



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1H1P  
Title : STRUCTURE OF HUMAN THR160-PHOSPHO CDK2/CYCLIN A COM-  
PLEXED WITH THE INHIBITOR NU2058  
Authors : Davies, T.G.; Noble, M.E.M.; Endicott, J.A.; Johnson, L.N.  
Deposited on : 2002-07-21  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

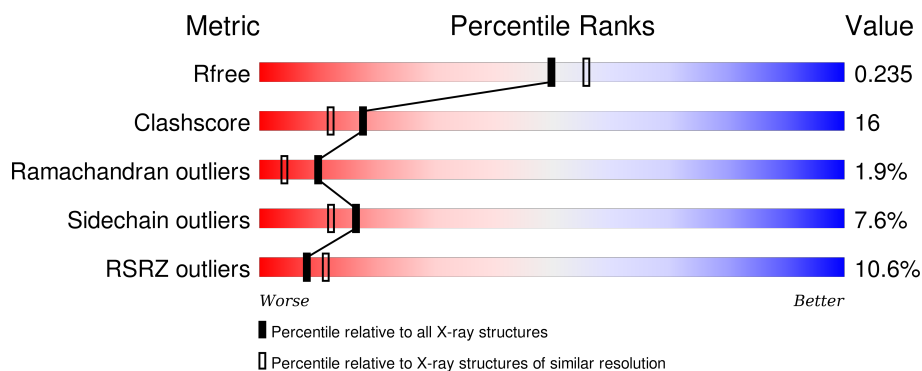
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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>8%</div> <div>56%</div> <div>28%</div> <div>8%</div> <div>6%</div> <div>.</div> </div>
1	C	303	<div> <div>14%</div> <div>62%</div> <div>28%</div> <div>6%</div> <div>.</div> <div>.</div> </div>
2	B	258	<div> <div>9%</div> <div>64%</div> <div>28%</div> <div>6%</div> <div>.</div> </div>
2	D	258	<div> <div>10%</div> <div>65%</div> <div>26%</div> <div>7%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9388 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.

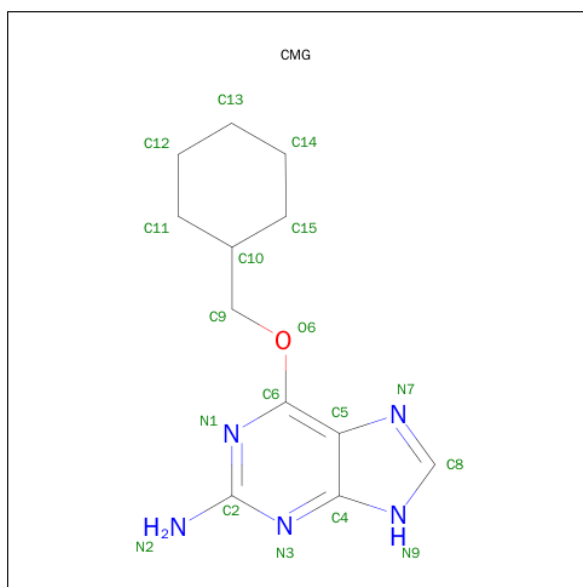
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

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-O-CYCLOHEXYLMETHYL GUANINE (three-letter code: CMG) (formula:  $C_{12}H_{17}N_5O$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	12	5	1		
3	C	1	Total	C	N	O	0	0
			18	12	5	1		

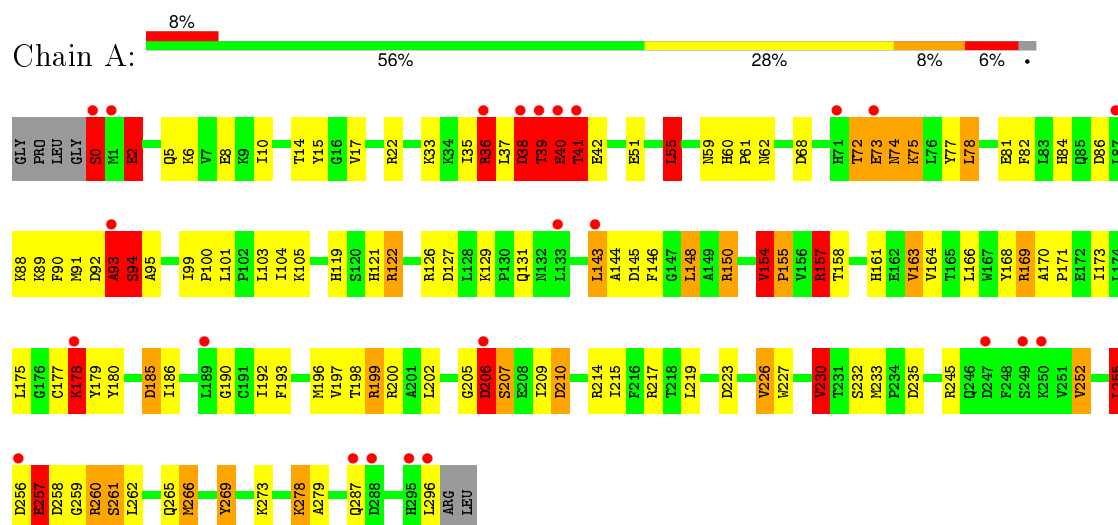
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	106	Total	O	0	0
			106	106		
4	C	107	Total	O	0	0
			107	107		
4	D	92	Total	O	0	0
			92	92		

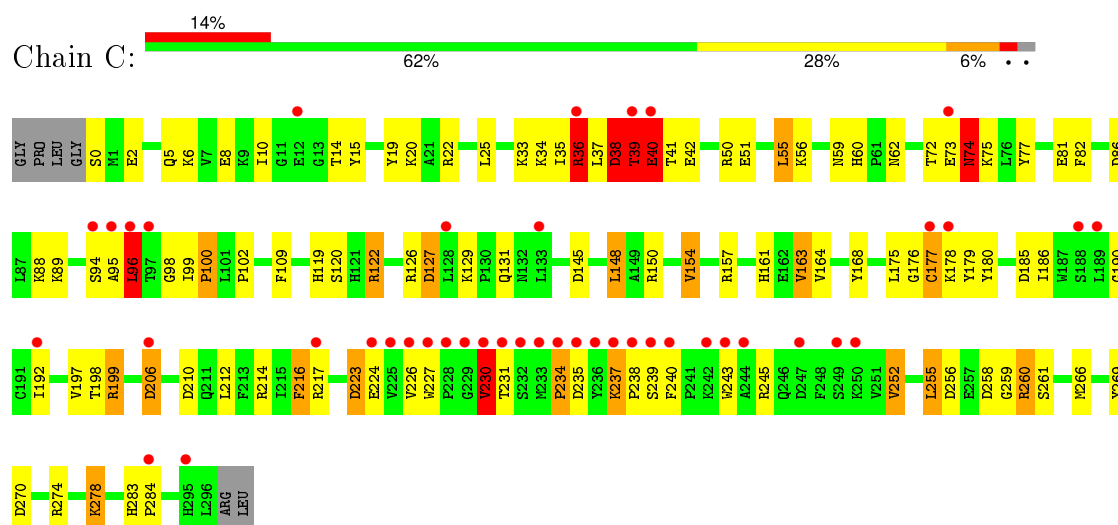
### 3 Residue-property plots

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

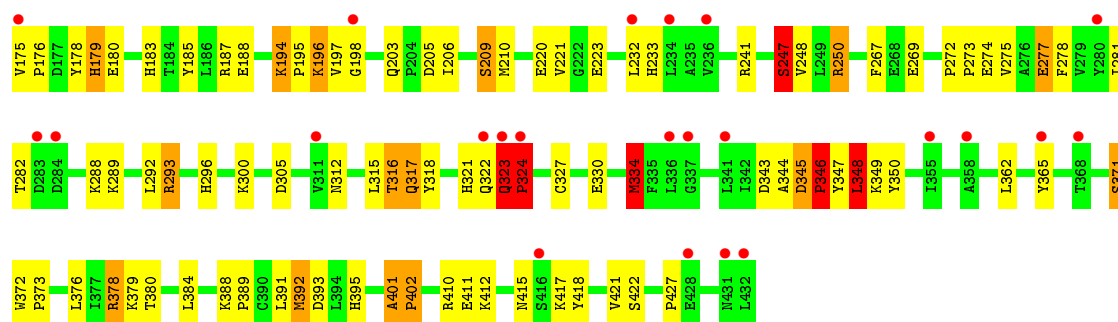


#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2

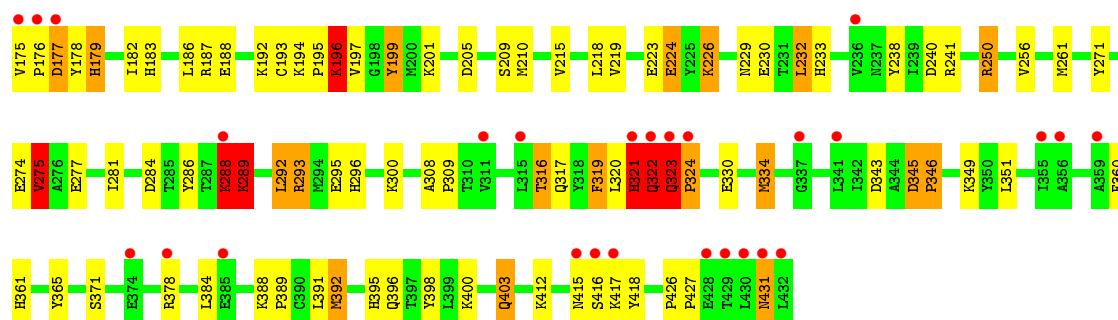


#### • Molecule 2: CYCLIN A2





• Molecule 2: CYCLIN A2



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.03Å 193.83Å 157.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 32.45 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.5 (20.00-2.10) 92.3 (32.45-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.222 , 0.258 0.203 , 0.235	Depositor DCC
$R_{free}$ test set	5068 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 62.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 101798 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9388	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: CMG, TPO

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	1.00	2/2438 (0.1%)	2.15	105/3308 (3.2%)
1	C	0.91	2/2438 (0.1%)	1.90	64/3308 (1.9%)
2	B	0.95	1/2133 (0.0%)	1.95	64/2897 (2.2%)
2	D	0.95	1/2133 (0.0%)	2.09	67/2897 (2.3%)
All	All	0.95	6/9142 (0.1%)	2.03	300/12410 (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	6
1	C	0	4
2	B	0	7
2	D	0	4
All	All	0	21

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	198	GLY	N-CA	7.17	1.56	1.46
1	A	93	ALA	C-N	6.66	1.49	1.34
1	A	93	ALA	CA-C	5.48	1.67	1.52
1	C	177	CYS	CB-SG	5.18	1.91	1.82
2	D	275	VAL	CB-CG2	-5.16	1.42	1.52
1	C	120	SER	CA-CB	5.01	1.60	1.52

All (300) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	322	GLN	C-N-CA	20.08	171.91	121.70
1	A	217	ARG	NE-CZ-NH2	18.57	129.58	120.30
2	B	378	ARG	NE-CZ-NH2	-17.88	111.36	120.30
2	D	323	GLN	N-CA-CB	17.10	141.39	110.60
1	A	217	ARG	NE-CZ-NH1	-16.95	111.83	120.30
2	B	241	ARG	NE-CZ-NH2	-16.20	112.20	120.30
2	D	321	HIS	C-N-CA	15.69	160.93	121.70
2	D	238	TYR	CB-CG-CD2	-15.29	111.82	121.00
1	C	256	ASP	CB-CG-OD2	14.90	131.71	118.30
1	A	206	ASP	CB-CA-C	14.29	138.97	110.40
1	A	178	LYS	CB-CG-CD	14.02	148.06	111.60
2	D	322	GLN	O-C-N	-13.57	100.99	122.70
1	C	270	ASP	CB-CG-OD1	12.87	129.88	118.30
1	A	126	ARG	NE-CZ-NH1	-12.77	113.92	120.30
2	D	226	LYS	CG-CD-CE	12.67	149.90	111.90
1	A	93	ALA	N-CA-CB	12.36	127.41	110.10
1	C	245	ARG	NE-CZ-NH2	-12.29	114.16	120.30
1	A	178	LYS	CG-CD-CE	11.93	147.69	111.90
1	A	36	ARG	NE-CZ-NH2	-11.82	114.39	120.30
2	B	241	ARG	NE-CZ-NH1	11.72	126.16	120.30
2	D	323	GLN	CB-CA-C	-11.54	87.33	110.40
2	D	241	ARG	NE-CZ-NH2	-11.50	114.55	120.30
2	B	277	GLU	OE1-CD-OE2	-11.47	109.54	123.30
2	D	230	GLU	OE1-CD-OE2	-11.27	109.77	123.30
2	B	293	ARG	NE-CZ-NH1	11.04	125.82	120.30
2	D	323	GLN	CA-CB-CG	11.04	137.68	113.40
1	A	122	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	A	169	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	A	92	ASP	CB-CG-OD1	10.67	127.91	118.30
2	D	378	ARG	NE-CZ-NH2	10.57	125.59	120.30
1	C	199	ARG	NE-CZ-NH1	10.55	125.57	120.30
2	D	284	ASP	CB-CG-OD2	10.50	127.75	118.30
2	B	293	ARG	CD-NE-CZ	10.31	138.03	123.60
1	A	230	VAL	CB-CA-C	-10.19	92.04	111.40
1	A	77	TYR	CB-CG-CD1	-10.18	114.89	121.00
2	D	321	HIS	O-C-N	-10.11	106.53	122.70
1	A	8	GLU	OE1-CD-OE2	-9.79	111.55	123.30
1	C	40	GLU	CA-C-O	-9.77	99.58	120.10
2	D	293	ARG	CD-NE-CZ	9.75	137.25	123.60
1	A	77	TYR	CB-CG-CD2	9.57	126.74	121.00
1	A	36	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	127	ASP	CB-CG-OD1	9.20	126.58	118.30
2	B	345	ASP	CA-C-O	-9.19	100.80	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	322	GLN	N-CA-C	9.16	135.72	111.00
1	A	41	THR	N-CA-CB	9.11	127.61	110.30
1	A	273	LYS	CA-CB-CG	9.10	133.41	113.40
2	D	345	ASP	CA-C-O	-9.00	101.21	120.10
1	A	93	ALA	CA-C-N	-8.94	97.52	117.20
1	A	199	ARG	NE-CZ-NH1	8.93	124.77	120.30
1	C	154	VAL	CA-C-O	-8.86	101.49	120.10
1	A	92	ASP	C-N-CA	8.73	143.53	121.70
1	C	8	GLU	OE1-CD-OE2	-8.70	112.86	123.30
1	C	230	VAL	CB-CA-C	-8.69	94.89	111.40
1	A	22	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	A	206	ASP	N-CA-C	-8.69	87.54	111.00
1	A	22	ARG	NE-CZ-NH2	-8.59	116.00	120.30
2	B	393	ASP	CB-CG-OD2	8.58	126.03	118.30
1	C	177	CYS	N-CA-CB	8.58	126.04	110.60
2	D	238	TYR	CB-CG-CD1	8.57	126.14	121.00
1	C	127	ASP	CB-CG-OD2	8.54	125.98	118.30
2	D	226	LYS	CD-CE-NZ	8.51	131.26	111.70
1	A	150	ARG	CA-CB-CG	8.49	132.08	113.40
2	B	323	GLN	CA-C-O	-8.48	102.29	120.10
2	D	275	VAL	CB-CA-C	-8.46	95.32	111.40
1	A	287	GLN	CA-CB-CG	8.40	131.89	113.40
1	C	40	GLU	N-CA-CB	8.27	125.49	110.60
1	A	154	VAL	CA-C-O	-8.19	102.91	120.10
1	C	270	ASP	CB-CG-OD2	-8.18	110.94	118.30
2	B	247	SER	O-C-N	-8.15	109.66	122.70
2	B	347	TYR	CB-CG-CD2	-8.14	116.12	121.00
1	A	257	GLU	N-CA-CB	-8.13	95.96	110.60
1	A	206	ASP	CA-C-O	-8.13	103.03	120.10
1	A	93	ALA	O-C-N	-8.12	109.71	122.70
2	D	321	HIS	CA-CB-CG	8.09	127.35	113.60
2	D	241	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	A	223	ASP	CB-CG-OD1	8.05	125.55	118.30
2	B	305	ASP	CB-CG-OD2	8.05	125.54	118.30
1	A	252	VAL	CG1-CB-CG2	-7.96	98.16	110.90
1	A	38	ASP	CB-CG-OD1	-7.93	111.16	118.30
2	B	324	PRO	CA-N-CD	-7.92	100.42	111.50
1	C	256	ASP	CB-CG-OD1	-7.91	111.18	118.30
2	D	187	ARG	NE-CZ-NH2	-7.89	116.35	120.30
2	D	343	ASP	CB-CG-OD2	7.86	125.38	118.30
2	D	224	GLU	OE1-CD-OE2	7.74	132.59	123.30
1	A	258	ASP	CB-CG-OD1	7.72	125.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	393	ASP	CB-CG-OD1	-7.65	111.42	118.30
2	B	343	ASP	CB-CG-OD1	7.56	125.10	118.30
1	C	237	LYS	CA-CB-CG	7.53	129.97	113.40
1	A	39	THR	N-CA-CB	7.53	124.61	110.30
1	C	258	ASP	CB-CG-OD2	7.48	125.03	118.30
2	B	316	THR	N-CA-CB	-7.42	96.19	110.30
1	C	81	GLU	OE1-CD-OE2	-7.41	114.41	123.30
2	D	197	VAL	CA-C-N	7.41	131.02	116.20
1	A	256	ASP	CB-CG-OD1	-7.41	111.63	118.30
1	A	205	GLY	C-N-CA	-7.40	103.20	121.70
2	B	241	ARG	CD-NE-CZ	7.34	133.87	123.60
2	B	293	ARG	NE-CZ-NH2	-7.27	116.67	120.30
2	B	345	ASP	CB-CG-OD1	7.26	124.83	118.30
2	D	334	MET	CG-SD-CE	-7.25	88.60	100.20
1	A	210	ASP	CB-CG-OD1	7.25	124.82	118.30
1	C	40	GLU	CA-C-N	7.24	133.13	117.20
1	A	81	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	A	163	VAL	N-CA-CB	-7.18	95.70	111.50
2	B	277	GLU	CB-CG-CD	7.13	133.46	114.20
1	A	235	ASP	CB-CG-OD1	7.12	124.71	118.30
2	D	403	GLN	CB-CA-C	-7.11	96.18	110.40
2	B	197	VAL	CA-C-N	7.09	130.38	116.20
1	C	261	SER	N-CA-CB	-7.08	99.89	110.50
1	C	126	ARG	NE-CZ-NH2	-7.06	116.77	120.30
2	D	322	GLN	CA-C-N	7.06	132.74	117.20
2	B	220	GLU	OE1-CD-OE2	-7.04	114.85	123.30
2	B	209	SER	N-CA-CB	-7.03	99.96	110.50
2	D	205	ASP	CB-CG-OD1	7.01	124.61	118.30
2	D	275	VAL	CG1-CB-CG2	7.01	122.11	110.90
1	A	260	ARG	NE-CZ-NH2	7.00	123.80	120.30
2	D	323	GLN	OE1-CD-NE2	-7.00	105.81	121.90
1	A	196	MET	CG-SD-CE	6.98	111.37	100.20
2	D	391	LEU	CA-CB-CG	6.96	131.31	115.30
1	A	169	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	206	ASP	O-C-N	-6.94	111.60	122.70
1	C	36	ARG	NE-CZ-NH1	-6.93	116.84	120.30
2	D	289	LYS	CA-CB-CG	6.92	128.62	113.40
2	B	209	SER	CB-CA-C	6.90	123.21	110.10
1	A	73	GLU	C-N-CA	6.88	138.89	121.70
1	A	200	ARG	NE-CZ-NH2	-6.85	116.88	120.30
2	D	345	ASP	CB-CG-OD2	-6.82	112.16	118.30
2	D	250	ARG	CA-CB-CG	6.82	128.40	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	226	VAL	CA-CB-CG1	6.81	121.11	110.90
1	C	163	VAL	N-CA-CB	-6.79	96.56	111.50
2	B	391	LEU	CA-CB-CG	6.76	130.85	115.30
2	D	324	PRO	N-CA-C	-6.76	94.52	112.10
2	B	194	LYS	CA-CB-CG	6.71	128.17	113.40
2	B	378	ARG	NH1-CZ-NH2	6.68	126.75	119.40
2	B	401	ALA	CB-CA-C	6.63	120.04	110.10
2	B	247	SER	CA-CB-OG	-6.62	93.32	111.20
2	B	197	VAL	C-N-CA	-6.58	108.47	122.30
2	D	320	LEU	C-N-CA	6.56	138.09	121.70
1	A	180	TYR	CB-CG-CD2	-6.54	117.07	121.00
1	A	256	ASP	CB-CG-OD2	6.54	124.19	118.30
2	B	347	TYR	CB-CG-CD1	6.49	124.89	121.00
1	A	199	ARG	NE-CZ-NH2	-6.46	117.07	120.30
2	B	327	CYS	CB-CA-C	6.45	123.31	110.40
1	A	266	MET	CG-SD-CE	6.45	110.52	100.20
2	D	196	LYS	CA-CB-CG	6.44	127.57	113.40
1	A	217	ARG	CD-NE-CZ	6.43	132.61	123.60
1	C	235	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	A	155	PRO	CA-N-CD	-6.42	102.51	111.50
1	A	40	GLU	CA-C-O	6.42	133.57	120.10
1	C	206	ASP	CB-CG-OD1	-6.41	112.53	118.30
1	A	210	ASP	OD1-CG-OD2	-6.38	111.17	123.30
2	B	410	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	257	GLU	OE1-CD-OE2	6.36	130.93	123.30
2	B	324	PRO	N-CA-CB	6.36	110.93	103.30
2	D	293	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	61	PRO	O-C-N	-6.35	112.53	122.70
2	B	346	PRO	CA-N-CD	-6.35	102.61	111.50
1	A	214	ARG	CD-NE-CZ	-6.34	114.72	123.60
2	D	271	TYR	CB-CG-CD1	-6.34	117.19	121.00
1	A	210	ASP	CB-CG-OD2	6.34	124.00	118.30
1	C	212	LEU	CB-CA-C	-6.32	98.20	110.20
1	A	269	TYR	CB-CG-CD1	-6.29	117.22	121.00
1	A	202	LEU	O-C-N	-6.29	112.64	122.70
1	A	94	SER	N-CA-CB	-6.29	101.07	110.50
1	A	206	ASP	N-CA-CB	6.28	121.90	110.60
1	A	206	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	A	2	GLU	CA-CB-CG	6.25	127.15	113.40
1	C	120	SER	CA-CB-OG	-6.24	94.34	111.20
1	C	176	GLY	CA-C-N	6.21	130.87	117.20
1	C	214	ARG	NE-CZ-NH2	-6.19	117.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	A	185	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	38	ASP	C-N-CA	6.16	137.09	121.70
2	D	323	GLN	CB-CG-CD	6.14	127.57	111.60
1	A	39	THR	CA-C-O	-6.14	107.22	120.10
1	A	205	GLY	CA-C-O	6.13	131.63	120.60
1	C	56	LYS	CA-CB-CG	-6.08	100.03	113.40
2	D	197	VAL	CA-C-O	-6.08	107.34	120.10
1	A	68	ASP	CB-CG-OD2	-6.07	112.84	118.30
2	B	205	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	75	LYS	CB-CA-C	-6.01	98.39	110.40
2	D	322	GLN	OE1-CD-NE2	6.00	135.71	121.90
2	D	319	PHE	CB-CG-CD2	-5.99	116.61	120.80
1	C	223	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	252	VAL	CG1-CB-CG2	-5.99	101.32	110.90
2	B	247	SER	CB-CA-C	5.98	121.47	110.10
2	D	403	GLN	CA-CB-CG	5.98	126.55	113.40
1	C	38	ASP	N-CA-CB	-5.96	99.86	110.60
2	D	316	THR	N-CA-CB	-5.93	99.03	110.30
1	C	50	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	81	GLU	CG-CD-OE2	5.93	130.16	118.30
2	D	209	SER	CB-CA-C	5.89	121.29	110.10
2	D	322	GLN	CB-CA-C	-5.88	98.63	110.40
1	C	39	THR	N-CA-CB	5.87	121.44	110.30
1	C	245	ARG	NH1-CZ-NH2	5.85	125.84	119.40
1	A	245	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	255	LEU	CA-C-O	5.83	132.34	120.10
2	B	318	TYR	CB-CG-CD2	-5.83	117.50	121.00
2	B	324	PRO	N-CD-CG	5.82	111.93	103.20
2	B	323	GLN	N-CA-C	5.81	126.69	111.00
1	C	223	ASP	CB-CG-OD1	5.79	123.52	118.30
1	C	176	GLY	CA-C-O	-5.78	110.19	120.60
2	D	199	TYR	CD1-CE1-CZ	-5.78	114.60	119.80
1	A	163	VAL	CB-CA-C	5.76	122.34	111.40
1	C	74	ASN	O-C-N	-5.76	113.49	122.70
1	A	126	ARG	NH1-CZ-NH2	5.71	125.68	119.40
2	D	187	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	C	210	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	230	VAL	N-CA-CB	5.68	124.00	111.50
2	D	281	ILE	N-CA-CB	5.64	123.77	110.80
1	C	40	GLU	N-CA-C	-5.63	95.80	111.00
2	D	361	HIS	CA-CB-CG	-5.63	104.03	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	365	TYR	CB-CG-CD1	-5.60	117.64	121.00
2	B	365	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	C	39	THR	CA-CB-CG2	-5.60	104.56	112.40
1	A	0	SER	N-CA-CB	5.58	118.88	110.50
1	A	163	VAL	CG1-CB-CG2	5.55	119.79	110.90
1	A	126	ARG	CD-NE-CZ	-5.54	115.84	123.60
1	A	287	GLN	O-C-N	-5.54	113.84	122.70
2	D	250	ARG	NE-CZ-NH1	-5.53	117.54	120.30
2	D	209	SER	N-CA-CB	-5.52	102.22	110.50
2	D	398	TYR	CA-CB-CG	5.52	123.89	113.40
1	A	226	VAL	N-CA-CB	-5.52	99.36	111.50
1	A	232	SER	CB-CA-C	-5.49	99.67	110.10
2	B	350	TYR	CG-CD1-CE1	5.48	125.69	121.30
1	C	258	ASP	CB-CG-OD1	-5.48	113.37	118.30
2	B	188	GLU	N-CA-CB	-5.47	100.76	110.60
2	D	322	GLN	N-CA-CB	-5.45	100.79	110.60
1	A	92	ASP	OD1-CG-OD2	-5.44	112.96	123.30
1	C	42	GLU	CG-CD-OE2	5.43	129.16	118.30
2	B	348	LEU	CA-CB-CG	5.42	127.78	115.30
2	B	362	LEU	O-C-N	-5.42	114.03	122.70
1	A	0	SER	O-C-N	-5.42	114.03	122.70
2	B	317	GLN	CG-CD-OE1	-5.41	110.77	121.60
1	C	199	ARG	O-C-N	-5.41	114.04	122.70
2	B	267	PHE	CB-CG-CD1	-5.40	117.02	120.80
1	A	94	SER	O-C-N	-5.39	114.07	122.70
1	C	5	GLN	CG-CD-OE1	-5.39	110.82	121.60
1	C	38	ASP	CA-C-O	-5.38	108.79	120.10
1	A	261	SER	N-CA-CB	-5.37	102.44	110.50
1	C	109	PHE	CA-CB-CG	5.35	126.75	113.90
1	C	127	ASP	OD1-CG-OD2	-5.33	113.17	123.30
1	A	55	LEU	CA-CB-CG	5.33	127.56	115.30
1	A	279	ALA	O-C-N	-5.32	114.19	122.70
1	A	207	SER	O-C-N	5.32	131.21	122.70
1	C	216	PHE	CB-CG-CD1	5.32	124.52	120.80
2	B	334	MET	CG-SD-CE	5.30	108.68	100.20
2	D	177	ASP	CA-CB-CG	5.28	125.01	113.40
2	B	185	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	C	269	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	A	105	LYS	CD-CE-NZ	-5.25	99.61	111.70
2	B	350	TYR	CD1-CE1-CZ	-5.24	115.08	119.80
2	B	250	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	C	37	LEU	CB-CA-C	-5.24	100.25	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	D	288	LYS	N-CA-CB	-5.23	101.19	110.60
2	B	248	VAL	CG1-CB-CG2	-5.22	102.54	110.90
2	B	269	GLU	CG-CD-OE2	5.22	128.75	118.30
1	A	168	TYR	CA-CB-CG	-5.22	103.48	113.40
2	B	269	GLU	OE1-CD-OE2	-5.22	117.04	123.30
1	C	168	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	A	157	ARG	NE-CZ-NH1	-5.19	117.70	120.30
2	B	422	SER	N-CA-CB	5.19	118.29	110.50
2	D	256	VAL	C-N-CA	5.19	133.20	122.30
2	D	286	TYR	CB-CG-CD1	-5.18	117.89	121.00
2	D	229	ASN	CA-CB-CG	-5.17	102.03	113.40
2	B	188	GLU	O-C-N	-5.16	114.44	122.70
2	D	345	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	155	PRO	N-CD-CG	5.15	110.92	103.20
2	B	305	ASP	OD1-CG-OD2	-5.14	113.53	123.30
1	A	143	LEU	CB-CA-C	-5.13	100.45	110.20
1	C	163	VAL	CA-CB-CG1	5.13	118.60	110.90
2	B	379	LYS	CD-CE-NZ	-5.13	99.90	111.70
1	C	96	LEU	CA-CB-CG	-5.13	103.51	115.30
1	C	199	ARG	CD-NE-CZ	5.13	130.78	123.60
1	A	209	ILE	O-C-N	-5.12	114.51	122.70
1	A	163	VAL	C-N-CA	5.12	134.49	121.70
1	C	175	LEU	O-C-N	-5.12	114.50	123.20
2	B	178	TYR	CD1-CE1-CZ	-5.11	115.20	119.80
2	D	346	PRO	CA-N-CD	-5.10	104.35	111.50
2	D	322	GLN	CA-CB-CG	-5.10	102.17	113.40
1	A	78	LEU	CA-CB-CG	5.09	127.01	115.30
1	A	185	ASP	CB-CG-OD2	-5.09	113.72	118.30
2	B	187	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	81	GLU	CG-CD-OE2	5.08	128.46	118.30
1	C	40	GLU	C-N-CA	-5.08	109.01	121.70
2	D	240	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	38	ASP	O-C-N	5.08	130.82	122.70
1	A	144	ALA	C-N-CA	5.07	134.38	121.70
1	A	17	VAL	CB-CA-C	-5.06	101.79	111.40
2	B	180	GLU	OE1-CD-OE2	-5.06	117.23	123.30
2	B	411	GLU	CG-CD-OE2	5.06	128.41	118.30
1	C	237	LYS	CB-CG-CD	5.05	124.74	111.60
1	C	180	TYR	N-CA-CB	5.05	119.69	110.60
2	B	321	HIS	CA-C-O	-5.04	109.51	120.10
1	C	260	ARG	NE-CZ-NH1	-5.04	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	C	96	LEU	CB-CA-C	5.03	119.76	110.20
1	A	214	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	255	LEU	O-C-N	-5.02	114.67	122.70
2	B	277	GLU	CA-CB-CG	5.02	124.44	113.40
2	D	197	VAL	C-N-CA	-5.01	111.78	122.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	0	SER	Mainchain
1	A	100	PRO	Mainchain
1	A	154	VAL	Mainchain,Peptide
1	A	206	ASP	Mainchain
1	A	93	ALA	Mainchain
2	B	323	GLN	Mainchain,Peptide
2	B	345	ASP	Mainchain,Peptide
2	B	348	LEU	Mainchain
2	B	349	LYS	Mainchain
2	B	380	THR	Mainchain
1	C	0	SER	Mainchain
1	C	100	PRO	Mainchain
1	C	154	VAL	Mainchain,Peptide
2	D	321	HIS	Mainchain
2	D	345	ASP	Mainchain,Peptide
2	D	349	LYS	Mainchain

## 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	92	3
1	C	2388	0	2430	88	2
2	B	2083	0	2107	60	0
2	D	2083	0	2105	71	1
3	A	18	0	17	0	0
3	C	18	0	17	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	105	0	0	4	0
4	B	106	0	0	12	0
4	C	107	0	0	8	0
4	D	92	0	0	3	0
All	All	9388	0	9106	287	3

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 16.

All (287) 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:323:GLN:HB3	2:D:324:PRO:CD	1.78	1.10
2:D:323:GLN:HB3	2:D:324:PRO:HD3	1.38	1.06
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.41	0.99
1:A:178:LYS:HD2	1:A:179:TYR:CZ	1.98	0.98
1:C:39:THR:HG21	2:D:289:LYS:HE3	1.42	0.98
1:A:158:THR:OG1	1:A:178:LYS:HD3	1.68	0.93
1:A:178:LYS:HD2	1:A:179:TYR:CE1	2.09	0.87
1:A:266:MET:SD	4:A:2075:HOH:O	2.31	0.87
1:C:197:VAL:HG11	1:C:252:VAL:HG13	1.56	0.86
2:D:175:VAL:HB	2:D:176:PRO:HD3	1.58	0.85
1:C:60:HIS:HD2	1:C:62:ASN:H	1.25	0.85
1:C:190:GLY:HA2	1:C:266:MET:HE3	1.59	0.84
1:C:88:LYS:NZ	1:C:131:GLN:HE21	1.75	0.84
2:D:275:VAL:HB	2:D:288:LYS:CE	2.08	0.84
1:A:60:HIS:HD2	1:A:62:ASN:H	1.25	0.82
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.62	0.81
1:A:190:GLY:HA2	1:A:266:MET:HE3	1.64	0.80
1:A:252:VAL:HG11	1:A:255:LEU:HD22	1.62	0.80
2:D:396:GLN:HE21	2:D:400:LYS:HE3	1.46	0.79
2:D:210:MET:HE3	2:D:250:ARG:HB2	1.63	0.79
2:B:334:MET:HE1	4:B:2073:HOH:O	1.83	0.78
1:C:266:MET:SD	4:C:2076:HOH:O	2.42	0.78
1:C:255:LEU:HG	1:C:259:GLY:HA3	1.66	0.77
2:B:334:MET:HE2	2:B:334:MET:HA	1.65	0.77
1:A:88:LYS:HD2	1:A:131:GLN:HG3	1.66	0.77
1:C:177:CYS:HB2	4:C:2067:HOH:O	1.83	0.77
1:C:72:THR:HG22	1:C:74:ASN:H	1.49	0.76
1:C:190:GLY:HA2	1:C:266:MET:CE	2.16	0.76
1:C:41:THR:HA	2:D:288:LYS:HZ1	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:CD2	1:C:62:ASN:H	2.04	0.76
2:D:210:MET:CE	2:D:250:ARG:HB2	2.16	0.75
2:B:312:ASN:HB2	4:B:2073:HOH:O	1.87	0.75
2:D:388:LYS:HB3	2:D:389:PRO:HD3	1.69	0.75
2:D:323:GLN:CB	2:D:324:PRO:HD3	2.17	0.74
1:C:96:LEU:O	1:C:199:ARG:NH1	2.21	0.74
1:C:177:CYS:SG	1:C:178:LYS:N	2.62	0.73
2:D:193:CYS:SG	4:D:2033:HOH:O	2.46	0.73
2:D:417:LYS:HD3	2:D:418:TYR:CE2	2.24	0.73
1:C:34:LYS:HG3	1:C:77:TYR:CE1	2.25	0.71
1:A:40:GLU:HA	2:B:288:LYS:HZ3	1.55	0.71
2:D:275:VAL:HB	2:D:288:LYS:HE2	1.71	0.71
1:C:252:VAL:HG12	1:C:252:VAL:O	1.89	0.70
2:B:206:ILE:HG22	2:B:210:MET:HE1	1.74	0.70
1:C:190:GLY:CA	1:C:266:MET:HE3	2.20	0.69
2:B:378:ARG:HH21	2:B:378:ARG:CB	2.04	0.69
1:A:39:THR:O	1:A:40:GLU:C	2.30	0.69
2:B:175:VAL:N	2:B:176:PRO:CD	2.54	0.69
2:B:175:VAL:N	2:B:176:PRO:HD2	2.08	0.68
1:A:39:THR:HG21	2:B:289:LYS:HD2	1.75	0.68
1:C:39:THR:HG21	2:D:289:LYS:CE	2.22	0.68
1:C:88:LYS:NZ	1:C:131:GLN:NE2	2.43	0.67
1:C:223:ASP:H	1:C:226:VAL:HG12	1.59	0.66
2:D:196:LYS:HG3	2:D:199:TYR:HB3	1.78	0.66
1:A:278:LYS:HZ3	1:A:278:LYS:HB2	1.61	0.66
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.78	0.66
1:C:252:VAL:HG12	1:C:255:LEU:HB2	1.78	0.66
2:D:275:VAL:CG2	2:D:288:LYS:HZ2	2.09	0.66
2:D:388:LYS:O	2:D:392:MET:HG2	1.96	0.66
2:B:296:HIS:CD2	2:B:300:LYS:HE2	2.31	0.66
1:C:41:THR:HA	2:D:288:LYS:NZ	2.09	0.65
1:A:93:ALA:C	1:A:94:SER:OG	2.34	0.65
1:C:227:TRP:HB3	1:C:230:VAL:HG22	1.78	0.65
1:A:41:THR:N	2:B:288:LYS:HZ1	1.93	0.65
1:C:15:TYR:HE2	1:C:35:ILE:HD11	1.60	0.65
1:C:88:LYS:HZ3	1:C:131:GLN:HE21	1.41	0.65
1:A:73:GLU:HB3	1:A:74:ASN:ND2	2.11	0.65
1:A:95:ALA:O	1:A:199:ARG:HD3	1.97	0.65
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.28	0.64
2:D:275:VAL:HG11	2:D:288:LYS:HD3	1.79	0.64
2:B:196:LYS:O	2:B:196:LYS:HG3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:ARG:NH2	2:B:378:ARG:CB	2.62	0.63
1:C:161:HIS:HD2	4:C:2021:HOH:O	1.81	0.63
2:D:275:VAL:CG2	2:D:288:LYS:NZ	2.62	0.63
2:D:275:VAL:HB	2:D:288:LYS:NZ	2.13	0.63
1:C:95:ALA:O	1:C:199:ARG:HD3	1.98	0.63
1:A:158:THR:OG1	1:A:178:LYS:CD	2.43	0.63
1:A:41:THR:H	2:B:288:LYS:HZ1	1.46	0.62
1:C:88:LYS:HZ2	1:C:131:GLN:NE2	1.97	0.62
1:A:177:CYS:HB2	4:A:2066:HOH:O	1.99	0.62
2:D:288:LYS:HD2	2:D:292:LEU:HD22	1.81	0.62
2:B:378:ARG:NH2	2:B:378:ARG:HB2	2.14	0.62
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.34	0.62
1:A:40:GLU:HA	2:B:288:LYS:NZ	2.13	0.62
1:C:51:GLU:O	1:C:55:LEU:HB2	2.00	0.62
1:C:15:TYR:CZ	1:C:33:LYS:HE2	2.35	0.61
1:A:278:LYS:HE2	4:B:2021:HOH:O	1.99	0.61
1:A:60:HIS:CD2	1:A:62:ASN:H	2.13	0.61
1:A:39:THR:HG21	2:B:289:LYS:CD	2.30	0.61
2:D:396:GLN:NE2	2:D:400:LYS:HE3	2.15	0.60
1:A:72:THR:HG22	1:A:73:GLU:H	1.66	0.60
2:B:210:MET:HE1	2:B:250:ARG:CB	2.32	0.60
1:A:190:GLY:HA2	1:A:266:MET:CE	2.30	0.60
1:A:252:VAL:CG1	1:A:255:LEU:HD22	2.30	0.60
2:B:296:HIS:NE2	2:B:300:LYS:HE2	2.17	0.60
2:D:176:PRO:HB2	2:D:179:HIS:CE1	2.37	0.59
2:B:274:GLU:HG2	2:B:277:GLU:HG3	1.83	0.59
1:A:178:LYS:HD2	1:A:179:TYR:CE2	2.36	0.59
2:D:175:VAL:HB	2:D:176:PRO:CD	2.31	0.59
1:C:39:THR:HA	2:D:292:LEU:HD23	1.84	0.59
2:D:395:HIS:HE1	2:D:427:PRO:O	1.85	0.59
1:C:40:GLU:HA	2:D:288:LYS:HG2	1.82	0.59
1:C:178:LYS:HD2	1:C:179:TYR:CZ	2.38	0.59
1:C:39:THR:CG2	2:D:292:LEU:HD23	2.33	0.58
2:B:210:MET:HE3	4:B:2051:HOH:O	2.02	0.58
2:B:206:ILE:HG22	2:B:210:MET:CE	2.33	0.58
1:A:39:THR:O	1:A:41:THR:N	2.37	0.58
1:C:22:ARG:HD2	4:C:2006:HOH:O	2.03	0.58
1:A:2:GLU:HG2	2:D:293:ARG:NH1	2.19	0.57
1:A:90:PHE:O	1:A:93:ALA:C	2.43	0.57
1:C:99:ILE:HG13	4:C:2038:HOH:O	2.03	0.57
1:A:36:ARG:HH11	1:A:36:ARG:HG2	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:OE1	2:B:275:VAL:HG23	2.04	0.57
2:D:223:GLU:OE1	2:D:412:LYS:HG3	2.05	0.56
2:D:275:VAL:HG23	2:D:288:LYS:NZ	2.21	0.56
1:A:74:ASN:ND2	1:A:74:ASN:N	2.52	0.56
1:C:39:THR:HG23	2:D:292:LEU:HD23	1.87	0.56
2:D:201:LYS:C	2:D:201:LYS:HD3	2.26	0.56
1:C:119:HIS:HE1	1:C:185:ASP:OD2	1.89	0.56
1:A:119:HIS:HE1	1:A:185:ASP:OD2	1.88	0.56
1:A:88:LYS:HD2	1:A:131:GLN:HE21	1.70	0.56
1:C:36:ARG:HH11	1:C:36:ARG:HG2	1.71	0.55
2:D:176:PRO:HB2	2:D:179:HIS:HE1	1.71	0.55
1:C:14:THR:CG2	1:C:148:LEU:HD22	2.36	0.55
1:C:88:LYS:HZ2	1:C:131:GLN:HE21	1.49	0.55
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.34	0.55
1:A:190:GLY:CA	1:A:266:MET:HE3	2.36	0.54
2:D:321:HIS:O	2:D:360:PHE:CZ	2.60	0.54
2:B:312:ASN:CB	4:B:2073:HOH:O	2.50	0.54
2:B:415:ASN:OD1	2:B:417:LYS:HB3	2.07	0.54
2:D:223:GLU:OE2	2:D:412:LYS:HE3	2.08	0.54
1:A:74:ASN:ND2	1:A:74:ASN:H	2.06	0.53
1:C:252:VAL:HG11	1:C:255:LEU:CD2	2.27	0.53
1:C:22:ARG:HD3	4:C:2003:HOH:O	2.08	0.53
2:B:395:HIS:HE1	2:B:427:PRO:O	1.92	0.53
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.90	0.53
1:C:72:THR:HG22	1:C:74:ASN:N	2.21	0.52
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.74	0.52
1:A:154:VAL:HG11	2:B:179:HIS:HB2	1.92	0.52
1:A:161:HIS:HD2	4:A:2067:HOH:O	1.92	0.52
2:B:322:GLN:NE2	2:B:330:GLU:OE2	2.43	0.52
1:C:227:TRP:O	1:C:230:VAL:HG22	2.10	0.51
1:A:2:GLU:OE2	1:C:73:GLU:OE2	2.28	0.51
1:A:178:LYS:CD	1:A:179:TYR:CE1	2.89	0.51
2:D:233:HIS:HD2	4:D:2068:HOH:O	1.93	0.51
1:A:198:THR:O	1:A:199:ARG:HB2	2.09	0.51
1:A:51:GLU:HG3	1:A:146:PHE:HB2	1.93	0.51
1:C:88:LYS:HD3	1:C:131:GLN:HG3	1.92	0.51
1:A:193:PHE:HD2	1:A:266:MET:HE2	1.75	0.51
1:A:15:TYR:CE1	1:A:33:LYS:HE2	2.46	0.51
1:A:86:ASP:OD2	1:A:89:LYS:HE3	2.10	0.50
1:A:88:LYS:CD	1:A:131:GLN:HE21	2.23	0.50
1:A:84:HIS:CD2	1:A:296:LEU:HD13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LYS:HA	1:C:192:ILE:HD11	1.94	0.50
1:A:166:LEU:CD2	1:A:206:ASP:O	2.60	0.50
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.93	0.50
2:D:322:GLN:HB3	2:D:360:PHE:HZ	1.76	0.50
1:C:216:PHE:HE2	1:C:240:PHE:CD2	2.30	0.50
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.92	0.50
1:C:119:HIS:HD2	4:D:2008:HOH:O	1.94	0.49
2:D:323:GLN:C	2:D:324:PRO:O	2.48	0.49
1:A:261:SER:O	1:A:265:GLN:HG3	2.12	0.49
1:A:41:THR:H	2:B:288:LYS:NZ	2.11	0.49
1:C:20:LYS:HG3	1:C:82:PHE:CE1	2.47	0.49
1:C:72:THR:CG2	1:C:73:GLU:N	2.76	0.49
1:A:37:LEU:O	1:A:38:ASP:HB2	2.12	0.49
2:D:296:HIS:CD2	2:D:300:LYS:HE2	2.48	0.49
2:B:388:LYS:O	2:B:392:MET:HG2	2.12	0.49
1:A:51:GLU:O	1:A:55:LEU:HB2	2.13	0.48
1:C:223:ASP:H	1:C:226:VAL:CG1	2.26	0.48
2:D:426:PRO:O	2:D:427:PRO:C	2.50	0.48
2:D:415:ASN:OD1	2:D:416:SER:N	2.46	0.48
2:B:371:SER:O	2:B:372:TRP:C	2.50	0.48
1:C:40:GLU:O	2:D:288:LYS:HG2	2.14	0.48
1:C:14:THR:HG22	1:C:148:LEU:HD22	1.95	0.48
2:B:223:GLU:OE2	2:B:412:LYS:HE3	2.14	0.48
2:B:373:PRO:HG2	2:B:376:LEU:HD12	1.95	0.48
1:C:197:VAL:CG1	1:C:252:VAL:HG13	2.36	0.48
1:A:93:ALA:C	1:A:94:SER:HG	2.14	0.48
2:B:194:LYS:HA	2:B:195:PRO:HD3	1.76	0.48
2:D:288:LYS:CD	2:D:292:LEU:HD22	2.44	0.48
2:D:210:MET:HE3	2:D:250:ARG:CB	2.39	0.48
1:C:72:THR:HG22	1:C:73:GLU:N	2.29	0.48
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.49	0.47
2:D:176:PRO:HD2	2:D:179:HIS:NE2	2.29	0.47
1:C:6:LYS:HE2	1:C:19:TYR:CD1	2.49	0.47
1:C:260:ARG:HD3	4:C:2086:HOH:O	2.15	0.47
1:A:178:LYS:HD2	1:A:179:TYR:CD1	2.49	0.47
1:A:278:LYS:HZ3	1:A:278:LYS:CB	2.24	0.47
2:B:221:VAL:HG22	2:B:281:ILE:HD12	1.96	0.47
1:A:178:LYS:HG2	1:A:179:TYR:N	2.24	0.47
1:C:86:ASP:OD2	1:C:89:LYS:HE3	2.14	0.47
2:D:431:ASN:HD22	2:D:431:ASN:HA	1.52	0.47
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD11	1:C:82:PHE:HE1	1.80	0.47
2:D:275:VAL:HG21	2:D:288:LYS:HZ2	1.78	0.46
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.80	0.46
2:B:183:HIS:HD2	4:B:2018:HOH:O	1.97	0.46
2:B:277:GLU:HB3	4:B:2063:HOH:O	2.15	0.46
1:A:41:THR:N	2:B:288:LYS:NZ	2.63	0.46
2:B:210:MET:CE	2:B:250:ARG:HB2	2.45	0.46
1:A:193:PHE:O	1:A:197:VAL:HG23	2.15	0.46
2:D:388:LYS:HB3	2:D:389:PRO:CD	2.43	0.46
1:A:206:ASP:N	1:A:210:ASP:OD2	2.35	0.45
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.51	0.45
1:C:100:PRO:HB2	1:C:102:PRO:HD2	1.98	0.45
1:A:215:ILE:HG23	1:A:219:LEU:HD12	1.99	0.45
2:B:323:GLN:HG2	2:B:324:PRO:N	2.32	0.45
2:B:277:GLU:O	2:B:281:ILE:HG23	2.16	0.45
1:C:278:LYS:HB2	1:C:278:LYS:HE2	1.61	0.45
1:C:40:GLU:CA	2:D:288:LYS:HG2	2.47	0.45
1:C:224:GLU:HG2	1:C:231:THR:HG23	1.98	0.45
1:C:38:ASP:OD1	1:C:41:THR:OG1	2.29	0.45
1:A:158:THR:OG1	1:A:178:LYS:CE	2.65	0.45
2:D:321:HIS:O	2:D:360:PHE:CE2	2.70	0.45
1:A:15:TYR:HE2	1:A:35:ILE:HD11	1.82	0.45
2:D:274:GLU:HG2	2:D:277:GLU:OE2	2.17	0.45
1:A:227:TRP:CE3	1:A:269:TYR:HB3	2.52	0.44
1:C:94:SER:O	1:C:98:GLY:N	2.51	0.44
1:C:198:THR:O	1:C:199:ARG:HB2	2.18	0.44
1:C:217:ARG:HG2	1:C:243:TRP:CE2	2.52	0.44
2:B:221:VAL:CG2	2:B:281:ILE:HD12	2.48	0.44
1:A:101:LEU:HD23	1:A:104:ILE:HD12	1.99	0.44
2:D:175:VAL:CB	2:D:176:PRO:CD	2.94	0.44
2:B:315:LEU:CD1	2:B:334:MET:HE2	2.48	0.44
1:A:14:THR:HG22	1:A:15:TYR:HD1	1.82	0.44
1:A:143:LEU:HD23	1:A:143:LEU:N	2.33	0.44
1:A:197:VAL:HG11	1:A:252:VAL:HG13	2.00	0.43
2:D:175:VAL:N	2:D:176:PRO:CD	2.81	0.43
1:A:41:THR:HB	1:A:42:GLU:H	1.54	0.43
1:C:15:TYR:CE1	1:C:33:LYS:HE2	2.53	0.43
2:B:418:TYR:O	2:B:421:VAL:HG13	2.19	0.43
1:C:127:ASP:HB2	1:C:148:LEU:HD23	1.99	0.43
1:A:278:LYS:NZ	4:A:2104:HOH:O	2.51	0.43
1:A:170:ALA:HB1	1:A:171:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LYS:HA	1:C:238:PRO:HD2	1.80	0.43
2:B:277:GLU:CB	4:B:2063:HOH:O	2.67	0.43
2:D:323:GLN:O	2:D:324:PRO:C	2.53	0.43
1:C:223:ASP:O	1:C:226:VAL:HG12	2.19	0.43
1:A:14:THR:CG2	1:A:148:LEU:HD13	2.48	0.43
1:A:186:ILE:HD13	1:A:186:ILE:HA	1.90	0.42
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.84	0.42
1:A:119:HIS:HD2	4:B:2016:HOH:O	2.02	0.42
2:B:272:PRO:HA	2:B:273:PRO:HD3	1.93	0.42
1:C:86:ASP:OD1	1:C:88:LYS:HB3	2.19	0.42
2:D:210:MET:CE	2:D:250:ARG:CB	2.90	0.42
1:C:122:ARG:HD2	1:C:122:ARG:HH11	1.67	0.42
2:D:275:VAL:HG23	2:D:288:LYS:HZ2	1.79	0.42
1:A:129:LYS:HA	1:A:192:ILE:HD11	2.00	0.42
1:A:175:LEU:HD13	1:A:233:MET:CE	2.50	0.42
1:A:175:LEU:CB	1:A:233:MET:HE3	2.49	0.42
2:D:175:VAL:N	2:D:176:PRO:HD3	2.35	0.42
1:C:15:TYR:HE2	1:C:35:ILE:CD1	2.28	0.42
2:B:293:ARG:NE	1:C:2:GLU:OE1	2.52	0.42
1:C:186:ILE:HA	1:C:186:ILE:HD13	1.87	0.42
2:B:384:LEU:HA	2:B:384:LEU:HD12	1.84	0.42
1:A:14:THR:HG23	1:A:148:LEU:HD13	2.01	0.42
2:D:194:LYS:HG2	2:D:195:PRO:HD2	2.02	0.42
1:A:262:LEU:O	1:A:266:MET:HG3	2.20	0.41
2:B:277:GLU:CG	4:B:2063:HOH:O	2.68	0.41
1:A:175:LEU:HD13	1:A:233:MET:HE2	2.02	0.41
1:A:10:ILE:HD11	1:A:82:PHE:HE1	1.85	0.41
2:B:378:ARG:CG	2:B:378:ARG:NH2	2.83	0.41
1:A:99:ILE:HG23	1:A:103:LEU:HD23	2.02	0.41
2:B:278:PHE:O	2:B:282:THR:HG23	2.20	0.41
1:A:178:LYS:HG3	1:A:178:LYS:O	2.20	0.41
1:A:36:ARG:HG2	1:A:36:ARG:NH1	2.33	0.41
1:C:224:GLU:HG2	1:C:231:THR:CG2	2.50	0.41
2:D:182:ILE:O	2:D:186:LEU:HG	2.21	0.41
2:B:401:ALA:N	2:B:402:PRO:CD	2.83	0.41
2:B:203:GLN:OE1	2:B:247:SER:HA	2.21	0.41
1:A:169:ARG:HD3	1:A:173:ILE:HG22	2.01	0.41
2:D:210:MET:HE1	2:D:250:ARG:HB2	2.01	0.41
1:C:266:MET:O	1:C:274:ARG:HD3	2.20	0.41
1:C:266:MET:CE	4:C:2076:HOH:O	2.67	0.41
2:D:319:PHE:CG	2:D:330:GLU:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLU:HG3	1:A:260:ARG:NH2	2.36	0.41
2:B:233:HIS:HD2	4:B:2071:HOH:O	2.04	0.41
2:B:233:HIS:HE1	4:B:2077:HOH:O	2.03	0.41
1:A:157:ARG:HB2	1:A:158:THR:H	1.79	0.41
1:C:178:LYS:HD2	1:C:179:TYR:CE1	2.55	0.41
1:C:239:SER:O	1:C:240:PHE:C	2.58	0.41
2:D:215:VAL:O	2:D:219:VAL:HG23	2.20	0.40
2:B:315:LEU:HD12	2:B:334:MET:CE	2.51	0.40
2:D:218:LEU:HD23	2:D:218:LEU:HA	1.83	0.40
1:C:99:ILE:HD13	1:C:99:ILE:HG21	1.76	0.40
1:A:40:GLU:OE1	2:B:288:LYS:NZ	2.52	0.40
2:D:351:LEU:HD23	2:D:351:LEU:HA	1.92	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:SER:N	1:C:237:LYS:NZ[6_555]	1.96	0.24
1:A:93:ALA:CA	1:C:237:LYS:NZ[6_555]	2.12	0.08
1:A:207:SER:N	2:D:226:LYS:NZ[6_555]	2.15	0.05

## 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%)	278 (95%)	8 (3%)	8 (3%)	6 2
1	C	294/303 (97%)	275 (94%)	14 (5%)	5 (2%)	11 5
2	B	256/258 (99%)	247 (96%)	6 (2%)	3 (1%)	16 10
2	D	256/258 (99%)	245 (96%)	6 (2%)	5 (2%)	9 4
All	All	1100/1122 (98%)	1045 (95%)	34 (3%)	21 (2%)	10 4



All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	41	THR
1	A	94	SER
2	D	177	ASP
2	D	322	GLN
2	D	323	GLN
1	A	38	ASP
1	A	40	GLU
1	A	164	VAL
2	B	324	PRO
2	B	346	PRO
1	C	40	GLU
1	C	96	LEU
1	C	164	VAL
2	D	346	PRO
1	A	72	THR
2	D	178	TYR
1	A	145	ASP
2	B	323	GLN
1	C	145	ASP
1	C	234	PRO

### 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%)	245 (94%)	16 (6%)	23	19
2	B	232/232 (100%)	218 (94%)	14 (6%)	24	20
2	D	232/232 (100%)	212 (91%)	20 (9%)	13	9
All	All	986/994 (99%)	911 (92%)	75 (8%)	16	12

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	2	GLU
1	A	5	GLN
1	A	6	LYS
1	A	36	ARG
1	A	41	THR
1	A	55	LEU
1	A	59	ASN
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	91	MET
1	A	121	HIS
1	A	122	ARG
1	A	148	LEU
1	A	150	ARG
1	A	155	PRO
1	A	157	ARG
1	A	163	VAL
1	A	178	LYS
1	A	226	VAL
1	A	230	VAL
1	A	255	LEU
1	A	257	GLU
1	A	278	LYS
2	B	179	HIS
2	B	196	LYS
2	B	209	SER
2	B	232	LEU
2	B	247	SER
2	B	292	LEU
2	B	316	THR
2	B	317	GLN
2	B	323	GLN
2	B	334	MET
2	B	346	PRO
2	B	371	SER
2	B	392	MET
2	B	402	PRO
1	C	36	ARG
1	C	38	ASP
1	C	39	THR
1	C	55	LEU

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Mol	Chain	Res	Type
1	C	59	ASN
1	C	74	ASN
1	C	75	LYS
1	C	122	ARG
1	C	148	LEU
1	C	150	ARG
1	C	163	VAL
1	C	206	ASP
1	C	230	VAL
1	C	234	PRO
1	C	255	LEU
1	C	278	LYS
2	D	179	HIS
2	D	188	GLU
2	D	192	LYS
2	D	196	LYS
2	D	224	GLU
2	D	232	LEU
2	D	261	MET
2	D	275	VAL
2	D	288	LYS
2	D	289	LYS
2	D	292	LEU
2	D	295	GLU
2	D	316	THR
2	D	321	HIS
2	D	334	MET
2	D	371	SER
2	D	384	LEU
2	D	392	MET
2	D	403	GLN
2	D	431	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	60	HIS
1	A	71	HIS
1	A	74	ASN
1	A	84	HIS
1	A	119	HIS

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Mol	Chain	Res	Type
1	A	121	HIS
1	A	131	GLN
2	B	183	HIS
2	B	254	GLN
2	B	317	GLN
2	B	323	GLN
2	B	370	GLN
2	B	395	HIS
2	B	431	ASN
1	C	5	GLN
1	C	60	HIS
1	C	71	HIS
1	C	113	GLN
1	C	119	HIS
1	C	131	GLN
1	C	265	GLN
2	D	254	GLN
2	D	395	HIS
2	D	396	GLN
2	D	431	ASN

### 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	0.98	0	7,14,16	1.07	0
1	TPO	C	160	1	8,10,11	1.08	1 (12%)	7,14,16	2.11	3 (42%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-O3P	2.03	1.62	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	O-C-CA	-3.54	116.09	125.44
1	C	160	TPO	CG2-CB-CA	2.15	117.55	113.17
1	C	160	TPO	OG1-P-O1P	2.46	113.25	107.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [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	CMG	A	1298	-	17,20,20	2.08	5 (29%)	17,27,27	4.03	11 (64%)
3	CMG	C	1298	-	17,20,20	2.40	4 (23%)	17,27,27	3.80	9 (52%)

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	CMG	A	1298	-	-	0/5/13/13	0/3/3/3
3	CMG	C	1298	-	-	0/5/13/13	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	CMG	C6-N1	-3.71	1.25	1.31
3	C	1298	CMG	C6-N1	-3.21	1.26	1.31
3	A	1298	CMG	C5-C4	-2.66	1.34	1.40
3	C	1298	CMG	C5-C4	-2.64	1.34	1.40
3	A	1298	CMG	O6-C6	-2.19	1.33	1.35
3	A	1298	CMG	C4-N3	3.44	1.42	1.36
3	C	1298	CMG	C4-N3	4.18	1.44	1.36
3	A	1298	CMG	C2-N1	4.78	1.43	1.35
3	C	1298	CMG	C2-N1	6.09	1.46	1.35

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	CMG	C4-C5-N7	-8.08	102.04	109.48
3	A	1298	CMG	N3-C2-N1	-6.94	116.88	127.44
3	C	1298	CMG	N3-C2-N1	-6.55	117.47	127.44
3	A	1298	CMG	C5-C6-N1	-5.65	113.83	123.81
3	C	1298	CMG	C9-O6-C6	-5.41	111.58	117.23
3	C	1298	CMG	C5-C6-N1	-4.97	115.04	123.81
3	C	1298	CMG	C4-C5-N7	-4.52	105.32	109.48
3	C	1298	CMG	O6-C9-C10	-3.07	100.89	107.97
3	A	1298	CMG	C11-C10-C9	-2.27	106.67	111.47
3	A	1298	CMG	C15-C10-C11	2.23	114.88	109.26
3	A	1298	CMG	O6-C9-C10	2.24	113.12	107.97
3	A	1298	CMG	C14-C15-C10	2.32	115.96	112.22
3	A	1298	CMG	O6-C6-C5	2.46	118.92	115.07
3	C	1298	CMG	C15-C10-C11	2.75	116.17	109.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	CMG	C9-O6-C6	2.98	120.34	117.23
3	C	1298	CMG	O6-C6-C5	3.31	120.25	115.07
3	A	1298	CMG	N2-C2-N3	3.90	125.28	117.80
3	C	1298	CMG	N2-C2-N3	5.33	128.02	117.80
3	C	1298	CMG	C2-N1-C6	8.05	127.11	116.03
3	A	1298	CMG	C2-N1-C6	8.75	128.07	116.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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%)	0.34	24 (8%) 15 20	29, 40, 63, 88	0
1	C	296/303 (97%)	0.65	43 (14%) 3 5	31, 43, 74, 87	0
2	B	258/258 (100%)	0.35	23 (8%) 12 16	29, 40, 60, 81	0
2	D	258/258 (100%)	0.52	27 (10%) 8 11	30, 44, 66, 92	0
All	All	1108/1122 (98%)	0.47	117 (10%) 8 11	29, 42, 66, 92	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	175	VAL	14.0
1	C	96	LEU	10.8
1	A	39	THR	9.2
1	C	234	PRO	9.0
1	C	240	PHE	9.0
1	C	40	GLU	8.9
2	D	176	PRO	8.9
1	A	93	ALA	7.9
2	B	323	GLN	7.9
1	C	95	ALA	7.8
1	C	238	PRO	7.6
1	C	236	TYR	7.6
1	A	296	LEU	7.2
1	C	232	SER	7.0
2	D	177	ASP	6.9
1	A	40	GLU	6.8
1	A	295	HIS	6.8
2	D	432	LEU	6.5
1	C	233	MET	6.1
2	D	322	GLN	5.5
1	C	225	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	175	VAL	5.2
1	C	94	SER	5.2
1	C	239	SER	5.1
1	A	206	ASP	5.1
2	D	321	HIS	5.0
1	C	231	THR	5.0
1	C	73	GLU	4.4
1	C	229	GLY	4.4
1	C	39	THR	4.3
2	B	432	LEU	4.2
2	D	428	GLU	4.1
2	B	280	TYR	4.1
1	C	36	ARG	3.9
2	D	429	THR	3.8
2	D	323	GLN	3.8
1	C	226	VAL	3.7
2	B	324	PRO	3.7
2	B	428	GLU	3.7
1	A	38	ASP	3.6
2	B	431	ASN	3.6
1	A	0	SER	3.6
1	C	177	CYS	3.6
2	D	324	PRO	3.5
1	C	235	ASP	3.5
1	A	247	ASP	3.4
1	A	250	LYS	3.4
1	A	36	ARG	3.4
1	A	41	THR	3.3
1	C	192	ILE	3.3
2	B	355	ILE	3.3
1	A	287	GLN	3.3
2	D	416	SER	3.2
2	B	284	ASP	3.1
2	B	341	LEU	3.1
2	D	341	LEU	3.1
2	D	431	ASN	3.0
1	C	230	VAL	3.0
1	C	224	GLU	2.9
1	C	128	LEU	2.9
1	C	228	PRO	2.8
1	C	189	LEU	2.8
1	C	243	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	133	LEU	2.8
2	D	355	ILE	2.8
2	D	378	ARG	2.8
2	D	374	GLU	2.7
2	D	315	LEU	2.7
1	C	237	LYS	2.7
1	C	295	HIS	2.7
2	B	368	THR	2.7
2	D	337	GLY	2.7
2	B	232	LEU	2.6
2	D	430	LEU	2.6
2	B	311	VAL	2.6
1	C	217	ARG	2.6
2	B	336	LEU	2.6
2	B	416	SER	2.5
1	C	244	ALA	2.5
1	C	250	LYS	2.5
2	D	288	LYS	2.5
1	A	73	GLU	2.5
1	A	249	SER	2.5
1	C	227	TRP	2.5
2	D	385	GLU	2.4
2	D	417	LYS	2.5
2	D	311	VAL	2.4
2	D	236	VAL	2.4
1	C	242	LYS	2.4
2	B	283	ASP	2.3
2	D	356	ALA	2.3
2	D	359	ALA	2.3
1	C	247	ASP	2.3
2	B	365	TYR	2.3
1	C	206	ASP	2.3
1	A	189	LEU	2.3
2	B	198	GLY	2.2
1	C	133	LEU	2.2
1	A	143	LEU	2.2
1	C	12	GLU	2.2
2	B	337	GLY	2.2
1	A	178	LYS	2.2
2	B	236	VAL	2.1
1	A	71	HIS	2.1
2	D	415	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	288	ASP	2.1
1	C	249	SER	2.1
2	B	322	GLN	2.1
2	B	234	LEU	2.1
2	B	358	ALA	2.1
1	A	87	LEU	2.0
1	C	97	THR	2.0
1	C	188	SER	2.0
1	A	1	MET	2.0
1	C	178	LYS	2.0
1	C	284	PRO	2.0
1	A	256	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
1	TPO	A	160	11/12	0.98	0.09	-	32,35,37,37	0
1	TPO	C	160	11/12	0.99	0.09	-	30,34,39,39	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(Å <sup>2</sup> )	Q<0.9
3	CMG	C	1298	18/18	0.95	0.08	-0.80	39,42,44,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CMG	A	1298	18/18	0.97	0.09	-0.90	41,43,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.