



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1H1R  
Title : STRUCTURE OF HUMAN THR160-PHOSPHO CDK2/CYCLIN A COM-  
PLEXED WITH THE INHIBITOR NU6086  
Authors : Davies, T.G.; Noble, M.E.M.; Endicott, J.A.; Johnson, L.N.  
Deposited on : 2002-07-21  
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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

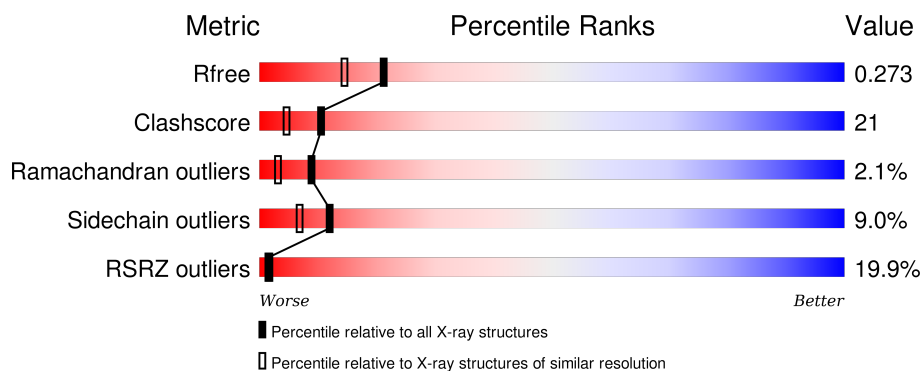
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. 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	303	<div> <div>6%</div> <div> <div></div> <div>64%</div> <div>25%</div> <div>6%</div> <div>• •</div> </div> </div>
1	C	303	<div> <div>32%</div> <div> <div></div> <div>48%</div> <div>39%</div> <div>8%</div> <div>• •</div> </div> </div>
2	B	258	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>5%</div> <div>•</div> </div> </div>
2	D	258	<div> <div>35%</div> <div> <div></div> <div>45%</div> <div>47%</div> <div>7%</div> <div>•</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9724 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.

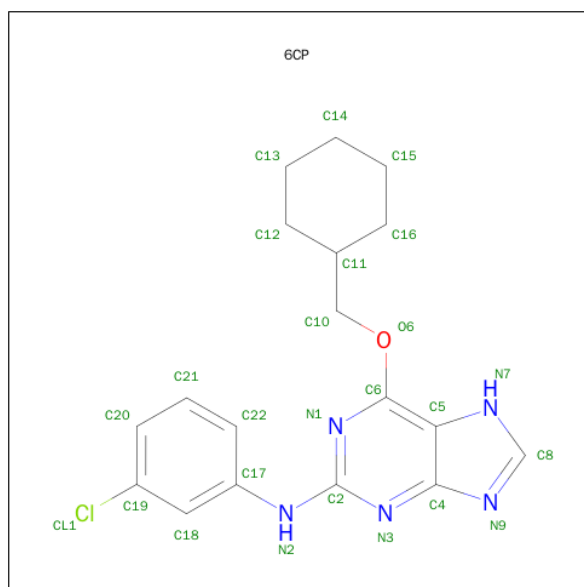
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

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			

- 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 6-CYCLOHEXYLMETHOXY-2-(3'-CHLOROANILINO) PURINE (three-letter code: 6CP) (formula: C<sub>18</sub>H<sub>20</sub>ClN<sub>5</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	1
			33	24	2	6	1		
3	C	1	Total	C	Cl	N	O	0	1
			26	18	2	5	1		

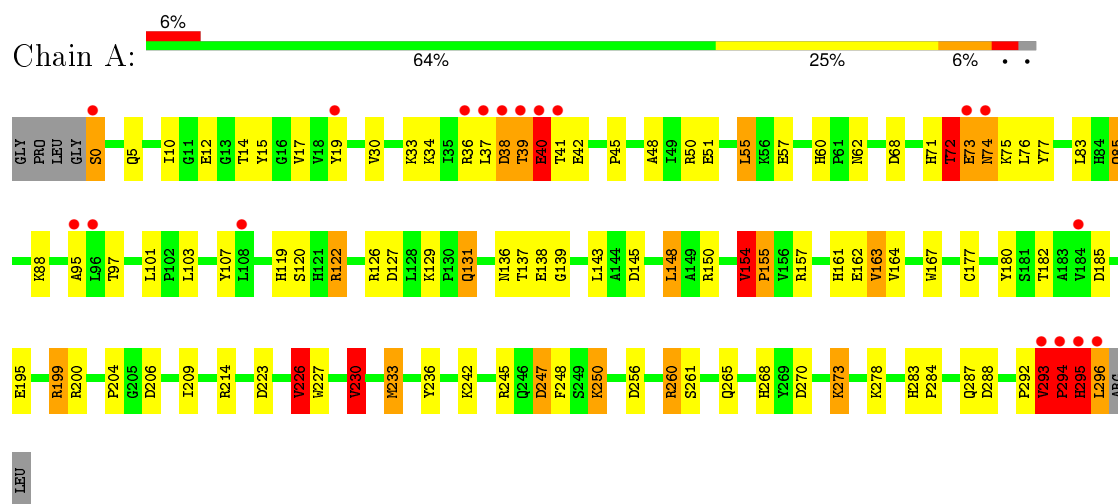
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	266	Total	O	0	0
			266	266		
4	B	229	Total	O	0	0
			229	229		
4	C	145	Total	O	0	0
			145	145		
4	D	83	Total	O	0	0
			83	83		

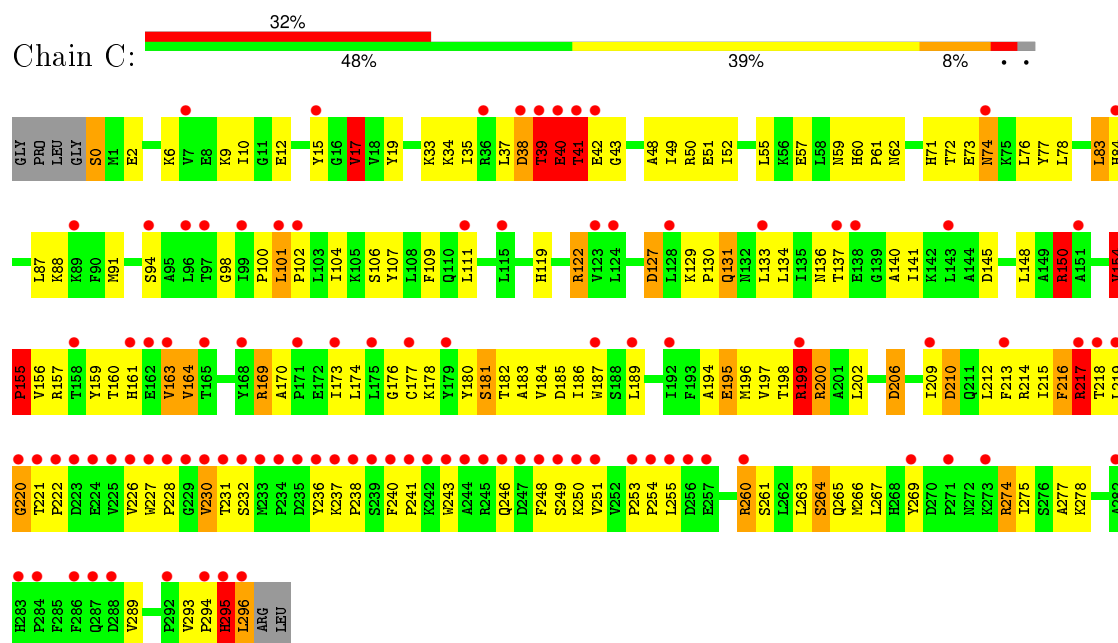
### 3 Residue-property plots

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

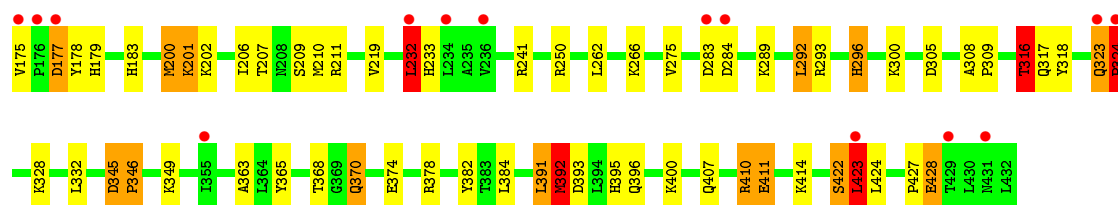
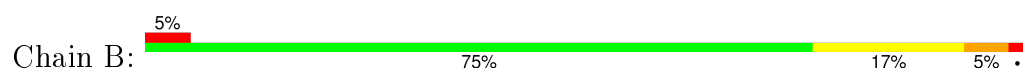
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



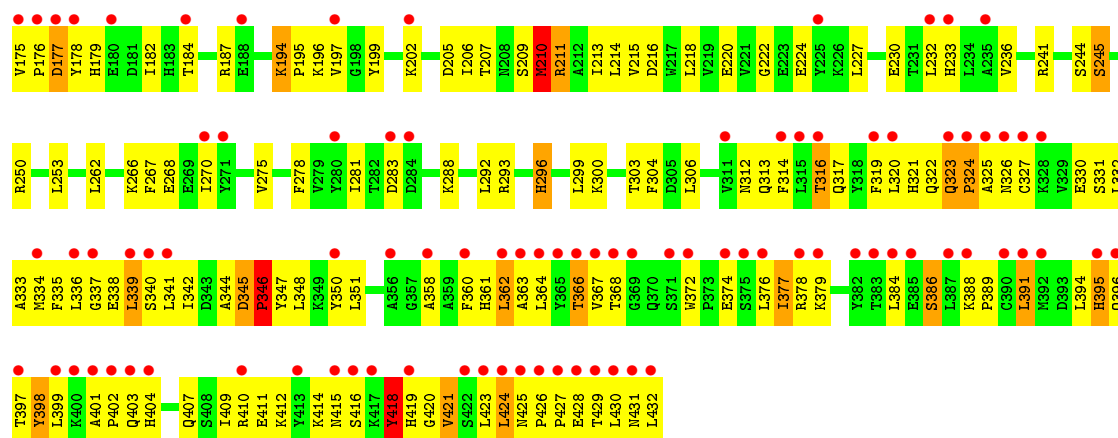
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



#### • 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, $\alpha$ , $\beta$ , $\gamma$	74.11Å 134.95Å 148.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 32.20 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (20.00-2.00) 92.8 (32.20-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.235 , 0.294 0.224 , 0.273	Depositor DCC
$R_{free}$ test set	4693 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 80.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 93678 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9724	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 6CP

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	0.87	2/2438 (0.1%)	2.02	70/3308 (2.1%)
1	C	0.62	0/2438	1.71	43/3308 (1.3%)
2	B	0.80	0/2133	1.72	36/2897 (1.2%)
2	D	0.62	0/2133	1.61	30/2897 (1.0%)
All	All	0.74	2/9142 (0.0%)	1.78	179/12410 (1.4%)

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	A	0	4
1	C	0	2
2	B	0	5
2	D	0	4
All	All	0	15

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	SER	CA-CB	5.75	1.61	1.52
1	A	293	VAL	N-CA	5.40	1.57	1.46

All (179) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ARG	CD-NE-CZ	27.03	161.44	123.60
1	A	199	ARG	CD-NE-CZ	24.57	158.00	123.60
1	C	217	ARG	CD-NE-CZ	24.00	157.20	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	PRO	C-N-CA	22.15	177.06	121.70
1	A	295	HIS	N-CA-CB	18.07	143.12	110.60
1	A	199	ARG	NE-CZ-NH2	-17.67	111.47	120.30
1	A	250	LYS	CG-CD-CE	15.88	159.54	111.90
2	B	423	LEU	CB-CA-C	15.57	139.78	110.20
1	A	295	HIS	CA-CB-CG	14.08	137.54	113.60
1	A	245	ARG	NE-CZ-NH2	-13.70	113.45	120.30
1	A	295	HIS	C-N-CA	13.17	154.62	121.70
2	D	241	ARG	NE-CZ-NH2	-12.70	113.95	120.30
2	D	378	ARG	NE-CZ-NH2	12.29	126.44	120.30
1	A	294	PRO	O-C-N	-12.23	103.13	122.70
1	A	293	VAL	CB-CA-C	12.18	134.54	111.40
2	D	378	ARG	CD-NE-CZ	11.91	140.28	123.60
2	B	177	ASP	CB-CG-OD1	11.90	129.01	118.30
2	D	296	HIS	CA-CB-CG	11.70	133.49	113.60
1	A	245	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	C	274	ARG	NE-CZ-NH1	11.44	126.02	120.30
2	D	345	ASP	CA-C-O	-11.15	96.68	120.10
1	C	200	ARG	NE-CZ-NH2	-11.03	114.78	120.30
1	A	294	PRO	CA-C-N	10.30	139.86	117.20
1	A	293	VAL	N-CA-CB	-10.14	89.18	111.50
1	A	295	HIS	CB-CA-C	-10.07	90.26	110.40
2	D	324	PRO	CA-N-CD	-9.54	98.14	111.50
2	B	423	LEU	CB-CG-CD1	9.44	127.05	111.00
1	A	260	ARG	NE-CZ-NH1	9.39	124.99	120.30
2	B	324	PRO	CA-N-CD	-9.33	98.44	111.50
1	A	270	ASP	CB-CG-OD1	9.28	126.65	118.30
1	A	295	HIS	CA-C-O	9.28	139.58	120.10
1	C	274	ARG	CD-NE-CZ	9.08	136.31	123.60
1	C	154	VAL	CA-C-O	-9.04	101.12	120.10
1	A	126	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	293	VAL	CA-CB-CG1	8.84	124.16	110.90
2	B	241	ARG	NE-CZ-NH1	8.81	124.70	120.30
2	D	323	GLN	CA-C-O	-8.48	102.28	120.10
2	B	382	TYR	CB-CG-CD2	-8.48	115.91	121.00
1	C	39	THR	C-N-CA	8.47	142.87	121.70
1	A	50	ARG	NE-CZ-NH2	-8.34	116.13	120.30
2	B	241	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	C	210	ASP	CB-CG-OD2	8.28	125.75	118.30
1	C	155	PRO	CA-N-CD	-8.02	100.27	111.50
1	C	217	ARG	CB-CG-CD	8.00	132.40	111.60
1	C	150	ARG	NE-CZ-NH2	-7.98	116.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	260	ARG	CD-NE-CZ	7.97	134.76	123.60
1	A	19	TYR	CB-CG-CD2	-7.96	116.22	121.00
1	C	169	ARG	NE-CZ-NH2	-7.96	116.32	120.30
2	B	323	GLN	CA-C-O	-7.96	103.39	120.10
1	C	50	ARG	NE-CZ-NH1	7.95	124.28	120.30
2	B	178	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	A	127	ASP	CB-CG-OD1	7.83	125.35	118.30
2	B	305	ASP	CB-CG-OD2	7.81	125.33	118.30
1	A	122	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	199	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	230	VAL	CB-CA-C	-7.67	96.82	111.40
1	C	122	ARG	CA-CB-CG	7.66	130.26	113.40
2	D	293	ARG	CD-NE-CZ	7.62	134.27	123.60
1	A	163	VAL	N-CA-CB	-7.56	94.86	111.50
2	B	392	MET	CG-SD-CE	7.40	112.04	100.20
1	A	122	ARG	CA-CB-CG	7.36	129.58	113.40
1	A	157	ARG	CD-NE-CZ	7.34	133.87	123.60
2	D	424	LEU	CA-CB-CG	7.23	131.94	115.30
1	C	199	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	C	50	ARG	NE-CZ-NH2	-7.17	116.72	120.30
2	D	216	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	A	157	ARG	CA-CB-CG	7.16	129.15	113.40
2	B	423	LEU	CA-CB-CG	7.15	131.74	115.30
2	B	378	ARG	NE-CZ-NH1	7.14	123.87	120.30
2	B	393	ASP	CB-CG-OD2	7.13	124.72	118.30
1	C	295	HIS	N-CA-CB	7.12	123.42	110.60
2	B	318	TYR	CB-CG-CD1	7.11	125.27	121.00
2	D	241	ARG	NH1-CZ-NH2	7.10	127.21	119.40
1	A	155	PRO	CA-N-CD	-7.05	101.63	111.50
2	B	316	THR	N-CA-CB	-7.02	96.96	110.30
2	B	422	SER	C-N-CA	-6.98	104.25	121.70
2	B	345	ASP	CA-C-O	-6.96	105.49	120.10
1	C	206	ASP	CB-CG-OD1	-6.93	112.06	118.30
2	D	395	HIS	CA-CB-CG	6.90	125.34	113.60
1	C	40	GLU	CA-C-O	6.89	134.56	120.10
1	A	145	ASP	CB-CG-OD1	6.88	124.50	118.30
1	C	50	ARG	CD-NE-CZ	-6.67	114.25	123.60
1	A	57	GLU	OE1-CD-OE2	-6.67	115.30	123.30
2	D	346	PRO	CA-N-CD	-6.66	102.17	111.50
1	C	127	ASP	CB-CG-OD1	6.65	124.28	118.30
1	C	155	PRO	N-CA-CB	6.65	111.28	103.30
1	A	230	VAL	N-CA-CB	6.61	126.04	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	288	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	40	GLU	C-N-CA	6.54	138.06	121.70
1	A	145	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	C	39	THR	N-CA-CB	6.50	122.64	110.30
1	A	292	PRO	O-C-N	-6.48	112.33	122.70
1	C	206	ASP	OD1-CG-OD2	6.41	135.48	123.30
2	B	411	GLU	CB-CA-C	-6.39	97.62	110.40
2	D	199	TYR	CB-CG-CD1	6.38	124.83	121.00
1	C	57	GLU	OE1-CD-OE2	-6.33	115.71	123.30
1	C	40	GLU	CA-C-N	-6.32	103.29	117.20
1	C	41	THR	N-CA-C	-6.32	93.93	111.00
1	A	154	VAL	CA-C-O	-6.30	106.87	120.10
2	B	318	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	A	233	MET	CG-SD-CE	6.23	110.17	100.20
1	C	195	GLU	OE1-CD-OE2	-6.23	115.83	123.30
1	A	295	HIS	CA-C-N	-6.21	103.54	117.20
1	A	209	ILE	O-C-N	-6.20	112.78	122.70
1	A	36	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	51	GLU	OE1-CD-OE2	-6.13	115.94	123.30
2	B	201	LYS	CA-CB-CG	6.13	126.89	113.40
1	A	180	TYR	CB-CG-CD2	-6.13	117.32	121.00
2	B	346	PRO	CA-N-CD	-6.09	102.97	111.50
1	A	85	GLN	N-CA-CB	-6.07	99.67	110.60
1	A	293	VAL	O-C-N	-6.04	109.61	121.10
1	C	17	VAL	CB-CA-C	-6.03	99.95	111.40
1	A	40	GLU	CA-C-O	5.98	132.66	120.10
1	A	143	LEU	CB-CG-CD1	5.94	121.10	111.00
2	D	220	GLU	OE1-CD-OE2	5.94	130.43	123.30
1	C	216	PHE	CB-CG-CD1	5.93	124.95	120.80
1	C	157	ARG	CD-NE-CZ	5.92	131.89	123.60
2	D	210	MET	CA-CB-CG	5.88	123.30	113.30
1	C	200	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	40	GLU	N-CA-CB	5.88	121.19	110.60
2	B	349	LYS	CA-CB-CG	5.87	126.31	113.40
1	C	157	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	73	GLU	CA-CB-CG	5.83	126.22	113.40
1	C	199	ARG	NE-CZ-NH1	-5.83	117.39	120.30
2	B	370	GLN	CA-CB-CG	5.82	126.19	113.40
1	C	127	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	30	VAL	CA-CB-CG2	5.80	119.60	110.90
2	D	211	ARG	NE-CZ-NH2	5.78	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	D	350	TYR	CB-CG-CD1	5.72	124.43	121.00
2	D	250	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	55	LEU	CB-CG-CD1	5.66	120.62	111.00
1	A	122	ARG	CD-NE-CZ	5.64	131.49	123.60
2	B	410	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	B	324	PRO	N-CD-CG	5.59	111.58	103.20
2	B	232	LEU	CB-CG-CD2	5.58	120.49	111.00
1	A	68	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	214	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	B	346	PRO	N-CA-CB	5.51	109.91	103.30
1	A	19	TYR	CB-CA-C	-5.50	99.41	110.40
2	D	177	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	120	SER	CA-CB-OG	-5.45	96.49	111.20
1	A	157	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	236	TYR	CB-CG-CD1	-5.42	117.75	121.00
2	D	205	ASP	CB-CG-OD2	5.41	123.17	118.30
2	D	199	TYR	CA-CB-CG	5.40	123.66	113.40
2	B	423	LEU	O-C-N	-5.40	114.06	122.70
1	A	247	ASP	N-CA-CB	-5.37	100.93	110.60
2	D	224	GLU	CA-CB-CG	5.36	125.19	113.40
1	A	157	ARG	CB-CA-C	-5.35	99.69	110.40
1	A	256	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	150	ARG	NH1-CZ-NH2	5.35	125.29	119.40
2	D	245	SER	CB-CA-C	-5.35	99.94	110.10
2	D	350	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	14	THR	CA-CB-CG2	-5.32	104.95	112.40
2	D	296	HIS	N-CA-CB	-5.32	101.03	110.60
1	A	250	LYS	CB-CG-CD	5.29	125.35	111.60
1	C	155	PRO	N-CD-CG	5.27	111.10	103.20
1	C	216	PHE	CB-CG-CD2	-5.25	117.12	120.80
2	D	253	LEU	CA-C-O	5.23	131.08	120.10
2	B	423	LEU	CB-CG-CD2	-5.21	102.15	111.00
2	B	200	MET	CG-SD-CE	5.20	108.53	100.20
1	A	39	THR	N-CA-CB	5.20	120.18	110.30
2	B	232	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	226	VAL	CG1-CB-CG2	-5.18	102.61	110.90
2	D	418	TYR	CA-CB-CG	5.18	123.24	113.40
1	C	150	ARG	CA-CB-CG	5.17	124.77	113.40
1	A	72	THR	N-CA-CB	-5.16	100.50	110.30
2	B	365	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	162	GLU	O-C-N	5.13	130.91	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	267	PHE	CB-CG-CD2	-5.11	117.22	120.80
2	B	422	SER	N-CA-CB	5.11	118.16	110.50
1	A	233	MET	CA-CB-CG	-5.11	104.62	113.30
1	A	288	ASP	CB-CG-OD2	-5.05	113.76	118.30
2	D	283	ASP	N-CA-CB	5.04	119.67	110.60
2	B	296	HIS	N-CA-CB	-5.04	101.53	110.60
2	B	391	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	230	VAL	CA-CB-CG1	5.00	118.40	110.90

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	SER	Mainchain
1	A	154	VAL	Mainchain,Peptide
1	A	293	VAL	Mainchain
2	B	323	GLN	Mainchain,Peptide
2	B	345	ASP	Mainchain,Peptide
2	B	423	LEU	Mainchain
1	C	154	VAL	Mainchain,Peptide
2	D	323	GLN	Mainchain,Peptide
2	D	345	ASP	Mainchain,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	A	2388	0	2428	83	0
1	C	2388	0	2429	151	0
2	B	2083	0	2107	59	0
2	D	2083	0	2107	110	0
3	A	33	0	9	1	0
3	C	26	0	0	0	0
4	A	266	0	0	16	0
4	B	229	0	0	12	0
4	C	145	0	0	46	0
4	D	83	0	0	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9724	0	9080	386	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 21.

All (386) 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:230:VAL:HA	1:A:233:MET:HE3	1.35	1.04
2:B:423:LEU:HB2	4:B:2222:HOH:O	1.63	0.98
1:A:177:CYS:HB2	4:A:2152:HOH:O	1.68	0.90
1:A:41:THR:HG22	1:A:42:GLU:H	1.39	0.88
2:B:177:ASP:HB2	4:B:2048:HOH:O	1.74	0.86
2:D:376:LEU:HD23	2:D:379:LYS:HD3	1.58	0.85
1:C:130:PRO:HA	4:C:2084:HOH:O	1.75	0.85
1:A:60:HIS:HD2	1:A:62:ASN:H	1.25	0.84
2:B:422:SER:OG	2:B:423:LEU:HD12	1.78	0.83
1:C:218:THR:HG22	1:C:219:LEU:HG	1.60	0.82
1:A:72:THR:HG22	1:A:75:LYS:H	1.43	0.82
1:A:41:THR:HA	4:A:2043:HOH:O	1.78	0.82
1:C:183:ALA:HB1	1:C:274:ARG:HH11	1.44	0.81
1:A:230:VAL:HA	1:A:233:MET:CE	2.12	0.80
2:D:275:VAL:HG11	2:D:292:LEU:HD21	1.64	0.80
1:C:277:ALA:HB3	4:D:2009:HOH:O	1.83	0.79
1:A:230:VAL:CA	1:A:233:MET:HE3	2.11	0.79
1:A:60:HIS:CD2	1:A:62:ASN:H	2.01	0.79
1:A:161:HIS:HD2	4:A:2136:HOH:O	1.65	0.79
1:C:83:LEU:HD13	1:C:134:LEU:HB2	1.65	0.78
1:C:174:LEU:HB3	1:C:212:LEU:HD21	1.64	0.78
2:D:194:LYS:HD3	2:D:351:LEU:HD23	1.66	0.78
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.66	0.77
2:B:414:LYS:HG2	2:B:423:LEU:HD13	1.66	0.77
2:B:414:LYS:HG2	2:B:423:LEU:CD1	2.15	0.77
1:C:156:VAL:HG11	1:C:181:SER:HB2	1.67	0.76
2:B:296:HIS:NE2	2:B:300:LYS:HE2	1.99	0.76
1:C:243:TRP:HA	4:C:2124:HOH:O	1.83	0.76
2:D:206:ILE:HG22	2:D:210:MET:HE1	1.69	0.75
2:B:328:LYS:NZ	2:B:424:LEU:HD21	2.02	0.75
2:B:316:THR:HG21	4:B:2023:HOH:O	1.87	0.74
2:D:175:VAL:N	2:D:176:PRO:CD	2.50	0.74
2:D:296:HIS:CD2	2:D:300:LYS:HE2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:LEU:O	1:C:38:ASP:HB2	1.86	0.73
1:C:227:TRP:O	1:C:230:VAL:HG22	1.88	0.73
1:A:139:GLY:CA	1:A:293:VAL:HA	2.18	0.73
1:C:0:SER:O	4:C:2002:HOH:O	2.07	0.73
2:B:423:LEU:CB	4:B:2222:HOH:O	2.28	0.72
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.71	0.72
1:C:263:LEU:HD12	4:C:2134:HOH:O	1.89	0.72
1:C:177:CYS:HB2	4:C:2102:HOH:O	1.90	0.72
1:C:218:THR:HA	1:C:246:GLN:HG3	1.70	0.72
2:D:322:GLN:NE2	2:D:326:ASN:H	1.88	0.71
1:A:88:LYS:HD3	1:A:131:GLN:HE22	1.56	0.71
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.73	0.71
1:A:39:THR:HG22	1:A:40:GLU:H	1.56	0.70
1:C:221:THR:HB	4:C:2111:HOH:O	1.90	0.70
1:C:41:THR:HB	4:C:2046:HOH:O	1.91	0.70
2:B:328:LYS:HZ1	2:B:424:LEU:HD21	1.57	0.70
1:C:0:SER:HA	4:C:2002:HOH:O	1.91	0.70
2:D:322:GLN:HE21	2:D:325:ALA:HA	1.55	0.69
1:C:181:SER:OG	1:C:182:THR:N	2.26	0.69
1:C:198:THR:O	1:C:199:ARG:HB2	1.91	0.69
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.75	0.69
1:C:267:LEU:HG	4:C:2134:HOH:O	1.92	0.69
1:C:238:PRO:HD3	4:C:2118:HOH:O	1.92	0.68
2:D:206:ILE:HG22	2:D:210:MET:CE	2.23	0.68
2:D:196:LYS:HG2	2:D:244:SER:HB3	1.75	0.68
1:A:138:GLU:HG2	4:A:2116:HOH:O	1.94	0.68
1:C:60:HIS:HD2	1:C:62:ASN:H	1.41	0.68
1:C:212:LEU:HD22	4:C:2108:HOH:O	1.95	0.67
2:D:358:ALA:HB1	2:D:391:LEU:HD13	1.76	0.67
2:D:418:TYR:HB2	4:D:2071:HOH:O	1.93	0.67
1:C:164:VAL:HG13	4:C:2082:HOH:O	1.95	0.67
1:A:74:ASN:ND2	1:A:74:ASN:H	1.92	0.67
1:C:42:GLU:HG3	4:C:2048:HOH:O	1.94	0.67
2:D:388:LYS:HG3	2:D:432:LEU:HD13	1.76	0.66
1:C:187:TRP:HB2	4:C:2139:HOH:O	1.95	0.66
1:C:155:PRO:HD3	2:D:320:LEU:HD21	1.78	0.66
1:A:137:THR:O	1:A:293:VAL:HG13	1.96	0.66
1:C:133:LEU:HD12	4:C:2084:HOH:O	1.94	0.65
1:C:87:LEU:HD23	4:C:2084:HOH:O	1.94	0.65
1:A:154:VAL:O	2:B:316:THR:HG23	1.96	0.65
2:D:321:HIS:ND1	2:D:376:LEU:HG	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:LYS:HG2	2:B:293:ARG:HH21	1.61	0.64
1:C:137:THR:HG22	1:C:296:LEU:CD1	2.28	0.64
2:D:429:THR:HA	4:D:2079:HOH:O	1.96	0.64
1:A:293:VAL:HG12	1:A:294:PRO:HD2	1.80	0.64
1:C:127:ASP:HA	4:C:2082:HOH:O	1.98	0.63
1:A:34:LYS:HE3	1:A:75:LYS:HD3	1.80	0.63
2:D:376:LEU:HA	2:D:379:LYS:HB3	1.81	0.62
1:C:60:HIS:CD2	1:C:62:ASN:H	2.17	0.62
1:A:248:PHE:HB2	4:A:2223:HOH:O	1.98	0.62
1:C:6:LYS:HG3	4:C:2007:HOH:O	1.99	0.62
2:D:430:LEU:HB2	4:D:2083:HOH:O	1.99	0.62
1:C:209:ILE:HD11	1:C:213:PHE:CZ	2.35	0.62
2:D:176:PRO:HA	2:D:179:HIS:CD2	2.34	0.62
1:C:34:LYS:HE3	1:C:77:TYR:OH	1.99	0.62
2:D:428:GLU:HG3	2:D:429:THR:HG23	1.82	0.61
2:D:321:HIS:HB2	2:D:376:LEU:HD11	1.80	0.61
1:C:195:GLU:HB2	4:C:2104:HOH:O	2.01	0.61
1:C:17:VAL:HG22	4:C:2011:HOH:O	2.00	0.61
1:C:154:VAL:O	2:D:316:THR:HG23	1.99	0.61
2:D:407:GLN:OE1	2:D:410:ARG:HD3	2.01	0.61
1:C:129:LYS:HG3	1:C:131:GLN:HG2	1.82	0.60
2:B:423:LEU:HB3	4:B:2220:HOH:O	2.01	0.60
1:A:34:LYS:HE3	1:A:75:LYS:CD	2.32	0.60
1:C:130:PRO:HG3	4:C:2105:HOH:O	2.01	0.60
2:D:425:ASN:HA	4:D:2073:HOH:O	2.00	0.60
1:C:52:ILE:HD11	1:C:78:LEU:CD2	2.31	0.60
2:D:336:LEU:HA	2:D:339:LEU:HD12	1.83	0.60
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.84	0.60
1:A:250:LYS:HD3	4:A:2090:HOH:O	2.01	0.59
1:C:84:HIS:CG	1:C:296:LEU:HD13	2.37	0.59
2:B:296:HIS:CD2	2:B:300:LYS:HE2	2.37	0.59
1:C:129:LYS:HB2	1:C:130:PRO:HD2	1.84	0.59
2:D:175:VAL:N	2:D:176:PRO:HD2	2.18	0.59
1:C:35:ILE:HA	4:C:2017:HOH:O	2.03	0.59
1:C:248:PHE:HA	1:C:251:VAL:HG23	1.85	0.58
2:B:392:MET:HA	2:B:392:MET:CE	2.34	0.58
2:D:278:PHE:O	2:D:281:ILE:HG12	2.03	0.58
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.39	0.58
2:D:427:PRO:HA	4:D:2076:HOH:O	2.03	0.58
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.84	0.58
2:D:399:LEU:HD23	2:D:426:PRO:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:337:GLY:O	2:D:340:SER:OG	2.23	0.57
1:C:88:LYS:HD3	1:C:131:GLN:NE2	2.20	0.57
1:C:183:ALA:HB1	1:C:274:ARG:NH1	2.16	0.57
1:C:261:SER:O	1:C:265:GLN:HG3	2.05	0.57
2:B:423:LEU:HD13	4:B:2222:HOH:O	2.05	0.57
1:A:41:THR:HG22	1:A:42:GLU:N	2.16	0.56
2:D:196:LYS:CG	2:D:244:SER:HB3	2.35	0.56
1:C:84:HIS:CD2	1:C:296:LEU:HD22	2.41	0.56
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.89	0.56
2:D:421:VAL:HA	2:D:424:LEU:HG	1.88	0.56
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.36	0.56
1:A:107:TYR:OH	1:A:294:PRO:HB3	2.06	0.56
2:B:210:MET:HE3	2:B:250:ARG:HB2	1.87	0.55
1:C:184:VAL:HB	4:C:2103:HOH:O	2.05	0.55
1:C:197:VAL:HG21	1:C:255:LEU:HD13	1.89	0.55
1:C:156:VAL:HB	1:C:159:TYR:CE2	2.42	0.55
2:D:288:LYS:O	2:D:292:LEU:HD23	2.07	0.55
1:C:228:PRO:HA	4:C:2113:HOH:O	2.07	0.55
1:C:91:MET:HE2	1:C:196:MET:HG3	1.89	0.55
2:D:321:HIS:CB	2:D:376:LEU:HD11	2.37	0.54
1:A:74:ASN:ND2	1:A:74:ASN:N	2.55	0.54
1:C:129:LYS:HB2	1:C:130:PRO:CD	2.37	0.54
1:C:84:HIS:CD2	1:C:296:LEU:HD13	2.42	0.54
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.89	0.54
1:A:39:THR:HG21	2:B:289:LYS:HE3	1.90	0.54
1:A:5:GLN:NE2	4:A:2005:HOH:O	2.40	0.54
1:A:227:TRP:O	1:A:230:VAL:HG22	2.07	0.54
1:C:215:ILE:HG23	4:C:2109:HOH:O	2.07	0.54
1:A:88:LYS:HD3	1:A:131:GLN:NE2	2.20	0.54
1:C:51:GLU:O	1:C:55:LEU:HB2	2.07	0.54
1:A:247:ASP:HB3	1:A:250:LYS:HG3	1.90	0.54
1:C:107:TYR:O	1:C:111:LEU:HG	2.08	0.54
1:A:74:ASN:N	1:A:74:ASN:HD22	2.05	0.54
2:B:392:MET:HE2	4:B:2197:HOH:O	2.07	0.54
2:B:207:THR:OG1	2:B:210:MET:HG3	2.08	0.54
1:C:91:MET:CE	1:C:196:MET:HG3	2.38	0.53
1:A:161:HIS:CD2	4:A:2136:HOH:O	2.50	0.53
2:D:209:SER:O	2:D:213:ILE:HG13	2.08	0.53
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.89	0.53
1:C:219:LEU:HD13	4:C:2135:HOH:O	2.08	0.53
1:C:220:GLY:HA2	1:C:243:TRP:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:SER:O	1:C:184:VAL:HG22	2.09	0.53
2:D:312:ASN:HB3	4:D:2055:HOH:O	2.07	0.53
1:A:139:GLY:HA3	1:A:293:VAL:HA	1.90	0.53
2:D:386:SER:O	2:D:389:PRO:HD2	2.08	0.53
1:A:230:VAL:CG1	1:A:233:MET:HE3	2.38	0.53
2:D:366:THR:OG1	2:D:427:PRO:HD3	2.09	0.53
1:C:84:HIS:NE2	1:C:296:LEU:HB3	2.23	0.53
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.44	0.53
1:C:137:THR:O	1:C:293:VAL:HG13	2.08	0.53
2:D:322:GLN:HE22	2:D:326:ASN:H	1.54	0.52
2:B:206:ILE:HA	2:B:210:MET:SD	2.49	0.52
1:C:0:SER:CA	4:C:2002:HOH:O	2.54	0.52
2:B:183:HIS:HD2	4:B:2058:HOH:O	1.92	0.52
1:A:136:ASN:O	1:A:294:PRO:HG3	2.09	0.52
2:D:211:ARG:O	2:D:215:VAL:HG23	2.08	0.52
2:D:366:THR:HG22	2:D:367:VAL:HG23	1.92	0.52
1:C:238:PRO:HB2	4:C:2120:HOH:O	2.10	0.52
2:D:313:GLN:O	2:D:316:THR:HG22	2.09	0.52
1:C:289:VAL:HA	4:C:2143:HOH:O	2.07	0.52
1:C:163:VAL:HG12	1:C:164:VAL:HG23	1.92	0.52
2:D:270:ILE:HG13	4:D:2036:HOH:O	2.10	0.52
2:B:233:HIS:HE1	4:B:2159:HOH:O	1.92	0.52
1:A:119:HIS:CD2	1:A:182:THR:HB	2.44	0.52
1:C:164:VAL:HA	4:C:2082:HOH:O	2.09	0.52
1:C:249:SER:HA	1:C:260:ARG:HD3	1.91	0.52
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.91	0.51
1:A:15:TYR:OH	1:A:48:ALA:HA	2.10	0.51
1:A:37:LEU:O	1:A:38:ASP:HB2	2.11	0.51
2:D:340:SER:HA	2:D:347:TYR:CD2	2.45	0.51
2:B:201:LYS:HD3	2:B:201:LYS:O	2.10	0.51
1:C:163:VAL:CG1	1:C:164:VAL:HG23	2.41	0.51
2:B:423:LEU:CD1	4:B:2222:HOH:O	2.58	0.51
1:C:83:LEU:HD13	1:C:134:LEU:CB	2.39	0.51
1:C:260:ARG:O	1:C:264:SER:OG	2.24	0.51
1:C:183:ALA:CB	1:C:274:ARG:HH11	2.18	0.51
1:A:119:HIS:HD2	4:B:2049:HOH:O	1.94	0.51
2:D:327:CYS:HB2	2:D:419:HIS:NE2	2.25	0.51
1:C:161:HIS:NE2	1:C:176:GLY:HA2	2.26	0.51
1:A:223:ASP:OD1	1:A:226:VAL:HG12	2.11	0.50
2:D:360:PHE:O	2:D:364:LEU:HB2	2.11	0.50
1:A:242:LYS:HB2	4:A:2209:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:399:LEU:CD2	2:D:426:PRO:HG2	2.42	0.50
1:C:101:LEU:N	1:C:102:PRO:HD2	2.27	0.50
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.46	0.50
1:C:219:LEU:HD12	4:C:2109:HOH:O	2.11	0.50
2:B:210:MET:CE	2:B:250:ARG:HB2	2.41	0.50
1:C:217:ARG:HG3	1:C:243:TRP:CD1	2.47	0.50
1:C:216:PHE:CE1	1:C:222:PRO:HD3	2.47	0.49
1:A:195:GLU:O	1:A:199:ARG:HA	2.11	0.49
1:C:231:THR:HA	1:C:236:TYR:CD1	2.47	0.49
1:C:227:TRP:CE3	1:C:269:TYR:HB3	2.47	0.49
1:A:74:ASN:H	1:A:74:ASN:HD22	1.60	0.49
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.47	0.49
1:A:39:THR:HG21	2:B:289:LYS:CE	2.42	0.49
2:B:392:MET:HA	2:B:392:MET:HE3	1.95	0.49
1:C:35:ILE:HB	1:C:76:LEU:HB3	1.94	0.49
1:C:186:ILE:HG13	1:C:275:ILE:O	2.12	0.49
2:D:430:LEU:O	2:D:431:ASN:HB2	2.13	0.49
2:B:423:LEU:CG	4:B:2222:HOH:O	2.58	0.49
1:A:60:HIS:HE1	4:A:2042:HOH:O	1.96	0.49
1:C:71:HIS:NE2	2:D:296:HIS:ND1	2.61	0.48
1:C:33:LYS:NZ	1:C:51:GLU:OE1	2.44	0.48
1:A:284:PRO:O	1:A:287:GLN:HG2	2.14	0.48
2:D:303:THR:O	2:D:304:PHE:HB2	2.13	0.48
1:C:217:ARG:HG3	1:C:243:TRP:CE2	2.48	0.48
2:B:395:HIS:HE1	2:B:427:PRO:O	1.96	0.48
1:C:129:LYS:HB3	4:C:2081:HOH:O	2.12	0.48
1:C:220:GLY:O	1:C:221:THR:C	2.49	0.48
1:C:74:ASN:H	1:C:74:ASN:ND2	2.11	0.48
2:D:401:ALA:HB3	2:D:402:PRO:CD	2.41	0.48
2:D:407:GLN:O	2:D:411:GLU:HG2	2.13	0.48
2:D:374:GLU:HA	2:D:377:ILE:CD1	2.44	0.48
1:C:194:ALA:CB	1:C:202:LEU:HD22	2.43	0.48
1:A:71:HIS:CD2	1:A:76:LEU:HD13	2.49	0.48
1:A:139:GLY:HA2	1:A:293:VAL:HA	1.92	0.48
2:B:289:LYS:CG	2:B:293:ARG:HH21	2.26	0.48
1:A:223:ASP:H	1:A:226:VAL:CG1	2.27	0.48
1:C:186:ILE:HD12	4:C:2141:HOH:O	2.13	0.48
2:D:362:LEU:HD21	2:D:395:HIS:HB2	1.96	0.48
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.97	0.48
2:B:211:ARG:HH11	2:B:211:ARG:HG2	1.79	0.48
1:A:97:THR:HG22	1:A:97:THR:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:THR:HG22	1:C:40:GLU:N	2.29	0.47
1:A:148:LEU:HD12	4:A:2119:HOH:O	2.14	0.47
1:C:150:ARG:NH2	1:C:160:TPO:O1P	2.47	0.47
2:D:332:LEU:HD12	2:D:335:PHE:CD2	2.50	0.47
2:B:211:ARG:NH1	2:B:211:ARG:HG2	2.29	0.47
1:A:85:GLN:OE1	1:A:296:LEU:HD22	2.13	0.47
2:D:332:LEU:HG	2:D:332:LEU:O	2.13	0.47
1:C:88:LYS:HD3	1:C:131:GLN:HE22	1.79	0.47
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.83	0.47
2:D:207:THR:OG1	2:D:210:MET:HG3	2.14	0.47
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.49	0.47
2:D:366:THR:HG22	2:D:367:VAL:N	2.29	0.47
1:C:174:LEU:HD13	1:C:212:LEU:HD23	1.97	0.47
1:C:212:LEU:HB3	4:C:2108:HOH:O	2.15	0.47
2:D:336:LEU:HA	2:D:339:LEU:CD1	2.45	0.47
1:C:150:ARG:HH21	1:C:160:TPO:P	2.37	0.47
2:D:347:TYR:OH	2:D:394:LEU:HA	2.15	0.47
2:D:233:HIS:CD2	2:D:341:LEU:HD21	2.49	0.47
2:D:414:LYS:HG2	2:D:423:LEU:HG	1.97	0.47
1:A:131:GLN:H	1:A:131:GLN:CD	2.19	0.46
2:B:414:LYS:HG2	2:B:423:LEU:HD11	1.97	0.46
1:C:194:ALA:HB3	1:C:202:LEU:HD22	1.97	0.46
1:A:72:THR:O	2:B:296:HIS:HE1	1.99	0.46
2:D:296:HIS:NE2	2:D:300:LYS:HE2	2.31	0.46
2:D:230:GLU:HA	4:D:2055:HOH:O	2.15	0.46
1:A:137:THR:O	1:A:293:VAL:CG1	2.63	0.46
1:C:231:THR:HA	1:C:236:TYR:CE1	2.51	0.46
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.51	0.46
1:C:17:VAL:HB	1:C:19:TYR:CE1	2.51	0.46
2:D:232:LEU:O	2:D:236:VAL:HG23	2.16	0.46
1:C:15:TYR:OH	1:C:48:ALA:HA	2.16	0.46
1:C:100:PRO:O	1:C:104:ILE:HG13	2.16	0.46
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.51	0.46
1:C:156:VAL:HG21	1:C:180:TYR:O	2.16	0.45
1:C:227:TRP:HA	1:C:228:PRO:HD2	1.63	0.45
1:C:98:GLY:HA2	1:C:199:ARG:NE	2.31	0.45
2:D:319:PHE:CZ	2:D:333:ALA:HB3	2.52	0.45
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.80	0.45
2:D:361:HIS:CD2	2:D:384:LEU:HD11	2.51	0.45
2:D:342:ILE:HG21	2:D:404:HIS:CE1	2.51	0.45
1:C:266:MET:HG2	4:C:2141:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:VAL:HA	4:C:2139:HOH:O	2.16	0.45
2:B:219:VAL:HG22	2:B:232:LEU:HD11	1.98	0.45
2:D:338:GLU:CD	2:D:412:LYS:HZ3	2.20	0.45
2:B:283:ASP:O	2:B:284:ASP:HB2	2.15	0.45
2:D:334:MET:O	2:D:335:PHE:C	2.55	0.45
2:D:409:ILE:O	2:D:412:LYS:HB3	2.15	0.45
2:D:396:GLN:O	2:D:399:LEU:N	2.50	0.45
1:C:169:ARG:HG2	1:C:173:ILE:HB	1.97	0.45
2:D:395:HIS:CD2	2:D:430:LEU:HG	2.52	0.45
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.99	0.45
2:D:402:PRO:HB2	2:D:403:GLN:NE2	2.32	0.45
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.32	0.45
1:C:174:LEU:CB	1:C:212:LEU:HD21	2.42	0.45
1:C:274:ARG:NH1	4:C:2139:HOH:O	2.49	0.44
1:A:103:LEU:HD13	1:A:293:VAL:O	2.17	0.44
2:D:415:ASN:OD1	2:D:416:SER:N	2.50	0.44
1:A:230:VAL:CG1	1:A:233:MET:CE	2.95	0.44
1:A:129:LYS:HG3	1:A:131:GLN:HG2	1.99	0.44
2:D:404:HIS:O	2:D:407:GLN:NE2	2.43	0.44
1:A:37:LEU:O	1:A:38:ASP:CB	2.65	0.44
1:C:236:TYR:HD2	4:C:2115:HOH:O	2.00	0.44
1:A:230:VAL:HG13	1:A:233:MET:CE	2.47	0.44
2:B:296:HIS:NE2	2:B:300:LYS:CE	2.77	0.44
1:C:106:SER:O	1:C:109:PHE:N	2.51	0.44
1:A:260:ARG:HD3	4:A:2230:HOH:O	2.16	0.44
2:D:332:LEU:CD2	2:D:363:ALA:HA	2.44	0.44
2:B:396:GLN:HE21	2:B:400:LYS:HE3	1.83	0.44
2:B:308:ALA:HA	2:B:309:PRO:HD3	1.86	0.44
2:D:210:MET:HE2	2:D:210:MET:HB2	1.84	0.44
1:A:39:THR:HG22	2:B:292:LEU:HD23	1.99	0.44
1:C:111:LEU:HD21	1:C:141:ILE:HD13	2.00	0.44
1:A:268:HIS:CD2	4:A:2192:HOH:O	2.70	0.43
2:B:289:LYS:HG3	2:B:293:ARG:HE	1.83	0.43
1:A:138:GLU:CG	4:A:2116:HOH:O	2.58	0.43
2:D:233:HIS:HB2	4:D:2055:HOH:O	2.18	0.43
1:C:295:HIS:C	1:C:295:HIS:ND1	2.70	0.43
2:D:275:VAL:HG23	4:D:2040:HOH:O	2.18	0.43
2:D:178:TYR:HB3	2:D:182:ILE:HG13	2.00	0.43
1:C:88:LYS:CD	1:C:131:GLN:HE22	2.32	0.43
2:D:206:ILE:HG21	2:D:206:ILE:HD13	1.77	0.43
1:A:154:VAL:O	2:B:316:THR:CG2	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:361:HIS:CE1	2:D:384:LEU:HD21	2.54	0.43
2:D:398:TYR:HD1	2:D:398:TYR:O	2.01	0.43
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.88	0.43
2:D:184:THR:O	2:D:187:ARG:HB2	2.19	0.43
1:C:109:PHE:HD2	4:C:2038:HOH:O	2.01	0.43
1:C:129:LYS:O	1:C:133:LEU:HG	2.19	0.43
2:B:332:LEU:HD23	2:B:363:ALA:HA	2.01	0.43
4:C:2044:HOH:O	2:D:292:LEU:HD23	2.19	0.42
1:C:71:HIS:NE2	2:D:296:HIS:CE1	2.87	0.42
1:A:39:THR:HG21	2:B:289:LYS:HD2	2.01	0.42
2:B:275:VAL:HG11	2:B:292:LEU:HD13	2.00	0.42
1:C:169:ARG:HD3	1:C:173:ILE:CG2	2.49	0.42
1:A:39:THR:CG2	2:B:292:LEU:HD23	2.50	0.42
1:A:17:VAL:O	1:A:33:LYS:HA	2.19	0.42
2:D:214:LEU:O	2:D:218:LEU:HG	2.19	0.42
1:C:170:ALA:HB2	4:C:2139:HOH:O	2.18	0.42
2:D:299:LEU:HD13	2:D:304:PHE:CE1	2.55	0.42
1:C:198:THR:O	1:C:199:ARG:CB	2.60	0.42
2:B:368:THR:CB	2:B:370:GLN:HE21	2.33	0.42
1:C:43:GLY:HA3	2:D:292:LEU:HD12	2.01	0.42
1:C:241:PRO:HG2	1:C:243:TRP:CH2	2.55	0.42
1:C:199:ARG:HG3	4:C:2106:HOH:O	2.19	0.42
2:D:314:PHE:HA	2:D:317:GLN:HG3	2.02	0.42
1:A:227:TRP:HB3	1:A:230:VAL:HG22	2.00	0.42
1:A:40:GLU:H	2:B:292:LEU:HD23	1.84	0.42
2:D:332:LEU:HB2	2:D:421:VAL:HB	2.02	0.42
2:D:332:LEU:CD2	2:D:366:THR:HG21	2.49	0.42
2:D:175:VAL:N	2:D:176:PRO:HD3	2.33	0.42
2:D:175:VAL:O	2:D:175:VAL:HG12	2.20	0.42
2:D:409:ILE:O	2:D:410:ARG:C	2.58	0.42
1:A:10:ILE:HD13	3:A:1298[A]:6CP:C18	2.50	0.42
1:C:217:ARG:HD3	1:C:243:TRP:NE1	2.35	0.41
2:D:361:HIS:HD2	2:D:391:LEU:HG	1.84	0.41
1:A:39:THR:O	1:A:40:GLU:C	2.58	0.41
4:A:2158:HOH:O	2:B:175:VAL:HG12	2.20	0.41
2:D:361:HIS:CE1	2:D:384:LEU:HD11	2.55	0.41
1:C:101:LEU:HB3	1:C:102:PRO:HD3	2.01	0.41
1:C:39:THR:HG22	4:C:2044:HOH:O	2.21	0.41
1:C:38:ASP:HA	4:C:2041:HOH:O	2.21	0.41
1:C:215:ILE:HG12	4:C:2109:HOH:O	2.19	0.41
1:C:237:LYS:HA	1:C:238:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:210:MET:O	2:D:213:ILE:HB	2.21	0.41
1:C:177:CYS:SG	1:C:178:LYS:N	2.94	0.41
1:C:209:ILE:HG23	1:C:210:ASP:N	2.35	0.41
1:C:156:VAL:HB	1:C:159:TYR:HE2	1.83	0.41
2:D:206:ILE:HA	2:D:210:MET:CE	2.51	0.41
2:B:428:GLU:HG2	2:B:428:GLU:H	1.56	0.41
1:A:261:SER:O	1:A:265:GLN:HG3	2.21	0.41
2:D:194:LYS:HA	2:D:195:PRO:HD3	1.92	0.41
2:B:424:LEU:HD23	2:B:424:LEU:HA	1.81	0.40
1:A:293:VAL:CG1	1:A:294:PRO:HD2	2.47	0.40
2:B:275:VAL:HG11	2:B:292:LEU:CD1	2.51	0.40
2:B:410:ARG:HH21	2:B:410:ARG:HD3	1.60	0.40
2:B:296:HIS:O	2:B:300:LYS:HG3	2.21	0.40
1:C:217:ARG:HG3	1:C:243:TRP:NE1	2.35	0.40
1:A:34:LYS:HD2	1:A:77:TYR:OH	2.21	0.40
1:C:72:THR:O	2:D:296:HIS:HE1	2.04	0.40
1:A:250:LYS:NZ	4:A:2229:HOH:O	2.54	0.40
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.85	0.40
1:C:72:THR:HG22	1:C:74:ASN:ND2	2.37	0.40
1:C:240:PHE:HD2	4:C:2119:HOH:O	2.02	0.40
1:C:101:LEU:HB3	1:C:102:PRO:CD	2.52	0.40
2:D:262:LEU:HD11	2:D:266:LYS:HE3	2.03	0.40
2:B:407:GLN:O	2:B:411:GLU:HG2	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	294/303 (97%)	280 (95%)	8 (3%)	6 (2%)	<b>9</b> <b>3</b>
1	C	294/303 (97%)	265 (90%)	18 (6%)	11 (4%)	<b>4</b> <b>1</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	256/258 (99%)	251 (98%)	3 (1%)	2 (1%)	24	15
2	D	256/258 (99%)	230 (90%)	22 (9%)	4 (2%)	12	5
All	All	1100/1122 (98%)	1026 (93%)	51 (5%)	23 (2%)	9	3

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	293	VAL
1	A	294	PRO
1	C	38	ASP
1	C	39	THR
2	D	346	PRO
2	B	324	PRO
1	C	164	VAL
1	C	294	PRO
1	C	295	HIS
2	D	420	GLY
1	A	164	VAL
2	B	346	PRO
1	C	155	PRO
1	C	181	SER
1	C	199	ARG
1	A	40	GLU
1	C	145	ASP
1	A	295	HIS
1	C	41	THR
2	D	421	VAL
1	C	220	GLY
2	D	372	TRP

### 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	261/265 (98%)	236 (90%)	25 (10%)	10	6
1	C	261/265 (98%)	232 (89%)	29 (11%)	8	4
2	B	232/232 (100%)	218 (94%)	14 (6%)	24	17
2	D	232/232 (100%)	211 (91%)	21 (9%)	12	6
All	All	986/994 (99%)	897 (91%)	89 (9%)	12	7

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	12	GLU
1	A	40	GLU
1	A	45	PRO
1	A	55	LEU
1	A	72	THR
1	A	73	GLU
1	A	74	ASN
1	A	83	LEU
1	A	101	LEU
1	A	122	ARG
1	A	131	GLN
1	A	148	LEU
1	A	150	ARG
1	A	155	PRO
1	A	163	VAL
1	A	200	ARG
1	A	206	ASP
1	A	226	VAL
1	A	230	VAL
1	A	273	LYS
1	A	278	LYS
1	A	294	PRO
1	A	295	HIS
1	A	296	LEU
2	B	179	HIS
2	B	200	MET
2	B	202	LYS
2	B	209	SER
2	B	232	LEU
2	B	292	LEU
2	B	316	THR
2	B	324	PRO

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Mol	Chain	Res	Type
2	B	374	GLU
2	B	384	LEU
2	B	391	LEU
2	B	392	MET
2	B	423	LEU
2	B	428	GLU
1	C	0	SER
1	C	2	GLU
1	C	9	LYS
1	C	12	GLU
1	C	17	VAL
1	C	40	GLU
1	C	41	THR
1	C	59	ASN
1	C	73	GLU
1	C	74	ASN
1	C	83	LEU
1	C	94	SER
1	C	101	LEU
1	C	122	ARG
1	C	131	GLN
1	C	148	LEU
1	C	150	ARG
1	C	163	VAL
1	C	199	ARG
1	C	200	ARG
1	C	206	ASP
1	C	217	ARG
1	C	226	VAL
1	C	230	VAL
1	C	232	SER
1	C	250	LYS
1	C	264	SER
1	C	278	LYS
1	C	296	LEU
2	D	177	ASP
2	D	194	LYS
2	D	197	VAL
2	D	202	LYS
2	D	210	MET
2	D	245	SER
2	D	268	GLU

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Mol	Chain	Res	Type
2	D	316	THR
2	D	324	PRO
2	D	331	SER
2	D	339	LEU
2	D	346	PRO
2	D	362	LEU
2	D	366	THR
2	D	368	THR
2	D	377	ILE
2	D	386	SER
2	D	391	LEU
2	D	397	THR
2	D	398	TYR
2	D	418	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	60	HIS
1	A	74	ASN
1	A	84	HIS
1	A	119	HIS
1	A	131	GLN
1	A	161	HIS
1	A	268	HIS
2	B	183	HIS
2	B	233	HIS
2	B	317	GLN
2	B	370	GLN
2	B	395	HIS
2	B	396	GLN
1	C	60	HIS
1	C	62	ASN
1	C	85	GLN
1	C	119	HIS
1	C	131	GLN
2	D	179	HIS
2	D	254	GLN
2	D	313	GLN
2	D	322	GLN
2	D	361	HIS

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Mol	Chain	Res	Type
2	D	403	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	TPO	A	160	1	8,10,11	1.27	1 (12%)	7,14,16	1.72	2 (28%)
1	TPO	C	160	1	8,10,11	1.47	2 (25%)	7,14,16	1.43	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	160	1	-	0/8/11/13	0/0/0/0
1	TPO	C	160	1	-	0/8/11/13	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	2.30	1.67	1.60
1	A	160	TPO	CG2-CB	2.64	1.58	1.51
1	C	160	TPO	P-O2P	2.68	1.64	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O-C-CA	-3.13	117.18	125.44
1	C	160	TPO	O-C-CA	-2.27	119.44	125.44
1	A	160	TPO	O3P-P-O2P	2.20	115.74	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	160	TPO	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 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	6CP	A	1298[A]	-	25,28,28	1.75	7 (28%)	29,38,38	3.17	9 (31%)
3	6CP	A	1298[B]	-	25,28,28	1.76	7 (28%)	29,38,38	3.58	11 (37%)
3	6CP	C	1298[A]	-	25,28,28	19.90	8 (32%)	29,38,38	12.30	13 (44%)
3	6CP	C	1298[B]	-	25,28,28	2.00	7 (28%)	29,38,38	3.49	11 (37%)

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	6CP	A	1298[A]	-	-	0/9/17/17	0/4/4/4
3	6CP	A	1298[B]	-	-	0/9/17/17	0/4/4/4
3	6CP	C	1298[A]	-	-	0/9/17/17	0/4/4/4
3	6CP	C	1298[B]	-	-	0/9/17/17	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298[B]	6CP	C6-N1	-3.97	1.24	1.31
3	C	1298[A]	6CP	C6-N1	-3.97	1.24	1.31
3	A	1298[B]	6CP	C2-N2	-3.53	1.30	1.36
3	A	1298[A]	6CP	C2-N2	-3.35	1.30	1.36
3	C	1298[B]	6CP	C5-C4	-3.09	1.33	1.40
3	C	1298[A]	6CP	C5-C4	-3.09	1.33	1.40
3	A	1298[B]	6CP	C17-N2	-2.52	1.35	1.40
3	A	1298[A]	6CP	C17-N2	-2.46	1.35	1.40
3	A	1298[B]	6CP	O6-C6	-2.36	1.33	1.35
3	A	1298[A]	6CP	O6-C6	-2.36	1.33	1.35
3	A	1298[B]	6CP	C5-C4	-2.35	1.35	1.40
3	A	1298[A]	6CP	C5-C4	-2.35	1.35	1.40
3	C	1298[B]	6CP	O6-C6	-2.18	1.33	1.35
3	C	1298[A]	6CP	O6-C6	-2.18	1.33	1.35
3	C	1298[B]	6CP	C2-N2	-2.04	1.32	1.36
3	C	1298[A]	6CP	C2-N2	-2.04	1.32	1.36
3	C	1298[B]	6CP	C12-C11	2.00	1.57	1.52
3	C	1298[A]	6CP	C12-C11	2.00	1.57	1.52
3	A	1298[B]	6CP	C14-C13	2.39	1.61	1.51
3	A	1298[A]	6CP	C14-C13	2.39	1.61	1.51
3	A	1298[B]	6CP	C2-N1	3.26	1.46	1.34
3	A	1298[A]	6CP	C2-N1	3.26	1.46	1.34
3	C	1298[B]	6CP	C2-N1	3.54	1.47	1.34
3	C	1298[A]	6CP	C2-N1	3.54	1.47	1.34
3	A	1298[B]	6CP	C4-N3	4.04	1.43	1.36
3	A	1298[A]	6CP	C4-N3	4.04	1.43	1.36
3	C	1298[B]	6CP	C4-N3	4.92	1.45	1.36
3	C	1298[A]	6CP	C4-N3	4.92	1.45	1.36
3	C	1298[A]	6CP	C19-CL1	99.02	4.00	1.74

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298[A]	6CP	C20-C19-CL1	-61.89	17.85	119.35
3	C	1298[A]	6CP	C18-C19-CL1	-14.40	101.26	119.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298[B]	6CP	C10-O6-C6	-11.60	105.11	117.23
3	A	1298[A]	6CP	C10-O6-C6	-11.60	105.11	117.23
3	C	1298[B]	6CP	N3-C2-N1	-7.95	114.02	126.22
3	C	1298[A]	6CP	N3-C2-N1	-7.95	114.02	126.22
3	A	1298[B]	6CP	C4-C5-N7	-6.45	103.54	109.48
3	A	1298[A]	6CP	C4-C5-N7	-6.45	103.54	109.48
3	C	1298[B]	6CP	C4-C5-N7	-5.33	104.58	109.48
3	C	1298[A]	6CP	C4-C5-N7	-5.33	104.58	109.48
3	A	1298[B]	6CP	N3-C2-N1	-4.97	118.60	126.22
3	A	1298[A]	6CP	N3-C2-N1	-4.97	118.60	126.22
3	C	1298[B]	6CP	C5-C6-N1	-4.62	115.65	123.81
3	C	1298[A]	6CP	C5-C6-N1	-4.62	115.65	123.81
3	C	1298[B]	6CP	C17-N2-C2	-3.59	119.67	129.19
3	C	1298[A]	6CP	C17-N2-C2	-3.59	119.67	129.19
3	C	1298[B]	6CP	C13-C12-C11	-2.97	107.43	112.22
3	C	1298[A]	6CP	C13-C12-C11	-2.97	107.43	112.22
3	A	1298[B]	6CP	C20-C19-C18	-2.90	117.65	121.53
3	C	1298[B]	6CP	C22-C17-C18	-2.73	116.42	119.69
3	C	1298[A]	6CP	C22-C17-C18	-2.73	116.42	119.69
3	A	1298[B]	6CP	O6-C10-C11	2.07	112.74	107.97
3	A	1298[A]	6CP	O6-C10-C11	2.07	112.74	107.97
3	A	1298[A]	6CP	C21-C22-C17	2.11	122.40	119.72
3	A	1298[B]	6CP	C14-C15-C16	2.41	116.49	111.44
3	A	1298[A]	6CP	C14-C15-C16	2.41	116.49	111.44
3	A	1298[B]	6CP	C13-C12-C11	2.57	116.37	112.22
3	A	1298[A]	6CP	C13-C12-C11	2.57	116.37	112.22
3	C	1298[B]	6CP	C14-C13-C12	3.27	118.30	111.44
3	C	1298[A]	6CP	C14-C13-C12	3.27	118.30	111.44
3	A	1298[B]	6CP	C2-N1-C6	3.47	120.27	115.32
3	A	1298[A]	6CP	C2-N1-C6	3.47	120.27	115.32
3	C	1298[B]	6CP	N2-C2-N3	4.74	131.36	116.93
3	C	1298[A]	6CP	N2-C2-N3	4.74	131.36	116.93
3	A	1298[B]	6CP	C18-C19-CL1	5.65	126.16	119.14
3	A	1298[B]	6CP	C2-N3-C4	5.87	122.16	115.09
3	A	1298[A]	6CP	C2-N3-C4	5.87	122.16	115.09
3	C	1298[B]	6CP	C17-C18-C19	6.12	123.62	118.65
3	C	1298[A]	6CP	C17-C18-C19	6.12	123.62	118.65
3	A	1298[B]	6CP	C17-C18-C19	6.17	123.66	118.65
3	C	1298[B]	6CP	C2-N3-C4	6.28	122.65	115.09
3	C	1298[A]	6CP	C2-N3-C4	6.28	122.65	115.09
3	C	1298[B]	6CP	C2-N1-C6	9.25	128.51	115.32
3	C	1298[A]	6CP	C2-N1-C6	9.25	128.51	115.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298[A]	6CP	1	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 ⓘ

### 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	296/303 (97%)	0.49	18 (6%) 25 26	19, 31, 61, 91	0
1	C	296/303 (97%)	2.00	98 (33%) 0 1	31, 54, 85, 99	0
2	B	258/258 (100%)	0.38	14 (5%) 29 31	21, 32, 50, 74	0
2	D	258/258 (100%)	1.65	90 (34%) 0 1	31, 58, 85, 96	0
All	All	1108/1122 (98%)	1.14	220 (19%) 1 2	19, 42, 81, 99	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	226	VAL	14.8
1	C	225	VAL	14.4
1	C	244	ALA	13.9
2	B	175	VAL	12.5
1	C	233	MET	12.5
1	C	296	LEU	11.4
1	C	227	TRP	11.1
1	C	236	TYR	11.0
1	C	230	VAL	11.0
1	A	295	HIS	10.6
1	C	243	TRP	10.2
1	C	235	ASP	9.2
1	A	40	GLU	9.2
1	C	232	SER	9.1
2	D	175	VAL	8.9
1	C	240	PHE	8.5
1	C	221	THR	7.9
1	C	223	ASP	7.7
2	D	432	LEU	7.6
1	C	231	THR	7.6
1	C	177	CYS	7.6

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Mol	Chain	Res	Type	RSRZ
1	C	234	PRO	7.6
2	D	367	VAL	7.4
1	C	241	PRO	7.4
2	D	176	PRO	7.4
1	A	39	THR	7.4
1	C	245	ARG	7.3
2	D	423	LEU	6.9
1	C	224	GLU	6.8
1	C	295	HIS	6.8
1	C	249	SER	6.7
2	D	429	THR	6.7
1	C	228	PRO	6.5
2	D	430	LEU	6.4
1	C	242	LYS	6.2
1	C	247	ASP	6.0
1	C	253	PRO	5.9
1	C	239	SER	5.9
2	D	384	LEU	5.9
2	D	364	LEU	5.8
1	C	246	GLN	5.7
1	A	96	LEU	5.7
2	D	402	PRO	5.7
2	D	311	VAL	5.7
2	D	327	CYS	5.6
1	A	293	VAL	5.6
2	D	388	LYS	5.5
1	A	36	ARG	5.5
1	C	217	ARG	5.4
2	B	423	LEU	5.4
2	D	382	TYR	5.3
2	D	390	CYS	5.3
2	D	428	GLU	5.1
2	D	401	ALA	5.0
1	C	248	PHE	4.9
1	C	38	ASP	4.9
1	C	250	LYS	4.9
2	D	383	THR	4.9
2	D	399	LEU	4.8
1	C	238	PRO	4.8
1	C	229	GLY	4.8
1	C	294	PRO	4.7
1	C	209	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	256	ASP	4.6
2	D	419	HIS	4.5
2	D	431	ASN	4.4
2	B	176	PRO	4.4
1	C	175	LEU	4.4
2	D	375	SER	4.4
2	D	425	ASN	4.4
2	D	184	THR	4.3
1	C	39	THR	4.3
2	D	372	TRP	4.2
2	D	416	SER	4.2
2	D	315	LEU	4.2
2	D	369	GLY	4.1
2	D	324	PRO	4.1
1	C	288	ASP	4.1
2	D	177	ASP	4.1
2	D	283	ASP	4.1
1	A	294	PRO	4.0
1	C	189	LEU	4.0
2	D	392	MET	4.0
2	D	284	ASP	4.0
2	D	427	PRO	3.9
1	C	179	TYR	3.9
1	C	287	GLN	3.8
1	A	38	ASP	3.8
1	C	165	THR	3.8
1	C	101	LEU	3.8
1	C	161	HIS	3.8
2	D	379	LYS	3.8
2	D	326	ASN	3.8
1	C	271	PRO	3.7
1	C	102	PRO	3.7
2	D	280	TYR	3.7
2	B	283	ASP	3.7
2	D	391	LEU	3.7
1	C	222	PRO	3.6
2	D	403	GLN	3.6
2	D	328	LYS	3.6
1	C	128	LEU	3.5
1	C	151	ALA	3.5
1	C	257	GLU	3.5
1	C	218	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	41	THR	3.4
1	C	41	THR	3.4
1	C	219	LEU	3.4
2	D	341	LEU	3.4
2	D	365	TYR	3.4
2	D	385	GLU	3.4
2	D	360	PHE	3.3
2	D	378	ARG	3.3
1	C	96	LEU	3.3
2	D	395	HIS	3.3
2	D	376	LEU	3.3
2	D	417	LYS	3.3
2	D	325	ALA	3.3
2	D	323	GLN	3.2
1	C	273	LYS	3.2
2	D	413	TYR	3.2
1	C	171	PRO	3.2
2	B	284	ASP	3.2
1	C	97	THR	3.2
1	A	95	ALA	3.1
1	C	251	VAL	3.1
2	D	415	ASN	3.0
1	C	143	LEU	3.0
2	D	320	LEU	3.0
2	D	356	ALA	3.0
2	D	422	SER	3.0
2	B	323	GLN	3.0
2	D	334	MET	2.9
2	D	368	THR	2.9
1	C	187	TRP	2.9
1	C	282	ALA	2.9
2	D	410	ARG	2.8
1	C	162	GLU	2.8
2	D	350	TYR	2.8
2	D	371	SER	2.8
1	C	84	HIS	2.8
2	B	431	ASN	2.7
1	A	296	LEU	2.7
1	C	7	VAL	2.7
2	B	234	LEU	2.7
2	D	387	LEU	2.7
2	B	236	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	199	ARG	2.7
2	D	358	ALA	2.7
1	C	40	GLU	2.7
2	D	339	LEU	2.6
1	C	99	ILE	2.6
2	D	336	LEU	2.6
1	C	292	PRO	2.6
2	D	363	ALA	2.6
1	C	36	ARG	2.6
1	C	237	LYS	2.5
1	C	111	LEU	2.5
1	C	284	PRO	2.5
1	C	269	TYR	2.5
1	C	123	VAL	2.5
1	C	260	ARG	2.5
1	C	133	LEU	2.5
2	B	324	PRO	2.5
2	D	396	GLN	2.5
1	A	19	TYR	2.4
2	D	337	GLY	2.4
1	C	220	GLY	2.4
1	A	108	LEU	2.4
1	C	286	PHE	2.4
1	C	158	THR	2.4
1	C	15	TYR	2.4
2	D	424	LEU	2.4
1	C	89	LYS	2.4
2	D	232	LEU	2.3
1	C	163	VAL	2.3
1	C	192	ILE	2.3
2	D	233	HIS	2.3
1	C	137	THR	2.3
2	D	180	GLU	2.3
2	D	202	LYS	2.3
1	C	115	LEU	2.3
2	D	178	TYR	2.3
1	A	0	SER	2.3
2	D	188	GLU	2.3
2	D	235	ALA	2.3
2	D	404	HIS	2.3
2	D	397	THR	2.3
1	C	168	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	225	TYR	2.2
2	D	366	THR	2.2
1	C	124	LEU	2.2
1	C	255	LEU	2.2
2	D	362	LEU	2.2
2	D	319	PHE	2.2
2	D	400	LYS	2.2
1	C	173	ILE	2.2
1	C	283	HIS	2.2
2	B	355	ILE	2.2
1	C	94	SER	2.2
1	A	74	ASN	2.2
2	D	197	VAL	2.2
1	A	37	LEU	2.1
2	B	177	ASP	2.1
2	D	316	THR	2.1
1	A	73	GLU	2.1
2	D	374	GLU	2.1
1	C	254	PRO	2.1
2	D	426	PRO	2.1
1	C	213	PHE	2.1
2	B	429	THR	2.1
2	B	232	LEU	2.1
1	C	42	GLU	2.1
2	D	340	SER	2.1
1	A	184	VAL	2.0
2	D	271	TYR	2.0
2	D	270	ILE	2.0
1	C	138	GLU	2.0
2	D	314	PHE	2.0
1	C	74	ASN	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TPO	C	160	11/12	0.92	0.15	-	34,44,50,52	0
1	TPO	A	160	11/12	0.99	0.10	-	24,26,27,27	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	6CP	A	1298[A]	25/25	0.92	0.15	1.89	29,35,39,40	8
3	6CP	A	1298[B]	25/25	0.92	0.15	1.17	29,34,37,37	8
3	6CP	C	1298[B]	25/25	0.93	0.16	-0.26	36,42,47,48	1
3	6CP	C	1298[A]	25/25	0.93	0.16	-1.00	36,42,47,48	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.