



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 08:07 pm BST

PDB ID : 1PKD  
Title : THE CRYSTAL STRUCTURE OF UCN-01 IN COMPLEX WITH  
PHOSPHO-CDK2/CYCLIN A  
Authors : Johnson, L.N.; De Moliner, E.; Brown, N.R.; Song, H.  
Deposited on : 2003-06-05  
Resolution : 2.30 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

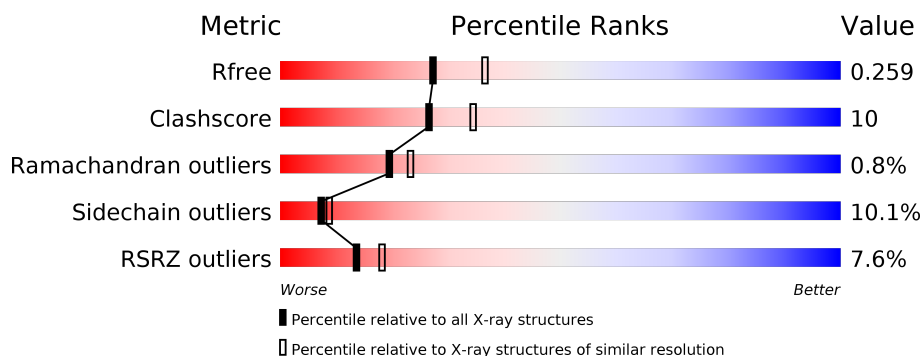
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	297	
1	C	297	
2	B	258	
2	D	258	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9416 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 Cell division protein kinase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2388	1550	404	425	1	8			

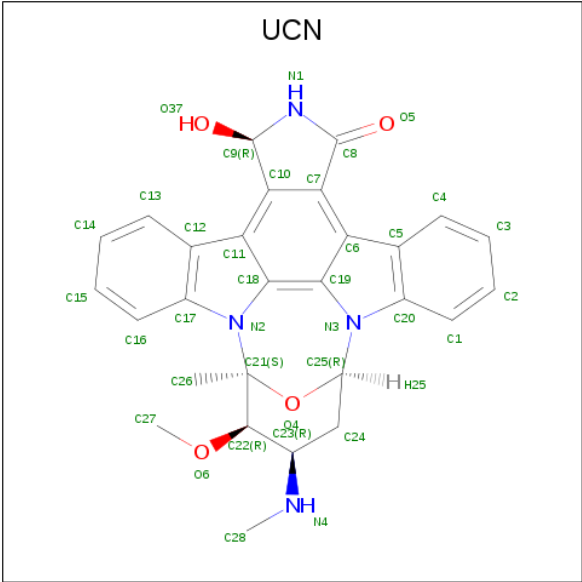
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	CLONING ARTIFACT	UNP P24941
A	160	TPO	THR	MODIFIED RESIDUE	UNP P24941
C	0	SER	-	CLONING ARTIFACT	UNP P24941
C	160	TPO	THR	MODIFIED RESIDUE	UNP P24941

- Molecule 2 is a protein called Cyclin A2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S		0	0	0
			2083	1350	339	383	11				
2	D	258	Total	C	N	O	S		0	0	0
			2083	1350	339	383	11				

- Molecule 3 is 7-HYDROXYSTAUROSPORINE (three-letter code: UCN) (formula: C<sub>28</sub>H<sub>26</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			36	28	4	4		
3	C	1	Total	C	N	O	0	0
			36	28	4	4		

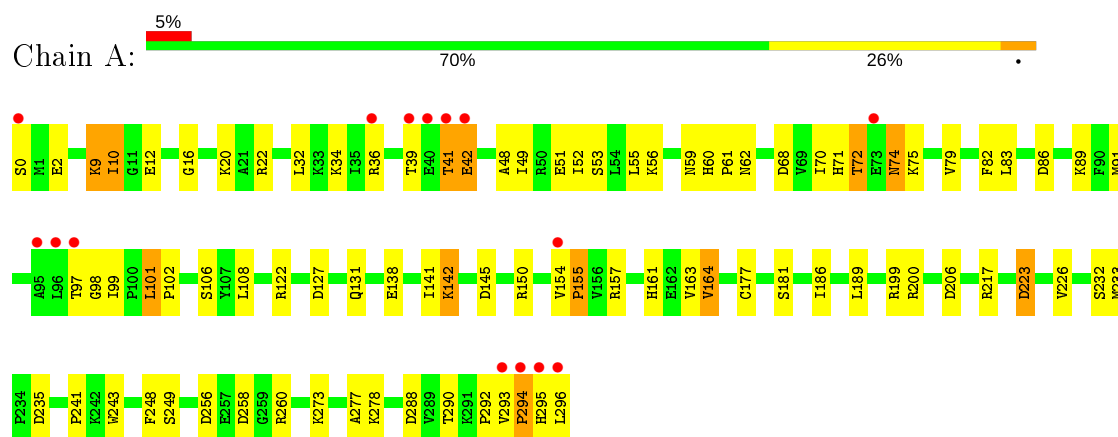
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total	O	0	0
			146	146		
4	B	110	Total	O	0	0
			110	110		
4	C	87	Total	O	0	0
			87	87		
4	D	59	Total	O	0	0
			59	59		

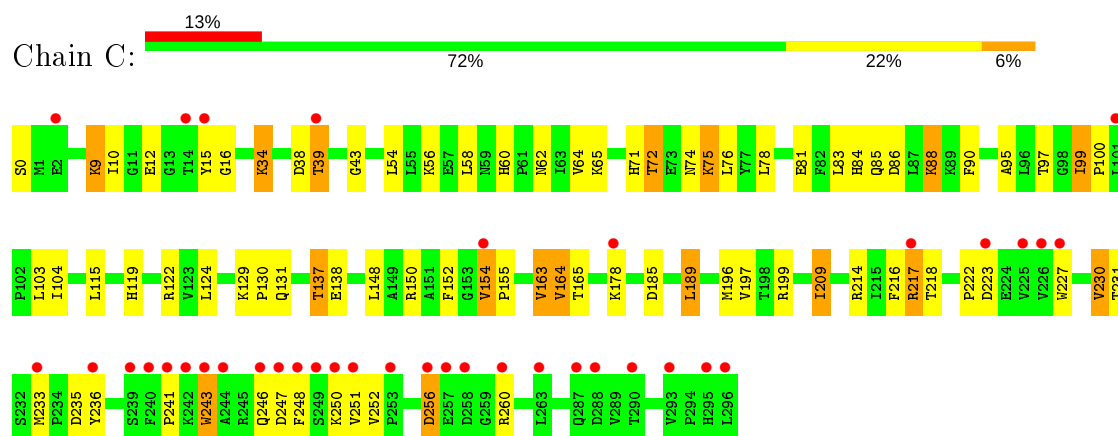
### 3 Residue-property plots [i](#)

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

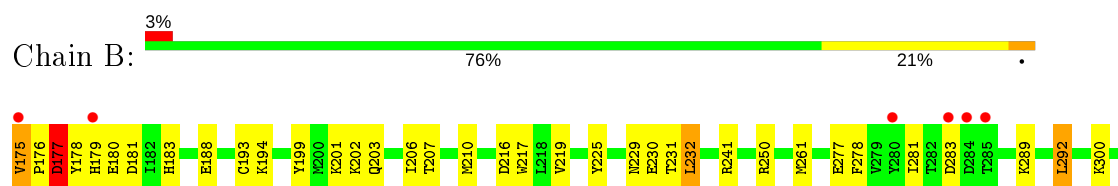
- Molecule 1: Cell division protein kinase 2



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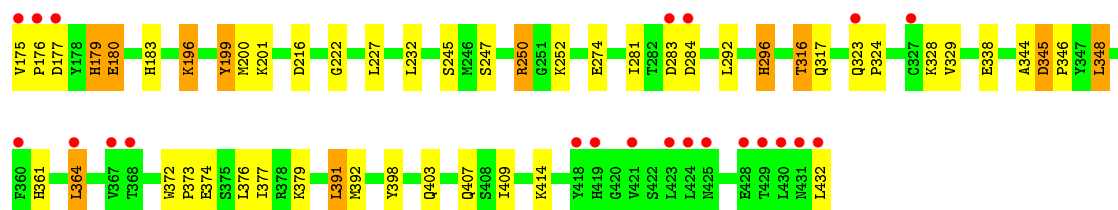
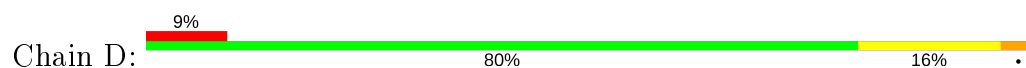


- Molecule 2: Cyclin A2





• Molecule 2: Cyclin A2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.62Å 134.57Å 147.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 64.83 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.0 (100.00-2.30) 87.0 (64.83-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, $R_{free}$	0.215 , 0.268 0.210 , 0.259	Depositor DCC
$R_{free}$ test set	2904 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

### 5.1 Standard geometry

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

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	0.50	0/2438	0.81	11/3308 (0.3%)
1	C	0.43	0/2438	0.73	4/3308 (0.1%)
2	B	0.47	0/2133	0.73	4/2897 (0.1%)
2	D	0.40	0/2133	0.70	3/2897 (0.1%)
All	All	0.45	0/9142	0.75	22/12410 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	256	ASP	CB-CG-OD2	7.08	124.68	118.30
2	B	177	ASP	CB-CG-OD2	6.44	124.10	118.30
1	A	256	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	235	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	86	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	127	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	155	PRO	N-CA-C	-5.79	97.05	112.10
2	B	216	ASP	CB-CG-OD2	5.78	123.51	118.30
2	D	216	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	145	ASP	CB-CG-OD2	5.46	123.22	118.30
1	C	223	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	223	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	288	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	235	ASP	CB-CG-OD2	5.36	123.13	118.30
1	C	86	ASP	CB-CG-OD2	5.30	123.07	118.30
2	D	284	ASP	CB-CG-OD2	5.28	123.05	118.30
2	D	283	ASP	CB-CG-OD2	5.26	123.03	118.30
2	B	343	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	68	ASP	CB-CG-OD2	5.22	122.99	118.30
1	A	258	ASP	CB-CG-OD2	5.16	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	345	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	206	ASP	CB-CG-OD2	5.05	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2388	0	2430	63	0
1	C	2388	0	2430	60	0
2	B	2083	0	2107	47	0
2	D	2083	0	2107	31	0
3	A	36	0	26	4	0
3	C	36	0	26	3	0
4	A	146	0	0	13	0
4	B	110	0	0	2	0
4	C	87	0	0	4	0
4	D	59	0	0	2	0
All	All	9416	0	9126	186	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (186) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PRO:HD2	4:A:424:HOH:O	1.39	1.18
1:A:155:PRO:CD	4:A:424:HOH:O	1.90	1.17
2:B:175:VAL:HB	2:B:176:PRO:HD2	1.31	1.06
1:C:154:VAL:HG21	2:D:317:GLN:HG2	1.34	1.05
2:D:345:ASP:HB3	2:D:346:PRO:HD3	1.35	1.04
2:D:250:ARG:HH21	2:D:250:ARG:HG3	1.18	1.03
1:A:56:LYS:HB2	1:A:56:LYS:NZ	1.76	0.99
2:B:175:VAL:HB	2:B:176:PRO:CD	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:SER:HB3	4:A:523:HOH:O	1.65	0.95
1:C:71:HIS:HD2	2:D:296:HIS:HE1	1.09	0.93
1:C:60:HIS:HD2	1:C:62:ASN:H	1.19	0.88
2:D:323:GLN:HB2	2:D:324:PRO:HD3	1.56	0.87
1:C:71:HIS:HD2	2:D:296:HIS:CE1	1.93	0.86
1:A:71:HIS:HE1	2:B:304:PHE:HE2	1.22	0.84
1:C:154:VAL:HG23	1:C:155:PRO:HD2	1.60	0.84
1:C:154:VAL:HG21	2:D:317:GLN:CG	2.08	0.84
2:B:345:ASP:HB3	2:B:346:PRO:HD3	1.60	0.83
2:B:175:VAL:O	2:B:178:TYR:N	2.10	0.83
1:A:98:GLY:HA2	1:A:199:ARG:HE	1.45	0.82
1:A:56:LYS:HB2	1:A:56:LYS:HZ3	1.47	0.79
2:B:345:ASP:HB3	2:B:346:PRO:CD	2.14	0.78
1:C:71:HIS:CD2	2:D:296:HIS:HE1	1.99	0.77
2:D:250:ARG:HG3	2:D:250:ARG:NH2	1.97	0.77
1:A:71:HIS:CE1	2:B:304:PHE:HE2	2.03	0.76
1:A:39:THR:O	2:B:292:LEU:HD23	1.87	0.75
1:C:71:HIS:O	1:C:75:LYS:O	2.05	0.74
1:C:217:ARG:HD2	4:C:497:HOH:O	1.89	0.73
1:C:60:HIS:CD2	1:C:62:ASN:H	2.04	0.73
1:A:56:LYS:HB2	1:A:56:LYS:HZ2	1.54	0.72
1:A:71:HIS:HE1	2:B:304:PHE:CE2	2.07	0.71
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.73	0.70
2:D:345:ASP:HB3	2:D:346:PRO:CD	2.19	0.70
2:D:373:PRO:HD2	2:D:376:LEU:HD12	1.74	0.70
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.74	0.69
1:C:38:ASP:O	1:C:39:THR:OG1	2.10	0.68
4:A:424:HOH:O	2:B:316:THR:CG2	2.42	0.67
1:A:161:HIS:HD2	4:A:466:HOH:O	1.77	0.67
4:A:424:HOH:O	2:B:316:THR:HG22	1.94	0.66
1:A:60:HIS:CD2	1:A:62:ASN:H	2.13	0.66
2:D:196:LYS:HG3	2:D:199:TYR:HB3	1.78	0.65
1:A:16:GLY:HA2	1:A:34:LYS:O	1.96	0.65
2:D:374:GLU:HA	2:D:377:ILE:HD12	1.79	0.64
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.79	0.64
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.80	0.63
1:C:154:VAL:HG23	2:D:316:THR:HG22	1.80	0.63
2:D:323:GLN:HB2	2:D:324:PRO:CD	2.28	0.63
1:C:71:HIS:O	1:C:72:THR:HB	1.98	0.63
3:A:410:UCN:H263	3:A:410:UCN:H16	1.79	0.62
1:C:197:VAL:HG11	1:C:252:VAL:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ALA:O	1:C:199:ARG:NH1	2.33	0.62
1:A:101:LEU:N	1:A:102:PRO:HD2	2.16	0.61
1:C:115:LEU:HD21	1:C:185:ASP:HB3	1.83	0.60
4:C:463:HOH:O	2:D:177:ASP:HB3	2.00	0.60
2:B:374:GLU:HA	2:B:377:ILE:HD12	1.82	0.60
2:B:231:THR:HG22	2:B:261:MET:HE3	1.83	0.60
1:C:241:PRO:HD2	1:C:243:TRP:HZ3	1.67	0.60
1:A:60:HIS:HD2	1:A:62:ASN:H	1.49	0.59
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.38	0.59
1:A:106:SER:HB2	1:A:292:PRO:HD2	1.84	0.59
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.68	0.58
1:C:84:HIS:HD2	1:C:137:THR:H	1.50	0.58
1:A:293:VAL:O	1:A:294:PRO:O	2.21	0.58
3:C:411:UCN:H263	3:C:411:UCN:H16	1.85	0.57
2:B:388:LYS:O	2:B:392:MET:HG2	2.05	0.57
2:B:231:THR:HG22	2:B:261:MET:CE	2.33	0.57
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.87	0.57
1:A:72:THR:HG22	1:A:75:LYS:H	1.70	0.57
1:C:72:THR:HG22	1:C:75:LYS:H	1.69	0.57
1:C:64:VAL:HG11	3:C:411:UCN:O37	2.05	0.57
1:C:218:THR:HG22	1:C:251:VAL:HG22	1.87	0.55
1:C:241:PRO:HD2	1:C:243:TRP:CZ3	2.41	0.55
2:B:407:GLN:O	2:B:411:GLU:HG2	2.07	0.55
1:A:51:GLU:O	1:A:55:LEU:HB2	2.07	0.54
1:A:10:ILE:HD11	1:A:82:PHE:HE1	1.72	0.54
1:C:104:ILE:HG12	1:C:196:MET:HB3	1.88	0.54
1:A:177:CYS:HB2	1:A:233:MET:CE	2.37	0.54
1:A:98:GLY:HA2	1:A:199:ARG:NE	2.19	0.54
1:C:214:ARG:O	1:C:217:ARG:HB2	2.08	0.54
2:B:175:VAL:CB	2:B:176:PRO:HD2	2.20	0.53
1:A:10:ILE:HD12	1:A:20:LYS:HB2	1.90	0.53
1:C:85:GLN:HE21	1:C:90:PHE:HB2	1.73	0.53
1:A:138:GLU:O	1:A:293:VAL:HG22	2.08	0.53
1:C:241:PRO:HG2	1:C:243:TRP:CH2	2.44	0.53
1:A:39:THR:O	2:B:292:LEU:CD2	2.57	0.52
1:A:72:THR:HG22	1:A:74:ASN:H	1.74	0.52
1:A:155:PRO:HD2	2:B:316:THR:CG2	2.37	0.52
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.91	0.52
4:A:480:HOH:O	2:B:316:THR:HG21	2.10	0.51
2:B:229:ASN:HB3	4:B:481:HOH:O	2.09	0.51
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LYS:HB3	4:C:475:HOH:O	2.09	0.51
2:D:345:ASP:CB	2:D:346:PRO:HD3	2.23	0.51
2:B:210:MET:CE	2:B:250:ARG:HB2	2.40	0.51
2:D:338:GLU:HG2	2:D:409:ILE:HD13	1.93	0.51
1:C:71:HIS:CD2	2:D:296:HIS:CE1	2.85	0.50
1:A:53:SER:HA	1:A:56:LYS:HE3	1.93	0.50
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.92	0.50
2:B:323:GLN:CB	2:B:324:PRO:CD	2.89	0.50
1:C:241:PRO:HG2	1:C:243:TRP:CZ3	2.47	0.50
2:B:277:GLU:O	2:B:281:ILE:HG23	2.12	0.49
1:A:83:LEU:HD21	1:A:142:LYS:HE2	1.93	0.49
2:B:175:VAL:O	2:B:177:ASP:N	2.45	0.49
1:A:131:GLN:HB3	3:A:410:UCN:H281	1.93	0.49
1:C:154:VAL:CG2	2:D:317:GLN:HG2	2.25	0.49
2:D:250:ARG:NE	4:D:439:HOH:O	2.44	0.49
1:A:60:HIS:HE1	4:A:425:HOH:O	1.96	0.49
2:B:395:HIS:HB2	2:B:430:LEU:HD11	1.94	0.49
1:A:83:LEU:O	3:A:410:UCN:H4	2.12	0.49
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.95	0.49
2:D:250:ARG:CG	2:D:250:ARG:HH21	2.07	0.49
1:A:61:PRO:O	1:A:142:LYS:HD3	2.13	0.48
2:B:323:GLN:HB3	2:B:324:PRO:HD3	1.95	0.48
2:D:176:PRO:HA	2:D:179:HIS:CG	2.49	0.48
1:A:10:ILE:CD1	1:A:82:PHE:HE1	2.26	0.48
2:B:345:ASP:CB	2:B:346:PRO:CD	2.85	0.48
1:A:249:SER:HA	1:A:260:ARG:HD3	1.96	0.48
1:C:163:VAL:CG1	1:C:164:VAL:HG23	2.44	0.48
1:A:154:VAL:CA	4:A:424:HOH:O	2.62	0.47
2:D:180:GLU:OE1	2:D:180:GLU:HA	2.13	0.47
1:C:248:PHE:HA	1:C:251:VAL:HB	1.97	0.47
1:A:260:ARG:HD3	4:A:532:HOH:O	2.15	0.47
1:C:241:PRO:CG	1:C:243:TRP:CZ3	2.98	0.47
1:C:252:VAL:HB	4:C:450:HOH:O	2.13	0.47
1:A:0:SER:HB3	1:A:70:ILE:CG2	2.44	0.47
1:C:54:LEU:O	1:C:58:LEU:HG	2.15	0.47
2:B:183:HIS:HD2	4:B:471:HOH:O	1.98	0.46
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.99	0.45
1:C:129:LYS:HE2	1:C:165:THR:OG1	2.17	0.45
1:C:38:ASP:HB2	1:C:43:GLY:H	1.81	0.45
1:C:216:PHE:CD1	1:C:222:PRO:HD3	2.52	0.45
1:A:32:LEU:HD23	1:A:79:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:VAL:HG22	1:C:83:LEU:HD13	1.99	0.45
1:C:154:VAL:CG2	1:C:155:PRO:HD2	2.37	0.45
1:C:154:VAL:HB	1:C:155:PRO:CD	2.47	0.44
1:C:16:GLY:HA2	1:C:34:LYS:O	2.17	0.44
1:C:227:TRP:O	1:C:230:VAL:HG23	2.18	0.44
1:C:119:HIS:HE1	1:C:185:ASP:OD2	2.00	0.44
1:A:141:ILE:C	1:A:142:LYS:HG2	2.37	0.44
2:B:207:THR:OG1	2:B:210:MET:HG3	2.17	0.44
1:C:252:VAL:HG12	1:C:252:VAL:O	2.17	0.44
2:B:230:GLU:HA	2:B:230:GLU:OE1	2.18	0.44
1:C:10:ILE:O	3:C:411:UCN:H25	2.17	0.44
1:C:209:ILE:HD12	1:C:209:ILE:HA	1.75	0.44
1:C:231:THR:HA	1:C:236:TYR:CD1	2.53	0.43
2:D:176:PRO:HA	2:D:179:HIS:ND1	2.34	0.43
1:A:56:LYS:CB	1:A:56:LYS:NZ	2.61	0.43
2:B:278:PHE:HA	2:B:281:ILE:HG12	1.99	0.43
1:A:9:LYS:NZ	1:A:12:GLU:HB2	2.34	0.43
2:B:371:SER:O	2:B:372:TRP:C	2.57	0.43
1:C:88:LYS:HE2	1:C:131:GLN:HE21	1.84	0.43
1:C:65:LYS:H	1:C:81:GLU:HG2	1.83	0.43
1:A:0:SER:HA	4:A:539:HOH:O	2.19	0.43
1:A:0:SER:CA	4:A:539:HOH:O	2.67	0.43
1:A:0:SER:HB3	1:A:70:ILE:HG23	2.01	0.43
1:A:241:PRO:HB2	1:A:243:TRP:CZ3	2.54	0.43
2:B:193:CYS:O	2:B:241:ARG:HD2	2.19	0.43
1:C:256:ASP:O	1:C:260:ARG:HG3	2.18	0.43
1:C:99:ILE:HA	1:C:100:PRO:HD2	1.87	0.42
1:C:72:THR:HG22	1:C:74:ASN:H	1.84	0.42
1:A:108:LEU:HD12	1:A:108:LEU:HA	1.81	0.42
1:A:163:VAL:CG1	1:A:164:VAL:HG23	2.48	0.42
1:A:48:ALA:O	1:A:52:ILE:HD12	2.20	0.42
1:C:163:VAL:HG13	1:C:164:VAL:HG23	2.01	0.42
2:D:329:VAL:HG11	2:D:364:LEU:HD12	2.02	0.42
1:A:278:LYS:NZ	2:B:181:ASP:OD2	2.46	0.42
2:B:217:TRP:CZ2	2:B:281:ILE:HD12	2.54	0.42
2:B:395:HIS:HE1	2:B:427:PRO:O	2.02	0.42
1:C:129:LYS:HB2	1:C:130:PRO:HD2	2.01	0.42
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.85	0.42
1:A:223:ASP:H	1:A:226:VAL:HG12	1.83	0.42
1:C:124:LEU:HG	1:C:152:PHE:CD1	2.55	0.42
1:C:9:LYS:HE3	1:C:12:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.85	0.42
1:A:49:ILE:HG23	2:B:306:LEU:HD12	2.02	0.41
2:B:203:GLN:HB3	2:B:206:ILE:HG12	2.03	0.41
2:B:225:TYR:HE1	2:B:281:ILE:CG2	2.31	0.41
1:A:217:ARG:HG2	1:A:243:TRP:CD2	2.56	0.41
1:C:154:VAL:CB	1:C:155:PRO:CD	2.98	0.41
1:A:55:LEU:HA	1:A:55:LEU:HD12	1.92	0.41
1:A:186:ILE:HD11	1:A:277:ALA:HB2	2.03	0.41
1:A:41:THR:HB	1:A:42:GLU:H	1.69	0.41
1:A:138:GLU:C	1:A:293:VAL:HG13	2.42	0.40
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.56	0.40
1:A:177:CYS:HB3	4:A:433:HOH:O	2.22	0.40
3:A:410:UCN:H263	3:A:410:UCN:C16	2.50	0.40
2:D:414:LYS:HA	4:D:437:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/297 (99%)	282 (96%)	9 (3%)	3 (1%)	15	17
1	C	294/297 (99%)	270 (92%)	21 (7%)	3 (1%)	15	17
2	B	256/258 (99%)	248 (97%)	7 (3%)	1 (0%)	34	42
2	D	256/258 (99%)	247 (96%)	7 (3%)	2 (1%)	19	23
All	All	1100/1110 (99%)	1047 (95%)	44 (4%)	9 (1%)	19	23

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	PRO

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Mol	Chain	Res	Type
1	A	72	THR
1	A	164	VAL
1	C	164	VAL
2	B	283	ASP
1	C	72	THR
1	C	99	ILE
2	D	372	TRP
2	D	345	ASP

### 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	261/261 (100%)	237 (91%)	24 (9%)	9	11
1	C	261/261 (100%)	233 (89%)	28 (11%)	6	7
2	B	232/232 (100%)	211 (91%)	21 (9%)	9	11
2	D	232/232 (100%)	205 (88%)	27 (12%)	5	6
All	All	986/986 (100%)	886 (90%)	100 (10%)	7	9

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	9	LYS
1	A	10	ILE
1	A	22	ARG
1	A	36	ARG
1	A	41	THR
1	A	42	GLU
1	A	59	ASN
1	A	74	ASN
1	A	89	LYS
1	A	97	THR
1	A	101	LEU
1	A	122	ARG

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Mol	Chain	Res	Type
1	A	142	LYS
1	A	150	ARG
1	A	157	ARG
1	A	189	LEU
1	A	200	ARG
1	A	232	SER
1	A	248	PHE
1	A	273	LYS
1	A	290	THR
1	A	295	HIS
1	A	296	LEU
2	B	175	VAL
2	B	177	ASP
2	B	180	GLU
2	B	188	GLU
2	B	194	LYS
2	B	199	TYR
2	B	201	LYS
2	B	202	LYS
2	B	232	LEU
2	B	289	LYS
2	B	292	LEU
2	B	300	LYS
2	B	316	THR
2	B	323	GLN
2	B	328	LYS
2	B	348	LEU
2	B	349	LYS
2	B	364	LEU
2	B	371	SER
2	B	374	GLU
2	B	384	LEU
1	C	0	SER
1	C	9	LYS
1	C	15	TYR
1	C	34	LYS
1	C	39	THR
1	C	56	LYS
1	C	75	LYS
1	C	76	LEU
1	C	78	LEU
1	C	88	LYS

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Mol	Chain	Res	Type
1	C	97	THR
1	C	103	LEU
1	C	122	ARG
1	C	137	THR
1	C	138	GLU
1	C	148	LEU
1	C	150	ARG
1	C	154	VAL
1	C	163	VAL
1	C	189	LEU
1	C	209	ILE
1	C	217	ARG
1	C	230	VAL
1	C	233	MET
1	C	243	TRP
1	C	246	GLN
1	C	247	ASP
1	C	250	LYS
2	D	175	VAL
2	D	179	HIS
2	D	180	GLU
2	D	196	LYS
2	D	199	TYR
2	D	200	MET
2	D	201	LYS
2	D	232	LEU
2	D	245	SER
2	D	247	SER
2	D	250	ARG
2	D	252	LYS
2	D	274	GLU
2	D	281	ILE
2	D	292	LEU
2	D	296	HIS
2	D	316	THR
2	D	328	LYS
2	D	348	LEU
2	D	364	LEU
2	D	379	LYS
2	D	391	LEU
2	D	392	MET
2	D	398	TYR

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Mol	Chain	Res	Type
2	D	403	GLN
2	D	407	GLN
2	D	432	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	71	HIS
1	A	131	GLN
1	A	161	HIS
1	A	268	HIS
1	A	295	HIS
2	B	183	HIS
2	B	254	GLN
2	B	317	GLN
2	B	395	HIS
2	B	396	GLN
2	B	431	ASN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	84	HIS
1	C	119	HIS
1	C	121	HIS
2	D	183	HIS
2	D	254	GLN
2	D	296	HIS
2	D	317	GLN
2	D	396	GLN
2	D	425	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](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
1	TPO	C	160	1	8,10,11	1.25	1 (12%)	10,14,16	0.70	0
1	TPO	A	160	1	8,10,11	1.09	1 (12%)	10,14,16	0.90	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
1	TPO	C	160	1	-	0/9/11/13	-
1	TPO	A	160	1	-	0/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-O1P	2.49	1.58	1.50
1	A	160	TPO	P-O1P	2.36	1.58	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

2 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	UCN	A	410	-	31,43,43	2.07	6 (19%)	36,70,70	2.17	11 (30%)
3	UCN	C	411	-	31,43,43	2.13	8 (25%)	36,70,70	2.29	11 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UCN	A	410	-	-	2/4/45/45	-
3	UCN	C	411	-	-	0/4/45/45	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	411	UCN	C11-C18	5.71	1.49	1.42
3	A	410	UCN	C11-C18	5.55	1.49	1.42
3	C	411	UCN	C12-C17	4.51	1.48	1.41
3	A	410	UCN	C12-C17	4.47	1.48	1.41
3	C	411	UCN	C5-C20	4.20	1.48	1.41
3	A	410	UCN	C7-C10	3.84	1.46	1.39
3	A	410	UCN	C5-C20	3.80	1.47	1.41
3	C	411	UCN	C6-C19	3.76	1.47	1.42
3	C	411	UCN	C7-C10	3.61	1.45	1.39
3	A	410	UCN	C6-C19	3.53	1.47	1.42
3	C	411	UCN	C7-C6	2.63	1.47	1.43
3	A	410	UCN	C7-C6	2.47	1.47	1.43
3	C	411	UCN	O37-C9	2.29	1.49	1.40
3	C	411	UCN	C16-C17	2.04	1.45	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	411	UCN	C7-C10-C11	-5.53	119.33	122.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	411	UCN	C16-C17-N2	5.31	138.71	132.29
3	A	410	UCN	O5-C8-C7	-4.89	123.52	129.32
3	C	411	UCN	O5-C8-C7	-4.79	123.64	129.32
3	A	410	UCN	C7-C10-C9	-4.70	107.26	109.42
3	A	410	UCN	C16-C17-N2	4.63	137.89	132.29
3	A	410	UCN	C7-C10-C11	-4.58	119.80	122.04
3	C	411	UCN	C16-C17-C12	-4.54	114.19	120.73
3	A	410	UCN	C16-C17-C12	-3.60	115.53	120.73
3	C	411	UCN	O5-C8-N1	3.55	129.06	125.98
3	C	411	UCN	C13-C12-C17	3.23	123.48	119.39
3	A	410	UCN	O37-C9-C10	3.12	121.64	112.29
3	A	410	UCN	O5-C8-N1	3.05	128.63	125.98
3	C	411	UCN	O37-C9-C10	-2.85	103.74	112.29
3	C	411	UCN	C3-C4-C5	-2.65	116.41	120.86
3	A	410	UCN	O37-C9-N1	2.65	115.65	112.06
3	A	410	UCN	C3-C4-C5	-2.60	116.49	120.86
3	C	411	UCN	C7-C10-C9	-2.46	108.29	109.42
3	A	410	UCN	C13-C12-C17	2.29	122.29	119.39
3	A	410	UCN	C4-C5-C20	2.13	122.08	119.39
3	C	411	UCN	C4-C5-C20	2.06	121.99	119.39
3	C	411	UCN	C14-C13-C12	-2.04	117.44	120.86

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	410	UCN	C24-C23-N4-C28
3	A	410	UCN	C22-C23-N4-C28

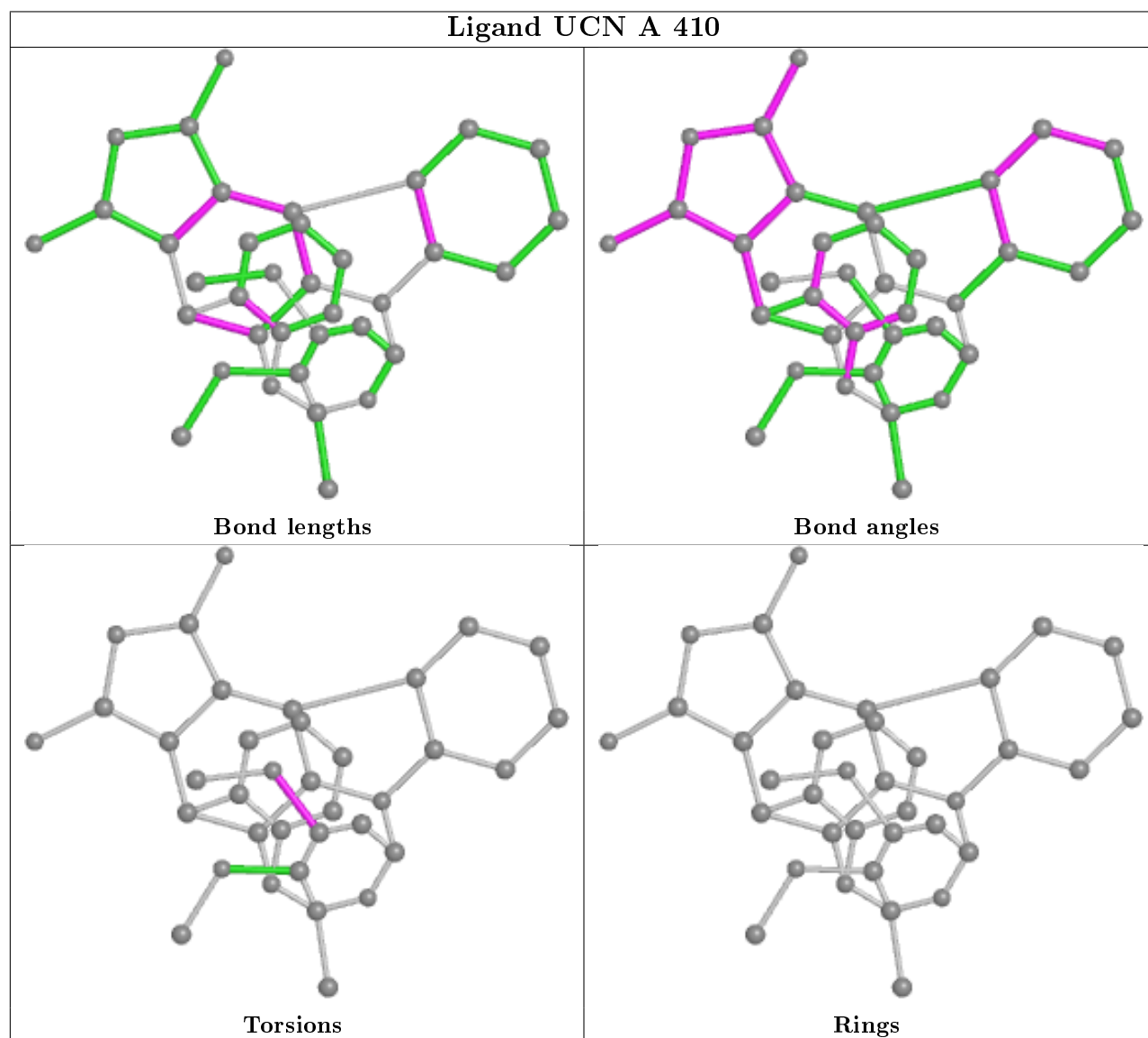
There are no ring outliers.

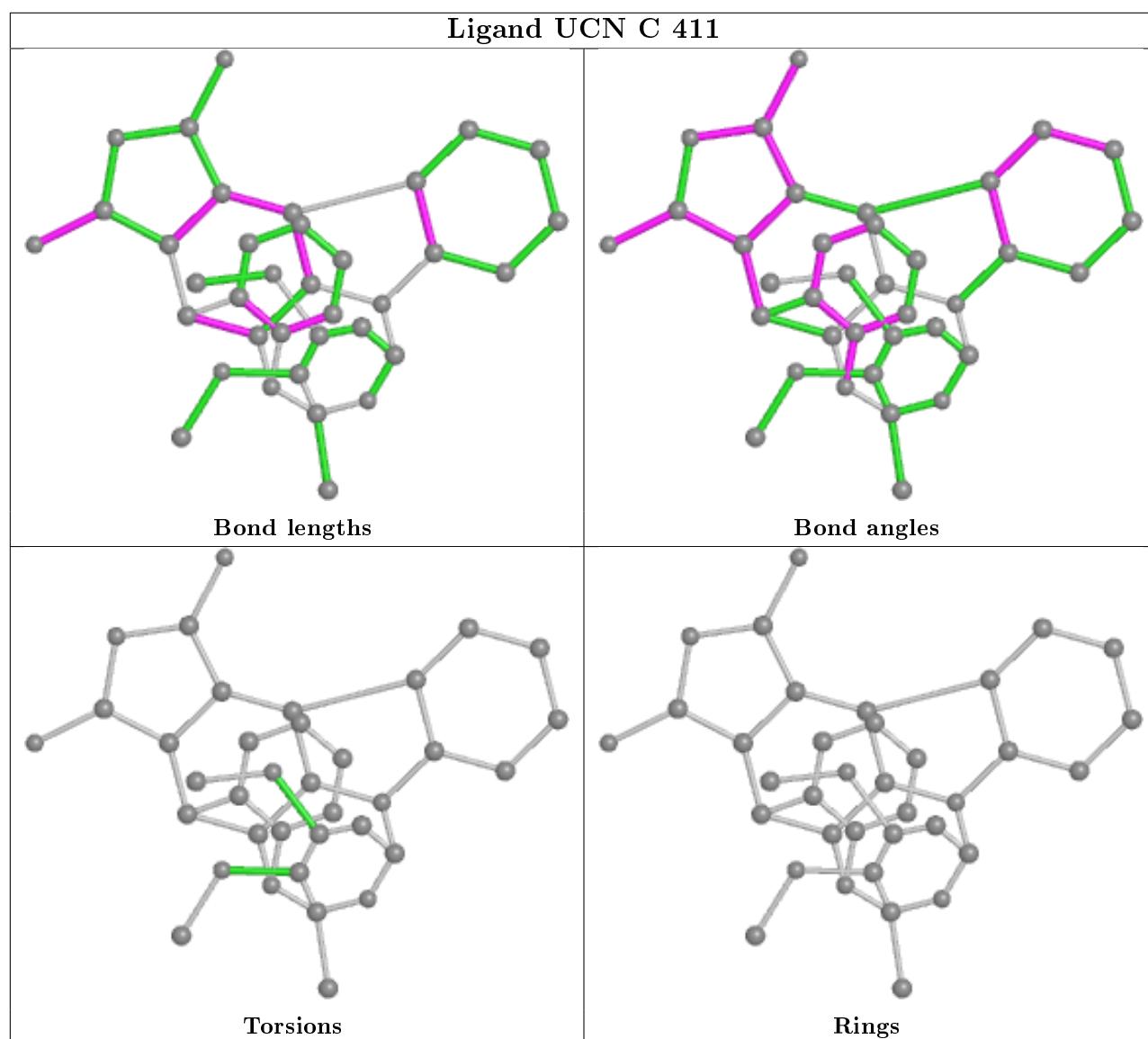
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	410	UCN	4	0
3	C	411	UCN	3	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.





## 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	296/297 (99%)	0.40	15 (5%) 28 35	16, 29, 69, 128	0
1	C	296/297 (99%)	0.70	38 (12%) 3 5	23, 46, 86, 109	0
2	B	258/258 (100%)	0.15	9 (3%) 44 51	17, 31, 52, 94	0
2	D	258/258 (100%)	0.57	22 (8%) 10 14	25, 49, 84, 120	0
All	All	1108/1110 (99%)	0.46	84 (7%) 13 18	16, 38, 82, 128	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	295	HIS	18.8
1	C	242	LYS	9.1
1	A	294	PRO	8.2
1	A	296	LEU	8.0
1	A	40	GLU	7.6
1	A	96	LEU	7.2
1	A	293	VAL	6.9
1	C	243	TRP	6.7
2	D	432	LEU	6.4
1	A	95	ALA	6.1
2	D	323	GLN	5.5
2	B	284	ASP	5.5
1	C	248	PHE	4.8
2	D	175	VAL	4.8
2	D	367	VAL	4.7
1	C	154	VAL	4.7
1	C	249	SER	4.7
1	C	233	MET	4.6
2	D	283	ASP	4.5
2	D	423	LEU	4.4
1	A	97	THR	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	430	LEU	4.1
1	C	223	ASP	4.1
1	C	241	PRO	3.9
2	D	364	LEU	3.9
2	B	283	ASP	3.9
1	C	244	ALA	3.8
1	C	296	LEU	3.7
1	C	217	ARG	3.6
1	A	154	VAL	3.4
2	B	432	LEU	3.4
1	C	288	ASP	3.3
1	A	39	THR	3.3
2	D	431	ASN	3.3
2	D	176	PRO	3.2
1	C	250	LYS	3.2
1	C	251	VAL	3.2
2	D	284	ASP	3.2
2	B	175	VAL	3.2
1	C	227	TRP	3.1
1	C	39	THR	3.1
2	B	345	ASP	3.1
1	C	225	VAL	3.0
1	C	290	THR	3.0
1	C	258	ASP	3.0
1	C	15	TYR	3.0
1	A	36	ARG	2.9
1	C	236	TYR	2.9
1	C	295	HIS	2.9
1	A	42	GLU	2.8
1	C	293	VAL	2.8
2	B	280	TYR	2.8
2	D	421	VAL	2.8
1	C	260	ARG	2.8
1	C	2	GLU	2.8
1	C	14	THR	2.8
1	C	247	ASP	2.7
2	D	418	TYR	2.7
1	C	287	GLN	2.7
2	D	428	GLU	2.7
2	B	327	CYS	2.6
1	C	240	PHE	2.6
2	D	368	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	101	LEU	2.6
2	D	327	CYS	2.6
1	A	0	SER	2.4
1	C	256	ASP	2.4
1	A	73	GLU	2.4
2	B	179	HIS	2.4
2	D	419	HIS	2.4
1	C	253	PRO	2.4
1	C	226	VAL	2.4
1	C	239	SER	2.4
1	A	41	THR	2.3
1	C	263	LEU	2.2
2	D	360	PHE	2.2
2	D	429	THR	2.2
2	D	424	LEU	2.2
1	C	257	GLU	2.1
2	B	285	THR	2.1
1	C	246	GLN	2.1
1	C	178	LYS	2.1
2	D	425	ASN	2.0
2	D	177	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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(Å <sup>2</sup> )	Q<0.9
1	TPO	C	160	11/12	0.98	0.12	36,41,44,44	0
1	TPO	A	160	11/12	0.99	0.13	20,25,29,30	0

## 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,

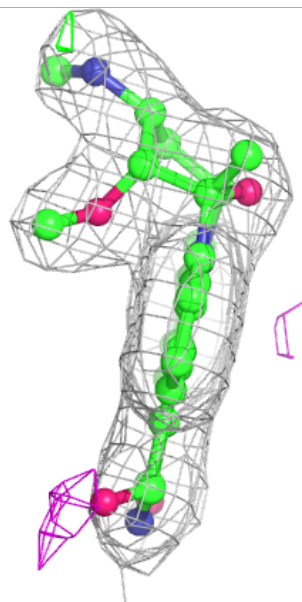
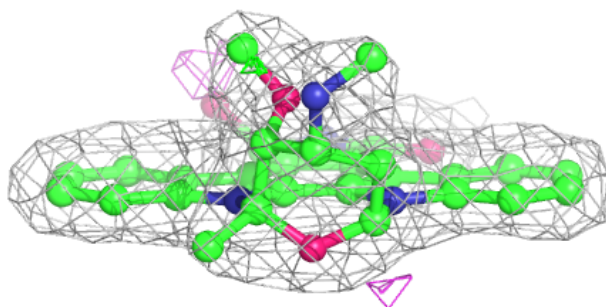
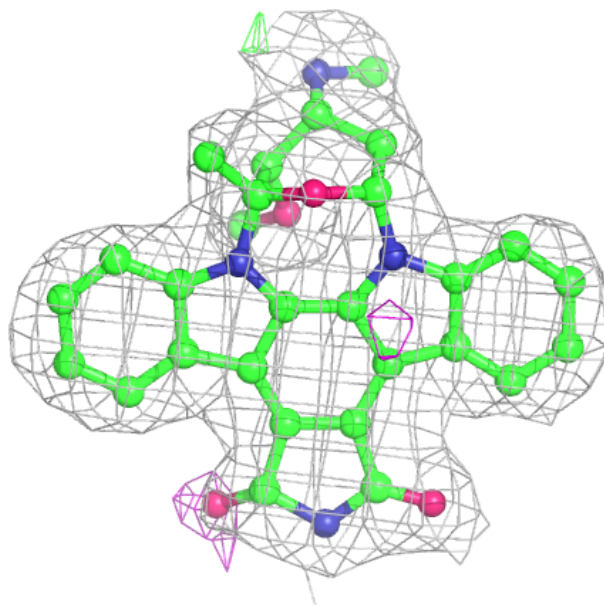
median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	UCN	A	410	36/36	0.96	0.13	23,28,33,44	0
3	UCN	C	411	36/36	0.96	0.14	33,34,40,44	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.

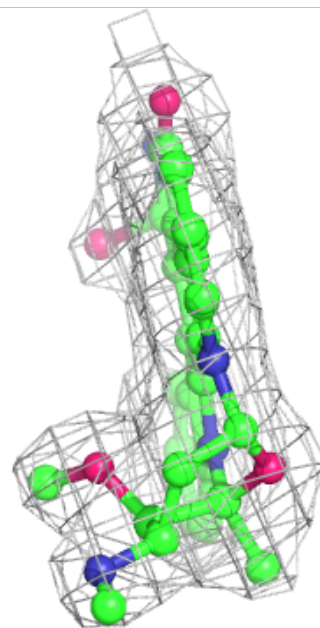
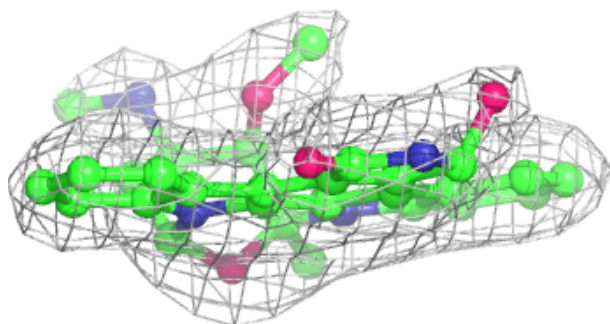
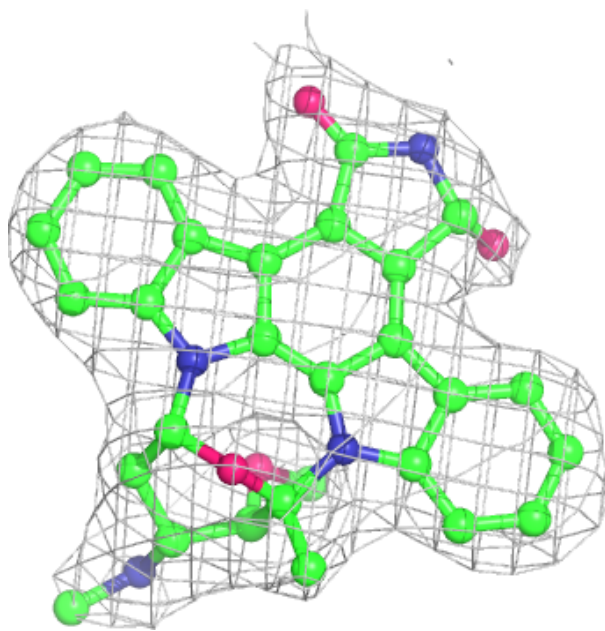
**Electron density around UCN A 410:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around UCN C 411:**

$2mF_o-DF_c$  (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.