



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:00 am BST

PDB ID : 3UGM  
Title : Structure of TAL effector PthXo1 bound to its DNA target  
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Deposited on : 2011-11-02  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

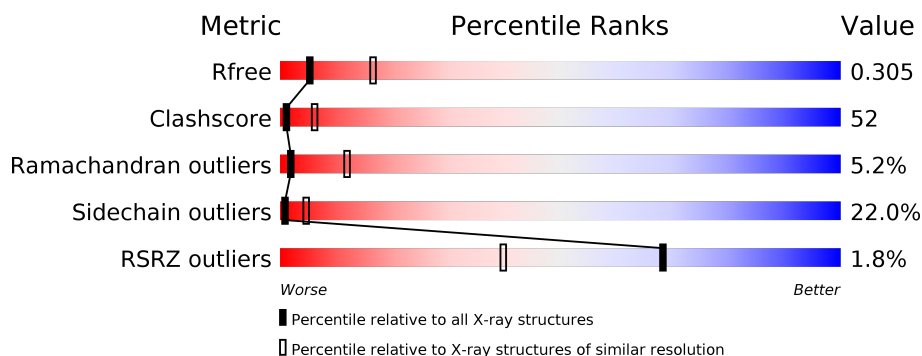
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1047	<div> <div> <div></div> <div>25%</div> <div>41%</div> <div>14%</div> <div>•</div> <div>18%</div> </div> </div>
2	B	38	<div> <div>5%</div> <div>26%</div> <div>61%</div> <div>13%</div> </div>
3	C	38	<div> <div>3%</div> <div>32%</div> <div>58%</div> <div>11%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7853 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 TAL effector AvrBs3/PthA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	854	Total	C	N	O	S	0	0	0
			6085	3792	1123	1147	23			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	MET	-	EXPRESSION TAG	UNP B2SU53
A	104	ALA	-	EXPRESSION TAG	UNP B2SU53
A	105	SER	-	EXPRESSION TAG	UNP B2SU53
A	106	SER	-	EXPRESSION TAG	UNP B2SU53
A	107	HIS	-	EXPRESSION TAG	UNP B2SU53
A	108	HIS	-	EXPRESSION TAG	UNP B2SU53
A	109	HIS	-	EXPRESSION TAG	UNP B2SU53
A	110	HIS	-	EXPRESSION TAG	UNP B2SU53
A	111	HIS	-	EXPRESSION TAG	UNP B2SU53
A	112	HIS	-	EXPRESSION TAG	UNP B2SU53
A	113	SER	-	EXPRESSION TAG	UNP B2SU53
A	114	SER	-	EXPRESSION TAG	UNP B2SU53
A	115	GLY	-	EXPRESSION TAG	UNP B2SU53
A	116	LEU	-	EXPRESSION TAG	UNP B2SU53
A	117	VAL	-	EXPRESSION TAG	UNP B2SU53
A	118	PRO	-	EXPRESSION TAG	UNP B2SU53
A	119	ARG	-	EXPRESSION TAG	UNP B2SU53
A	120	GLY	-	EXPRESSION TAG	UNP B2SU53
A	121	SER	-	EXPRESSION TAG	UNP B2SU53
A	122	SER	-	EXPRESSION TAG	UNP B2SU53
A	123	GLY	-	EXPRESSION TAG	UNP B2SU53
A	124	SER	-	EXPRESSION TAG	UNP B2SU53
A	125	SER	-	EXPRESSION TAG	UNP B2SU53
A	126	MET	-	EXPRESSION TAG	UNP B2SU53
A	173	ARG	GLY	ENGINEERED MUTATION	UNP B2SU53
A	198	GLN	ARG	ENGINEERED MUTATION	UNP B2SU53
A	209	THR	LYS	ENGINEERED MUTATION	UNP B2SU53

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Chain	Residue	Modelled	Actual	Comment	Reference
A	212	HIS	ASP	ENGINEERED MUTATION	UNP B2SU53
A	213	ILE	MET	ENGINEERED MUTATION	UNP B2SU53
A	215	THR	ALA	ENGINEERED MUTATION	UNP B2SU53
A	244	ASP	VAL	ENGINEERED MUTATION	UNP B2SU53
A	272	MET	VAL	ENGINEERED MUTATION	UNP B2SU53

- Molecule 2 is a DNA chain called DNA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	38	Total	C	N	O	P	0	0	0
			764	367	137	223	37			

- Molecule 3 is a DNA chain called DNA-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	38	Total	C	N	O	P	0	0	0
			788	376	146	229	37			

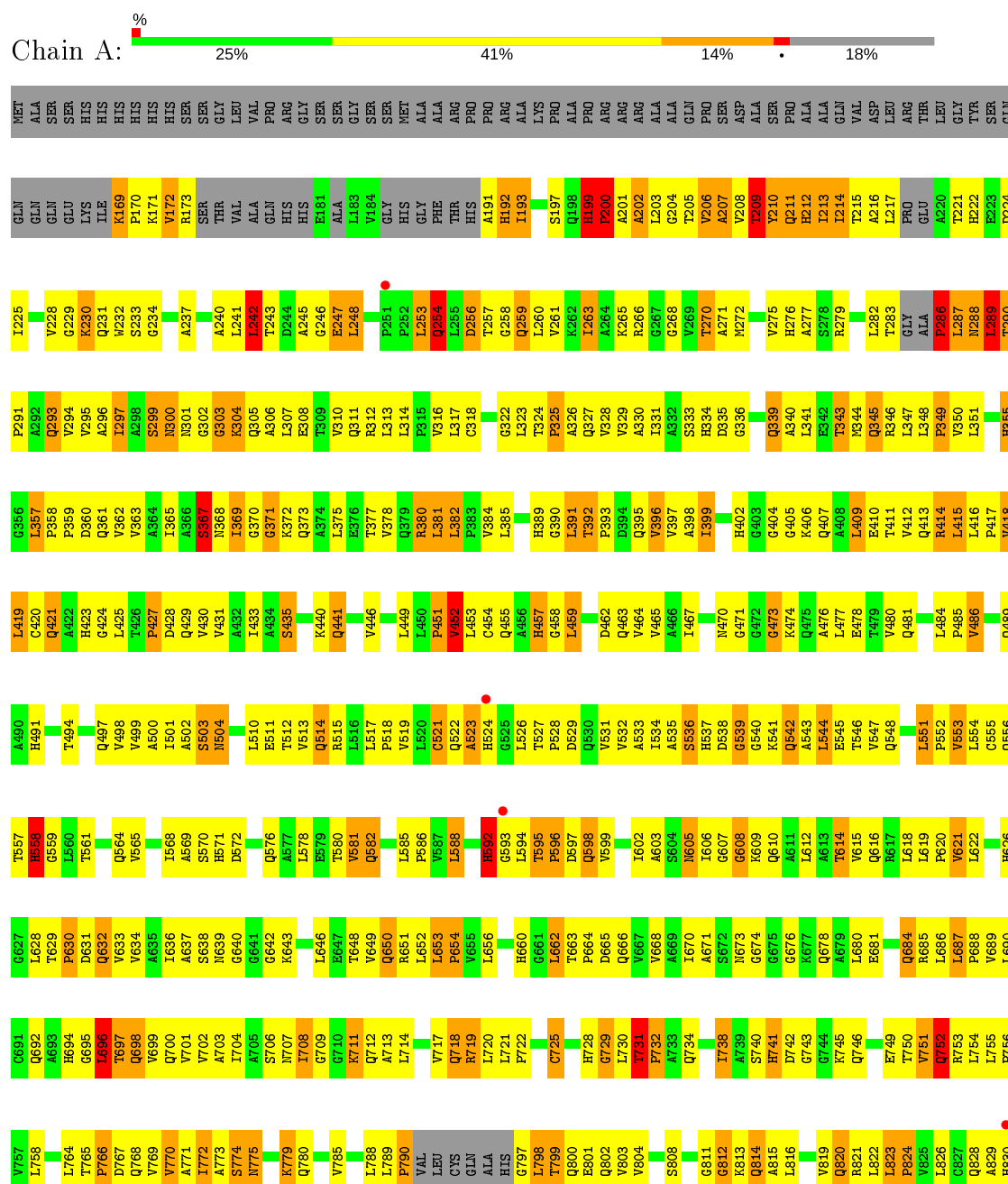
- Molecule 4 is water.

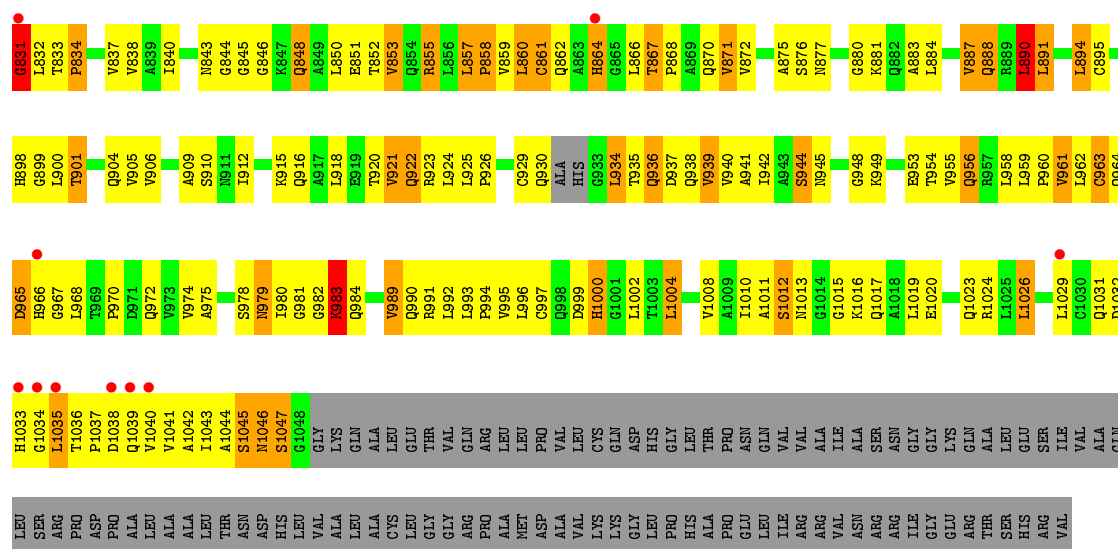
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total	O	0	0
			159	159		
4	B	23	Total	O	0	0
			23	23		
4	C	34	Total	O	0	0
			34	34		

### 3 Residue-property plots

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

- Molecule 1: TAL effector AvrBs3/PthA





### • Molecule 2: DNA-1



### • Molecule 3: DNA-2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.58 Å   248.48 Å   54.65 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	50.00 – 3.00 44.60 – 3.01	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-3.00) 95.9 (44.60-3.01)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 3.01 Å)	Xtriage
Refinement program	REFMAC, CNS	Depositor
R, $R_{free}$	0.266   ,   0.294 0.267   ,   0.305	Depositor DCC
$R_{free}$ test set	1326 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.4	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 105.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	7853	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.50% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	1.07	42/6153 (0.7%)	1.18	64/8397 (0.8%)
2	B	1.44	4/855 (0.5%)	1.22	2/1314 (0.2%)
3	C	1.36	6/885 (0.7%)	1.11	0/1368
All	All	1.15	52/7893 (0.7%)	1.18	66/11079 (0.6%)

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	9

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ALA	CA-CB	-15.15	1.20	1.52
1	A	169	LYS	CA-CB	-14.67	1.21	1.53
1	A	210	TYR	CE2-CZ	-10.88	1.24	1.38
1	A	212	HIS	CA-CB	-10.45	1.30	1.53
1	A	210	TYR	CG-CD1	-9.62	1.26	1.39
1	A	170	PRO	CA-CB	-9.46	1.34	1.53
1	A	191	ALA	C-O	-9.21	1.05	1.23
1	A	216	ALA	CA-CB	-9.21	1.33	1.52
1	A	171	LYS	CA-CB	-9.19	1.33	1.53
1	A	201	ALA	CA-C	-8.75	1.30	1.52
1	A	200	PRO	C-O	-8.72	1.05	1.23
1	A	200	PRO	CA-C	-8.68	1.35	1.52
1	A	210	TYR	CD2-CE2	-8.50	1.26	1.39
1	A	214	ILE	CA-C	-8.44	1.31	1.52
1	A	202	ALA	CA-CB	-8.42	1.34	1.52
1	A	193	ILE	CA-CB	-8.39	1.35	1.54
1	A	210	TYR	CB-CG	-7.89	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	VAL	C-O	-7.88	1.08	1.23
1	A	201	ALA	N-CA	-7.74	1.30	1.46
1	A	207	ALA	CA-CB	-7.72	1.36	1.52
1	A	214	ILE	C-O	-7.70	1.08	1.23
1	A	210	TYR	CD1-CE1	-7.65	1.27	1.39
1	A	210	TYR	CG-CD2	-7.02	1.30	1.39
1	A	191	ALA	CA-C	-6.93	1.34	1.52
3	C	16	DG	C6-O6	-6.79	1.18	1.24
1	A	170	PRO	CA-C	-6.67	1.39	1.52
1	A	210	TYR	CE1-CZ	-6.66	1.29	1.38
1	A	171	LYS	C-O	-6.62	1.10	1.23
1	A	963	CYS	CB-SG	6.48	1.93	1.82
3	C	35	DT	C4-C5	6.08	1.50	1.45
1	A	1047	SER	CA-CB	-5.93	1.44	1.52
3	C	25	DG	C5-C4	-5.90	1.34	1.38
1	A	191	ALA	N-CA	-5.89	1.34	1.46
1	A	210	TYR	N-CA	-5.88	1.34	1.46
1	A	1045	SER	CB-OG	-5.87	1.34	1.42
2	B	8	DC	C4-N4	-5.87	1.28	1.33
2	B	18	DA	N9-C8	5.80	1.42	1.37
1	A	173	ARG	CA-CB	-5.76	1.41	1.53
1	A	1046	ASN	CA-CB	-5.61	1.38	1.53
1	A	209	THR	C-O	-5.60	1.12	1.23
1	A	216	ALA	N-CA	-5.56	1.35	1.46
1	A	170	PRO	N-CA	-5.47	1.38	1.47
3	C	26	DA	C5-C4	-5.46	1.34	1.38
1	A	209	THR	N-CA	-5.44	1.35	1.46
2	B	13	DA	C6-N6	-5.42	1.29	1.33
3	C	22	DG	C6-N1	5.42	1.43	1.39
3	C	21	DG	C6-O6	5.33	1.28	1.24
1	A	207	ALA	C-O	-5.26	1.13	1.23
2	B	11	DC	N3-C4	5.13	1.37	1.33
1	A	861	CYS	CB-SG	-5.10	1.73	1.81
1	A	192	HIS	CA-CB	-5.08	1.42	1.53
1	A	287	LEU	CA-CB	-5.06	1.42	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ALA	CB-CA-C	9.49	124.34	110.10
1	A	202	ALA	N-CA-CB	-8.41	98.33	110.10
1	A	774	SER	CB-CA-C	-7.60	95.66	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ASN	C-N-CA	7.46	140.35	121.70
1	A	559	GLY	N-CA-C	7.44	131.70	113.10
1	A	209	THR	N-CA-CB	7.36	124.28	110.30
1	A	289	LEU	N-CA-CB	-7.31	95.78	110.40
1	A	216	ALA	CB-CA-C	-7.25	99.23	110.10
1	A	696	LEU	CA-CB-CG	7.21	131.89	115.30
1	A	171	LYS	N-CA-C	-7.19	91.58	111.00
1	A	201	ALA	N-CA-CB	7.08	120.02	110.10
1	A	831	GLY	N-CA-C	7.07	130.78	113.10
1	A	740	SER	N-CA-C	7.06	130.07	111.00
1	A	965	ASP	N-CA-C	7.05	130.04	111.00
1	A	593	GLY	N-CA-C	7.01	130.63	113.10
1	A	593	GLY	C-N-CA	6.99	139.18	121.70
1	A	731	THR	N-CA-C	-6.97	92.18	111.00
1	A	216	ALA	N-CA-C	6.94	129.74	111.00
1	A	214	ILE	N-CA-CB	-6.92	94.88	110.80
1	A	210	TYR	N-CA-CB	-6.80	98.35	110.60
1	A	253	LEU	N-CA-C	-6.75	92.79	111.00
1	A	1046	ASN	N-CA-C	-6.68	92.95	111.00
1	A	205	THR	N-CA-C	6.66	128.97	111.00
1	A	206	VAL	N-CA-C	6.63	128.91	111.00
1	A	775	ASN	N-CA-C	-6.61	93.16	111.00
1	A	200	PRO	N-CA-CB	-6.58	95.36	102.60
1	A	558	HIS	CB-CA-C	-6.57	97.26	110.40
1	A	214	ILE	N-CA-C	6.54	128.66	111.00
1	A	206	VAL	N-CA-CB	-6.53	97.13	111.50
1	A	743	GLY	N-CA-C	6.53	129.43	113.10
1	A	696	LEU	N-CA-CB	-6.46	97.49	110.40
1	A	202	ALA	N-CA-C	-6.45	93.60	111.00
1	A	210	TYR	CA-CB-CG	-6.40	101.23	113.40
1	A	1047	SER	N-CA-CB	-6.37	100.94	110.50
1	A	592	HIS	N-CA-C	-6.36	93.83	111.00
1	A	197	SER	N-CA-C	-6.28	94.05	111.00
1	A	390	GLY	N-CA-C	6.21	128.64	113.10
1	A	287	LEU	N-CA-CB	6.17	122.75	110.40
1	A	569	ALA	CB-CA-C	-6.12	100.92	110.10
1	A	201	ALA	C-N-CA	6.08	136.90	121.70
1	A	662	LEU	N-CA-C	6.05	127.32	111.00
1	A	254	GLN	N-CA-CB	-5.97	99.86	110.60
1	A	457	HIS	CB-CA-C	-5.96	98.49	110.40
1	A	798	LEU	CB-CA-C	5.92	121.44	110.20
1	A	890	LEU	CA-CB-CG	5.89	128.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	457	HIS	N-CA-C	-5.80	95.33	111.00
1	A	503	SER	CB-CA-C	5.79	121.10	110.10
1	A	457	HIS	N-CA-CB	5.77	120.99	110.60
2	B	12	DT	C1'-O4'-C4'	-5.74	104.36	110.10
1	A	287	LEU	C-N-CA	-5.65	107.58	121.70
1	A	963	CYS	CB-CA-C	5.61	121.63	110.40
1	A	741	HIS	CB-CA-C	5.58	121.57	110.40
1	A	209	THR	C-N-CA	5.57	135.61	121.70
1	A	290	THR	CB-CA-C	-5.55	96.61	111.60
1	A	210	TYR	N-CA-C	5.53	125.94	111.00
1	A	788	LEU	N-CA-C	5.53	125.93	111.00
1	A	415	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	732	PRO	CA-N-CD	-5.49	103.82	111.50
1	A	242	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	523	ALA	CB-CA-C	5.45	118.27	110.10
2	B	15	DT	C1'-O4'-C4'	-5.38	104.72	110.10
1	A	638	SER	CB-CA-C	5.35	120.27	110.10
1	A	458	GLY	N-CA-C	-5.16	100.21	113.10
1	A	207	ALA	N-CA-CB	5.14	117.30	110.10
1	A	253	LEU	CB-CA-C	5.07	119.83	110.20
1	A	855	ARG	NE-CZ-NH2	-5.07	117.77	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	LYS	Peptide
1	A	200	PRO	Mainchain
1	A	209	THR	Peptide
1	A	211	GLN	Peptide
1	A	215	THR	Peptide
1	A	286	PRO	Mainchain,Peptide
1	A	731	THR	Mainchain
1	A	831	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6085	0	6242	687	0
2	B	764	0	427	52	0
3	C	788	0	432	49	0
4	A	159	0	0	88	0
4	B	23	0	0	12	0
4	C	34	0	0	12	0
All	All	7853	0	7101	772	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 52.

All (772) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:CYS:HA	1:A:457:HIS:O	1.26	1.27
1:A:729:GLY:O	1:A:730:LEU:HD23	1.14	1.26
1:A:1008:VAL:HG11	4:A:101:HOH:O	1.37	1.21
1:A:684:GLN:HB2	4:A:1175:HOH:O	1.43	1.16
1:A:389:HIS:CE1	1:A:416:LEU:HD23	1.79	1.16
1:A:391:LEU:HD21	1:A:396:VAL:CG2	1.78	1.14
1:A:697:THR:OG1	1:A:700:GLN:HB2	1.49	1.13
1:A:200:PRO:HG3	1:A:222:HIS:CE1	1.83	1.13
1:A:288:ASN:HB3	1:A:289:LEU:HG	1.26	1.12
1:A:966:HIS:HB2	1:A:993:LEU:HD23	1.30	1.09
3:C:37:DA:H2''	3:C:38:DC:C5	1.88	1.09
3:C:36:DA:H4'	4:C:43:HOH:O	1.53	1.09
1:A:200:PRO:CG	1:A:222:HIS:CE1	2.36	1.08
1:A:200:PRO:CG	1:A:222:HIS:HE1	1.66	1.08
1:A:199:HIS:HB3	1:A:200:PRO:HD3	1.34	1.06
1:A:602:ILE:CG2	1:A:637:ALA:HB1	1.87	1.05
1:A:866:LEU:HD23	1:A:871:VAL:HG23	1.35	1.04
1:A:254:GLN:HG2	4:A:1173:HOH:O	1.57	1.03
1:A:622:LEU:HA	1:A:626:HIS:HB2	1.40	1.03
1:A:1046:ASN:CB	1:A:1047:SER:HA	1.89	1.03
1:A:360:ASP:HA	4:A:1205:HOH:O	1.55	1.02
1:A:729:GLY:O	1:A:730:LEU:CD2	2.06	1.02
3:C:32:DA:H2''	3:C:33:DT:H5''	1.42	1.01
1:A:206:VAL:C	1:A:208:VAL:H	1.56	0.99
1:A:953:GLU:HG2	4:A:1154:HOH:O	1.61	0.99
1:A:966:HIS:CB	1:A:993:LEU:HD23	1.91	0.99
1:A:916:GLN:HB3	1:A:949:LYS:HD3	1.46	0.98
1:A:966:HIS:HB2	1:A:993:LEU:CD2	1.94	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:VAL:HG12	1:A:1040:VAL:O	1.63	0.98
1:A:753:ARG:HD2	4:A:1156:HOH:O	1.63	0.97
1:A:362:VAL:HA	1:A:365:ILE:HD12	1.45	0.96
1:A:989:VAL:HG23	1:A:1019:LEU:HD11	1.49	0.95
1:A:351:LEU:HD22	4:A:1215:HOH:O	1.66	0.95
1:A:391:LEU:HD21	1:A:396:VAL:HG22	1.46	0.95
1:A:212:HIS:CB	1:A:214:ILE:HG13	1.97	0.95
1:A:607:GLY:HA3	4:A:1153:HOH:O	1.65	0.94
1:A:686:LEU:HD23	1:A:718:GLN:HG2	1.48	0.94
1:A:620:PRO:HD3	4:A:87:HOH:O	1.66	0.94
1:A:670:ILE:HD11	1:A:702:VAL:HG23	1.49	0.93
3:C:37:DA:H2''	3:C:38:DC:H5	1.25	0.93
4:A:1232:HOH:O	3:C:19:DG:H2''	1.68	0.93
2:B:-1:DA:H2''	2:B:0:DT:H5'	1.51	0.92
1:A:217:LEU:HG	4:A:1187:HOH:O	1.69	0.91
1:A:656:LEU:O	1:A:660:HIS:HB2	1.71	0.91
1:A:966:HIS:CB	1:A:993:LEU:CD2	2.49	0.91
1:A:663:THR:HG22	1:A:666:GLN:HE21	1.34	0.90
1:A:286:PRO:HB3	1:A:287:LEU:HA	1.52	0.90
1:A:588:LEU:HD21	1:A:615:VAL:CG1	2.02	0.90
1:A:208:VAL:HG12	1:A:208:VAL:O	1.69	0.90
1:A:654:PRO:HG3	4:A:85:HOH:O	1.70	0.89
1:A:425:LEU:HD22	1:A:429:GLN:OE1	1.74	0.88
1:A:539:GLY:HA3	4:A:102:HOH:O	1.72	0.88
1:A:708:ILE:HB	1:A:742:ASP:CG	1.95	0.87
2:B:-6:DT:H2''	2:B:-5:DA:C8	2.10	0.86
1:A:588:LEU:HD21	1:A:615:VAL:HG11	1.56	0.86
1:A:217:LEU:HD13	4:A:1166:HOH:O	1.76	0.86
1:A:339:GLN:HE21	1:A:339:GLN:N	1.73	0.85
1:A:614:THR:HG22	1:A:618:LEU:HD12	1.57	0.85
1:A:866:LEU:HG	1:A:870:GLN:HB2	1.58	0.85
1:A:602:ILE:HG23	1:A:637:ALA:HB1	1.58	0.85
1:A:721:LEU:HB3	1:A:722:PRO:HD3	1.57	0.85
1:A:512:THR:OG1	1:A:541:LYS:HG3	1.77	0.85
1:A:351:LEU:CD2	4:A:1215:HOH:O	2.24	0.84
1:A:953:GLU:HA	4:A:1154:HOH:O	1.76	0.84
1:A:248:LEU:HD12	1:A:253:LEU:HB3	1.58	0.84
3:C:37:DA:C2'	3:C:38:DC:C5	2.61	0.84
2:B:-1:DA:H2''	2:B:0:DT:C5'	2.07	0.84
1:A:200:PRO:HG2	1:A:222:HIS:CE1	2.13	0.83
1:A:454:CYS:CA	1:A:457:HIS:O	2.20	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:PRO:CD	4:A:87:HOH:O	2.24	0.83
1:A:289:LEU:HB3	1:A:293:GLN:HG3	1.60	0.83
1:A:864:HIS:CE1	1:A:866:LEU:HB2	2.14	0.83
3:C:21:DG:H2"	3:C:22:DG:H5'	1.59	0.82
1:A:206:VAL:C	1:A:208:VAL:N	2.30	0.82
1:A:708:ILE:HB	1:A:742:ASP:OD2	1.79	0.82
1:A:823:LEU:HB3	1:A:824:PRO:HD3	1.63	0.80
1:A:725:CYS:HB3	1:A:730:LEU:O	1.82	0.80
1:A:389:HIS:CE1	1:A:416:LEU:CD2	2.64	0.80
1:A:680:LEU:CB	4:A:73:HOH:O	2.30	0.80
1:A:270:THR:HG21	2:B:0:DT:OP2	1.82	0.79
1:A:212:HIS:HA	1:A:213:ILE:C	2.03	0.79
1:A:912:ILE:HG23	4:A:1176:HOH:O	1.82	0.79
1:A:385:LEU:HD23	1:A:389:HIS:CD2	2.17	0.79
1:A:1046:ASN:CB	1:A:1047:SER:CA	2.58	0.79
1:A:287:LEU:O	1:A:288:ASN:HB2	1.81	0.79
1:A:811:GLY:HA3	4:A:1219:HOH:O	1.82	0.78
1:A:799:THR:HG23	1:A:802:GLN:OE1	1.82	0.78
3:C:2:DT:H2"	3:C:3:DT:H5'	1.66	0.78
1:A:441:GLN:HB3	1:A:474:LYS:HE3	1.64	0.78
1:A:656:LEU:CD1	4:A:1175:HOH:O	2.31	0.78
1:A:391:LEU:HD21	1:A:396:VAL:HG21	1.63	0.77
1:A:1040:VAL:CG1	1:A:1040:VAL:O	2.32	0.77
1:A:254:GLN:CG	4:A:1173:HOH:O	2.23	0.77
1:A:391:LEU:HD12	1:A:395:GLN:HB2	1.67	0.77
1:A:345:GLN:HB3	1:A:346:ARG:NH1	2.00	0.77
1:A:288:ASN:CB	1:A:289:LEU:HG	2.10	0.77
1:A:314:LEU:HD23	4:A:1201:HOH:O	1.84	0.77
1:A:680:LEU:HB3	4:A:73:HOH:O	1.85	0.76
1:A:200:PRO:HG2	1:A:222:HIS:HE1	1.49	0.75
1:A:389:HIS:ND1	1:A:416:LEU:CD2	2.49	0.75
1:A:992:LEU:HD11	1:A:1020:GLU:HG2	1.68	0.75
1:A:861:CYS:CB	4:A:1168:HOH:O	2.32	0.75
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.02	0.74
1:A:857:LEU:HB3	1:A:858:PRO:HD3	1.69	0.74
1:A:257:THR:O	1:A:260:LEU:N	2.21	0.74
1:A:588:LEU:O	1:A:592:HIS:HD2	1.70	0.74
1:A:1017:GLN:HG3	4:B:129:HOH:O	1.88	0.74
1:A:391:LEU:CD1	1:A:395:GLN:HB2	2.18	0.74
1:A:650:GLN:CG	1:A:651:ARG:N	2.51	0.74
1:A:200:PRO:HG3	1:A:222:HIS:ND1	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:LEU:HB3	1:A:756:PRO:HD3	1.70	0.73
1:A:253:LEU:HG	4:A:1173:HOH:O	1.88	0.73
1:A:769:VAL:HA	1:A:772:ILE:HD12	1.70	0.73
1:A:960:PRO:O	1:A:964:GLN:HG2	1.88	0.73
1:A:602:ILE:HG23	1:A:637:ALA:CB	2.19	0.73
1:A:861:CYS:HB2	4:A:1168:HOH:O	1.88	0.73
2:B:14:DC:H2"	2:B:15:DT:O5'	1.88	0.73
4:A:1232:HOH:O	3:C:19:DG:C2'	2.30	0.73
1:A:797:GLY:O	1:A:798:LEU:HB2	1.86	0.73
1:A:470:ASN:ND2	4:A:1220:HOH:O	2.20	0.73
1:A:556:GLN:HG3	4:A:1180:HOH:O	1.88	0.73
1:A:351:LEU:HA	1:A:355:HIS:CD2	2.24	0.73
1:A:866:LEU:HD23	1:A:871:VAL:CG2	2.17	0.73
1:A:663:THR:CG2	1:A:666:GLN:HE21	2.02	0.73
1:A:859:VAL:CG1	4:A:1231:HOH:O	2.36	0.73
1:A:656:LEU:HD12	4:A:1175:HOH:O	1.89	0.72
1:A:595:THR:OG1	1:A:598:GLN:HB3	1.89	0.72
1:A:199:HIS:CB	1:A:200:PRO:HD3	2.07	0.72
1:A:405:GLY:O	1:A:409:LEU:HD12	1.89	0.72
1:A:789:LEU:HB3	1:A:790:PRO:CD	2.19	0.72
3:C:36:DA:H1'	4:C:133:HOH:O	1.90	0.72
1:A:615:VAL:HG12	1:A:616:GLN:N	2.05	0.71
3:C:37:DA:C2'	3:C:38:DC:H5	1.98	0.71
3:C:3:DT:H2"	3:C:4:DT:H5"	1.71	0.71
1:A:602:ILE:HG21	1:A:637:ALA:HB1	1.71	0.71
1:A:1029:LEU:HD12	1:A:1040:VAL:HG21	1.72	0.71
1:A:313:LEU:O	1:A:317:LEU:HG	1.89	0.71
1:A:848:GLN:HA	1:A:848:GLN:NE2	2.05	0.71
2:B:11:DC:H2"	2:B:12:DT:O5'	1.90	0.71
2:B:9:DC:H2"	2:B:10:DC:O5'	1.89	0.71
1:A:389:HIS:ND1	1:A:416:LEU:HD23	2.05	0.71
1:A:741:HIS:NE2	1:A:774:SER:O	2.23	0.71
1:A:348:LEU:HD13	1:A:362:VAL:HG21	1.73	0.70
1:A:609:LYS:HE3	1:A:610:GLN:HE22	1.55	0.70
1:A:517:LEU:HB3	1:A:518:PRO:CD	2.21	0.70
1:A:673:ASN:HB3	1:A:708:ILE:HG12	1.73	0.70
1:A:399:ILE:CG2	1:A:399:ILE:O	2.39	0.70
3:C:23:DG:N7	4:C:104:HOH:O	2.24	0.70
1:A:1045:SER:O	1:A:1046:ASN:C	2.24	0.70
1:A:596:PRO:O	1:A:599:VAL:N	2.23	0.70
1:A:1045:SER:O	1:A:1046:ASN:CB	2.29	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:HD12	1:A:395:GLN:CB	2.22	0.70
1:A:454:CYS:HB3	1:A:459:LEU:O	1.92	0.70
1:A:607:GLY:CA	4:A:1153:HOH:O	2.30	0.70
1:A:954:THR:OG1	1:A:983:LYS:HG2	1.91	0.69
1:A:228:VAL:HG22	1:A:265:LYS:HA	1.71	0.69
1:A:558:HIS:HD1	1:A:585:LEU:HD22	1.56	0.69
1:A:602:ILE:CG2	1:A:637:ALA:CB	2.70	0.69
1:A:864:HIS:CD2	1:A:866:LEU:HD13	2.27	0.69
3:C:21:DG:H2''	3:C:22:DG:C5'	2.23	0.69
1:A:697:THR:HG1	1:A:700:GLN:HB2	1.55	0.69
1:A:690:LEU:HD13	1:A:701:VAL:HG21	1.73	0.69
1:A:199:HIS:HB3	1:A:200:PRO:CD	2.18	0.69
1:A:286:PRO:CB	1:A:287:LEU:HA	2.15	0.69
1:A:295:VAL:O	1:A:299:SER:HB3	1.92	0.69
1:A:753:ARG:CD	4:A:1156:HOH:O	2.32	0.68
1:A:861:CYS:SG	4:A:1168:HOH:O	2.51	0.68
1:A:282:LEU:HD23	1:A:288:ASN:OD1	1.94	0.68
1:A:925:LEU:HD13	1:A:939:VAL:HG11	1.73	0.68
1:A:256:ASP:HB3	1:A:259:GLN:HB2	1.76	0.68
1:A:843:ASN:ND2	1:A:876:SER:O	2.27	0.68
1:A:237:ALA:O	1:A:272:MET:HE1	1.93	0.68
1:A:212:HIS:CB	1:A:214:ILE:CG1	2.71	0.68
1:A:348:LEU:HB3	1:A:349:PRO:HD3	1.74	0.68
3:C:32:DA:C2'	3:C:33:DT:H5''	2.22	0.68
3:C:28:DG:N7	4:C:44:HOH:O	2.26	0.68
1:A:639:ASN:OD1	1:A:640:GLY:N	2.27	0.67
1:A:780:GLN:HE21	1:A:813:LYS:NZ	1.92	0.67
1:A:391:LEU:HD21	1:A:396:VAL:CG1	2.24	0.67
1:A:829:ALA:C	1:A:831:GLY:H	1.96	0.67
1:A:232:TRP:CE3	1:A:233:SER:HB3	2.30	0.67
3:C:13:DA:H2''	3:C:14:DC:H5'	1.75	0.67
1:A:537:HIS:CE1	1:A:570:SER:O	2.48	0.67
1:A:864:HIS:NE2	1:A:866:LEU:HD13	2.09	0.67
3:C:13:DA:H4'	3:C:14:DC:OP1	1.94	0.67
1:A:347:LEU:HD23	1:A:350:VAL:HB	1.77	0.67
1:A:202:ALA:O	1:A:203:LEU:HG	1.95	0.67
1:A:915:LYS:HD3	1:A:916:GLN:OE1	1.95	0.66
1:A:966:HIS:HB3	1:A:993:LEU:CD2	2.23	0.66
2:B:-4:DG:H5'	4:B:72:HOH:O	1.96	0.66
1:A:1029:LEU:HD12	1:A:1040:VAL:CG2	2.25	0.66
1:A:686:LEU:CD2	1:A:718:GLN:HG2	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:ASP:C	1:A:965:ASP:OD2	2.33	0.66
1:A:721:LEU:HB3	1:A:722:PRO:CD	2.26	0.66
1:A:831:GLY:HA3	1:A:832:LEU:HD12	1.76	0.66
1:A:396:VAL:HA	1:A:399:ILE:HB	1.77	0.65
1:A:663:THR:HG22	1:A:666:GLN:NE2	2.08	0.65
3:C:37:DA:H2''	3:C:38:DC:C6	2.31	0.65
1:A:392:THR:HB	1:A:395:GLN:HG3	1.78	0.65
1:A:650:GLN:HG2	1:A:651:ARG:N	2.11	0.65
1:A:288:ASN:N	1:A:288:ASN:HD22	1.90	0.65
1:A:419:LEU:O	1:A:424:GLY:N	2.28	0.65
2:B:-5:DA:H1'	4:B:72:HOH:O	1.96	0.65
1:A:192:HIS:O	1:A:193:ILE:C	2.32	0.65
1:A:317:LEU:HD21	1:A:345:GLN:OE1	1.96	0.65
1:A:554:LEU:HD23	1:A:558:HIS:CD2	2.32	0.65
1:A:282:LEU:HA	1:A:288:ASN:OD1	1.97	0.64
1:A:406:LYS:HE3	1:A:410:GLU:OE1	1.96	0.64
1:A:741:HIS:CD2	1:A:774:SER:O	2.51	0.64
1:A:916:GLN:HB3	1:A:949:LYS:CD	2.24	0.64
1:A:412:VAL:HG12	1:A:413:GLN:N	2.11	0.64
1:A:453:LEU:O	1:A:457:HIS:HB2	1.98	0.64
1:A:217:LEU:CG	4:A:1187:HOH:O	2.36	0.64
1:A:260:LEU:HA	1:A:263:ILE:HG12	1.80	0.64
1:A:1023:GLN:NE2	1:A:1024:ARG:HG2	2.12	0.63
1:A:966:HIS:HB3	1:A:993:LEU:HD21	1.81	0.63
1:A:966:HIS:CB	1:A:993:LEU:HD21	2.27	0.63
1:A:288:ASN:N	1:A:288:ASN:ND2	2.43	0.63
1:A:564:GLN:O	1:A:568:ILE:HG13	1.99	0.63
1:A:552:PRO:HB3	4:A:1180:HOH:O	1.97	0.63
3:C:21:DG:H8	3:C:21:DG:H5''	1.63	0.63
1:A:312:ARG:HG2	1:A:313:LEU:CD2	2.29	0.63
1:A:848:GLN:HG3	1:A:881:LYS:HD3	1.78	0.63
1:A:707:ASN:ND2	1:A:741:HIS:HA	2.12	0.63
1:A:263:ILE:HD13	1:A:295:VAL:HG13	1.81	0.63
2:B:29:DA:H2''	2:B:30:DG:C8	2.34	0.63
1:A:528:PRO:O	1:A:532:VAL:HG23	1.99	0.62
1:A:535:ALA:HB2	1:A:544:LEU:HD11	1.80	0.62
1:A:729:GLY:C	1:A:730:LEU:HD23	2.11	0.62
2:B:1:DG:N3	4:B:183:HOH:O	2.31	0.62
1:A:823:LEU:HB3	1:A:824:PRO:CD	2.29	0.62
1:A:939:VAL:HG12	1:A:940:VAL:N	2.13	0.62
1:A:1017:GLN:N	1:A:1017:GLN:OE1	2.23	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:VAL:HG12	4:A:1162:HOH:O	1.99	0.62
1:A:521:CYS:SG	1:A:522:GLN:HG3	2.40	0.62
1:A:270:THR:CG2	1:A:271:ALA:N	2.63	0.62
1:A:473:GLY:O	1:A:476:ALA:HB3	1.98	0.62
1:A:536:SER:O	1:A:537:HIS:CD2	2.53	0.62
1:A:1035:LEU:HD23	1:A:1036:THR:H	1.64	0.62
1:A:953:GLU:CA	4:A:1154:HOH:O	2.39	0.62
2:B:18:DA:H2''	2:B:19:DC:C5'	2.29	0.61
1:A:696:LEU:HD12	1:A:701:VAL:HG23	1.81	0.61
1:A:242:LEU:O	1:A:242:LEU:HD22	2.01	0.60
1:A:391:LEU:CD2	1:A:396:VAL:HG22	2.29	0.60
1:A:538:ASP:O	1:A:539:GLY:C	2.36	0.60
1:A:900:LEU:HA	1:A:904:GLN:NE2	2.16	0.60
2:B:-5:DA:H1'	2:B:-4:DG:H5'	1.83	0.60
1:A:270:THR:HG22	1:A:271:ALA:N	2.17	0.60
1:A:380:ARG:HD3	1:A:380:ARG:N	2.17	0.60
1:A:557:THR:HG22	1:A:558:HIS:N	2.16	0.60
1:A:921:VAL:CG1	1:A:922:GLN:N	2.63	0.60
1:A:540:GLY:HA3	4:A:1206:HOH:O	2.01	0.60
1:A:392:THR:O	1:A:395:GLN:HB2	2.01	0.60
1:A:381:LEU:HD11	1:A:413:GLN:HG3	1.83	0.60
1:A:814:GLN:NE2	2:B:15:DT:OP1	2.27	0.60
1:A:243:THR:O	1:A:247:GLU:HB2	2.02	0.59
1:A:385:LEU:O	1:A:389:HIS:N	2.35	0.59
1:A:751:VAL:HG12	1:A:752:GLN:N	2.16	0.59
1:A:428:ASP:HA	1:A:431:VAL:HB	1.85	0.59
1:A:912:ILE:CG2	4:A:1176:HOH:O	2.47	0.59
1:A:666:GLN:HB3	1:A:702:VAL:HG21	1.84	0.59
2:B:28:DA:N1	3:C:2:DT:O4	2.35	0.59
1:A:610:GLN:HE21	2:B:9:DC:H5''	1.68	0.59
1:A:317:LEU:HD21	1:A:345:GLN:CD	2.23	0.59
1:A:628:LEU:HA	1:A:632:GLN:OE1	2.02	0.59
1:A:681:GLU:N	4:A:73:HOH:O	2.36	0.59
3:C:12:DT:H73	4:C:189:HOH:O	2.03	0.59
1:A:256:ASP:O	1:A:260:LEU:HD23	2.01	0.59
1:A:393:PRO:O	1:A:397:VAL:HG23	2.02	0.59
2:B:-3:DA:H2''	2:B:-2:DT:H5'	1.84	0.59
1:A:247:GLU:O	1:A:253:LEU:HD22	2.02	0.59
1:A:299:SER:OG	1:A:299:SER:O	2.19	0.59
1:A:359:PRO:O	1:A:362:VAL:HG22	2.02	0.59
3:C:21:DG:C2'	3:C:22:DG:O5'	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:HIS:CB	1:A:214:ILE:CD1	2.80	0.59
1:A:339:GLN:HB3	1:A:372:LYS:HD2	1.85	0.59
1:A:860:LEU:O	1:A:864:HIS:ND1	2.32	0.59
1:A:287:LEU:O	1:A:288:ASN:C	2.38	0.58
1:A:389:HIS:ND1	1:A:416:LEU:HD21	2.17	0.58
1:A:304:LYS:O	1:A:308:GLU:HG2	2.03	0.58
1:A:875:ALA:HB2	1:A:884:LEU:HD21	1.86	0.58
3:C:12:DT:C7	4:C:189:HOH:O	2.50	0.58
1:A:207:ALA:O	1:A:209:THR:HG22	2.04	0.58
1:A:712:GLN:HG2	2:B:12:DT:H5''	1.86	0.58
1:A:499:VAL:HA	4:A:50:HOH:O	2.03	0.58
1:A:704:ILE:HG21	1:A:714:LEU:HD23	1.84	0.58
1:A:923:ARG:NH2	4:A:60:HOH:O	2.36	0.58
3:C:37:DA:H2''	3:C:38:DC:OP2	2.04	0.58
1:A:407:GLN:HB3	1:A:440:LYS:HZ3	1.69	0.58
1:A:621:VAL:HB	4:A:1211:HOH:O	2.02	0.58
1:A:960:PRO:O	1:A:964:GLN:CG	2.52	0.58
1:A:1013:ASN:ND2	4:A:27:HOH:O	2.37	0.58
1:A:391:LEU:CD1	1:A:395:GLN:CB	2.79	0.57
1:A:738:ILE:HA	1:A:774:SER:OG	2.03	0.57
1:A:765:THR:O	1:A:768:GLN:N	2.24	0.57
1:A:898:HIS:O	1:A:936:GLN:NE2	2.37	0.57
1:A:260:LEU:HA	1:A:263:ILE:CG1	2.34	0.57
1:A:517:LEU:HB3	1:A:518:PRO:HD3	1.86	0.57
3:C:13:DA:H2'	3:C:14:DC:C6	2.39	0.57
1:A:192:HIS:C	1:A:193:ILE:O	2.36	0.57
1:A:270:THR:HG22	1:A:271:ALA:H	1.68	0.57
1:A:293:GLN:O	1:A:297:ILE:HD13	2.05	0.57
1:A:616:GLN:HA	1:A:616:GLN:OE1	2.05	0.57
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.69	0.57
1:A:399:ILE:HG23	1:A:399:ILE:O	2.04	0.57
1:A:598:GLN:HE22	1:A:634:VAL:HB	1.69	0.57
1:A:378:VAL:O	1:A:382:LEU:N	2.38	0.56
1:A:419:LEU:HA	1:A:423:HIS:CD2	2.40	0.56
1:A:620:PRO:HB3	4:A:87:HOH:O	2.05	0.56
1:A:1041:VAL:HA	1:A:1042:ALA:C	2.25	0.56
1:A:925:LEU:HB3	1:A:926:PRO:HD3	1.87	0.56
1:A:993:LEU:HB3	1:A:994:PRO:CD	2.36	0.56
1:A:207:ALA:HB1	4:A:88:HOH:O	2.05	0.56
1:A:491:HIS:NE2	4:A:66:HOH:O	2.32	0.56
2:B:24:DC:H2''	2:B:25:DC:O5'	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:LYS:HE2	1:A:407:GLN:OE1	2.05	0.56
1:A:918:LEU:O	1:A:921:VAL:N	2.39	0.56
1:A:391:LEU:CD2	1:A:396:VAL:CG1	2.83	0.56
1:A:690:LEU:HD22	1:A:696:LEU:HG	1.87	0.56
1:A:751:VAL:HG13	1:A:755:LEU:HB2	1.86	0.56
1:A:302:GLY:O	1:A:303:GLY:C	2.41	0.56
1:A:819:VAL:HG13	1:A:823:LEU:HD23	1.87	0.56
2:B:23:DA:H2'	2:B:23:DA:OP2	2.06	0.56
1:A:212:HIS:HA	1:A:213:ILE:O	2.05	0.56
1:A:789:LEU:HB3	1:A:790:PRO:HD2	1.87	0.56
1:A:942:ILE:HD11	1:A:974:VAL:HG22	1.86	0.56
1:A:224:ASP:HB3	1:A:261:VAL:HG11	1.87	0.56
1:A:753:ARG:HG2	4:A:1156:HOH:O	2.05	0.56
2:B:18:DA:H2''	2:B:19:DC:H5'	1.87	0.56
1:A:830:HIS:CE1	4:A:1168:HOH:O	2.59	0.55
1:A:866:LEU:HD11	1:A:906:VAL:HG21	1.88	0.55
1:A:378:VAL:HG12	4:A:1215:HOH:O	2.06	0.55
1:A:554:LEU:HD23	1:A:558:HIS:HD2	1.69	0.55
1:A:769:VAL:HA	1:A:772:ILE:CD1	2.35	0.55
3:C:36:DA:H5''	4:C:43:HOH:O	2.06	0.55
1:A:391:LEU:HD11	1:A:396:VAL:N	2.22	0.55
1:A:821:ARG:NH2	1:A:851:GLU:OE1	2.38	0.55
1:A:920:THR:OG1	1:A:949:LYS:HG3	2.06	0.55
1:A:441:GLN:CB	1:A:474:LYS:HE3	2.36	0.55
1:A:941:ALA:HA	1:A:944:SER:OG	2.06	0.55
1:A:288:ASN:HA	4:A:1201:HOH:O	2.06	0.55
1:A:653:LEU:HD23	1:A:654:PRO:HD3	1.89	0.55
1:A:648:THR:HG22	1:A:680:LEU:HD13	1.89	0.55
1:A:351:LEU:HA	1:A:355:HIS:HD2	1.69	0.55
1:A:719:ARG:NH1	4:A:55:HOH:O	2.35	0.55
1:A:588:LEU:O	1:A:592:HIS:CD2	2.57	0.55
2:B:22:DC:N4	4:B:178:HOH:O	2.23	0.55
2:B:-3:DA:H1'	2:B:-2:DT:H5'	1.88	0.55
1:A:350:VAL:O	1:A:355:HIS:CD2	2.60	0.55
1:A:543:ALA:O	1:A:544:LEU:C	2.45	0.55
1:A:632:GLN:HG2	1:A:668:VAL:HG21	1.88	0.55
1:A:1044:ALA:O	1:A:1046:ASN:O	2.25	0.55
1:A:318:CYS:HA	1:A:323:LEU:H	1.72	0.55
2:B:10:DC:H42	3:C:20:DG:H1	1.54	0.55
2:B:7:DC:N4	4:B:99:HOH:O	2.40	0.55
1:A:568:ILE:CG2	1:A:603:ALA:HB1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:VAL:CG1	1:A:616:GLN:N	2.69	0.54
1:A:578:LEU:O	1:A:581:VAL:HG12	2.06	0.54
1:A:293:GLN:CD	4:A:1217:HOH:O	2.45	0.54
1:A:312:ARG:HG2	1:A:313:LEU:HD23	1.88	0.54
1:A:871:VAL:HG12	1:A:872:VAL:N	2.23	0.54
1:A:901:THR:H	1:A:904:GLN:NE2	2.06	0.54
1:A:758:LEU:HB3	1:A:764:LEU:HD12	1.90	0.54
1:A:848:GLN:HB3	1:A:881:LYS:HB2	1.90	0.54
1:A:945:ASN:ND2	1:A:978:SER:O	2.40	0.54
1:A:678:GLN:HG3	2:B:11:DC:O3'	2.07	0.54
1:A:494:THR:OG1	1:A:497:GLN:HG3	2.07	0.54
1:A:780:GLN:HG3	1:A:813:LYS:HD2	1.89	0.54
1:A:504:ASN:O	1:A:538:ASP:HA	2.06	0.54
1:A:840:ILE:HA	1:A:876:SER:HA	1.90	0.54
1:A:348:LEU:HB3	1:A:349:PRO:CD	2.38	0.54
1:A:894:LEU:HD13	1:A:905:VAL:HG22	1.90	0.54
1:A:993:LEU:HB3	1:A:994:PRO:HD3	1.90	0.54
2:B:28:DA:H5''	4:B:65:HOH:O	2.08	0.54
3:C:38:DC:OP2	3:C:38:DC:C6	2.61	0.54
1:A:398:ALA:O	1:A:435:SER:HB3	2.07	0.53
2:B:-3:DA:C2'	2:B:-2:DT:H5'	2.38	0.53
1:A:738:ILE:HD11	1:A:773:ALA:HB3	1.89	0.53
1:A:686:LEU:O	1:A:690:LEU:HD12	2.07	0.53
1:A:751:VAL:HG13	1:A:755:LEU:HD12	1.89	0.53
2:B:-6:DT:H2''	2:B:-5:DA:N7	2.24	0.53
1:A:568:ILE:HG23	1:A:603:ALA:HB1	1.90	0.53
1:A:880:GLY:O	1:A:883:ALA:N	2.41	0.53
1:A:371:GLY:HA3	4:A:71:HOH:O	2.08	0.53
1:A:325:PRO:O	1:A:329:VAL:HG22	2.09	0.53
1:A:534:ILE:HD13	1:A:547:VAL:HG21	1.91	0.53
1:A:610:GLN:O	1:A:614:THR:OG1	2.22	0.53
1:A:662:LEU:O	1:A:663:THR:C	2.47	0.53
1:A:860:LEU:O	1:A:864:HIS:N	2.42	0.53
1:A:358:PRO:O	1:A:361:GLN:HB2	2.09	0.53
1:A:363:VAL:O	1:A:367:SER:HB2	2.08	0.53
1:A:470:ASN:ND2	1:A:503:SER:O	2.42	0.53
1:A:630:PRO:O	1:A:634:VAL:HG13	2.09	0.53
1:A:753:ARG:NE	4:A:81:HOH:O	2.24	0.53
2:B:28:DA:H3'	4:B:65:HOH:O	2.09	0.53
3:C:13:DA:H2''	3:C:14:DC:C5'	2.39	0.53
1:A:674:GLY:O	1:A:676:GLY:N	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LYS:HB3	1:A:231:GLN:NE2	2.24	0.52
1:A:385:LEU:HD21	1:A:413:GLN:HA	1.90	0.52
1:A:491:HIS:CG	1:A:517:LEU:HG	2.43	0.52
1:A:864:HIS:NE2	1:A:866:LEU:HB2	2.24	0.52
1:A:789:LEU:HB3	1:A:790:PRO:HD3	1.90	0.52
1:A:958:LEU:O	1:A:962:LEU:HD23	2.09	0.52
1:A:1011:ALA:HA	1:A:1015:GLY:HA2	1.90	0.52
3:C:2:DT:H2''	3:C:3:DT:C5'	2.39	0.52
1:A:412:VAL:O	1:A:416:LEU:HB2	2.10	0.52
1:A:440:LYS:HD2	1:A:441:GLN:NE2	2.24	0.52
1:A:906:VAL:O	1:A:910:SER:OG	2.25	0.52
1:A:953:GLU:CG	4:A:1154:HOH:O	2.36	0.52
1:A:620:PRO:CB	4:A:87:HOH:O	2.56	0.52
2:B:-5:DA:C2	4:B:170:HOH:O	2.54	0.52
3:C:11:DG:H2''	3:C:12:DT:OP2	2.08	0.52
3:C:36:DA:C4'	4:C:43:HOH:O	2.31	0.52
1:A:674:GLY:H	1:A:708:ILE:HG12	1.75	0.52
1:A:680:LEU:C	4:A:73:HOH:O	2.48	0.52
2:B:-6:DT:C2'	2:B:-5:DA:N7	2.73	0.52
1:A:287:LEU:O	1:A:288:ASN:CB	2.44	0.51
2:B:-5:DA:C2	3:C:36:DA:C2	2.98	0.51
1:A:542:GLN:HA	1:A:542:GLN:NE2	2.25	0.51
1:A:619:LEU:HD12	4:A:87:HOH:O	2.09	0.51
1:A:753:ARG:CG	4:A:1156:HOH:O	2.58	0.51
1:A:921:VAL:HG12	1:A:922:GLN:H	1.76	0.51
1:A:965:ASP:O	1:A:965:ASP:OD2	2.28	0.51
1:A:240:ALA:HB3	1:A:272:MET:HE3	1.91	0.51
1:A:275:VAL:C	1:A:277:ALA:H	2.13	0.51
1:A:829:ALA:C	1:A:831:GLY:N	2.63	0.51
1:A:297:ILE:HG22	1:A:333:SER:HA	1.92	0.51
1:A:527:THR:O	1:A:531:VAL:HG23	2.11	0.51
1:A:619:LEU:HD13	1:A:619:LEU:C	2.30	0.51
1:A:246:GLY:C	1:A:248:LEU:H	2.13	0.51
1:A:571:HIS:O	1:A:572:ASP:C	2.46	0.51
1:A:775:ASN:ND2	1:A:808:SER:O	2.43	0.51
1:A:247:GLU:OE2	1:A:253:LEU:HD13	2.11	0.51
1:A:254:GLN:CB	4:A:1173:HOH:O	2.54	0.51
1:A:254:GLN:NE2	1:A:283:THR:OG1	2.43	0.51
1:A:368:ASN:ND2	1:A:402:HIS:CA	2.73	0.51
1:A:499:VAL:O	1:A:500:ALA:C	2.48	0.51
3:C:38:DC:OP2	3:C:38:DC:H6	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:GLN:H	1:A:1017:GLN:CD	2.11	0.51
1:A:257:THR:C	1:A:259:GLN:N	2.62	0.51
1:A:499:VAL:CG2	4:A:50:HOH:O	2.59	0.51
1:A:995:VAL:O	1:A:999:ASP:HB2	2.11	0.51
1:A:370:GLY:O	1:A:371:GLY:C	2.49	0.51
1:A:391:LEU:CD2	1:A:396:VAL:HG13	2.41	0.51
1:A:537:HIS:O	1:A:538:ASP:C	2.47	0.51
1:A:830:HIS:O	1:A:868:PRO:HG3	2.10	0.51
1:A:831:GLY:HA2	1:A:868:PRO:CB	2.41	0.51
1:A:299:SER:O	1:A:300:ASN:OD1	2.29	0.50
1:A:341:LEU:O	1:A:344:MET:HB3	2.11	0.50
1:A:620:PRO:C	1:A:622:LEU:H	2.14	0.50
1:A:860:LEU:C	1:A:862:GLN:H	2.15	0.50
1:A:192:HIS:O	1:A:193:ILE:O	2.29	0.50
1:A:336:GLY:O	1:A:340:ALA:N	2.33	0.50
1:A:853:VAL:O	1:A:857:LEU:N	2.44	0.50
1:A:207:ALA:O	1:A:208:VAL:C	2.50	0.50
1:A:866:LEU:HD12	1:A:870:GLN:OE1	2.11	0.50
1:A:834:PRO:O	1:A:838:VAL:HG23	2.12	0.50
1:A:680:LEU:HB2	4:A:73:HOH:O	2.06	0.50
1:A:670:ILE:CD1	1:A:702:VAL:HG23	2.30	0.50
1:A:694:HIS:O	1:A:695:GLY:C	2.49	0.50
1:A:751:VAL:O	1:A:755:LEU:N	2.32	0.50
1:A:895:CYS:HA	1:A:900:LEU:O	2.11	0.50
1:A:486:VAL:CG2	1:A:514:GLN:HE22	2.24	0.50
1:A:966:HIS:O	1:A:1004:LEU:HD21	2.11	0.50
1:A:975:ALA:O	1:A:1012:SER:OG	2.29	0.50
3:C:38:DC:H5''	4:C:41:HOH:O	2.11	0.50
1:A:653:LEU:N	1:A:654:PRO:CD	2.75	0.50
3:C:36:DA:C5'	4:C:43:HOH:O	2.58	0.50
1:A:741:HIS:CD2	1:A:774:SER:C	2.85	0.49
1:A:254:GLN:OE1	1:A:254:GLN:N	2.45	0.49
1:A:339:GLN:CA	1:A:339:GLN:HE21	2.25	0.49
1:A:339:GLN:NE2	1:A:339:GLN:CA	2.75	0.49
1:A:648:THR:HG21	4:A:73:HOH:O	2.11	0.49
1:A:848:GLN:HG3	1:A:881:LYS:CD	2.41	0.49
1:A:689:VAL:HG12	1:A:689:VAL:O	2.13	0.49
1:A:780:GLN:HE21	1:A:813:LYS:HZ2	1.60	0.49
1:A:608:GLY:O	1:A:612:LEU:HG	2.13	0.49
1:A:738:ILE:HG13	1:A:770:VAL:HG12	1.95	0.49
1:A:268:GLY:HA2	4:A:1208:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:LYS:HG3	1:A:712:GLN:NE2	2.27	0.49
1:A:768:GLN:HB3	1:A:804:VAL:HG21	1.93	0.49
1:A:997:CYS:HA	1:A:1002:LEU:H	1.76	0.49
1:A:629:THR:HB	1:A:630:PRO:HD2	1.95	0.49
1:A:963:CYS:SG	1:A:970:PRO:HD3	2.52	0.49
1:A:848:GLN:HA	1:A:848:GLN:HE21	1.76	0.49
1:A:859:VAL:HG13	4:A:1231:HOH:O	2.05	0.49
1:A:912:ILE:HG22	1:A:912:ILE:O	2.10	0.49
1:A:213:ILE:C	1:A:214:ILE:HG13	2.33	0.48
1:A:391:LEU:HG	1:A:391:LEU:O	2.13	0.48
1:A:407:GLN:OE1	1:A:407:GLN:HA	2.14	0.48
1:A:850:LEU:HA	1:A:853:VAL:HG23	1.95	0.48
1:A:294:VAL:O	1:A:295:VAL:C	2.51	0.48
1:A:649:VAL:O	1:A:650:GLN:C	2.49	0.48
1:A:996:LEU:HD21	1:A:1023:GLN:HA	1.96	0.48
3:C:33:DT:H2''	3:C:34:DC:C6	2.48	0.48
1:A:660:HIS:O	1:A:698:GLN:OE1	2.32	0.48
1:A:688:PRO:C	1:A:690:LEU:H	2.15	0.48
1:A:780:GLN:CG	1:A:813:LYS:HD2	2.44	0.48
1:A:924:LEU:CD2	4:A:1154:HOH:O	2.60	0.48
3:C:21:DG:C2'	3:C:22:DG:C5'	2.91	0.48
1:A:690:LEU:HD23	1:A:694:HIS:HD2	1.78	0.48
1:A:771:ALA:C	1:A:773:ALA:H	2.16	0.48
1:A:305:GLN:O	1:A:306:ALA:C	2.52	0.48
1:A:850:LEU:O	1:A:853:VAL:HG23	2.14	0.48
1:A:291:PRO:O	1:A:295:VAL:HG23	2.14	0.48
1:A:552:PRO:HA	1:A:555:CYS:HB2	1.95	0.48
1:A:867:THR:OG1	1:A:870:GLN:HG3	2.13	0.48
1:A:293:GLN:NE2	4:A:1217:HOH:O	2.46	0.48
1:A:552:PRO:O	1:A:556:GLN:N	2.46	0.48
1:A:652:LEU:O	1:A:656:LEU:HB2	2.13	0.48
1:A:664:PRO:O	1:A:665:ASP:C	2.51	0.48
1:A:718:GLN:CA	1:A:718:GLN:NE2	2.77	0.48
2:B:-1:DA:C2'	2:B:0:DT:H5''	2.43	0.48
1:A:558:HIS:ND1	1:A:585:LEU:HD22	2.26	0.48
1:A:821:ARG:HB3	1:A:822:LEU:CD2	2.44	0.48
1:A:875:ALA:C	1:A:877:ASN:H	2.16	0.48
1:A:900:LEU:HA	1:A:904:GLN:HE22	1.79	0.48
1:A:989:VAL:HG23	1:A:1019:LEU:CD1	2.34	0.48
1:A:324:THR:HB	1:A:326:ALA:H	1.79	0.47
1:A:749:GLU:HB3	1:A:753:ARG:HH22	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:LEU:HD23	1:A:888:GLN:HA	1.95	0.47
1:A:925:LEU:O	1:A:926:PRO:C	2.51	0.47
1:A:344:MET:O	1:A:348:LEU:HB2	2.14	0.47
1:A:674:GLY:HA3	2:B:12:DT:H72	1.96	0.47
1:A:253:LEU:HD12	1:A:253:LEU:HA	1.87	0.47
1:A:845:GLY:N	4:A:64:HOH:O	2.48	0.47
1:A:714:LEU:O	1:A:717:VAL:HG22	2.14	0.47
1:A:966:HIS:CG	1:A:993:LEU:HD23	2.47	0.47
1:A:687:LEU:CB	1:A:688:PRO:HD3	2.45	0.47
1:A:746:GLN:HB3	1:A:779:LYS:HB3	1.96	0.47
1:A:811:GLY:CA	4:A:1219:HOH:O	2.52	0.47
1:A:826:LEU:C	1:A:828:GLN:H	2.18	0.47
1:A:812:GLY:O	1:A:815:ALA:HB3	2.15	0.47
1:A:257:THR:C	1:A:259:GLN:H	2.18	0.47
1:A:954:THR:HG23	1:A:958:LEU:HD12	1.97	0.47
1:A:979:ASN:HB3	1:A:981:GLY:H	1.79	0.47
2:B:-1:DA:C2'	2:B:0:DT:C5'	2.85	0.47
2:B:29:DA:N1	3:C:1:DT:C4	2.82	0.47
1:A:260:LEU:HD13	1:A:263:ILE:HG13	1.96	0.47
1:A:417:PRO:O	1:A:418:VAL:C	2.53	0.47
1:A:901:THR:H	1:A:904:GLN:HE21	1.62	0.47
1:A:720:LEU:HD22	1:A:752:GLN:CB	2.45	0.47
1:A:629:THR:HB	1:A:630:PRO:CD	2.44	0.47
2:B:-1:DA:H2''	2:B:0:DT:H5''	1.93	0.47
3:C:27:DT:H2''	3:C:28:DG:OP2	2.14	0.47
1:A:707:ASN:O	1:A:709:GLY:N	2.48	0.46
1:A:769:VAL:C	1:A:771:ALA:H	2.16	0.46
1:A:948:GLY:O	1:A:949:LYS:C	2.51	0.46
1:A:467:ILE:O	1:A:467:ILE:HG22	2.15	0.46
1:A:470:ASN:O	1:A:471:GLY:C	2.54	0.46
1:A:962:LEU:HD22	1:A:962:LEU:N	2.30	0.46
1:A:666:GLN:CB	1:A:702:VAL:HG21	2.46	0.46
1:A:813:LYS:C	1:A:815:ALA:H	2.18	0.46
1:A:880:GLY:O	1:A:881:LYS:C	2.54	0.46
1:A:497:GLN:O	1:A:498:VAL:C	2.52	0.46
1:A:764:LEU:HD23	1:A:800:GLN:OE1	2.16	0.46
1:A:232:TRP:CZ3	1:A:233:SER:HB3	2.50	0.46
1:A:581:VAL:CG1	1:A:582:GLN:N	2.78	0.46
1:A:370:GLY:O	1:A:373:GLN:N	2.49	0.46
1:A:410:GLU:O	1:A:414:ARG:HB2	2.16	0.46
1:A:324:THR:OG1	1:A:327:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:848:GLN:CA	1:A:848:GLN:NE2	2.76	0.46
1:A:955:VAL:O	1:A:956:GLN:C	2.54	0.46
1:A:961:VAL:HB	1:A:962:LEU:HD22	1.98	0.46
1:A:266:ARG:HD2	4:C:74:HOH:O	2.14	0.46
1:A:602:ILE:HB	1:A:612:LEU:HD21	1.97	0.46
1:A:642:GLY:O	1:A:646:LEU:HD12	2.16	0.46
1:A:785:VAL:HG13	1:A:789:LEU:HD12	1.98	0.46
1:A:972:GLN:HB3	1:A:1008:VAL:HG21	1.98	0.46
1:A:257:THR:O	1:A:259:GLN:N	2.49	0.46
1:A:485:PRO:O	1:A:489:GLN:HB2	2.16	0.46
1:A:730:LEU:HA	1:A:734:GLN:OE1	2.16	0.46
1:A:925:LEU:HB3	1:A:926:PRO:CD	2.45	0.46
1:A:391:LEU:HD21	1:A:396:VAL:CB	2.42	0.45
1:A:831:GLY:HA2	1:A:868:PRO:HB2	1.98	0.45
1:A:929:CYS:HA	1:A:934:LEU:O	2.15	0.45
2:B:1:DG:H2''	2:B:2:DC:O5'	2.16	0.45
1:A:872:VAL:O	1:A:876:SER:HB3	2.15	0.45
1:A:1037:PRO:O	4:A:45:HOH:O	2.21	0.45
1:A:357:LEU:HD21	1:A:382:LEU:HD11	1.98	0.45
1:A:543:ALA:O	1:A:545:GLU:N	2.49	0.45
1:A:654:PRO:CG	4:A:85:HOH:O	2.43	0.45
1:A:1017:GLN:CB	4:B:129:HOH:O	2.65	0.45
1:A:451:PRO:HG2	1:A:452:VAL:H	1.81	0.45
1:A:821:ARG:HB3	1:A:822:LEU:HD23	1.98	0.45
1:A:996:LEU:O	1:A:1002:LEU:HB2	2.16	0.45
1:A:391:LEU:CD1	1:A:396:VAL:HG13	2.46	0.45
2:B:6:DT:H73	4:B:165:HOH:O	2.17	0.45
1:A:551:LEU:HB3	1:A:552:PRO:HD3	1.99	0.45
1:A:755:LEU:HB3	1:A:756:PRO:CD	2.44	0.45
1:A:254:GLN:NE2	4:A:91:HOH:O	2.43	0.45
1:A:417:PRO:O	1:A:421:GLN:N	2.46	0.45
1:A:924:LEU:HD22	4:A:1154:HOH:O	2.17	0.45
1:A:982:GLY:C	1:A:984:GLN:H	2.20	0.45
1:A:995:VAL:HG13	1:A:999:ASP:HB2	1.99	0.45
1:A:210:TYR:O	1:A:211:GLN:C	2.55	0.45
1:A:217:LEU:CD2	4:A:1187:HOH:O	2.63	0.45
1:A:803:VAL:O	1:A:804:VAL:C	2.54	0.45
1:A:471:GLY:HA3	2:B:6:DT:H72	1.99	0.45
1:A:826:LEU:HD13	1:A:837:VAL:HG22	1.98	0.44
1:A:351:LEU:CA	1:A:355:HIS:HD2	2.30	0.44
1:A:361:GLN:OE1	1:A:397:VAL:HG21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:VAL:HG12	1:A:616:GLN:H	1.80	0.44
1:A:632:GLN:HE21	1:A:668:VAL:HG11	1.82	0.44
1:A:684:GLN:HA	4:A:1175:HOH:O	2.17	0.44
1:A:859:VAL:HG12	4:A:1231:HOH:O	2.08	0.44
3:C:22:DG:H2"	3:C:23:DG:OP2	2.17	0.44
1:A:551:LEU:HD23	1:A:565:VAL:HG11	1.99	0.44
1:A:746:GLN:HG3	1:A:779:LYS:HD2	1.99	0.44
1:A:339:GLN:NE2	1:A:339:GLN:N	2.54	0.44
1:A:347:LEU:O	1:A:348:LEU:C	2.56	0.44
1:A:425:LEU:HD11	1:A:465:VAL:HG22	1.98	0.44
1:A:543:ALA:O	1:A:546:THR:N	2.50	0.44
1:A:837:VAL:O	1:A:840:ILE:HB	2.17	0.44
1:A:433:ILE:HG22	1:A:433:ILE:O	2.18	0.44
1:A:494:THR:HG1	1:A:497:GLN:HG3	1.82	0.44
1:A:610:GLN:HA	1:A:610:GLN:OE1	2.17	0.44
1:A:1000:HIS:CD2	1:A:1026:LEU:HD22	2.53	0.44
1:A:521:CYS:HA	1:A:526:LEU:HB2	1.99	0.44
1:A:634:VAL:C	1:A:636:ILE:H	2.20	0.44
1:A:698:GLN:O	1:A:699:VAL:C	2.56	0.44
1:A:738:ILE:HD13	1:A:773:ALA:O	2.17	0.44
1:A:328:VAL:C	1:A:330:ALA:H	2.22	0.44
1:A:494:THR:HG1	1:A:497:GLN:CG	2.30	0.44
1:A:499:VAL:O	1:A:502:ALA:N	2.50	0.44
1:A:853:VAL:HG12	1:A:857:LEU:HD22	1.99	0.44
2:B:18:DA:H2"	2:B:19:DC:H5"	1.99	0.44
1:A:822:LEU:O	1:A:823:LEU:C	2.56	0.44
1:A:899:GLY:O	1:A:900:LEU:C	2.56	0.44
1:A:499:VAL:HG22	4:A:50:HOH:O	2.18	0.43
1:A:501:ILE:HG13	1:A:532:VAL:HG13	2.00	0.43
1:A:918:LEU:O	1:A:920:THR:N	2.50	0.43
1:A:203:LEU:HA	1:A:204:GLY:C	2.38	0.43
1:A:392:THR:HA	1:A:393:PRO:HD2	1.66	0.43
1:A:477:LEU:O	1:A:478:GLU:C	2.57	0.43
1:A:513:VAL:HG23	1:A:544:LEU:CD1	2.48	0.43
1:A:962:LEU:O	1:A:968:LEU:N	2.49	0.43
1:A:993:LEU:HD11	1:A:1004:LEU:HD23	1.99	0.43
1:A:519:VAL:O	1:A:523:ALA:HB3	2.18	0.43
1:A:674:GLY:C	1:A:676:GLY:H	2.17	0.43
1:A:996:LEU:HD21	1:A:1023:GLN:HB2	1.98	0.43
1:A:1010:ILE:O	1:A:1015:GLY:N	2.49	0.43
1:A:517:LEU:N	1:A:518:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:VAL:O	1:A:533:ALA:C	2.54	0.43
1:A:578:LEU:HA	1:A:578:LEU:HD23	1.75	0.43
1:A:633:VAL:HA	1:A:636:ILE:HG13	2.00	0.43
1:A:648:THR:CG2	4:A:73:HOH:O	2.64	0.43
1:A:921:VAL:HG13	1:A:922:GLN:N	2.33	0.43
2:B:29:DA:N1	3:C:1:DT:O4	2.51	0.43
3:C:33:DT:H2"	3:C:34:DC:H6	1.83	0.43
1:A:1013:ASN:OD1	1:A:1013:ASN:C	2.57	0.43
1:A:334:HIS:HB3	1:A:369:ILE:HD12	2.00	0.43
1:A:921:VAL:HG12	1:A:922:GLN:N	2.34	0.43
1:A:607:GLY:C	4:A:1153:HOH:O	2.50	0.43
2:B:28:DA:H2"	2:B:29:DA:H5"	1.99	0.43
1:A:451:PRO:O	1:A:453:LEU:N	2.51	0.43
1:A:551:LEU:HB3	1:A:552:PRO:CD	2.49	0.43
1:A:720:LEU:HD22	1:A:752:GLN:HB2	2.00	0.43
1:A:844:GLY:O	1:A:846:GLY:N	2.47	0.43
1:A:860:LEU:CD2	1:A:887:VAL:HG12	2.48	0.43
1:A:852:THR:HG22	1:A:884:LEU:HD12	2.01	0.43
2:B:10:DC:N4	3:C:20:DG:H1	2.16	0.43
1:A:294:VAL:O	1:A:296:ALA:N	2.51	0.43
1:A:433:ILE:HD13	1:A:446:VAL:HG21	2.00	0.43
1:A:524:HIS:HB3	1:A:551:LEU:CD1	2.49	0.43
1:A:606:ILE:HG23	4:A:1200:HOH:O	2.17	0.43
1:A:547:VAL:O	1:A:548:GLN:C	2.57	0.43
1:A:598:GLN:HE22	1:A:634:VAL:CB	2.32	0.43
1:A:766:PRO:O	1:A:770:VAL:HG23	2.19	0.43
1:A:816:LEU:O	1:A:819:VAL:N	2.51	0.43
1:A:877:ASN:ND2	1:A:910:SER:O	2.51	0.43
1:A:935:THR:HG23	1:A:938:GLN:OE1	2.19	0.43
1:A:259:GLN:NE2	1:A:295:VAL:HG21	2.33	0.43
1:A:288:ASN:OD1	1:A:311:GLN:NE2	2.52	0.43
1:A:289:LEU:HD22	1:A:329:VAL:HG11	2.01	0.43
1:A:663:THR:O	1:A:666:GLN:HB2	2.19	0.43
1:A:685:ARG:HB3	1:A:686:LEU:HD13	2.00	0.43
1:A:866:LEU:HG	1:A:870:GLN:CB	2.39	0.43
1:A:598:GLN:NE2	1:A:634:VAL:HB	2.33	0.42
1:A:711:LYS:CG	1:A:712:GLN:NE2	2.83	0.42
1:A:728:HIS:NE2	1:A:756:PRO:HG3	2.34	0.42
1:A:463:GLN:O	1:A:464:VAL:C	2.57	0.42
1:A:639:ASN:CG	1:A:640:GLY:H	2.22	0.42
1:A:887:VAL:O	1:A:891:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:DC:H2''	2:B:10:DC:C5'	2.48	0.42
1:A:206:VAL:O	1:A:208:VAL:N	2.52	0.42
1:A:232:TRP:O	1:A:232:TRP:CG	2.72	0.42
1:A:912:ILE:HG13	4:A:1207:HOH:O	2.18	0.42
1:A:334:HIS:HD2	1:A:368:ASN:HA	1.84	0.42
1:A:696:LEU:CD1	1:A:701:VAL:HG23	2.47	0.42
1:A:819:VAL:HG12	1:A:820:GLN:N	2.34	0.42
1:A:263:ILE:HG12	1:A:263:ILE:H	1.73	0.42
1:A:385:LEU:HD23	1:A:389:HIS:HD2	1.77	0.42
1:A:391:LEU:HD11	1:A:395:GLN:HB2	1.97	0.42
1:A:391:LEU:HD11	1:A:396:VAL:H	1.82	0.42
1:A:698:GLN:O	1:A:701:VAL:N	2.48	0.42
1:A:964:GLN:H	1:A:964:GLN:HG2	1.33	0.42
1:A:301:ASN:C	1:A:303:GLY:H	2.23	0.42
1:A:367:SER:O	1:A:368:ASN:OD1	2.38	0.42
1:A:614:THR:HB	1:A:646:LEU:HD13	2.01	0.42
1:A:639:ASN:CG	1:A:640:GLY:N	2.72	0.42
1:A:229:GLY:HA2	1:A:234:GLY:HA3	2.02	0.42
1:A:323:LEU:HA	1:A:327:GLN:OE1	2.20	0.42
1:A:660:HIS:ND1	1:A:687:LEU:HD13	2.34	0.42
1:A:663:THR:O	1:A:666:GLN:N	2.48	0.42
1:A:864:HIS:NE2	1:A:866:LEU:HD22	2.35	0.42
1:A:954:THR:OG1	1:A:983:LYS:CG	2.62	0.42
1:A:316:VAL:HG12	1:A:316:VAL:O	2.18	0.42
1:A:343:THR:OG1	1:A:372:LYS:HG3	2.20	0.42
1:A:429:GLN:O	1:A:430:VAL:C	2.57	0.42
2:B:1:DG:C2	3:C:30:DA:C2	3.08	0.42
2:B:-5:DA:N1	3:C:35:DT:O4	2.53	0.42
1:A:288:ASN:HD22	1:A:288:ASN:H	1.67	0.42
1:A:909:ALA:HB2	1:A:918:LEU:HD11	2.00	0.42
1:A:419:LEU:O	1:A:423:HIS:N	2.47	0.42
1:A:556:GLN:CG	4:A:1180:HOH:O	2.58	0.42
1:A:984:GLN:HG2	1:A:1016:LYS:HD3	2.01	0.42
1:A:245:ALA:O	1:A:248:LEU:HB3	2.20	0.41
1:A:558:HIS:HE1	1:A:586:PRO:HD3	1.85	0.41
1:A:596:PRO:O	1:A:597:ASP:C	2.57	0.41
1:A:241:LEU:HD11	1:A:260:LEU:HB3	2.03	0.41
1:A:449:LEU:O	1:A:453:LEU:HG	2.20	0.41
1:A:527:THR:C	1:A:529:ASP:H	2.23	0.41
1:A:605:ASN:OD1	1:A:605:ASN:N	2.53	0.41
2:B:-5:DA:N3	4:B:170:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:996:LEU:HD21	1:A:1023:GLN:CB	2.50	0.41
1:A:713:ALA:O	1:A:714:LEU:C	2.58	0.41
1:A:813:LYS:C	1:A:815:ALA:N	2.73	0.41
1:A:331:ILE:HG22	1:A:340:ALA:HB1	2.02	0.41
1:A:558:HIS:CE1	1:A:586:PRO:HD3	2.55	0.41
1:A:741:HIS:O	1:A:742:ASP:C	2.59	0.41
1:A:1036:THR:OG1	1:A:1037:PRO:HD2	2.21	0.41
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.85	0.41
1:A:404:GLY:O	1:A:407:GLN:N	2.54	0.41
1:A:419:LEU:HG	1:A:419:LEU:H	1.57	0.41
1:A:552:PRO:O	1:A:553:VAL:C	2.58	0.41
1:A:212:HIS:CB	1:A:214:ILE:HD11	2.51	0.41
1:A:407:GLN:HB3	1:A:440:LYS:NZ	2.34	0.41
1:A:568:ILE:HG23	1:A:603:ALA:CB	2.50	0.41
1:A:275:VAL:C	1:A:277:ALA:N	2.74	0.41
1:A:588:LEU:HD21	1:A:615:VAL:HG13	1.95	0.41
1:A:209:THR:C	1:A:210:TYR:CD1	2.94	0.41
1:A:717:VAL:O	1:A:718:GLN:C	2.57	0.41
1:A:361:GLN:HG2	1:A:397:VAL:HG11	2.02	0.41
1:A:471:GLY:HA3	2:B:6:DT:C7	2.50	0.41
1:A:704:ILE:CG2	1:A:714:LEU:CD2	2.98	0.41
1:A:890:LEU:O	1:A:890:LEU:HD13	2.21	0.41
1:A:1032:ASP:CG	1:A:1033:HIS:H	2.23	0.41
1:A:339:GLN:O	1:A:343:THR:OG1	2.39	0.41
1:A:427:PRO:N	4:A:1209:HOH:O	2.53	0.41
1:A:510:LEU:O	1:A:511:GLU:C	2.57	0.41
1:A:476:ALA:O	1:A:477:LEU:C	2.59	0.41
2:B:7:DC:C2	2:B:8:DC:C5	3.09	0.41
1:A:521:CYS:SG	1:A:522:GLN:NE2	2.94	0.40
1:A:222:HIS:HD2	1:A:225:ILE:HD11	1.86	0.40
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.52	0.40
1:A:553:VAL:O	1:A:557:THR:HB	2.21	0.40
1:A:610:GLN:HB3	1:A:643:LYS:HD2	2.03	0.40
1:A:681:GLU:O	1:A:684:GLN:NE2	2.52	0.40
1:A:701:VAL:C	1:A:703:ALA:N	2.73	0.40
1:A:775:ASN:HB3	4:A:1196:HOH:O	2.21	0.40
1:A:797:GLY:O	1:A:798:LEU:CB	2.59	0.40
3:C:25:DG:H8	4:C:181:HOH:O	2.05	0.40
1:A:636:ILE:HG23	1:A:671:ALA:O	2.21	0.40
1:A:704:ILE:C	1:A:706:SER:H	2.25	0.40
1:A:918:LEU:C	1:A:920:THR:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASN:HB3	1:A:289:LEU:CG	2.19	0.40
1:A:427:PRO:CA	4:A:1209:HOH:O	2.69	0.40
2:B:-5:DA:H8	2:B:-5:DA:OP2	2.05	0.40
1:A:629:THR:OG1	1:A:632:GLN:HB2	2.21	0.40
1:A:734:GLN:NE2	1:A:767:ASP:OD1	2.51	0.40
3:C:37:DA:C1'	3:C:38:DC:C5	3.03	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	839/1047 (80%)	549 (65%)	246 (29%)	44 (5%)	2	12

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	PRO
1	A	303	GLY
1	A	371	GLY
1	A	1034	GLY
1	A	221	THR
1	A	473	GLY
1	A	596	PRO
1	A	697	THR
1	A	812	GLY
1	A	967	GLY
1	A	452	VAL
1	A	539	GLY
1	A	632	GLN
1	A	766	PRO
1	A	833	THR

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Mol	Chain	Res	Type
1	A	1004	LEU
1	A	199	HIS
1	A	420	CYS
1	A	544	LEU
1	A	731	THR
1	A	752	GLN
1	A	983	LYS
1	A	991	ARG
1	A	1043	ILE
1	A	367	SER
1	A	427	PRO
1	A	558	HIS
1	A	630	PRO
1	A	729	GLY
1	A	834	PRO
1	A	276	HIS
1	A	322	GLY
1	A	418	VAL
1	A	961	VAL
1	A	172	VAL
1	A	858	PRO
1	A	258	GLY
1	A	451	PRO
1	A	553	VAL
1	A	213	ILE
1	A	608	GLY
1	A	824	PRO
1	A	621	VAL
1	A	654	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	635/816 (78%)	495 (78%)	140 (22%)	<b>1</b> <b>4</b>



All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
1	A	230	LYS
1	A	242	LEU
1	A	247	GLU
1	A	248	LEU
1	A	254	GLN
1	A	256	ASP
1	A	259	GLN
1	A	263	ILE
1	A	270	THR
1	A	279	ARG
1	A	286	PRO
1	A	289	LEU
1	A	290	THR
1	A	293	GLN
1	A	297	ILE
1	A	299	SER
1	A	300	ASN
1	A	304	LYS
1	A	307	LEU
1	A	310	VAL
1	A	325	PRO
1	A	335	ASP
1	A	339	GLN
1	A	343	THR
1	A	345	GLN
1	A	349	PRO
1	A	355	HIS
1	A	357	LEU
1	A	367	SER
1	A	369	ILE
1	A	377	THR
1	A	380	ARG
1	A	381	LEU
1	A	382	LEU
1	A	384	VAL
1	A	391	LEU
1	A	392	THR
1	A	396	VAL
1	A	399	ILE
1	A	409	LEU
1	A	411	THR

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Mol	Chain	Res	Type
1	A	414	ARG
1	A	415	LEU
1	A	419	LEU
1	A	421	GLN
1	A	435	SER
1	A	441	GLN
1	A	452	VAL
1	A	455	GLN
1	A	459	LEU
1	A	462	ASP
1	A	480	VAL
1	A	481	GLN
1	A	484	LEU
1	A	486	VAL
1	A	504	ASN
1	A	514	GLN
1	A	515	ARG
1	A	521	CYS
1	A	536	SER
1	A	542	GLN
1	A	551	LEU
1	A	561	THR
1	A	576	GLN
1	A	580	THR
1	A	581	VAL
1	A	582	GLN
1	A	588	LEU
1	A	592	HIS
1	A	594	LEU
1	A	595	THR
1	A	598	GLN
1	A	605	ASN
1	A	614	THR
1	A	631	ASP
1	A	650	GLN
1	A	653	LEU
1	A	684	GLN
1	A	687	LEU
1	A	692	GLN
1	A	696	LEU
1	A	698	GLN
1	A	708	ILE

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Mol	Chain	Res	Type
1	A	711	LYS
1	A	718	GLN
1	A	719	ARG
1	A	725	CYS
1	A	732	PRO
1	A	738	ILE
1	A	745	LYS
1	A	750	THR
1	A	751	VAL
1	A	752	GLN
1	A	754	LEU
1	A	770	VAL
1	A	772	ILE
1	A	779	LYS
1	A	790	PRO
1	A	799	THR
1	A	801	GLU
1	A	814	GLN
1	A	820	GLN
1	A	823	LEU
1	A	848	GLN
1	A	853	VAL
1	A	855	ARG
1	A	857	LEU
1	A	860	LEU
1	A	864	HIS
1	A	867	THR
1	A	871	VAL
1	A	887	VAL
1	A	888	GLN
1	A	890	LEU
1	A	891	LEU
1	A	894	LEU
1	A	901	THR
1	A	921	VAL
1	A	922	GLN
1	A	930	GLN
1	A	934	LEU
1	A	936	GLN
1	A	937	ASP
1	A	939	VAL
1	A	944	SER

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Mol	Chain	Res	Type
1	A	956	GLN
1	A	959	LEU
1	A	979	ASN
1	A	980	ILE
1	A	983	LYS
1	A	989	VAL
1	A	990	GLN
1	A	1000	HIS
1	A	1012	SER
1	A	1026	LEU
1	A	1031	GLN
1	A	1035	LEU
1	A	1038	ASP
1	A	1039	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
1	A	222	HIS
1	A	231	GLN
1	A	259	GLN
1	A	288	ASN
1	A	311	GLN
1	A	334	HIS
1	A	339	GLN
1	A	355	HIS
1	A	368	ASN
1	A	470	ASN
1	A	475	GLN
1	A	504	ASN
1	A	514	GLN
1	A	537	HIS
1	A	542	GLN
1	A	582	GLN
1	A	592	HIS
1	A	610	GLN
1	A	650	GLN
1	A	666	GLN
1	A	694	HIS
1	A	707	ASN
1	A	718	GLN

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Mol	Chain	Res	Type
1	A	760	GLN
1	A	775	ASN
1	A	780	GLN
1	A	848	GLN
1	A	904	GLN
1	A	945	ASN
1	A	1023	GLN
1	A	1039	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](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	854/1047 (81%)	-0.23	14 (1%) 72 44	27, 84, 153, 200	0
2	B	38/38 (100%)	0.08	2 (5%) 26 10	31, 46, 132, 137	0
3	C	38/38 (100%)	0.02	1 (2%) 56 27	43, 70, 129, 135	0
All	All	930/1123 (82%)	-0.20	17 (1%) 68 40	27, 83, 153, 200	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1040	VAL	4.7
1	A	593	GLY	4.4
1	A	966	HIS	4.0
2	B	31	DT	3.9
1	A	1033	HIS	3.7
3	C	1	DT	3.3
1	A	864	HIS	3.2
1	A	831	GLY	2.9
1	A	1034	GLY	2.7
2	B	-6	DT	2.7
1	A	830	HIS	2.5
1	A	1039	GLN	2.5
1	A	524	HIS	2.4
1	A	251	PRO	2.4
1	A	1038	ASP	2.2
1	A	1029	LEU	2.1
1	A	1035	LEU	2.1

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.