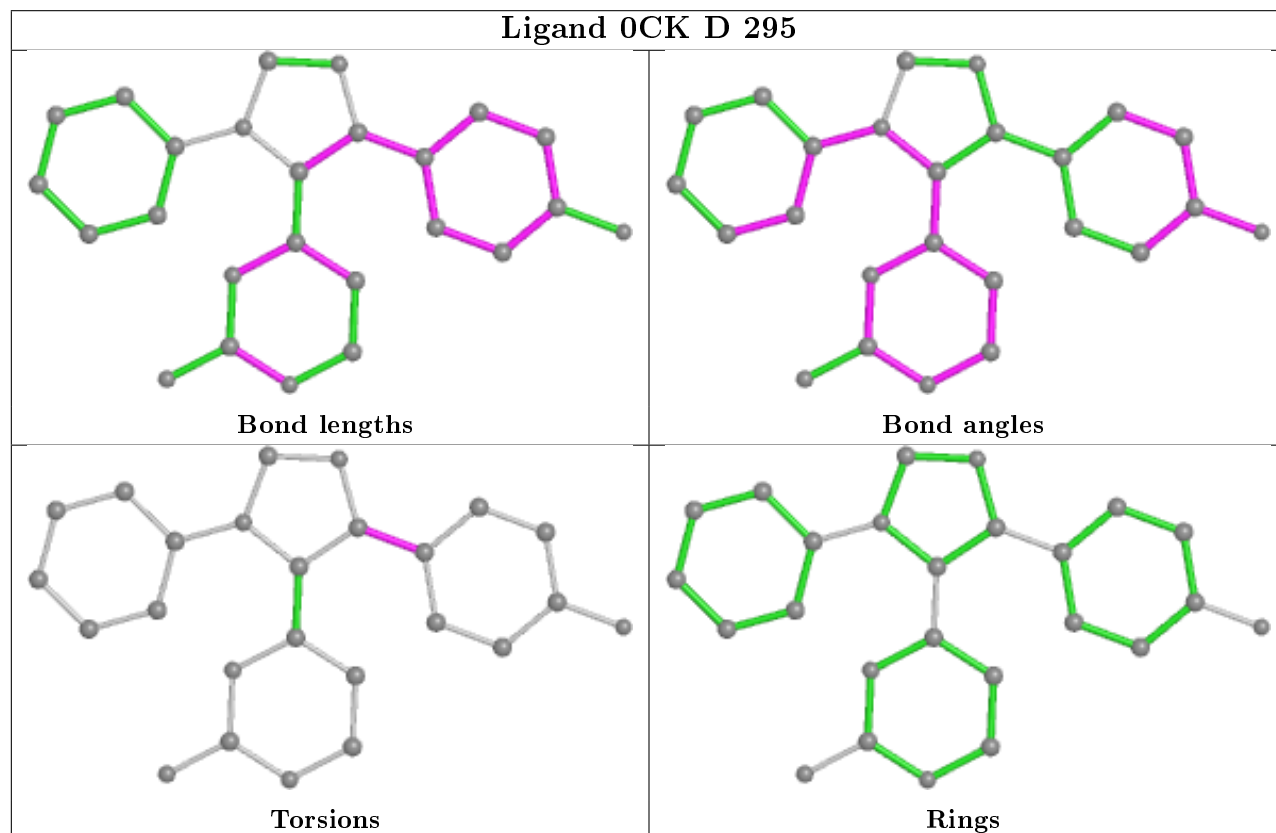
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

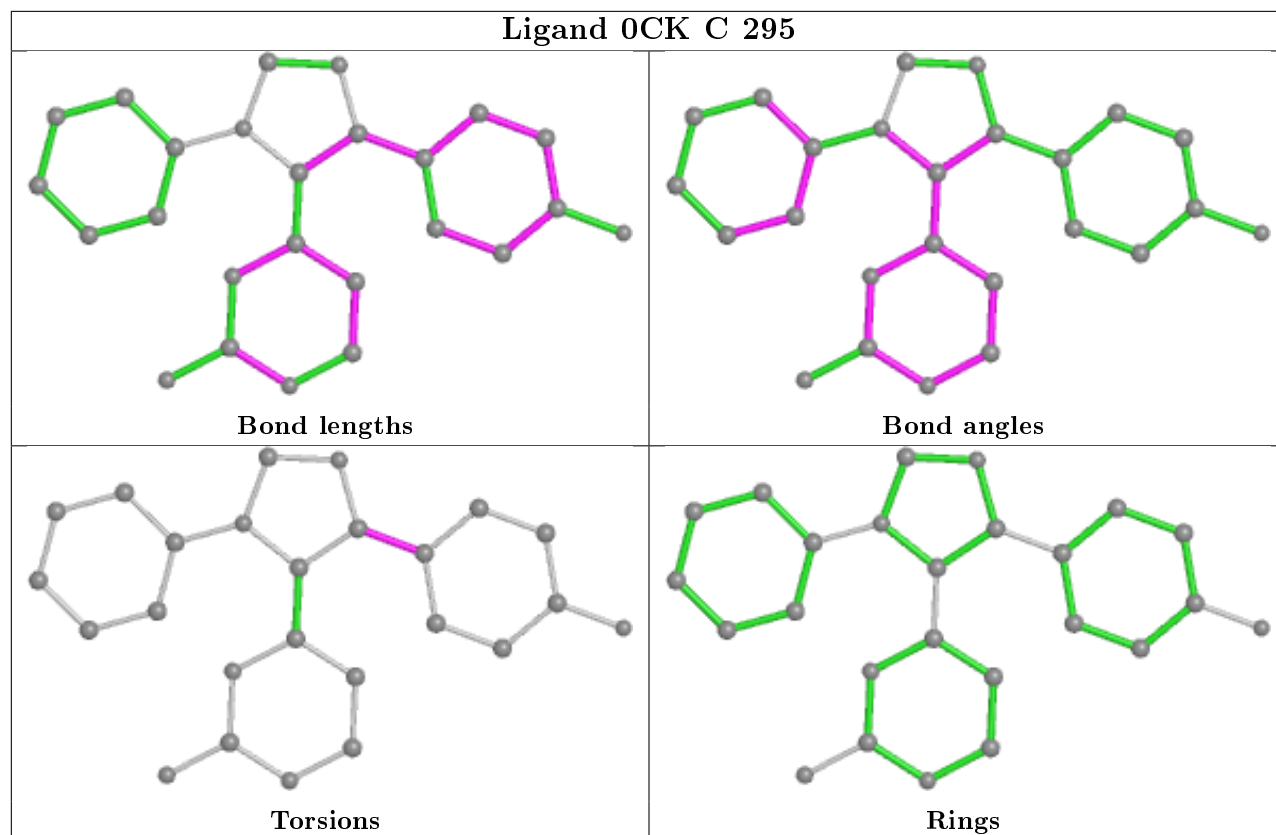


## Ligand 0CK A 295



## Ligand 0CK D 295





## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	287/296 (96%)	0.16	15 (5%)	27 26	20, 33, 52, 63	1 (0%)
1	B	286/296 (96%)	0.33	23 (8%)	12 11	21, 35, 59, 71	1 (0%)
1	C	286/296 (96%)	0.35	21 (7%)	15 14	20, 33, 67, 80	1 (0%)
1	D	268/296 (90%)	0.05	9 (3%)	45 44	19, 32, 51, 61	1 (0%)
All	All	1127/1184 (95%)	0.22	68 (6%)	21 20	19, 33, 57, 80	4 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	170	ASN	9.9
1	C	166	PRO	8.5
1	C	218	ALA	7.3
1	C	165	ILE	7.1
1	B	222	ARG	6.5
1	C	217	LYS	6.1
1	C	158	ASP	6.0
1	C	219	ALA	6.0
1	B	170	ASN	5.9
1	D	225	TYR	5.7
1	C	225	TYR	5.6
1	C	220	THR	5.1
1	C	167	TYR	5.1
1	C	173	LEU	4.3
1	D	294	LYS	4.2
1	C	172	ASN	4.0
1	C	223	GLN	4.0
1	B	220	THR	3.5
1	A	74	GLU	3.5
1	B	42	VAL	3.4
1	A	294	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	74	GLU	3.3
1	B	217	LYS	3.3
1	A	217	LYS	3.2
1	B	218	ALA	3.2
1	C	221	LYS	3.1
1	A	170	ASN	3.1
1	A	172	ASN	3.1
1	D	215	GLY	3.1
1	C	168	ARG	3.0
1	C	174	THR	2.9
1	B	166	PRO	2.8
1	C	216	LEU	2.8
1	D	216	LEU	2.7
1	A	216	LEU	2.7
1	C	157	ARG	2.6
1	B	225	TYR	2.6
1	A	6	GLY	2.6
1	A	41	CYS	2.6
1	B	41	CYS	2.6
1	C	215	GLY	2.6
1	B	50	HIS	2.5
1	D	46	HIS	2.5
1	B	223	GLN	2.4
1	B	168	ARG	2.4
1	B	71	CYS	2.3
1	B	169	GLU	2.2
1	B	75	GLY	2.2
1	B	219	ALA	2.2
1	A	199	LEU	2.2
1	A	95	PHE	2.2
1	A	168	ARG	2.2
1	B	199	LEU	2.1
1	D	224	LYS	2.1
1	B	167	TYR	2.1
1	B	73	ALA	2.1
1	C	164	HIS	2.1
1	A	223	GLN	2.1
1	D	7	ASN	2.1
1	B	221	LYS	2.1
1	A	76	ASP	2.0
1	B	292	MET	2.0
1	A	225	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	73	ALA	2.0
1	C	5	VAL	2.0
1	D	4	ARG	2.0
1	D	6	GLY	2.0
1	B	216	LEU	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

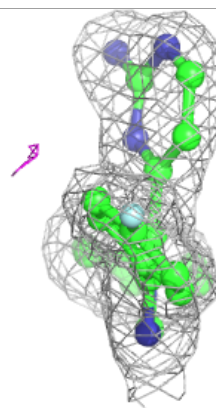
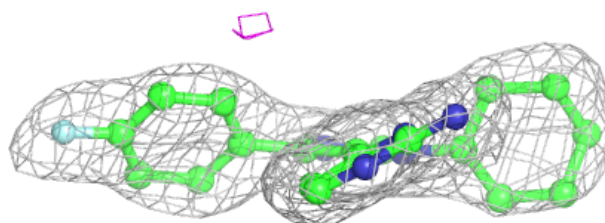
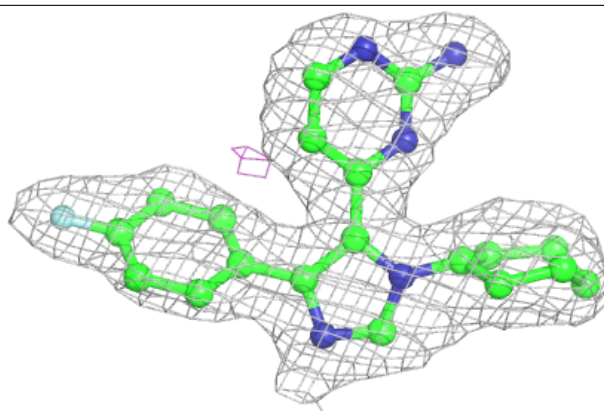
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	OCK	B	295	25/25	0.89	0.14	29,35,39,39	0
2	OCK	C	295	25/25	0.91	0.14	25,29,33,33	0
2	OCK	D	295	25/25	0.93	0.14	26,28,32,33	0
2	OCK	A	295	25/25	0.93	0.11	27,30,32,32	0
3	SO4	C	296	5/5	0.93	0.12	53,53,54,55	0
3	SO4	A	297	5/5	0.95	0.10	54,55,56,57	0
3	SO4	A	296	5/5	0.96	0.11	47,48,49,50	0
3	SO4	B	296	5/5	0.96	0.09	51,52,53,53	0
3	SO4	C	297	5/5	0.97	0.14	55,57,57,58	0
3	SO4	D	297	5/5	0.98	0.13	47,48,48,49	0
3	SO4	D	296	5/5	0.98	0.09	51,52,52,52	0

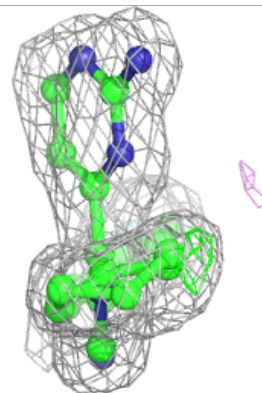
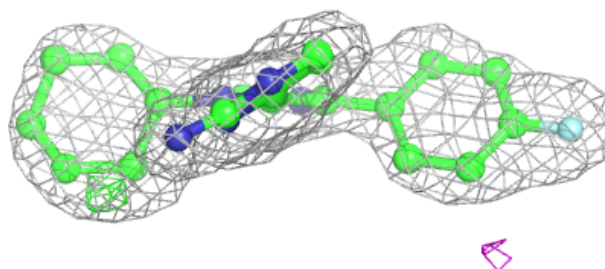
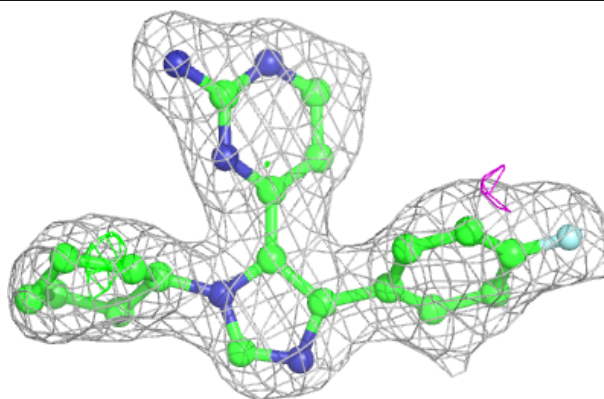
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 0CK B 295:**

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

**Electron density around 0CK C 295:**

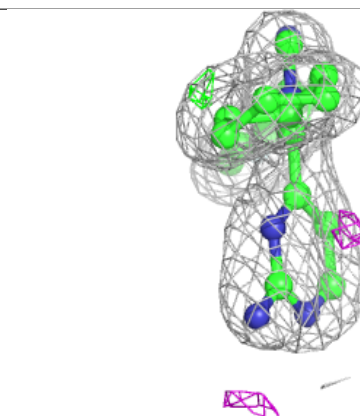
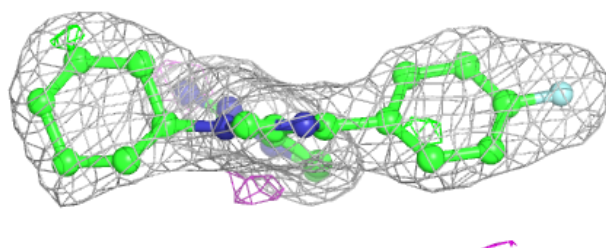
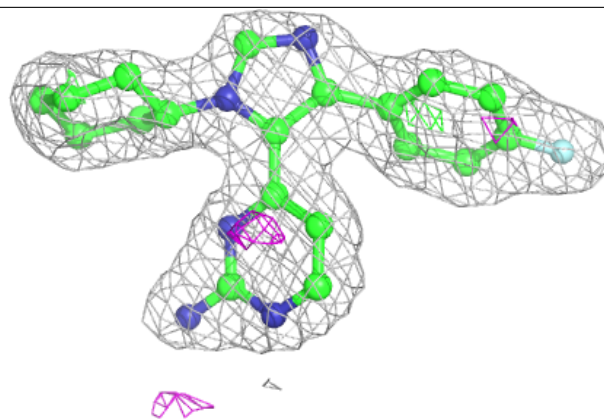
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



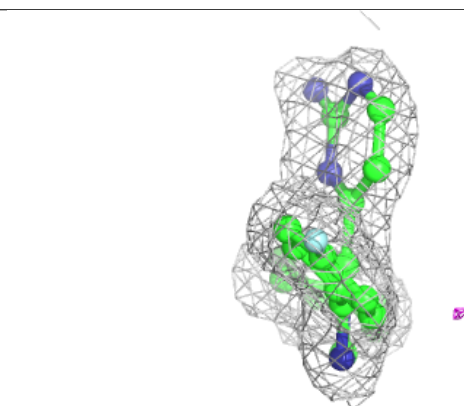
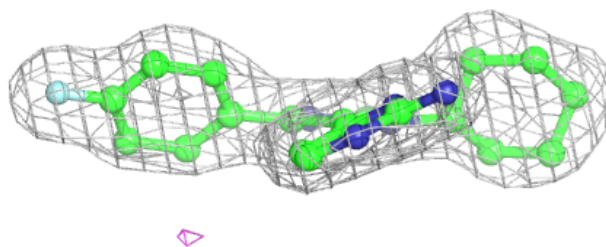
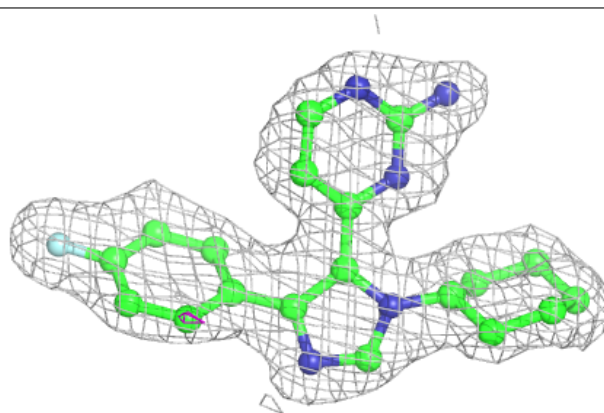


**Electron density around 0CK D 295:**

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

**Electron density around 0CK A 295:**

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



## 6.5 Other polymers

There are no such residues in this entry.