



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 09:03 am GMT

PDB ID : 1H1Q  
Title : Structure of human Thr160-phospho CDK2/cyclin A complexed with the inhibitor NU6094  
Authors : Davies, T.G.; Noble, M.E.M.; Endicott, J.A.; Johnson, L.N.  
Deposited on : 2002-07-21  
Resolution : 2.50 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

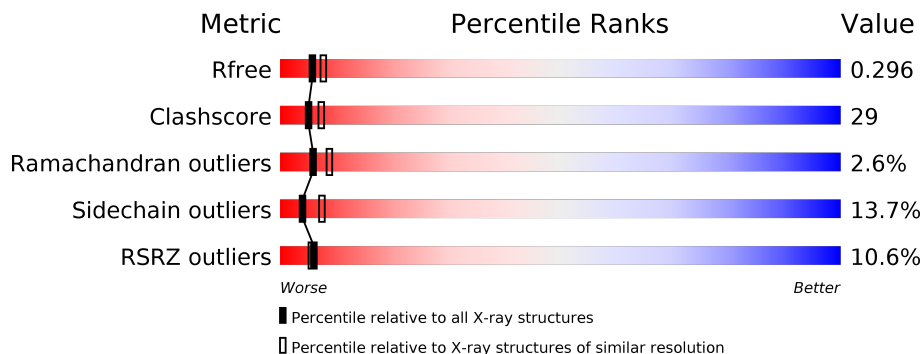
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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	 6% (poor fit), 45% (0 outliers), 39% (1 outlier), 11% (2 outliers), 0% (3+ outliers), 0% (not modelled)
1	C	303	 15% (poor fit), 31% (0 outliers), 51% (1 outlier), 14% (2 outliers), 0% (3+ outliers), 0% (not modelled)
2	B	258	 2% (poor fit), 50% (0 outliers), 36% (1 outlier), 11% (2 outliers), 0% (3+ outliers), 0% (not modelled)
2	D	258	 19% (poor fit), 33% (0 outliers), 43% (1 outlier), 19% (2 outliers), 5% (3+ outliers), 0% (not modelled)

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9325 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.

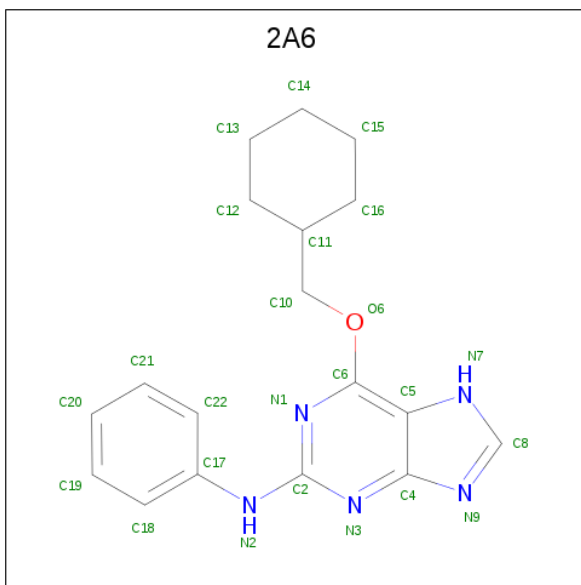
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

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

- Molecule 2 is a protein called CYCLIN A2.

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

- Molecule 3 is 2-ANILINO-6-CYCLOHEXYLMETHOXPURINE (three-letter code: 2A6) (formula: C<sub>18</sub>H<sub>21</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	18	5	1		
3	C	1	Total	C	N	O	0	0
			24	18	5	1		

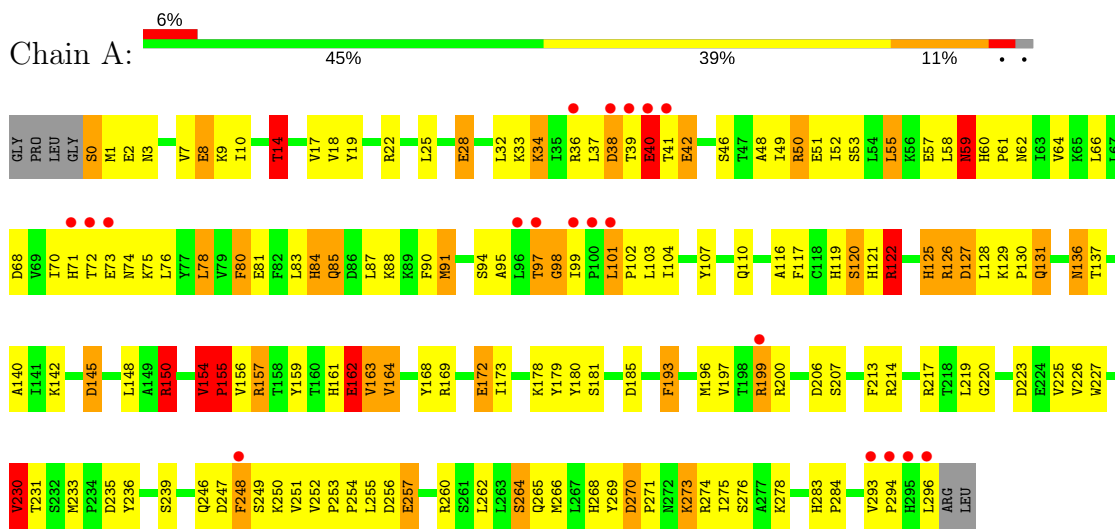
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	87	Total	O	0	0
			87	87		
4	C	74	Total	O	0	0
			74	74		
4	D	57	Total	O	0	0
			57	57		

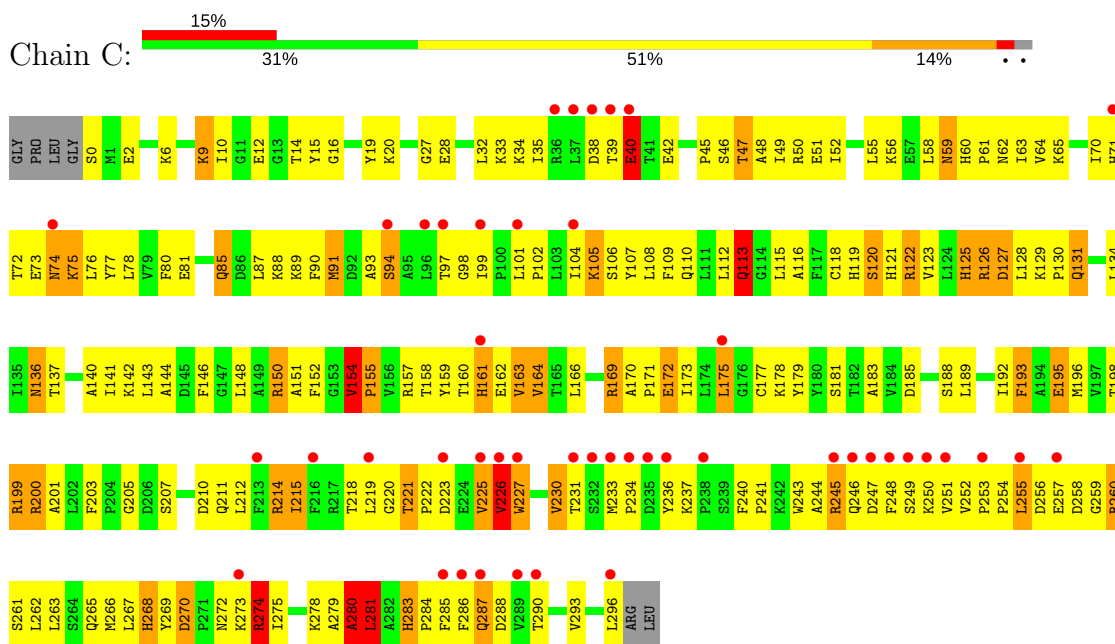
### 3 Residue-property plots [i](#)

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.

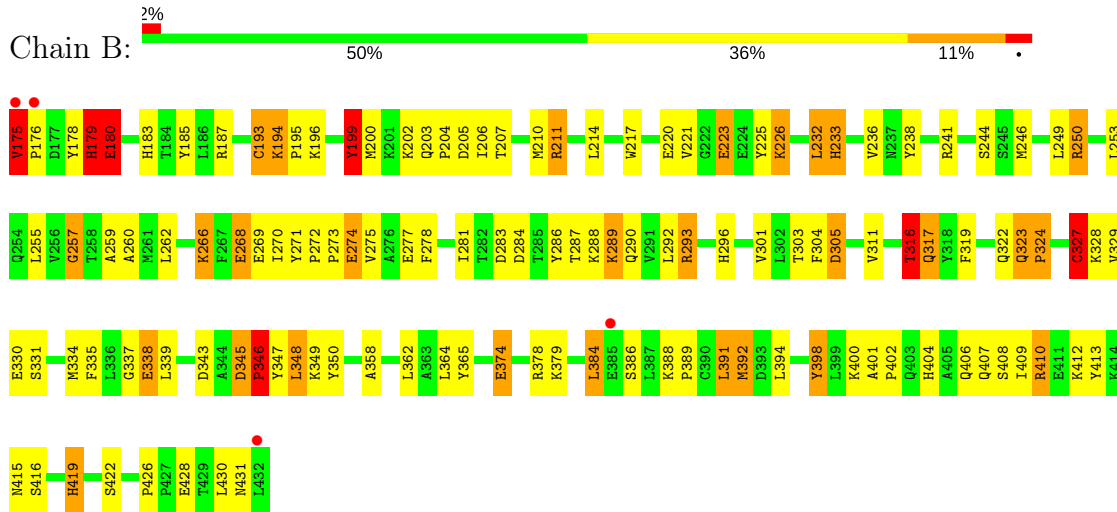
- Molecule 1: CELL DIVISION PROTEIN KINASE 2



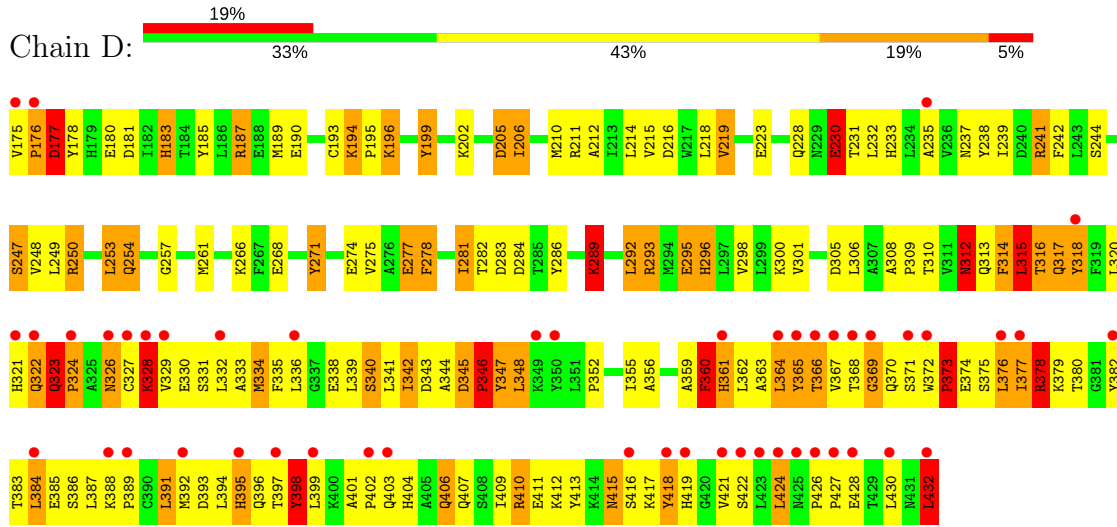
- Molecule 1: CELL DIVISION PROTEIN KINASE 2



- 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, $\alpha$ , $\beta$ , $\gamma$	73.99Å 134.73Å 148.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 39.28 – 2.52	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.50) 94.6 (39.28-2.52)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.66 (at 2.51Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.238 , 0.332 0.230 , 0.296	Depositor DCC
$R_{free}$ test set	2455 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.3	Xtrriage
Anisotropy	0.050	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 62.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9325	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: TPO, 2A6

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	0.66	0/2438	2.05	73/3308 (2.2%)
1	C	0.60	0/2438	1.98	62/3308 (1.9%)
2	B	0.67	0/2133	2.04	75/2897 (2.6%)
2	D	0.62	0/2133	2.18	85/2897 (2.9%)
All	All	0.64	0/9142	2.06	295/12410 (2.4%)

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	3
2	B	0	4
2	D	0	4
All	All	0	15

There are no bond length outliers.

All (295) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ARG	CD-NE-CZ	38.36	177.31	123.60
1	C	199	ARG	CD-NE-CZ	21.52	153.73	123.60
1	C	169	ARG	CD-NE-CZ	20.88	152.84	123.60
1	A	38	ASP	CA-CB-CG	18.99	155.18	113.40
2	D	241	ARG	NE-CZ-NH2	-18.02	111.29	120.30
2	D	318	TYR	CB-CG-CD1	15.44	130.26	121.00
2	D	318	TYR	CB-CG-CD2	-15.11	111.93	121.00
2	D	410	ARG	NE-CZ-NH2	14.32	127.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	187	ARG	NE-CZ-NH2	-14.01	113.30	120.30
1	C	260	ARG	NE-CZ-NH1	13.09	126.84	120.30
1	A	122	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	C	169	ARG	NE-CZ-NH1	13.03	126.81	120.30
1	C	150	ARG	NE-CZ-NH1	-12.59	114.00	120.30
2	D	398	TYR	CB-CG-CD1	12.55	128.53	121.00
2	D	378	ARG	NE-CZ-NH2	12.48	126.54	120.30
1	A	154	VAL	CA-C-O	-12.31	94.26	120.10
2	B	293	ARG	NE-CZ-NH2	12.27	126.44	120.30
1	A	157	ARG	NE-CZ-NH2	-11.64	114.48	120.30
1	C	155	PRO	CA-N-CD	-11.59	95.27	111.50
2	B	211	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	C	274	ARG	NE-CZ-NH1	-11.21	114.69	120.30
2	B	250	ARG	NE-CZ-NH1	-11.12	114.74	120.30
2	D	398	TYR	CB-CG-CD2	-10.91	114.45	121.00
1	A	169	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	C	214	ARG	NE-CZ-NH2	10.80	125.70	120.30
2	D	378	ARG	CD-NE-CZ	10.79	138.70	123.60
2	D	361	HIS	CA-CB-CG	-10.70	95.41	113.60
1	C	214	ARG	CD-NE-CZ	10.60	138.44	123.60
2	B	324	PRO	CA-N-CD	-10.48	96.82	111.50
2	B	345	ASP	CA-C-O	-10.47	98.11	120.10
1	A	217	ARG	NE-CZ-NH1	-10.42	115.09	120.30
2	B	293	ARG	NE-CZ-NH1	-10.38	115.11	120.30
1	C	150	ARG	NE-CZ-NH2	10.21	125.41	120.30
1	C	260	ARG	CD-NE-CZ	10.01	137.61	123.60
2	B	211	ARG	NE-CZ-NH2	-9.71	115.45	120.30
2	B	398	TYR	CB-CG-CD2	-9.59	115.25	121.00
2	B	413	TYR	CB-CG-CD1	-9.58	115.25	121.00
2	D	324	PRO	CA-N-CD	-9.58	98.09	111.50
2	D	283	ASP	N-CA-CB	9.49	127.68	110.60
2	D	345	ASP	CA-C-O	-9.45	100.26	120.10
2	B	193	CYS	CB-CA-C	9.37	129.13	110.40
2	B	187	ARG	CD-NE-CZ	9.33	136.66	123.60
2	D	376	LEU	CA-CB-CG	9.32	136.73	115.30
1	A	180	TYR	CB-CG-CD2	-9.09	115.54	121.00
1	A	50	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	C	154	VAL	CA-C-O	-8.92	101.37	120.10
1	C	280	ALA	CA-C-N	8.90	136.78	117.20
1	C	107	TYR	CB-CG-CD1	8.87	126.32	121.00
2	B	205	ASP	CB-CG-OD2	8.86	126.28	118.30
1	A	122	ARG	NE-CZ-NH2	-8.82	115.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	347	TYR	CB-CG-CD2	-8.81	115.72	121.00
2	D	293	ARG	NE-CZ-NH1	-8.79	115.91	120.30
2	D	322	GLN	CA-CB-CG	8.63	132.38	113.40
1	A	214	ARG	NE-CZ-NH2	-8.63	115.99	120.30
2	B	293	ARG	CD-NE-CZ	8.62	135.68	123.60
1	A	126	ARG	NE-CZ-NH1	-8.60	116.00	120.30
2	D	323	GLN	CA-C-O	-8.60	102.04	120.10
2	D	187	ARG	NE-CZ-NH1	8.59	124.59	120.30
2	B	413	TYR	CB-CG-CD2	8.59	126.15	121.00
1	A	159	TYR	CB-CG-CD1	-8.57	115.86	121.00
2	D	398	TYR	CA-CB-CG	8.50	129.54	113.40
1	C	107	TYR	CA-CB-CG	8.45	129.46	113.40
1	C	230	VAL	CB-CA-C	-8.44	95.37	111.40
1	A	59	ASN	CB-CA-C	8.33	127.06	110.40
2	B	274	GLU	CB-CA-C	8.29	126.99	110.40
2	D	410	ARG	CD-NE-CZ	8.26	135.16	123.60
1	C	255	LEU	CA-CB-CG	8.23	134.23	115.30
2	D	283	ASP	CB-CG-OD1	8.16	125.64	118.30
1	C	161	HIS	CA-CB-CG	-8.15	99.75	113.60
2	D	289	LYS	CA-CB-CG	8.14	131.31	113.40
2	D	347	TYR	CB-CG-CD1	8.12	125.87	121.00
2	D	346	PRO	CA-N-CD	-8.08	100.19	111.50
2	B	350	TYR	CB-CG-CD1	7.97	125.78	121.00
1	C	169	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	246	GLN	CA-CB-CG	7.85	130.68	113.40
1	C	50	ARG	NE-CZ-NH1	7.85	124.22	120.30
2	D	241	ARG	NH1-CZ-NH2	7.84	128.03	119.40
2	D	323	GLN	CA-CB-CG	7.84	130.65	113.40
1	A	180	TYR	CB-CG-CD1	7.80	125.68	121.00
1	C	19	TYR	CB-CG-CD2	-7.80	116.32	121.00
1	A	155	PRO	CA-N-CD	-7.79	100.60	111.50
2	D	378	ARG	NE-CZ-NH1	-7.75	116.43	120.30
2	D	328	LYS	CA-CB-CG	7.74	130.44	113.40
2	D	410	ARG	NE-CZ-NH1	-7.73	116.44	120.30
1	C	155	PRO	N-CA-CB	7.70	112.54	103.30
2	D	183	HIS	CA-CB-CG	7.68	126.67	113.60
2	D	305	ASP	CB-CG-OD2	-7.67	111.39	118.30
1	A	199	ARG	CD-NE-CZ	7.66	134.32	123.60
2	D	295	GLU	OE1-CD-OE2	-7.64	114.13	123.30
1	C	185	ASP	CB-CG-OD2	7.56	125.10	118.30
2	D	340	SER	CA-C-N	7.53	133.76	117.20
1	C	19	TYR	CB-CA-C	-7.52	95.36	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	A	3	ASN	CA-C-N	7.51	133.72	117.20
2	B	283	ASP	CA-C-O	7.50	135.84	120.10
1	A	84	HIS	CA-CB-CG	-7.46	100.91	113.60
2	D	391	LEU	CA-CB-CG	7.42	132.38	115.30
2	D	403	GLN	CA-CB-CG	7.41	129.70	113.40
2	B	311	VAL	CA-CB-CG2	-7.38	99.82	110.90
1	C	126	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	D	428	GLU	CA-CB-CG	7.34	129.55	113.40
2	B	323	GLN	CA-C-O	-7.32	104.73	120.10
1	A	68	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	3	ASN	CA-C-O	-7.16	105.07	120.10
1	C	260	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	280	ALA	CA-C-O	-7.09	105.20	120.10
2	B	271	TYR	CB-CG-CD1	7.07	125.24	121.00
1	C	28	GLU	OE1-CD-OE2	7.05	131.76	123.30
1	A	161	HIS	CA-CB-CG	-7.04	101.62	113.60
2	B	378	ARG	NE-CZ-NH2	7.04	123.82	120.30
2	D	318	TYR	CA-CB-CG	7.02	126.74	113.40
2	B	283	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	19	TYR	CB-CA-C	-6.97	96.45	110.40
1	A	180	TYR	N-CA-CB	6.92	123.06	110.60
1	A	230	VAL	CB-CA-C	-6.92	98.25	111.40
2	B	268	GLU	N-CA-CB	-6.91	98.16	110.60
2	B	223	GLU	OE1-CD-OE2	6.87	131.55	123.30
1	A	28	GLU	OE1-CD-OE2	-6.86	115.07	123.30
2	D	339	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	40	GLU	CA-CB-CG	6.84	128.44	113.40
1	C	59	ASN	CB-CA-C	6.84	124.08	110.40
2	D	177	ASP	N-CA-CB	6.83	122.89	110.60
1	A	150	ARG	O-C-N	6.81	133.59	122.70
2	B	199	TYR	CB-CG-CD2	-6.81	116.92	121.00
2	B	200	MET	CA-CB-CG	6.79	124.84	113.30
2	B	346	PRO	CA-N-CD	-6.77	102.03	111.50
1	A	122	ARG	CD-NE-CZ	6.75	133.05	123.60
1	C	91	MET	CA-CB-CG	6.72	124.73	113.30
1	A	162	GLU	CB-CG-CD	6.72	132.35	114.20
1	C	270	ASP	CB-CA-C	6.69	123.78	110.40
2	D	296	HIS	N-CA-CB	-6.69	98.56	110.60
2	B	179	HIS	CA-CB-CG	6.68	124.96	113.60
1	A	193	PHE	CB-CG-CD1	6.67	125.47	120.80
1	C	237	LYS	CA-CB-CG	6.55	127.81	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	122	ARG	CG-CD-NE	6.54	125.53	111.80
2	D	406	GLN	CA-CB-CG	6.52	127.75	113.40
1	A	274	ARG	CD-NE-CZ	6.50	132.70	123.60
2	B	419	HIS	CA-CB-CG	-6.48	102.58	113.60
1	C	230	VAL	N-CA-CB	6.48	125.76	111.50
1	A	90	PHE	CB-CG-CD2	6.47	125.33	120.80
1	C	175	LEU	CB-CA-C	6.44	122.44	110.20
2	B	327	CYS	CB-CA-C	6.44	123.27	110.40
2	D	328	LYS	N-CA-CB	6.42	122.16	110.60
2	B	211	ARG	CD-NE-CZ	6.38	132.53	123.60
1	A	80	PHE	CA-CB-CG	6.36	129.15	113.90
2	D	282	THR	C-N-CA	6.35	137.57	121.70
2	D	254	GLN	CG-CD-OE1	-6.33	108.94	121.60
1	A	40	GLU	CA-C-O	6.29	133.31	120.10
2	B	277	GLU	OE1-CD-OE2	6.29	130.84	123.30
2	B	187	ARG	NE-CZ-NH1	6.27	123.44	120.30
2	B	241	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	D	293	ARG	CD-NE-CZ	6.21	132.29	123.60
1	C	159	TYR	CB-CG-CD2	6.20	124.72	121.00
1	C	283	HIS	CB-CA-C	6.19	122.77	110.40
1	A	155	PRO	N-CA-CB	6.17	110.70	103.30
2	D	326	ASN	N-CA-CB	6.16	121.69	110.60
2	B	283	ASP	N-CA-CB	6.15	121.67	110.60
2	D	277	GLU	OE1-CD-OE2	6.13	130.66	123.30
2	B	196	LYS	CA-CB-CG	6.13	126.89	113.40
2	D	321	HIS	CB-CA-C	6.13	122.66	110.40
2	B	269	GLU	OE1-CD-OE2	6.12	130.64	123.30
1	C	122	ARG	CA-CB-CG	6.10	126.83	113.40
1	A	157	ARG	CB-CA-C	-6.09	98.22	110.40
1	A	97	THR	CA-CB-CG2	-6.07	103.90	112.40
2	D	323	GLN	CB-CA-C	6.07	122.54	110.40
2	D	324	PRO	N-CD-CG	6.07	112.30	103.20
2	B	365	TYR	CB-CG-CD1	-6.07	117.36	121.00
2	D	230	GLU	CB-CG-CD	6.07	130.58	114.20
2	B	316	THR	N-CA-CB	-6.05	98.80	110.30
1	C	107	TYR	CB-CG-CD2	-6.05	117.37	121.00
2	D	365	TYR	CB-CG-CD2	-6.01	117.39	121.00
2	B	343	ASP	N-CA-CB	-6.01	99.79	110.60
2	D	373	PRO	CA-C-O	5.98	134.56	120.20
2	B	220	GLU	CA-CB-CG	5.98	126.56	113.40
2	D	278	PHE	CB-CG-CD2	-5.96	116.63	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	PHE	CB-CG-CD2	-5.94	116.64	120.80
2	D	355	ILE	N-CA-CB	5.92	124.42	110.80
2	B	392	MET	CB-CA-C	-5.89	98.62	110.40
1	A	239	SER	CA-C-N	5.88	130.14	117.20
2	B	374	GLU	OE1-CD-OE2	5.88	130.36	123.30
2	D	418	TYR	CB-CG-CD1	5.87	124.52	121.00
2	B	349	LYS	CA-CB-CG	5.87	126.30	113.40
1	A	157	ARG	CA-CB-CG	5.83	126.22	113.40
2	D	223	GLU	CB-CA-C	-5.82	98.76	110.40
1	A	155	PRO	N-CD-CG	5.82	111.93	103.20
2	D	187	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	A	217	ARG	CG-CD-NE	5.80	123.98	111.80
2	D	317	GLN	C-N-CA	5.79	136.19	121.70
1	A	76	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	230	VAL	N-CA-CB	5.78	124.21	111.50
2	D	314	PHE	CB-CG-CD1	-5.78	116.76	120.80
2	D	230	GLU	CA-CB-CG	5.77	126.09	113.40
2	B	232	LEU	CB-CA-C	5.76	121.14	110.20
2	B	233	HIS	CA-C-N	5.76	129.87	117.20
1	A	37	LEU	CB-CA-C	5.74	121.11	110.20
2	B	345	ASP	CB-CG-OD2	-5.74	113.14	118.30
2	B	422	SER	N-CA-CB	5.73	119.09	110.50
2	D	314	PHE	CB-CG-CD2	5.72	124.81	120.80
2	B	365	TYR	CB-CG-CD2	5.70	124.42	121.00
2	B	337	GLY	N-CA-C	-5.68	98.91	113.10
1	A	199	ARG	CG-CD-NE	5.67	123.71	111.80
2	B	350	TYR	CB-CG-CD2	-5.67	117.60	121.00
2	D	301	VAL	CA-CB-CG2	-5.67	102.40	110.90
2	D	278	PHE	CA-C-O	-5.66	108.21	120.10
2	B	271	TYR	CB-CG-CD2	-5.66	117.60	121.00
2	D	205	ASP	CB-CG-OD1	5.65	123.38	118.30
2	B	323	GLN	CB-CA-C	5.64	121.67	110.40
2	B	338	GLU	OE1-CD-OE2	-5.63	116.55	123.30
2	D	432	LEU	N-CA-CB	5.60	121.60	110.40
2	B	350	TYR	CA-C-O	5.59	131.84	120.10
2	D	293	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	C	281	LEU	N-CA-CB	5.58	121.56	110.40
1	C	20	LYS	CA-CB-CG	5.58	125.67	113.40
1	C	125	HIS	CA-CB-CG	5.56	123.05	113.60
1	C	113	GLN	CA-CB-CG	5.55	125.61	113.40
2	B	349	LYS	CB-CA-C	-5.54	99.32	110.40
2	D	314	PHE	CB-CA-C	5.53	121.47	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	340	SER	CA-C-O	-5.51	108.53	120.10
1	A	19	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	C	283	HIS	CA-CB-CG	5.49	122.94	113.60
1	A	85	GLN	N-CA-CB	-5.49	100.72	110.60
2	D	205	ASP	CB-CG-OD2	-5.49	113.36	118.30
2	D	312	ASN	CB-CA-C	5.49	121.37	110.40
2	D	189	MET	N-CA-CB	5.48	120.47	110.60
1	C	195	GLU	CA-CB-CG	5.47	125.43	113.40
2	D	395	HIS	CA-CB-CG	-5.46	104.32	113.60
2	D	241	ARG	CD-NE-CZ	5.45	131.23	123.60
2	D	379	LYS	CA-CB-CG	5.45	125.39	113.40
2	D	366	THR	N-CA-CB	5.45	120.65	110.30
2	B	338	GLU	CG-CD-OE2	5.42	129.15	118.30
2	B	250	ARG	CA-C-N	5.41	127.03	116.20
2	B	266	LYS	N-CA-CB	5.41	120.34	110.60
2	B	345	ASP	CB-CG-OD1	5.41	123.17	118.30
2	B	232	LEU	CB-CG-CD2	5.40	120.18	111.00
2	B	194	LYS	CB-CG-CD	5.39	125.62	111.60
2	B	233	HIS	CA-C-O	-5.39	108.78	120.10
2	D	346	PRO	N-CD-CG	5.38	111.27	103.20
1	C	40	GLU	CA-CB-CG	5.37	125.22	113.40
1	A	214	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	169	ARG	NH1-CZ-NH2	5.37	125.30	119.40
2	B	410	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	C	214	ARG	NE-CZ-NH1	-5.35	117.63	120.30
2	D	369	GLY	N-CA-C	5.35	126.46	113.10
2	D	360	PHE	CA-C-N	-5.32	105.49	117.20
1	A	206	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	22	ARG	CB-CA-C	-5.31	99.78	110.40
1	C	59	ASN	N-CA-CB	-5.31	101.04	110.60
1	A	213	PHE	CB-CG-CD1	5.31	124.52	120.80
2	D	320	LEU	CB-CA-C	5.30	120.28	110.20
2	B	180	GLU	N-CA-CB	5.30	120.14	110.60
1	A	136	ASN	CB-CA-C	5.30	121.00	110.40
2	B	199	TYR	CB-CG-CD1	5.30	124.18	121.00
1	C	50	ARG	CD-NE-CZ	-5.29	116.19	123.60
1	A	168	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	A	125	HIS	CA-C-O	5.28	131.19	120.10
1	A	257	GLU	CA-CB-CG	5.28	125.02	113.40
1	A	172	GLU	CB-CA-C	-5.28	99.85	110.40
2	D	384	LEU	CB-CA-C	5.26	120.19	110.20
1	C	38	ASP	CB-CG-OD1	5.25	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	GLY	CA-C-O	-5.25	111.15	120.60
2	B	193	CYS	O-C-N	-5.25	114.30	122.70
2	D	194	LYS	N-CA-CB	-5.23	101.18	110.60
1	C	85	GLN	CB-CG-CD	-5.23	98.01	111.60
1	A	14	THR	N-CA-CB	5.22	120.21	110.30
1	C	77	TYR	CA-CB-CG	-5.21	103.50	113.40
1	A	262	LEU	CB-CG-CD2	5.20	119.84	111.00
1	A	270	ASP	CB-CG-OD1	5.19	122.97	118.30
2	D	395	HIS	N-CA-CB	-5.18	101.27	110.60
1	A	156	VAL	C-N-CA	5.17	134.63	121.70
1	C	129	LYS	CB-CA-C	5.17	120.73	110.40
1	C	77	TYR	CB-CG-CD2	-5.16	117.91	121.00
2	D	271	TYR	N-CA-CB	5.16	119.88	110.60
2	B	305	ASP	CB-CG-OD1	5.15	122.93	118.30
1	C	80	PHE	CB-CA-C	-5.15	100.11	110.40
2	D	315	LEU	CA-CB-CG	-5.12	103.53	115.30
1	C	227	TRP	CA-CB-CG	5.11	123.41	113.70
1	C	77	TYR	CB-CA-C	-5.09	100.22	110.40
1	C	70	ILE	CB-CA-C	5.09	121.77	111.60
2	B	205	ASP	CB-CG-OD1	-5.08	113.72	118.30
2	B	175	VAL	CA-CB-CG1	5.08	118.52	110.90
1	C	150	ARG	CD-NE-CZ	5.08	130.72	123.60
2	B	178	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	C	230	VAL	CA-CB-CG2	5.06	118.49	110.90
1	C	118	CYS	CA-CB-SG	5.05	123.09	114.00
1	A	172	GLU	CA-CB-CG	5.05	124.50	113.40
1	A	273	LYS	CA-C-O	-5.04	109.52	120.10
1	A	85	GLN	CA-CB-CG	5.04	124.48	113.40
1	A	235	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	59	ASN	OD1-CG-ND2	5.03	133.46	121.90
1	C	245	ARG	N-CA-C	5.01	124.53	111.00
1	A	22	ARG	CA-CB-CG	5.01	124.42	113.40
2	B	407	GLN	CA-CB-CG	5.00	124.41	113.40
2	B	257	GLY	CA-C-O	-5.00	111.60	120.60
2	B	317	GLN	OE1-CD-NE2	5.00	133.40	121.90

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	SER	Mainchain
1	A	122	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	A	154	VAL	Mainchain,Peptide
2	B	323	GLN	Mainchain,Peptide
2	B	345	ASP	Mainchain,Peptide
1	C	0	SER	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	2430	123	0
1	C	2388	0	2429	184	0
2	B	2083	0	2107	84	0
2	D	2083	0	2107	164	0
3	A	24	0	21	2	0
3	C	24	0	21	2	0
4	A	117	0	0	13	0
4	B	87	0	0	7	0
4	C	74	0	0	13	0
4	D	57	0	0	12	0
All	All	9325	0	9115	520	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 29.

All (520) 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)
2:D:367:VAL:HG12	2:D:368:THR:HG23	1.43	0.99
1:A:84:HIS:HD2	1:A:136:ASN:HA	1.31	0.95
2:D:378:ARG:HB2	2:D:378:ARG:HH21	1.33	0.91
1:C:64:VAL:HG21	1:C:144:ALA:HB2	1.52	0.90
1:A:14:THR:HG21	1:A:148:LEU:HD22	1.54	0.88
1:C:60:HIS:HD2	1:C:62:ASN:H	1.21	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:LEU:HG	2:D:356:ALA:HB1	1.57	0.86
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.58	0.85
2:D:210:MET:HE1	2:D:250:ARG:HD3	1.60	0.84
1:C:116:ALA:O	1:C:120:SER:HB2	1.76	0.84
1:C:115:LEU:HD22	1:C:189:LEU:HD12	1.62	0.82
1:C:223:ASP:H	1:C:226:VAL:HG13	1.44	0.81
2:D:315:LEU:HG	2:D:356:ALA:CB	2.10	0.81
1:A:39:THR:HB	2:B:289:LYS:HE3	1.62	0.80
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.62	0.79
1:A:60:HIS:HD2	1:A:62:ASN:H	1.30	0.78
1:C:113:GLN:HB3	4:C:2023:HOH:O	1.85	0.77
2:D:377:ILE:HG13	2:D:382:TYR:O	1.84	0.77
1:A:181:SER:HB3	4:A:2073:HOH:O	1.85	0.76
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.51	0.75
1:C:88:LYS:HD2	1:C:131:GLN:HE21	1.51	0.75
2:D:233:HIS:CE1	4:D:2036:HOH:O	2.39	0.74
1:A:60:HIS:CD2	1:A:62:ASN:H	2.05	0.73
2:D:424:LEU:HD23	2:D:424:LEU:H	1.52	0.73
2:D:216:ASP:OD2	2:D:406:GLN:HB3	1.89	0.72
2:D:183:HIS:HB2	2:D:317:GLN:NE2	2.05	0.71
1:A:84:HIS:CD2	1:A:136:ASN:HA	2.22	0.71
2:D:401:ALA:N	2:D:402:PRO:HD2	2.07	0.69
2:D:206:ILE:HG21	2:D:253:LEU:HD22	1.74	0.69
1:C:128:LEU:HD12	1:C:189:LEU:HG	1.73	0.69
1:C:45:PRO:HB2	1:C:47:THR:HG23	1.75	0.68
2:D:210:MET:CE	2:D:250:ARG:HB2	2.23	0.68
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.74	0.68
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.75	0.68
2:B:207:THR:OG1	2:B:210:MET:HG3	1.94	0.68
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.29	0.68
1:C:170:ALA:HB1	1:C:172:GLU:OE2	1.94	0.67
1:C:280:ALA:O	1:C:286:PHE:HE2	1.77	0.67
1:A:25:LEU:HD11	2:D:293:ARG:HB3	1.76	0.67
2:B:175:VAL:N	2:B:176:PRO:HD3	2.09	0.67
1:A:10:ILE:HD12	1:A:18:VAL:HG12	1.75	0.67
1:C:231:THR:HG22	1:C:236:TYR:CZ	2.29	0.67
1:C:203:PHE:HB3	4:C:2058:HOH:O	1.95	0.67
1:C:52:ILE:HD11	1:C:78:LEU:HD21	1.76	0.67
1:C:214:ARG:HB2	4:C:2058:HOH:O	1.95	0.67
1:C:246:GLN:HG2	1:C:251:VAL:HG23	1.76	0.67
1:A:88:LYS:HB2	1:A:130:PRO:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.31	0.66
1:A:137:THR:HG22	1:A:296:LEU:HD12	1.76	0.66
1:A:53:SER:HB3	2:B:304:PHE:O	1.96	0.66
1:C:60:HIS:CD2	1:C:62:ASN:H	2.11	0.66
2:D:326:ASN:HD21	2:D:328:LYS:HD3	1.61	0.66
1:A:51:GLU:O	1:A:55:LEU:HB2	1.96	0.66
1:C:154:VAL:O	2:D:316:THR:HG23	1.95	0.66
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.78	0.65
1:C:33:LYS:HD2	1:C:78:LEU:HD12	1.79	0.65
2:D:368:THR:O	2:D:370:GLN:HG3	1.97	0.65
1:C:126:ARG:NH2	1:C:160:TPO:O3P	2.29	0.65
2:D:327:CYS:HB3	4:D:2034:HOH:O	1.97	0.65
2:D:375:SER:HA	2:D:378:ARG:CZ	2.27	0.65
1:C:223:ASP:H	1:C:226:VAL:CG1	2.10	0.64
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.79	0.64
2:D:377:ILE:HD11	2:D:383:THR:HG22	1.78	0.64
2:D:218:LEU:HD22	2:D:261:MET:SD	2.38	0.64
1:A:219:LEU:HD23	4:A:2085:HOH:O	1.98	0.64
2:D:230:GLU:OE1	2:D:312:ASN:ND2	2.32	0.63
2:D:347:TYR:OH	2:D:394:LEU:HA	1.99	0.63
1:C:178:LYS:HG2	4:C:2048:HOH:O	1.97	0.63
2:B:327:CYS:HB2	4:B:2057:HOH:O	1.98	0.63
1:C:58:LEU:HB3	1:C:63:ILE:HD12	1.80	0.62
1:C:49:ILE:HG23	2:D:306:LEU:HD12	1.82	0.62
2:D:344:ALA:HA	2:D:348:LEU:HD22	1.81	0.62
1:C:195:GLU:HG2	1:C:201:ALA:HA	1.80	0.62
1:A:18:VAL:HA	1:A:32:LEU:O	1.99	0.62
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.64	0.62
1:C:287:GLN:HG2	1:C:288:ASP:N	2.13	0.62
2:D:378:ARG:HB2	2:D:378:ARG:NH2	2.11	0.62
1:C:227:TRP:O	1:C:230:VAL:HG23	2.00	0.62
1:C:241:PRO:HG2	1:C:243:TRP:CH2	2.34	0.62
2:D:187:ARG:NH2	2:D:382:TYR:OH	2.32	0.62
1:C:261:SER:O	1:C:265:GLN:HG3	2.00	0.61
2:D:364:LEU:HD21	2:D:370:GLN:CD	2.19	0.61
2:D:395:HIS:CG	2:D:430:LEU:HD11	2.34	0.61
1:C:88:LYS:HD2	1:C:131:GLN:NE2	2.13	0.61
1:A:116:ALA:O	1:A:120:SER:HB2	2.00	0.61
2:D:211:ARG:O	2:D:215:VAL:HG23	2.01	0.61
1:A:33:LYS:HD2	1:A:80:PHE:HE1	1.66	0.61
1:A:9:LYS:NZ	1:A:17:VAL:HG11	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:PRO:HA	2:B:179:HIS:CG	2.36	0.61
2:B:176:PRO:HA	2:B:179:HIS:ND1	2.16	0.61
2:D:289:LYS:HE2	2:D:293:ARG:NH2	2.16	0.61
1:A:154:VAL:HG13	2:B:179:HIS:CE1	2.36	0.61
2:D:233:HIS:HE1	4:D:2036:HOH:O	1.78	0.60
2:D:426:PRO:HG3	4:D:2048:HOH:O	2.00	0.60
2:D:364:LEU:HD22	2:D:370:GLN:HB2	1.84	0.59
2:B:358:ALA:HA	2:B:391:LEU:HD22	1.83	0.59
1:C:160:TPO:HG23	1:C:162:GLU:O	2.01	0.59
2:D:210:MET:HE1	2:D:250:ARG:CD	2.32	0.59
1:A:137:THR:HG22	1:A:296:LEU:CD1	2.32	0.59
1:A:39:THR:HB	2:B:289:LYS:CE	2.30	0.59
2:D:406:GLN:HB2	4:D:2050:HOH:O	2.03	0.59
1:A:75:LYS:HB2	4:A:2031:HOH:O	2.02	0.59
2:D:314:PHE:O	2:D:315:LEU:C	2.40	0.59
1:C:40:GLU:HA	2:D:292:LEU:HD23	1.84	0.59
2:D:235:ALA:O	2:D:239:ILE:HG13	2.02	0.59
2:D:315:LEU:CG	2:D:356:ALA:HB1	2.30	0.59
2:B:194:LYS:HG3	2:B:195:PRO:HD2	1.85	0.59
2:D:364:LEU:CD2	2:D:370:GLN:HB2	2.33	0.59
1:C:15:TYR:CE1	1:C:33:LYS:HE2	2.38	0.58
2:D:404:HIS:HB3	4:D:2049:HOH:O	2.04	0.58
1:A:7:VAL:O	1:A:8:GLU:HB3	2.03	0.58
2:D:342:ILE:HD11	2:D:409:ILE:HD12	1.83	0.58
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.86	0.58
2:B:194:LYS:HG3	2:B:195:PRO:CD	2.34	0.58
2:B:287:THR:N	2:B:290:GLN:OE1	2.30	0.58
2:D:374:GLU:O	2:D:377:ILE:HG22	2.04	0.58
2:B:233:HIS:HD2	4:B:2050:HOH:O	1.87	0.58
2:D:313:GLN:O	2:D:316:THR:HG22	2.04	0.58
1:A:154:VAL:HB	2:B:317:GLN:HG3	1.86	0.57
1:C:125:HIS:CE1	1:C:128:LEU:HD23	2.38	0.57
1:A:163:VAL:HG12	1:A:173:ILE:HD13	1.85	0.57
1:A:1:MET:SD	1:A:70:ILE:HD13	2.44	0.57
1:C:112:LEU:HB2	1:C:281:LEU:CD2	2.34	0.57
1:C:87:LEU:O	1:C:91:MET:HG2	2.03	0.57
1:A:40:GLU:HB3	2:B:288:LYS:HD3	1.86	0.57
1:C:183:ALA:HB1	1:C:274:ARG:NH1	2.20	0.57
2:D:205:ASP:OD2	2:D:250:ARG:HB3	2.04	0.57
1:A:72:THR:HA	4:A:2029:HOH:O	2.04	0.57
1:C:272:ASN:H	1:C:272:ASN:ND2	2.01	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:ASP:O	1:C:214:ARG:HG3	2.03	0.57
1:C:273:LYS:O	1:C:274:ARG:C	2.42	0.57
1:C:72:THR:HB	1:C:75:LYS:O	2.03	0.57
1:C:231:THR:HA	1:C:236:TYR:CD1	2.40	0.57
1:C:137:THR:HG23	4:C:2038:HOH:O	2.03	0.57
1:C:219:LEU:HB3	1:C:269:TYR:HE2	1.70	0.57
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.40	0.56
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.87	0.56
1:A:17:VAL:HB	4:A:2011:HOH:O	2.03	0.56
1:C:42:GLU:OE1	2:D:275:VAL:HG23	2.06	0.56
1:C:193:PHE:HD2	1:C:266:MET:HE3	1.70	0.56
2:D:364:LEU:HD21	2:D:370:GLN:NE2	2.20	0.56
1:A:58:LEU:HA	1:A:117:PHE:HE2	1.71	0.56
1:C:188:SER:O	1:C:192:ILE:HG13	2.05	0.56
2:D:315:LEU:HD22	2:D:333:ALA:HB1	1.86	0.56
1:A:64:VAL:HG11	3:A:1298:2A6:H8	1.88	0.56
2:B:388:LYS:O	2:B:392:MET:HG2	2.05	0.56
1:A:172:GLU:HG3	1:A:271:PRO:HG3	1.88	0.56
2:D:421:VAL:HA	2:D:424:LEU:HD21	1.88	0.56
1:C:90:PHE:O	1:C:94:SER:HB2	2.06	0.56
2:D:175:VAL:N	2:D:176:PRO:HD3	2.22	0.55
1:C:115:LEU:HG	1:C:119:HIS:CD2	2.42	0.55
2:D:233:HIS:CE1	2:D:341:LEU:HD11	2.41	0.55
1:C:115:LEU:CD2	1:C:189:LEU:HD12	2.35	0.55
2:D:331:SER:OG	2:D:418:TYR:HA	2.05	0.55
2:D:329:VAL:HG21	2:D:364:LEU:HA	1.89	0.55
1:A:223:ASP:H	1:A:226:VAL:CG1	2.19	0.55
1:C:64:VAL:CG2	1:C:144:ALA:HB2	2.30	0.55
2:D:404:HIS:O	2:D:407:GLN:NE2	2.40	0.55
1:C:104:ILE:O	1:C:108:LEU:N	2.37	0.54
1:C:115:LEU:HD22	1:C:189:LEU:CD1	2.33	0.54
1:C:198:THR:HG22	1:C:252:VAL:HG13	1.88	0.54
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.90	0.54
2:D:346:PRO:HD2	2:D:347:TYR:CE2	2.42	0.54
2:D:395:HIS:ND1	2:D:430:LEU:HD21	2.22	0.54
1:C:85:GLN:O	1:C:134:LEU:HA	2.06	0.54
2:D:360:PHE:CD2	2:D:376:LEU:HD11	2.43	0.54
2:D:424:LEU:HD23	2:D:424:LEU:N	2.21	0.54
1:C:46:SER:HB3	2:D:266:LYS:HB3	1.89	0.54
1:A:172:GLU:CG	1:A:271:PRO:HG3	2.38	0.54
1:C:62:ASN:HA	1:C:142:LYS:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:HIS:CE1	2:B:406:GLN:HB2	2.43	0.54
2:B:362:LEU:HD13	2:B:430:LEU:HD21	1.89	0.54
1:C:64:VAL:HG23	1:C:143:LEU:O	2.07	0.54
2:D:187:ARG:HD3	4:D:2003:HOH:O	2.08	0.54
2:D:426:PRO:HB2	2:D:427:PRO:HD2	1.89	0.54
1:A:193:PHE:CD2	1:A:266:MET:HE1	2.42	0.54
1:C:112:LEU:HB2	1:C:281:LEU:HD21	1.90	0.54
1:A:84:HIS:HD2	1:A:136:ASN:CA	2.14	0.53
2:B:401:ALA:HB1	2:B:410:ARG:HD2	1.90	0.53
2:D:242:PHE:CD1	2:D:298:VAL:HG22	2.42	0.53
2:D:411:GLU:O	2:D:412:LYS:C	2.44	0.53
2:D:328:LYS:HB2	2:D:421:VAL:HG12	1.89	0.53
1:A:9:LYS:HZ2	1:A:17:VAL:HG11	1.73	0.53
1:A:98:GLY:HA3	1:A:199:ARG:NH1	2.24	0.53
1:C:240:PHE:O	1:C:241:PRO:C	2.47	0.53
1:C:255:LEU:HG	1:C:259:GLY:HA3	1.89	0.53
1:C:115:LEU:HG	1:C:119:HIS:NE2	2.24	0.53
1:C:51:GLU:HG3	1:C:146:PHE:HB2	1.89	0.53
1:C:253:PRO:HD2	1:C:254:PRO:HD2	1.91	0.53
1:A:40:GLU:H	2:B:292:LEU:HD23	1.74	0.53
2:B:305:ASP:HA	4:B:2047:HOH:O	2.08	0.53
2:D:233:HIS:HB3	2:D:310:THR:HG21	1.91	0.53
2:B:180:GLU:OE1	2:B:379:LYS:NZ	2.40	0.53
2:D:289:LYS:HE2	2:D:293:ARG:HH22	1.74	0.53
1:A:33:LYS:HD2	1:A:80:PHE:CE1	2.44	0.52
2:D:274:GLU:H	2:D:277:GLU:HG3	1.74	0.52
1:A:260:ARG:O	1:A:264:SER:HB3	2.09	0.52
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.74	0.52
2:B:303:THR:O	2:B:304:PHE:HB2	2.09	0.52
2:B:347:TYR:OH	2:B:394:LEU:HA	2.09	0.52
1:C:200:ARG:NH1	1:C:200:ARG:HG3	2.23	0.52
1:C:231:THR:HA	1:C:236:TYR:CG	2.44	0.52
1:C:40:GLU:HA	2:D:292:LEU:CD2	2.40	0.52
2:D:395:HIS:NE2	2:D:399:LEU:HD11	2.25	0.52
2:B:419:HIS:HB3	4:B:2082:HOH:O	2.09	0.52
2:D:401:ALA:O	2:D:402:PRO:C	2.48	0.52
2:D:342:ILE:HD11	2:D:409:ILE:CD1	2.40	0.52
2:D:415:ASN:OD1	2:D:416:SER:N	2.42	0.52
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.24	0.52
2:D:332:LEU:O	2:D:336:LEU:HG	2.10	0.51
2:D:194:LYS:NZ	2:D:195:PRO:HD2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:328:LYS:HB2	2:D:421:VAL:CG1	2.40	0.51
1:C:108:LEU:HD22	1:C:193:PHE:CG	2.46	0.51
1:A:95:ALA:HA	1:A:199:ARG:HD2	1.93	0.51
2:D:331:SER:HB3	2:D:421:VAL:HG21	1.92	0.51
2:B:262:LEU:O	2:B:266:LYS:HG3	2.10	0.51
1:C:175:LEU:HG	1:C:212:LEU:HD21	1.93	0.51
1:C:227:TRP:CD2	1:C:230:VAL:HG22	2.46	0.51
1:C:249:SER:O	1:C:253:PRO:HA	2.10	0.51
1:C:42:GLU:OE1	2:D:274:GLU:HB2	2.11	0.51
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.92	0.51
1:C:137:THR:HA	1:C:296:LEU:CD1	2.41	0.51
1:C:74:ASN:HB2	1:C:75:LYS:HD2	1.92	0.51
1:C:154:VAL:HB	2:D:317:GLN:HG3	1.92	0.51
1:C:215:ILE:HD13	4:C:2058:HOH:O	2.10	0.51
1:C:6:LYS:HE3	1:C:32:LEU:CD1	2.41	0.51
2:D:315:LEU:HG	2:D:356:ALA:HB2	1.90	0.51
1:C:109:PHE:CE1	1:C:281:LEU:HB3	2.46	0.51
2:D:335:PHE:CD2	2:D:336:LEU:HD23	2.46	0.51
2:D:372:TRP:HB3	2:D:384:LEU:HD11	1.92	0.51
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.93	0.51
1:C:161:HIS:HB3	1:C:162:GLU:OE2	2.11	0.51
2:D:317:GLN:HA	4:D:2032:HOH:O	2.10	0.51
2:D:365:TYR:HB2	2:D:370:GLN:O	2.11	0.51
1:A:230:VAL:HA	1:A:233:MET:SD	2.51	0.50
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.46	0.50
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.46	0.50
1:C:109:PHE:HE1	1:C:281:LEU:HB3	1.75	0.50
2:B:232:LEU:O	2:B:236:VAL:HG23	2.11	0.50
2:D:230:GLU:O	2:D:233:HIS:HB2	2.11	0.50
1:A:95:ALA:HA	1:A:199:ARG:CD	2.42	0.50
2:D:175:VAL:HG22	2:D:177:ASP:OD2	2.12	0.50
1:A:178:LYS:HG3	1:A:179:TYR:CE2	2.46	0.50
1:C:200:ARG:HH11	1:C:200:ARG:HG3	1.76	0.50
1:C:15:TYR:CE2	1:C:48:ALA:HB2	2.47	0.50
1:A:162:GLU:H	1:A:162:GLU:CD	2.15	0.50
2:D:368:THR:O	2:D:370:GLN:N	2.41	0.50
2:D:371:SER:O	2:D:372:TRP:C	2.50	0.50
2:D:187:ARG:NH2	2:D:382:TYR:CZ	2.80	0.50
1:A:98:GLY:HA2	1:A:199:ARG:HD3	1.94	0.49
1:C:131:GLN:H	1:C:131:GLN:CD	2.14	0.49
2:D:361:HIS:ND1	2:D:372:TRP:N	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:LYS:HG3	1:A:131:GLN:HG2	1.94	0.49
2:B:289:LYS:HA	2:B:289:LYS:CE	2.41	0.49
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.37	0.49
1:C:227:TRP:CZ3	1:C:269:TYR:HD1	2.31	0.49
1:C:52:ILE:O	1:C:56:LYS:HG3	2.12	0.49
1:C:65:LYS:HB3	1:C:81:GLU:HG2	1.93	0.49
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.95	0.49
1:C:72:THR:HG22	1:C:73:GLU:H	1.77	0.49
2:B:211:ARG:HG2	2:B:211:ARG:HH11	1.77	0.49
1:C:198:THR:CG2	1:C:252:VAL:HG13	2.42	0.49
1:C:256:ASP:OD2	1:C:259:GLY:N	2.39	0.49
1:C:278:LYS:HB2	2:D:178:TYR:CE1	2.48	0.49
1:C:121:HIS:HD2	2:D:185:TYR:CE1	2.31	0.48
2:D:407:GLN:OE1	2:D:410:ARG:HG3	2.12	0.48
1:A:178:LYS:HG3	1:A:179:TYR:CD2	2.48	0.48
1:A:0:SER:C	1:A:2:GLU:H	2.16	0.48
2:B:327:CYS:SG	2:B:419:HIS:NE2	2.86	0.48
1:C:210:ASP:CG	1:C:214:ARG:HD2	2.34	0.48
2:D:418:TYR:O	2:D:419:HIS:HB2	2.13	0.48
1:A:99:ILE:HG23	1:A:103:LEU:HD23	1.95	0.48
1:A:1:MET:SD	1:A:70:ILE:HG21	2.53	0.48
2:B:194:LYS:NZ	2:B:195:PRO:O	2.46	0.48
1:C:278:LYS:NZ	2:D:181:ASP:OD2	2.47	0.48
1:C:227:TRP:CE3	1:C:269:TYR:HD1	2.32	0.48
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.39	0.48
2:D:421:VAL:O	2:D:424:LEU:HG	2.13	0.48
1:A:57:GLU:OE1	2:B:185:TYR:OH	2.29	0.48
2:D:193:CYS:O	2:D:241:ARG:HD2	2.13	0.48
2:D:210:MET:HE1	2:D:250:ARG:CB	2.39	0.48
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.47	0.48
1:A:34:LYS:HB3	4:A:2011:HOH:O	2.13	0.48
1:A:40:GLU:CB	2:B:288:LYS:HD3	2.44	0.48
1:C:101:LEU:N	1:C:102:PRO:HD2	2.28	0.48
2:D:370:GLN:HB2	4:D:2040:HOH:O	2.12	0.48
1:C:137:THR:HA	1:C:296:LEU:HD12	1.94	0.48
1:C:33:LYS:HD3	1:C:35:ILE:HD11	1.96	0.48
2:D:196:LYS:HG2	2:D:199:TYR:HB3	1.95	0.48
2:D:237:ASN:O	2:D:238:TYR:C	2.52	0.48
2:D:401:ALA:N	2:D:402:PRO:CD	2.74	0.48
1:A:94:SER:O	1:A:98:GLY:N	2.47	0.47
2:B:289:LYS:HA	2:B:289:LYS:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:SER:O	1:C:110:GLN:HG3	2.14	0.47
3:C:1298:2A6:N1	3:C:1298:2A6:C22	2.76	0.47
1:C:193:PHE:CD2	1:C:266:MET:HE3	2.48	0.47
2:D:254:GLN:HG2	2:D:286:TYR:HE2	1.78	0.47
1:C:262:LEU:O	1:C:265:GLN:N	2.47	0.47
1:A:14:THR:HG23	1:A:145:ASP:OD1	2.15	0.47
1:C:58:LEU:HD21	1:C:123:VAL:HG21	1.96	0.47
2:D:375:SER:HA	2:D:378:ARG:NH2	2.29	0.47
1:A:193:PHE:HD2	1:A:266:MET:HE1	1.80	0.47
2:D:329:VAL:HG13	2:D:363:ALA:CB	2.45	0.47
1:C:15:TYR:CZ	1:C:33:LYS:HE2	2.49	0.47
1:C:171:PRO:HD2	1:C:172:GLU:OE2	2.14	0.47
1:C:193:PHE:CZ	1:C:255:LEU:HD11	2.49	0.47
1:C:178:LYS:HE2	1:C:179:TYR:CE2	2.49	0.47
1:C:223:ASP:O	1:C:226:VAL:HG13	2.14	0.47
2:D:296:HIS:CD2	2:D:300:LYS:HZ1	2.29	0.47
1:A:125:HIS:ND1	1:A:128:LEU:HD23	2.29	0.47
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.44	0.47
1:A:59:ASN:HA	4:A:2024:HOH:O	2.14	0.47
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.96	0.47
2:B:404:HIS:ND1	2:B:406:GLN:HB2	2.30	0.47
1:C:250:LYS:O	1:C:251:VAL:C	2.52	0.47
1:C:193:PHE:CE1	1:C:255:LEU:HD11	2.49	0.47
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.95	0.46
2:B:322:GLN:NE2	2:B:330:GLU:OE2	2.47	0.46
2:D:338:GLU:HG2	2:D:409:ILE:HD13	1.96	0.46
1:A:231:THR:HG22	1:A:236:TYR:CZ	2.50	0.46
2:D:239:ILE:CD1	2:D:257:GLY:HA2	2.46	0.46
2:D:315:LEU:CD2	2:D:356:ALA:HB1	2.45	0.46
2:D:375:SER:HA	2:D:378:ARG:NH1	2.29	0.46
1:A:52:ILE:HD11	1:A:78:LEU:CD2	2.45	0.46
2:B:329:VAL:HG11	2:B:364:LEU:HD12	1.98	0.46
1:C:231:THR:HG22	1:C:236:TYR:CE2	2.51	0.46
1:C:157:ARG:HD3	2:D:228:GLN:OE1	2.16	0.46
1:A:154:VAL:O	2:B:316:THR:CG2	2.63	0.46
2:B:384:LEU:HA	2:B:384:LEU:HD12	1.90	0.46
1:C:207:SER:H	1:C:210:ASP:HB3	1.79	0.46
2:D:266:LYS:NZ	2:D:295:GLU:OE2	2.34	0.46
2:D:329:VAL:CG2	2:D:364:LEU:HA	2.45	0.46
1:A:178:LYS:HG2	4:A:2071:HOH:O	2.15	0.46
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.99	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LEU:HD13	4:C:2070:HOH:O	2.16	0.46
2:B:175:VAL:N	2:B:176:PRO:CD	2.79	0.46
2:B:335:PHE:CZ	2:B:339:LEU:HD11	2.51	0.46
1:C:225:VAL:O	1:C:227:TRP:N	2.49	0.46
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.98	0.46
1:C:259:GLY:O	1:C:260:ARG:C	2.52	0.46
1:A:223:ASP:H	1:A:226:VAL:HG12	1.81	0.46
1:A:249:SER:O	1:A:253:PRO:HA	2.16	0.46
1:A:270:ASP:HB3	1:A:273:LYS:HG2	1.97	0.46
1:A:48:ALA:O	1:A:52:ILE:HG13	2.16	0.46
1:C:244:ALA:HB2	4:C:2066:HOH:O	2.16	0.46
1:A:62:ASN:HA	1:A:142:LYS:HG2	1.96	0.46
1:A:253:PRO:CB	1:A:254:PRO:HD3	2.46	0.46
2:B:288:LYS:O	2:B:292:LEU:HB2	2.16	0.45
1:C:163:VAL:HG12	1:C:164:VAL:HG23	1.98	0.45
1:C:272:ASN:HB3	4:C:2072:HOH:O	2.16	0.45
1:A:265:GLN:HB3	1:A:275:ILE:HB	1.98	0.45
1:C:99:ILE:HD13	1:C:196:MET:HG2	1.97	0.45
2:B:330:GLU:O	2:B:334:MET:HG3	2.16	0.45
1:C:6:LYS:HE3	1:C:32:LEU:HD13	1.99	0.45
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.51	0.45
3:C:1298:2A6:H22	3:C:1298:2A6:N1	2.31	0.45
1:C:169:ARG:HD3	1:C:173:ILE:HG21	1.98	0.45
2:D:388:LYS:HD2	2:D:432:LEU:HD13	1.98	0.45
1:A:131:GLN:H	1:A:131:GLN:CD	2.19	0.45
2:B:316:THR:HG21	4:B:2053:HOH:O	2.16	0.45
1:C:172:GLU:OE1	1:C:274:ARG:NH1	2.30	0.45
1:C:258:ASP:OD2	1:C:284:PRO:HB2	2.15	0.45
1:C:94:SER:O	1:C:98:GLY:N	2.49	0.45
1:A:39:THR:CB	2:B:289:LYS:HZ2	2.29	0.45
1:C:137:THR:O	1:C:293:VAL:HG13	2.16	0.45
1:C:87:LEU:HB3	1:C:130:PRO:CB	2.46	0.45
2:D:214:LEU:HD12	2:D:214:LEU:O	2.17	0.45
2:D:383:THR:N	2:D:386:SER:OG	2.49	0.45
2:D:360:PHE:HD2	2:D:376:LEU:HD11	1.81	0.45
2:B:415:ASN:OD1	2:B:416:SER:N	2.50	0.45
1:C:205:GLY:HA2	1:C:210:ASP:OD2	2.17	0.45
2:B:210:MET:CE	2:B:250:ARG:HB2	2.48	0.45
1:C:225:VAL:O	1:C:226:VAL:C	2.55	0.45
1:C:51:GLU:O	1:C:55:LEU:HB2	2.17	0.45
1:C:257:GLU:HA	1:C:260:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:216:ASP:HA	2:D:219:VAL:HG23	1.98	0.44
2:D:248:VAL:HG12	2:D:249:LEU:O	2.17	0.44
2:D:335:PHE:HD2	2:D:336:LEU:HD23	1.82	0.44
2:D:340:SER:O	2:D:341:LEU:C	2.55	0.44
1:C:178:LYS:HG3	1:C:179:TYR:CD2	2.52	0.44
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.83	0.44
2:D:387:LEU:O	2:D:391:LEU:HB2	2.17	0.44
1:C:279:ALA:O	1:C:281:LEU:N	2.50	0.44
2:D:391:LEU:HD12	4:D:2044:HOH:O	2.17	0.44
2:D:418:TYR:O	2:D:421:VAL:HG13	2.18	0.44
1:A:51:GLU:HG3	1:A:55:LEU:HD22	2.00	0.44
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.85	0.44
1:A:81:GLU:HB2	4:A:2034:HOH:O	2.17	0.44
2:B:217:TRP:O	2:B:221:VAL:HG23	2.17	0.44
2:B:249:LEU:HG	1:C:27:GLY:HA3	1.99	0.44
2:B:338:GLU:HG2	2:B:409:ILE:HD13	1.98	0.44
1:C:93:ALA:HB3	4:C:2034:HOH:O	2.17	0.44
2:D:315:LEU:O	2:D:318:TYR:HB2	2.18	0.44
1:C:222:PRO:HD3	1:C:269:TYR:CE1	2.52	0.44
1:A:103:LEU:HD11	1:A:107:TYR:CZ	2.52	0.44
1:C:101:LEU:N	1:C:102:PRO:CD	2.80	0.44
2:D:332:LEU:HD21	2:D:398:TYR:OH	2.18	0.44
1:C:220:GLY:O	1:C:221:THR:C	2.56	0.44
2:B:400:LYS:O	2:B:401:ALA:C	2.56	0.44
1:C:126:ARG:O	1:C:127:ASP:HB2	2.17	0.44
2:D:338:GLU:HG2	2:D:409:ILE:CD1	2.47	0.44
2:B:255:LEU:HB2	2:B:286:TYR:CZ	2.53	0.43
1:A:207:SER:HB3	4:A:2080:HOH:O	2.17	0.43
1:A:283:HIS:CE1	1:A:284:PRO:HG2	2.52	0.43
1:A:72:THR:HG22	1:A:73:GLU:H	1.83	0.43
1:C:192:ILE:HG22	1:C:196:MET:CE	2.48	0.43
2:D:212:ALA:HA	2:D:342:ILE:HG22	2.00	0.43
1:A:130:PRO:HD2	1:A:131:GLN:OE1	2.18	0.43
1:C:128:LEU:HD22	1:C:143:LEU:HD22	1.99	0.43
1:C:263:LEU:HD11	1:C:267:LEU:HD11	1.98	0.43
1:C:286:PHE:O	1:C:287:GLN:C	2.57	0.43
2:D:190:GLU:HG3	2:D:352:PRO:HD2	2.00	0.43
1:A:283:HIS:CG	1:A:284:PRO:HD2	2.53	0.43
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.53	0.43
1:C:163:VAL:O	1:C:164:VAL:O	2.37	0.43
2:B:319:PHE:O	2:B:322:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LEU:O	1:C:215:ILE:HG12	2.19	0.43
1:A:154:VAL:HB	2:B:317:GLN:CG	2.49	0.43
2:B:401:ALA:HB3	2:B:402:PRO:HD3	2.01	0.43
1:C:210:ASP:OD1	1:C:214:ARG:HD2	2.19	0.43
1:A:157:ARG:NH2	2:B:268:GLU:OE2	2.45	0.43
1:C:233:MET:HA	1:C:234:PRO:HD3	1.88	0.43
1:C:74:ASN:HA	4:C:2033:HOH:O	2.18	0.43
1:A:28:GLU:HG3	2:D:247:SER:HB3	2.01	0.43
1:A:110:GLN:OE1	1:A:140:ALA:HA	2.19	0.43
1:A:193:PHE:O	1:A:197:VAL:HG23	2.19	0.43
1:A:293:VAL:HA	1:A:294:PRO:HD2	1.88	0.43
2:B:225:TYR:O	2:B:226:LYS:HB2	2.19	0.43
1:A:101:LEU:N	1:A:102:PRO:CD	2.82	0.42
1:C:222:PRO:HD3	1:C:269:TYR:CZ	2.53	0.42
2:B:238:TYR:CD1	2:B:238:TYR:N	2.87	0.42
2:B:270:ILE:HG13	4:B:2040:HOH:O	2.19	0.42
1:C:189:LEU:HA	1:C:189:LEU:HD23	1.80	0.42
1:C:40:GLU:HG3	2:D:289:LYS:HZ1	1.84	0.42
1:C:268:HIS:O	1:C:269:TYR:C	2.58	0.42
2:D:277:GLU:O	2:D:278:PHE:C	2.57	0.42
2:D:364:LEU:C	2:D:364:LEU:HD23	2.40	0.42
1:A:150:ARG:HG2	4:A:2050:HOH:O	2.19	0.42
2:D:331:SER:HA	2:D:334:MET:HG3	2.00	0.42
1:A:50:ARG:HD3	4:A:2049:HOH:O	2.19	0.42
1:C:172:GLU:CD	1:C:274:ARG:HH22	2.22	0.42
2:D:230:GLU:HG3	2:D:268:GLU:CD	2.39	0.42
2:D:409:ILE:O	2:D:410:ARG:C	2.58	0.42
1:A:126:ARG:O	1:A:127:ASP:HB2	2.19	0.42
1:C:158:THR:HA	1:C:178:LYS:O	2.20	0.42
1:C:105:LYS:NZ	1:C:285:PHE:O	2.51	0.42
1:C:60:HIS:HB3	1:C:63:ILE:HG13	2.02	0.42
2:D:230:GLU:O	2:D:233:HIS:N	2.53	0.42
2:D:296:HIS:NE2	2:D:300:LYS:NZ	2.54	0.42
2:D:347:TYR:N	2:D:347:TYR:CD2	2.86	0.42
1:A:101:LEU:CB	1:A:102:PRO:HD3	2.50	0.42
1:A:98:GLY:HA3	1:A:199:ARG:HH11	1.84	0.42
1:C:171:PRO:O	1:C:173:ILE:N	2.53	0.42
1:C:280:ALA:O	1:C:286:PHE:CE2	2.66	0.42
1:C:283:HIS:HA	1:C:284:PRO:HD2	1.72	0.42
2:D:371:SER:O	2:D:373:PRO:N	2.53	0.42
1:A:87:LEU:O	1:A:91:MET:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:MET:HB2	1:C:236:TYR:HB2	2.02	0.42
1:C:63:ILE:O	1:C:64:VAL:C	2.58	0.42
2:B:430:LEU:O	2:B:431:ASN:HB2	2.20	0.42
1:A:269:TYR:O	1:A:271:PRO:HD3	2.20	0.41
1:C:268:HIS:HD2	1:C:270:ASP:H	1.67	0.41
2:D:254:GLN:HB3	2:D:286:TYR:OH	2.20	0.41
1:A:53:SER:HB2	4:B:2048:HOH:O	2.20	0.41
2:B:259:ALA:O	2:B:260:ALA:C	2.55	0.41
1:C:253:PRO:CB	1:C:254:PRO:CD	2.97	0.41
1:C:88:LYS:O	1:C:89:LYS:C	2.58	0.41
2:D:194:LYS:HZ2	2:D:195:PRO:HD2	1.84	0.41
2:B:203:GLN:HA	2:B:204:PRO:HD2	1.92	0.41
2:D:327:CYS:HA	2:D:330:GLU:HB2	2.01	0.41
1:A:52:ILE:HG12	1:A:78:LEU:CD1	2.51	0.41
1:A:52:ILE:HG12	1:A:78:LEU:HD11	2.03	0.41
1:C:269:TYR:O	1:C:274:ARG:NH2	2.49	0.41
2:D:383:THR:H	2:D:386:SER:CB	2.33	0.41
2:B:211:ARG:HG2	2:B:211:ARG:NH1	2.35	0.41
2:D:343:ASP:O	2:D:344:ALA:C	2.58	0.41
1:C:9:LYS:HG2	1:C:10:ILE:N	2.34	0.41
2:B:246:MET:HG3	2:B:301:VAL:HG21	2.01	0.41
1:A:101:LEU:N	1:A:102:PRO:HD2	2.36	0.41
1:A:121:HIS:HD2	2:B:185:TYR:CE1	2.38	0.41
1:A:57:GLU:CD	2:B:185:TYR:HH	2.24	0.41
1:C:273:LYS:HD3	1:C:273:LYS:HA	1.90	0.41
1:A:40:GLU:HA	2:B:288:LYS:CE	2.50	0.41
1:C:162:GLU:O	1:C:163:VAL:HG23	2.20	0.41
1:C:227:TRP:CG	1:C:230:VAL:HG22	2.55	0.41
1:A:98:GLY:CA	1:A:199:ARG:NH1	2.84	0.41
2:B:223:GLU:CD	2:B:412:LYS:HG3	2.41	0.41
1:C:150:ARG:HG2	1:C:151:ALA:O	2.21	0.41
1:C:210:ASP:OD2	1:C:214:ARG:HD2	2.21	0.41
2:D:228:GLN:O	2:D:231:THR:HB	2.21	0.41
2:D:359:ALA:O	2:D:360:PHE:C	2.58	0.41
1:C:166:LEU:HD11	1:C:211:GLN:HB2	2.03	0.41
1:C:173:ILE:HG21	4:C:2042:HOH:O	2.21	0.41
2:D:219:VAL:HG21	2:D:409:ILE:HG13	2.02	0.41
1:A:219:LEU:HA	4:A:2085:HOH:O	2.21	0.40
1:A:223:ASP:OD1	1:A:225:VAL:N	2.54	0.40
2:B:214:LEU:HD11	2:B:257:GLY:HA3	2.02	0.40
2:D:366:THR:HG23	4:D:2056:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:PRO:HD3	4:C:2046:HOH:O	2.21	0.40
2:D:175:VAL:N	2:D:176:PRO:CD	2.83	0.40
1:C:49:ILE:CG2	2:D:306:LEU:HD12	2.50	0.40
2:D:329:VAL:HA	2:D:367:VAL:HG21	2.03	0.40
2:D:395:HIS:HE2	2:D:399:LEU:HD11	1.85	0.40
2:B:255:LEU:HA	2:B:255:LEU:HD12	1.88	0.40
1:C:134:LEU:O	1:C:141:ILE:HA	2.21	0.40
1:C:275:ILE:O	1:C:275:ILE:HG23	2.20	0.40
2:D:219:VAL:HG11	2:D:409:ILE:HG12	2.04	0.40
2:D:335:PHE:CE1	2:D:422:SER:HB3	2.56	0.40
1:A:85:GLN:HA	3:A:1298:2A6:C20	2.52	0.40
1:A:136:ASN:ND2	1:A:140:ALA:HB3	2.35	0.40
1:A:42:GLU:OE1	2:B:275:VAL:HG23	2.21	0.40
2:B:272:PRO:HA	2:B:273:PRO:HD3	1.94	0.40
1:A:72:THR:O	2:B:296:HIS:HE1	2.05	0.40
2:B:327:CYS:SG	2:B:419:HIS:CE1	3.14	0.40
1:C:274:ARG:HD2	1:C:274:ARG:HH11	1.39	0.40
2:D:241:ARG:O	2:D:244:SER:HB2	2.21	0.40
2:D:314:PHE:O	2:D:317:GLN:N	2.52	0.40
2:D:397:THR:HG23	4:D:2047:HOH:O	2.20	0.40
1:A:104:ILE:HG23	1:A:196:MET:HE3	2.04	0.40
1:C:284:PRO:O	1:C:285:PHE:C	2.60	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%)	274 (93%)	11 (4%)	9 (3%)	<b>4</b> <b>6</b>
1	C	294/303 (97%)	251 (85%)	33 (11%)	10 (3%)	<b>4</b> <b>5</b>
2	B	256/258 (99%)	244 (95%)	9 (4%)	3 (1%)	<b>14</b> <b>26</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	256/258 (99%)	219 (86%)	30 (12%)	7 (3%)	5	8
All	All	1100/1122 (98%)	988 (90%)	83 (8%)	29 (3%)	6	9

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	VAL
1	C	225	VAL
2	D	346	PRO
2	D	369	GLY
1	A	38	ASP
1	A	98	GLY
1	A	127	ASP
1	A	164	VAL
1	A	248	PHE
2	B	346	PRO
1	C	172	GLU
1	C	226	VAL
1	C	280	ALA
1	A	8	GLU
1	A	162	GLU
1	C	127	ASP
1	C	245	ARG
2	D	177	ASP
2	B	324	PRO
1	C	155	PRO
1	C	274	ARG
2	D	315	LEU
1	A	41	THR
2	D	176	PRO
1	A	155	PRO
2	B	281	ILE
1	C	16	GLY
2	D	281	ILE
2	D	373	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/265 (98%)	229 (88%)	32 (12%)	5	10
1	C	261/265 (98%)	224 (86%)	37 (14%)	3	7
2	B	232/232 (100%)	207 (89%)	25 (11%)	7	13
2	D	232/232 (100%)	191 (82%)	41 (18%)	2	3
All	All	986/994 (99%)	851 (86%)	135 (14%)	4	7

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	34	LYS
1	A	36	ARG
1	A	40	GLU
1	A	42	GLU
1	A	46	SER
1	A	49	ILE
1	A	55	LEU
1	A	59	ASN
1	A	66	LEU
1	A	74	ASN
1	A	78	LEU
1	A	91	MET
1	A	97	THR
1	A	101	LEU
1	A	120	SER
1	A	122	ARG
1	A	131	GLN
1	A	150	ARG
1	A	162	GLU
1	A	163	VAL
1	A	200	ARG
1	A	230	VAL
1	A	247	ASP
1	A	248	PHE
1	A	250	LYS
1	A	255	LEU
1	A	256	ASP
1	A	257	GLU
1	A	264	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	276	SER
1	A	278	LYS
2	B	175	VAL
2	B	179	HIS
2	B	180	GLU
2	B	193	CYS
2	B	199	TYR
2	B	202	LYS
2	B	206	ILE
2	B	226	LYS
2	B	244	SER
2	B	274	GLU
2	B	284	ASP
2	B	289	LYS
2	B	293	ARG
2	B	316	THR
2	B	327	CYS
2	B	328	LYS
2	B	331	SER
2	B	346	PRO
2	B	348	LEU
2	B	374	GLU
2	B	384	LEU
2	B	386	SER
2	B	391	LEU
2	B	408	SER
2	B	428	GLU
1	C	2	GLU
1	C	9	LYS
1	C	12	GLU
1	C	14	THR
1	C	34	LYS
1	C	39	THR
1	C	40	GLU
1	C	47	THR
1	C	59	ASN
1	C	74	ASN
1	C	75	LYS
1	C	94	SER
1	C	97	THR
1	C	105	LYS
1	C	113	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	120	SER
1	C	122	ARG
1	C	131	GLN
1	C	136	ASN
1	C	148	LEU
1	C	152	PHE
1	C	163	VAL
1	C	177	CYS
1	C	181	SER
1	C	193	PHE
1	C	199	ARG
1	C	200	ARG
1	C	215	ILE
1	C	218	THR
1	C	221	THR
1	C	226	VAL
1	C	247	ASP
1	C	248	PHE
1	C	268	HIS
1	C	281	LEU
1	C	287	GLN
1	C	290	THR
2	D	177	ASP
2	D	180	GLU
2	D	196	LYS
2	D	199	TYR
2	D	202	LYS
2	D	206	ILE
2	D	219	VAL
2	D	230	GLU
2	D	232	LEU
2	D	247	SER
2	D	250	ARG
2	D	253	LEU
2	D	271	TYR
2	D	281	ILE
2	D	284	ASP
2	D	289	LYS
2	D	292	LEU
2	D	312	ASN
2	D	316	THR
2	D	322	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	323	GLN
2	D	324	PRO
2	D	328	LYS
2	D	334	MET
2	D	342	ILE
2	D	346	PRO
2	D	348	LEU
2	D	360	PHE
2	D	364	LEU
2	D	377	ILE
2	D	378	ARG
2	D	380	THR
2	D	385	GLU
2	D	392	MET
2	D	393	ASP
2	D	396	GLN
2	D	398	TYR
2	D	415	ASN
2	D	417	LYS
2	D	424	LEU
2	D	432	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	60	HIS
1	A	84	HIS
1	A	119	HIS
1	A	265	GLN
2	B	254	GLN
2	B	317	GLN
2	B	431	ASN
1	C	60	HIS
1	C	84	HIS
1	C	85	GLN
1	C	113	GLN
1	C	265	GLN
1	C	268	HIS
1	C	272	ASN
2	D	312	ASN
2	D	313	GLN
2	D	317	GLN

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Mol	Chain	Res	Type
2	D	370	GLN

### 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	A	160	1	9,10,11	1.28	0	11,14,16	1.30	1 (9%)
1	TPO	C	160	1	9,10,11	1.98	2 (22%)	11,14,16	1.40	2 (18%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	CA-C	2.59	1.53	1.50
1	C	160	TPO	P-OG1	4.03	1.66	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	TPO	O-C-CA	-4.08	115.59	125.09
1	C	160	TPO	P-OG1-CB	-2.24	116.44	123.21
1	C	160	TPO	O3P-P-O1P	3.05	122.50	110.60

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](#)

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	2A6	A	1298	-	25,27,27	1.65	7 (28%)	27,36,36	3.97	10 (37%)
3	2A6	C	1298	-	25,27,27	2.38	9 (36%)	27,36,36	2.96	8 (29%)

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	2A6	A	1298	-	-	0/9/17/17	0/4/4/4
3	2A6	C	1298	-	-	0/9/17/17	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298	2A6	O6-C10	-7.27	1.22	1.44
3	A	1298	2A6	C2-N2	-3.16	1.30	1.36
3	C	1298	2A6	C5-C4	-3.08	1.33	1.40
3	C	1298	2A6	C4-N9	-2.81	1.29	1.34
3	C	1298	2A6	C2-N2	-2.76	1.31	1.36
3	A	1298	2A6	C5-C4	-2.71	1.34	1.40
3	C	1298	2A6	C6-N1	-2.67	1.26	1.31
3	A	1298	2A6	C17-N2	-2.40	1.35	1.40
3	A	1298	2A6	C4-N9	-2.38	1.30	1.34
3	C	1298	2A6	C2-N3	-2.33	1.27	1.34
3	A	1298	2A6	C2-N3	-2.32	1.27	1.34
3	C	1298	2A6	O6-C6	-2.03	1.33	1.35
3	A	1298	2A6	C4-N3	3.02	1.42	1.36
3	C	1298	2A6	C4-N3	3.57	1.44	1.36
3	C	1298	2A6	C2-N1	3.59	1.46	1.34
3	A	1298	2A6	C2-N1	3.67	1.46	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	2A6	C10-O6-C6	-14.19	103.95	117.50
3	A	1298	2A6	C4-C5-N7	-8.86	100.85	109.41
3	C	1298	2A6	N3-C2-N1	-7.51	115.08	126.23
3	A	1298	2A6	N3-C2-N1	-5.51	118.05	126.23
3	C	1298	2A6	C4-C5-N7	-4.88	104.70	109.41
3	A	1298	2A6	C17-N2-C2	-3.65	119.79	129.23
3	A	1298	2A6	C12-C11-C10	-2.21	106.83	111.41
3	C	1298	2A6	C12-C11-C10	-2.19	106.87	111.41
3	C	1298	2A6	C14-C13-C12	2.08	115.64	111.42
3	A	1298	2A6	C14-C13-C12	2.10	115.68	111.42
3	A	1298	2A6	C6-C5-C4	2.29	119.47	117.26
3	C	1298	2A6	N2-C2-N3	2.62	125.67	116.88
3	A	1298	2A6	N2-C2-N1	3.78	129.55	116.87
3	C	1298	2A6	C10-O6-C6	4.13	121.45	117.50
3	C	1298	2A6	C2-N1-C6	4.34	122.84	115.18
3	A	1298	2A6	C2-N1-C6	4.37	122.89	115.18
3	A	1298	2A6	C2-N3-C4	6.01	121.97	115.11
3	C	1298	2A6	C2-N3-C4	9.26	125.68	115.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298	2A6	2	0
3	C	1298	2A6	2	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%)	0.23	19 (6%) 19 20	25, 43, 121, 177	0
1	C	296/303 (97%)	0.66	46 (15%) 2 1	36, 61, 119, 178	0
2	B	258/258 (100%)	-0.14	4 (1%) 72 74	24, 40, 75, 143	0
2	D	258/258 (100%)	0.80	49 (18%) 1 1	32, 58, 87, 148	0
All	All	1108/1122 (98%)	0.39	118 (10%) 6 5	24, 52, 105, 178	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	40	GLU	7.2
2	D	367	VAL	6.9
2	D	175	VAL	6.5
1	C	231	THR	6.4
2	D	372	TRP	6.0
1	C	225	VAL	5.9
2	D	421	VAL	5.5
2	D	430	LEU	5.5
2	D	399	LEU	4.9
1	C	296	LEU	4.7
2	B	175	VAL	4.7
1	C	251	VAL	4.6
1	A	296	LEU	4.6
1	A	295	HIS	4.4
2	D	361	HIS	4.4
1	C	227	TRP	4.4
1	A	39	THR	4.2
2	D	432	LEU	4.2
1	A	36	ARG	4.2
1	C	40	GLU	4.1
2	D	418	TYR	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	294	PRO	4.0
2	D	427	PRO	4.0
2	B	176	PRO	3.9
2	D	336	LEU	3.7
1	C	248	PHE	3.6
1	A	73	GLU	3.6
1	C	250	LYS	3.6
1	A	99	ILE	3.6
2	D	329	VAL	3.5
2	D	327	CYS	3.5
1	C	257	GLU	3.5
2	D	322	GLN	3.4
1	C	39	THR	3.4
2	D	365	TYR	3.4
2	D	382	TYR	3.4
1	C	290	THR	3.4
2	D	423	LEU	3.4
1	C	247	ASP	3.3
2	D	426	PRO	3.3
1	C	246	GLN	3.3
1	A	38	ASP	3.3
2	D	376	LEU	3.2
1	C	233	MET	3.2
1	C	38	ASP	3.2
1	C	223	ASP	3.2
2	D	424	LEU	3.2
2	D	328	LYS	3.1
2	D	326	ASN	3.1
1	C	234	PRO	3.1
1	C	101	LEU	3.1
2	D	428	GLU	3.0
1	C	236	TYR	3.0
1	C	37	LEU	3.0
1	C	255	LEU	3.0
1	C	175	LEU	2.9
2	D	366	THR	2.9
1	A	293	VAL	2.9
1	C	219	LEU	2.9
1	C	213	PHE	2.9
2	B	432	LEU	2.9
1	C	96	LEU	2.9
1	C	74	ASN	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	71	HIS	2.8
2	D	402	PRO	2.8
2	D	425	ASN	2.8
1	A	100	PRO	2.7
1	C	99	ILE	2.7
2	D	368	THR	2.7
1	C	287	GLN	2.7
2	D	324	PRO	2.7
2	D	422	SER	2.7
2	D	321	HIS	2.7
1	A	96	LEU	2.7
1	A	199	ARG	2.6
1	C	226	VAL	2.6
1	C	253	PRO	2.6
2	D	332	LEU	2.6
1	A	248	PHE	2.6
2	D	392	MET	2.6
1	C	36	ARG	2.6
1	A	72	THR	2.6
1	A	97	THR	2.6
2	D	350	TYR	2.6
1	C	235	ASP	2.5
1	C	249	SER	2.5
2	D	416	SER	2.5
2	D	388	LYS	2.5
1	C	238	PRO	2.5
2	D	384	LEU	2.5
2	D	371	SER	2.5
2	D	369	GLY	2.4
2	B	385	GLU	2.4
1	C	285	PHE	2.4
2	D	389	PRO	2.4
2	D	419	HIS	2.4
1	A	101	LEU	2.4
2	D	377	ILE	2.3
2	D	395	HIS	2.3
1	C	104	ILE	2.2
2	D	364	LEU	2.2
2	D	318	TYR	2.2
1	A	41	THR	2.2
1	C	232	SER	2.2
1	C	161	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	97	THR	2.2
2	D	397	THR	2.2
1	C	94	SER	2.2
1	C	71	HIS	2.1
2	D	403	GLN	2.1
2	D	235	ALA	2.1
1	C	286	PHE	2.1
1	C	289	VAL	2.1
2	D	176	PRO	2.1
1	C	245	ARG	2.1
2	D	349	LYS	2.1
1	C	216	PHE	2.1
1	C	273	LYS	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	0.94	0.18	20,20,20,20	0
1	TPO	A	160	11/12	0.98	0.12	38,40,52,53	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	2A6	C	1298	24/24	0.93	0.17	47,51,54,55	0
3	2A6	A	1298	24/24	0.95	0.17	53,54,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.