



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:03 AM UTC

PDB ID : 3UGM / pdb_00003ugm
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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

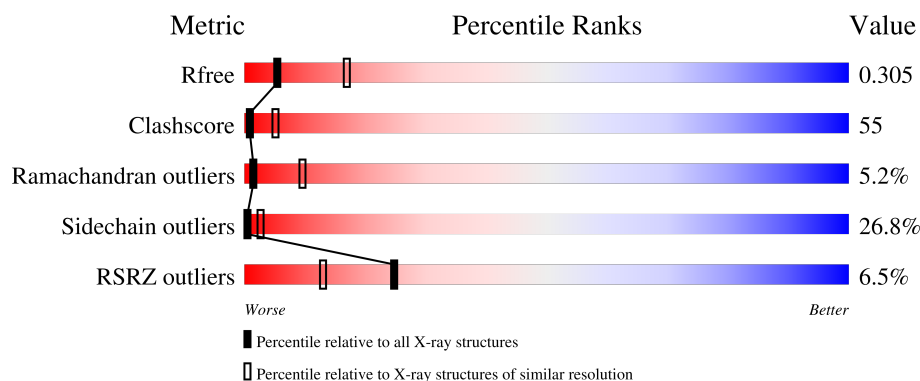
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	5% 20% 37% 21% • 18%
2	B	38	8% 29% 61% 11%
3	C	38	3% 34% 63% •

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			

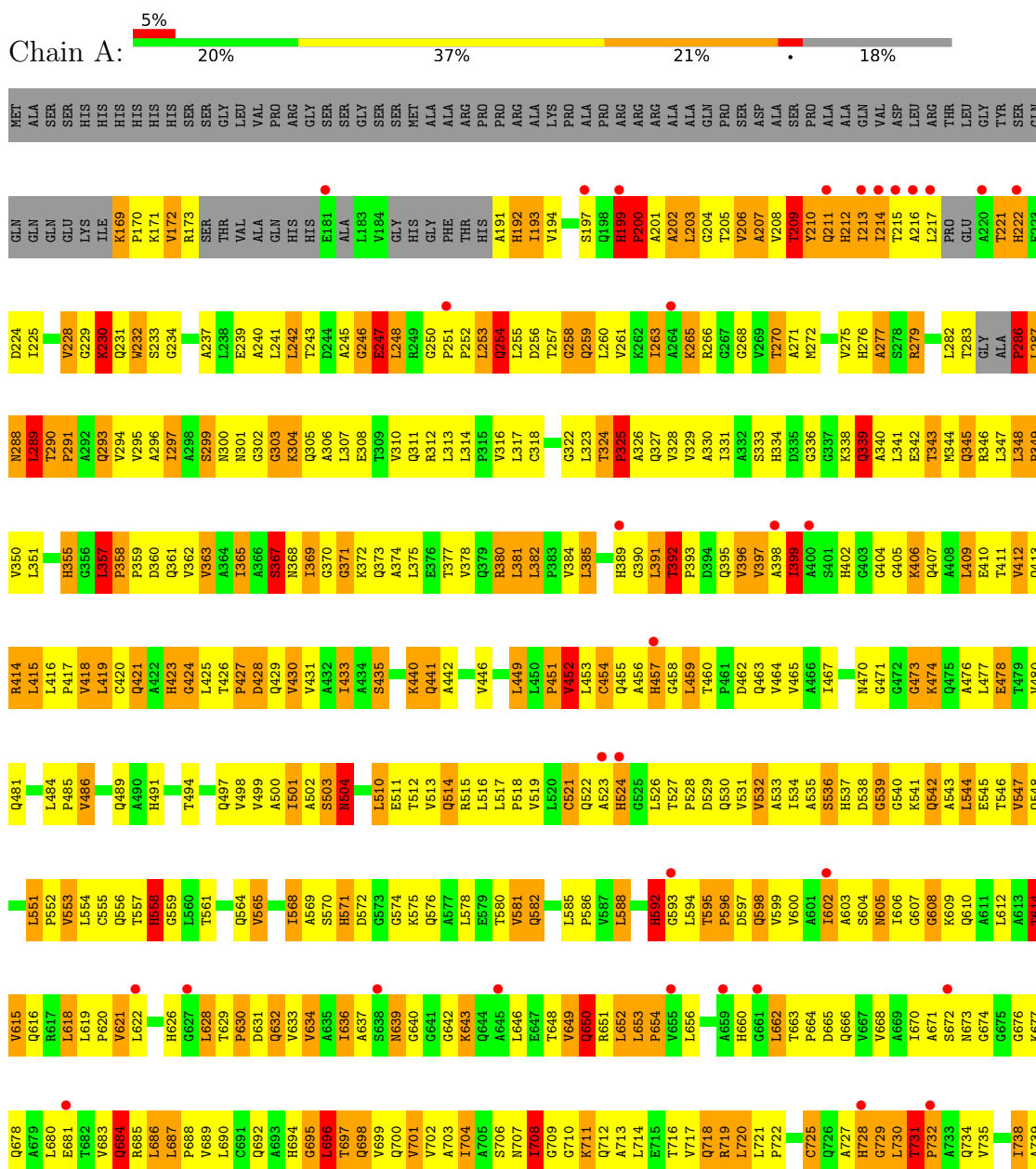
- Molecule 4 is water.

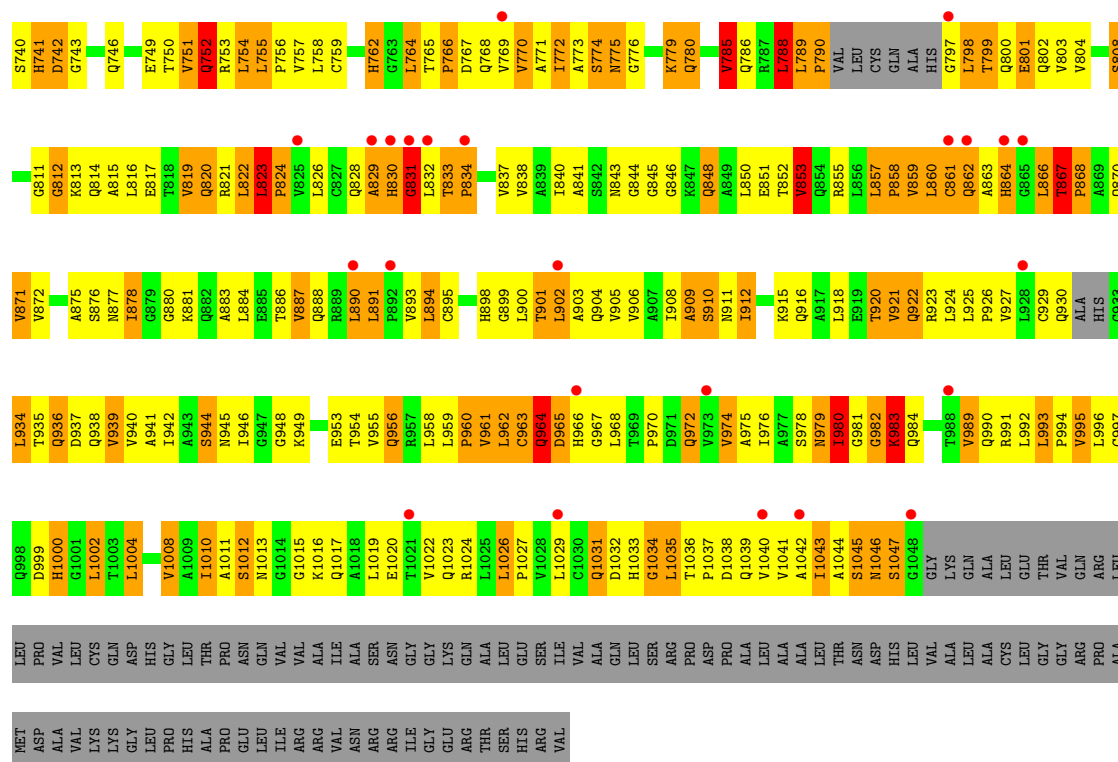
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	159	Total	O	0	0
			159	159		
4	B	23	Total	O	0	0
			23	23		
4	C	34	Total	O	0	0
			34	34		

3 Residue-property plots

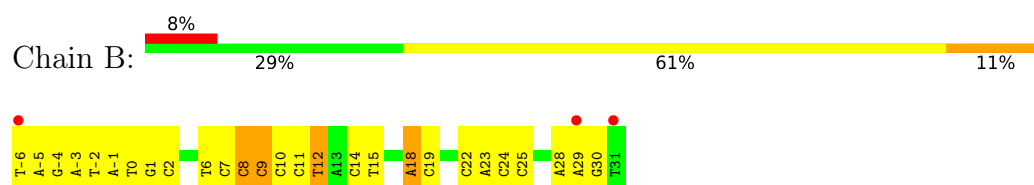
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

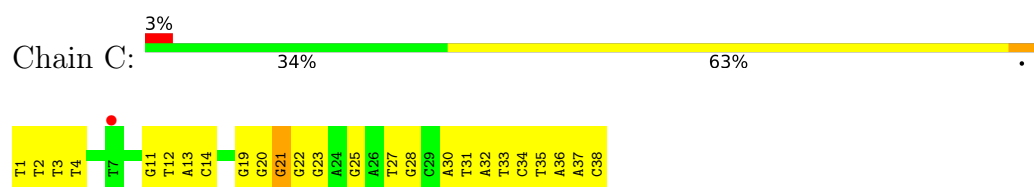




• Molecule 2: DNA-1



• Molecule 3: DNA-2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.58Å 248.48Å 54.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-3.00) 95.8 (50.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 3.01Å)	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 (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 114.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.48	69/6153 (1.1%)	1.70	205/8397 (2.4%)
2	B	0.78	0/855	1.16	5/1314 (0.4%)
3	C	0.67	0/885	1.05	2/1368 (0.1%)
All	All	1.35	69/7893 (0.9%)	1.57	212/11079 (1.9%)

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 (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	ILE	CA-C	-18.32	1.31	1.52
1	A	201	ALA	CA-C	-17.63	1.30	1.52
1	A	169	LYS	CA-CB	-15.88	1.21	1.53
1	A	214	ILE	C-O	-15.04	1.08	1.24
1	A	212	HIS	CA-CB	-14.63	1.30	1.53
1	A	200	PRO	C-O	-13.97	1.05	1.24
1	A	193	ILE	CA-CB	-13.90	1.35	1.54
1	A	170	PRO	CA-CB	-13.47	1.34	1.53
1	A	172	VAL	C-O	-13.19	1.08	1.24
1	A	202	ALA	CA-CB	-12.79	1.34	1.52
1	A	201	ALA	N-CA	-12.57	1.30	1.46
1	A	210	TYR	N-CA	-12.32	1.34	1.46
1	A	216	ALA	CA-CB	-12.04	1.33	1.53
1	A	200	PRO	CA-C	-11.90	1.35	1.52
1	A	171	LYS	CA-CB	-11.68	1.33	1.53
1	A	207	ALA	CA-CB	-11.67	1.36	1.53
1	A	171	LYS	C-O	-10.49	1.10	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	191	ALA	CA-CB	-9.67	1.20	1.52
1	A	202	ALA	CA-C	-9.12	1.42	1.53
1	A	170	PRO	CA-C	-9.07	1.39	1.52
1	A	210	TYR	CA-C	-9.05	1.45	1.52
1	A	209	THR	C-O	-8.95	1.12	1.24
1	A	191	ALA	C-O	-8.85	1.05	1.23
1	A	171	LYS	CA-C	-8.84	1.41	1.52
1	A	202	ALA	C-O	-8.68	1.14	1.23
1	A	191	ALA	CA-C	-8.58	1.34	1.52
1	A	216	ALA	N-CA	-8.50	1.35	1.46
1	A	210	TYR	CA-CB	-8.34	1.43	1.53
1	A	209	THR	N-CA	-8.32	1.35	1.46
1	A	203	LEU	C-O	-7.41	1.14	1.23
1	A	170	PRO	N-CA	-7.33	1.38	1.47
1	A	200	PRO	C-N	-7.28	1.24	1.33
1	A	1008	VAL	CA-CB	7.25	1.62	1.54
1	A	1046	ASN	C-O	-6.83	1.17	1.24
1	A	287	LEU	CA-CB	-6.72	1.42	1.53
1	A	207	ALA	C-O	-6.67	1.13	1.24
1	A	399	ILE	CA-CB	-6.62	1.46	1.54
1	A	207	ALA	N-CA	-6.54	1.36	1.46
1	A	1045	SER	C-O	-6.48	1.16	1.23
1	A	732	PRO	CA-C	6.44	1.61	1.52
1	A	399	ILE	C-O	-6.38	1.17	1.24
1	A	212	HIS	CA-C	-6.34	1.44	1.52
1	A	192	HIS	CA-CB	-6.33	1.42	1.53
1	A	212	HIS	C-O	-6.28	1.16	1.23
1	A	1046	ASN	CA-C	-6.25	1.46	1.53
1	A	191	ALA	N-CA	-6.15	1.34	1.46
1	A	170	PRO	C-O	-6.13	1.16	1.24
1	A	173	ARG	CA-CB	-6.09	1.41	1.53
1	A	210	TYR	CG-CD1	-6.05	1.26	1.39
1	A	708	ILE	CA-CB	5.98	1.62	1.54
1	A	912	ILE	CA-CB	-5.98	1.47	1.53
1	A	571	HIS	CA-C	5.91	1.59	1.52
1	A	203	LEU	N-CA	5.85	1.53	1.46
1	A	731	THR	CA-CB	5.81	1.62	1.53
1	A	193	ILE	C-O	-5.78	1.17	1.24
1	A	210	TYR	CE2-CZ	-5.77	1.24	1.38
1	A	1046	ASN	N-CA	-5.75	1.37	1.47
1	A	650	GLN	CA-C	-5.72	1.45	1.52
1	A	201	ALA	C-O	-5.71	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	THR	C-N	-5.67	1.27	1.33
1	A	202	ALA	N-CA	-5.54	1.39	1.46
1	A	193	ILE	CA-C	-5.53	1.45	1.52
1	A	474	LYS	CA-C	-5.52	1.45	1.52
1	A	212	HIS	N-CA	-5.48	1.38	1.46
1	A	775	ASN	CA-C	5.47	1.59	1.52
1	A	210	TYR	CB-CG	-5.38	1.39	1.51
1	A	216	ALA	CA-C	-5.25	1.45	1.52
1	A	762	HIS	CA-C	5.19	1.60	1.52
1	A	1046	ASN	CA-CB	-5.10	1.38	1.51

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	740	SER	N-CA-C	16.14	130.07	112.97
1	A	214	ILE	N-CA-C	14.02	128.66	108.48
1	A	207	ALA	N-CA-C	-12.29	99.07	113.21
1	A	853	VAL	N-CA-C	-12.23	98.96	110.82
1	A	593	GLY	CA-C-N	12.04	139.18	121.72
1	A	593	GLY	C-N-CA	12.04	139.18	121.72
1	A	636	ILE	N-CA-C	-11.88	102.14	112.12
1	A	592	HIS	N-CA-C	-11.13	93.83	108.19
1	A	209	THR	CA-C-N	10.88	135.61	121.90
1	A	209	THR	C-N-CA	10.88	135.61	121.90
1	A	788	LEU	N-CA-C	10.87	125.93	112.23
1	A	253	LEU	N-CA-C	-10.80	92.79	110.17
1	A	964	GLN	N-CA-C	10.57	124.08	111.82
1	A	775	ASN	N-CA-C	-10.55	93.16	109.52
1	A	1046	ASN	N-CA-C	-10.17	92.95	108.00
1	A	210	TYR	N-CA-C	9.80	125.94	111.34
1	A	259	GLN	N-CA-C	-9.76	100.33	110.97
1	A	963	CYS	N-CA-C	-9.70	100.67	111.14
1	A	995	VAL	N-CA-C	9.64	119.59	110.53
1	A	289	LEU	N-CA-CB	-9.63	95.78	110.42
1	A	214	ILE	N-CA-CB	-9.49	94.88	111.39
1	A	1010	ILE	N-CA-C	-9.48	104.13	111.62
1	A	423	HIS	N-CA-C	-9.45	102.85	114.75
1	A	206	VAL	N-CA-C	9.41	128.91	109.34
1	A	289	LEU	N-CA-C	9.37	124.18	110.59
1	A	774	SER	CB-CA-C	-9.18	95.66	111.45
1	A	201	ALA	CA-C-N	9.15	136.90	122.26
1	A	201	ALA	C-N-CA	9.15	136.90	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	ASN	CA-C-N	9.11	140.35	122.03
1	A	288	ASN	C-N-CA	9.11	140.35	122.03
1	A	980	ILE	N-CA-C	-9.07	99.89	112.50
1	A	965	ASP	N-CA-C	9.03	130.04	110.80
1	A	171	LYS	N-CA-C	-9.03	91.58	110.80
1	A	255	LEU	N-CA-C	9.01	124.08	109.85
1	A	397	VAL	N-CA-C	-8.92	101.86	110.42
1	A	216	ALA	N-CA-C	8.89	129.74	110.80
1	A	742	ASP	N-CA-C	-8.63	97.56	110.24
1	A	325	PRO	N-CA-C	-8.61	102.03	113.65
1	A	202	ALA	N-CA-C	-8.58	93.60	108.52
1	A	206	VAL	N-CA-CB	-8.55	97.13	111.23
1	A	614	THR	N-CA-C	-8.54	102.64	113.23
1	A	202	ALA	N-CA-CB	-8.51	98.33	110.58
1	A	785	VAL	N-CA-C	-8.27	102.80	110.82
2	B	18	DA	C4'-C3'-O3'	-8.23	97.65	110.00
1	A	192	HIS	N-CA-C	8.17	122.37	110.28
1	A	390	GLY	N-CA-C	8.16	128.64	114.76
1	A	209	THR	N-CA-CB	8.16	124.28	110.49
1	A	222	HIS	N-CA-C	-8.02	101.83	111.69
1	A	696	LEU	N-CA-CB	-8.00	97.49	110.21
1	A	731	THR	N-CA-C	-7.98	92.18	109.81
1	A	201	ALA	CB-CA-C	7.96	124.34	110.64
1	A	197	SER	N-CA-C	-7.92	94.05	107.99
1	A	731	THR	CA-C-N	-7.90	109.96	119.84
1	A	731	THR	C-N-CA	-7.90	109.96	119.84
1	A	720	LEU	N-CA-C	7.85	124.20	113.37
1	A	618	LEU	N-CA-C	7.85	122.67	113.18
1	A	559	GLY	N-CA-C	7.81	131.70	113.18
1	A	704	ILE	N-CA-C	-7.76	105.60	112.12
1	A	662	LEU	N-CA-C	7.76	127.32	110.80
1	A	246	GLY	N-CA-C	-7.76	102.84	112.77
1	A	993	LEU	N-CA-C	-7.67	102.31	112.75
1	A	392	THR	CA-C-N	7.54	128.21	119.47
1	A	392	THR	C-N-CA	7.54	128.21	119.47
1	A	1031	GLN	N-CA-C	7.52	122.59	113.41
1	A	516	LEU	N-CA-C	7.52	122.58	112.88
1	A	200	PRO	N-CA-CB	-7.51	95.36	103.25
1	A	831	GLY	N-CA-C	7.43	130.78	113.18
1	A	593	GLY	N-CA-C	7.36	130.63	113.18
1	A	867	THR	N-CA-C	-7.27	99.46	110.01
1	A	457	HIS	N-CA-C	-7.26	95.33	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	LEU	N-CA-CB	7.25	122.75	110.49
1	A	191	ALA	CA-C-N	7.23	131.14	120.87
1	A	191	ALA	C-N-CA	7.23	131.14	120.87
1	A	686	LEU	N-CA-C	7.20	120.93	112.72
1	A	449	LEU	N-CA-C	7.18	122.34	113.50
1	A	762	HIS	N-CA-C	7.11	121.98	113.16
1	A	290	THR	CB-CA-C	-7.09	96.61	109.45
1	A	210	TYR	CA-CB-CG	-7.04	101.23	113.90
1	A	442	ALA	N-CA-C	-7.03	103.23	111.03
1	A	569	ALA	N-CA-C	6.90	120.93	112.23
1	A	743	GLY	N-CA-C	6.86	129.43	113.18
1	A	739	ALA	N-CA-C	6.84	121.63	113.28
1	A	460	THR	N-CA-C	6.84	117.46	109.60
1	A	963	CYS	CB-CA-C	6.79	121.63	110.90
1	A	501	ILE	CB-CA-C	-6.79	102.85	112.22
1	A	169	LYS	CA-C-N	6.77	128.30	119.84
1	A	169	LYS	C-N-CA	6.77	128.30	119.84
1	A	912	ILE	CB-CA-C	-6.75	104.64	111.80
1	A	365	ILE	CB-CA-C	-6.75	103.44	111.94
1	A	684	GLN	N-CA-C	-6.73	103.19	111.33
1	A	232	TRP	N-CA-C	-6.68	100.82	110.24
1	A	893	VAL	N-CA-C	6.66	117.35	110.36
1	A	829	ALA	N-CA-C	-6.65	100.13	110.17
1	A	247	GLU	N-CA-C	-6.62	104.20	113.20
1	A	558	HIS	CB-CA-C	-6.61	97.26	110.42
1	A	764	LEU	N-CA-C	-6.61	98.46	108.96
1	A	982	GLY	N-CA-C	6.59	123.33	111.34
1	A	503	SER	CB-CA-C	6.58	121.10	110.96
1	A	200	PRO	CA-C-N	-6.47	112.40	122.37
1	A	200	PRO	C-N-CA	-6.47	112.40	122.37
1	A	776	GLY	N-CA-C	6.45	121.84	113.27
1	A	454	CYS	N-CA-C	6.43	119.10	111.71
1	A	504	ASN	N-CA-CB	-6.43	101.70	110.95
1	A	205	THR	N-CA-C	6.42	128.97	111.00
1	A	277	ALA	N-CA-C	-6.41	101.28	111.02
1	A	841	ALA	N-CA-C	6.34	121.02	113.28
1	A	201	ALA	O-C-N	6.33	129.85	122.19
1	A	291	PRO	N-CA-C	-6.32	105.12	113.65
1	A	202	ALA	CA-C-O	-6.30	114.79	122.41
1	A	652	LEU	N-CA-C	6.27	120.97	112.88
1	A	672	SER	N-CA-C	6.26	120.96	112.88
1	A	530	GLN	N-CA-C	-6.23	104.55	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	972	GLN	N-CA-C	-6.22	104.50	111.28
1	A	457	HIS	N-CA-CB	6.21	120.99	110.49
1	A	287	LEU	CA-C-N	-6.20	107.58	121.53
1	A	287	LEU	C-N-CA	-6.20	107.58	121.53
1	A	210	TYR	N-CA-CB	-6.18	98.35	111.21
1	A	808	SER	N-CA-C	6.17	120.54	113.19
1	A	399	ILE	N-CA-C	-6.14	104.66	113.07
1	A	823	LEU	N-CA-C	-6.11	105.70	113.77
1	A	253	LEU	CB-CA-C	6.11	119.83	109.50
1	A	1022	VAL	N-CA-C	-6.10	104.39	110.30
1	A	324	THR	CB-CA-C	-6.09	99.96	109.22
1	A	741	HIS	CB-CA-C	6.03	121.57	110.24
1	A	433	ILE	N-CA-C	-6.01	103.63	112.04
1	A	457	HIS	CB-CA-C	-6.00	98.49	110.42
1	A	863	ALA	N-CA-C	-6.00	107.20	114.75
1	A	727	ALA	N-CA-C	5.96	119.74	112.23
1	A	754	LEU	N-CA-C	5.96	120.68	113.17
1	A	604	SER	N-CA-C	5.91	123.39	110.80
1	A	735	VAL	N-CA-C	-5.90	105.96	111.45
1	A	524	HIS	CB-CA-C	-5.90	102.15	111.17
1	A	920	THR	N-CA-C	-5.88	106.23	113.41
1	A	279	ARG	N-CA-C	5.88	117.36	111.07
1	A	1046	ASN	CB-CA-C	-5.86	108.14	116.34
1	A	252	PRO	CA-C-N	-5.85	112.70	122.64
1	A	252	PRO	C-N-CA	-5.85	112.70	122.64
1	A	732	PRO	CA-N-CD	-5.84	103.82	112.00
1	A	853	VAL	CB-CA-C	-5.83	104.40	112.04
1	A	798	LEU	CB-CA-C	5.79	121.44	110.56
1	A	801	GLU	N-CA-C	-5.79	104.17	111.11
1	A	426	THR	CA-C-N	-5.76	112.64	119.84
1	A	426	THR	C-N-CA	-5.76	112.64	119.84
1	A	250	GLY	CA-C-N	5.75	126.31	120.38
1	A	250	GLY	C-N-CA	5.75	126.31	120.38
1	A	424	GLY	N-CA-C	5.75	123.18	114.61
1	A	643	LYS	N-CA-C	-5.75	98.55	110.80
3	C	31	DT	C2'-C3'-O3'	5.75	120.12	111.50
1	A	254	GLN	N-CA-CB	-5.75	99.86	110.32
1	A	415	LEU	N-CA-C	5.67	119.92	112.89
1	A	902	LEU	N-CA-C	-5.63	102.31	111.04
1	A	628	LEU	N-CA-C	-5.63	100.71	109.72
1	A	216	ALA	CB-CA-C	-5.62	99.23	110.42
1	A	759	CYS	N-CA-C	-5.62	106.97	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1047	SER	N-CA-CB	-5.62	100.94	110.50
2	B	9	DC	O3'-P-O5'	5.61	112.41	104.00
1	A	474	LYS	N-CA-C	-5.61	105.17	111.28
1	A	253	LEU	CA-C-N	5.56	131.33	120.99
1	A	253	LEU	C-N-CA	5.56	131.33	120.99
1	A	374	ALA	N-CA-C	-5.55	104.08	111.24
1	A	201	ALA	N-CA-C	-5.55	105.11	112.94
2	B	8	DC	C2'-C3'-O3'	-5.54	103.19	111.50
2	B	9	DC	C2'-C3'-O3'	5.52	119.78	111.50
1	A	730	LEU	N-CA-C	-5.50	100.38	108.79
1	A	428	ASP	N-CA-C	5.49	119.47	112.34
1	A	201	ALA	N-CA-CB	5.48	120.02	110.98
1	A	458	GLY	N-CA-C	-5.47	100.21	113.18
1	A	911	ASN	N-CA-C	-5.46	102.09	109.95
1	A	430	VAL	N-CA-C	-5.46	104.63	110.36
1	A	861	CYS	N-CA-C	-5.43	105.87	113.37
1	A	194	VAL	N-CA-C	5.39	120.56	109.34
1	A	172	VAL	CA-C-N	5.39	131.40	121.70
1	A	172	VAL	C-N-CA	5.39	131.40	121.70
1	A	193	ILE	N-CA-C	-5.39	98.13	109.34
1	A	251	PRO	N-CA-C	5.38	117.27	110.70
1	A	600	VAL	N-CA-C	-5.38	105.14	110.62
1	A	324	THR	N-CA-C	5.37	118.43	109.09
1	A	990	GLN	N-CA-C	-5.35	104.87	111.40
1	A	833	THR	N-CA-C	-5.34	98.00	109.81
1	A	695	GLY	CA-C-N	5.34	129.53	122.42
1	A	695	GLY	C-N-CA	5.34	129.53	122.42
1	A	976	ILE	N-CA-C	-5.27	105.99	111.58
1	A	878	ILE	CB-CA-C	-5.27	103.00	111.59
1	A	960	PRO	N-CA-C	5.27	121.00	113.47
1	A	358	PRO	CA-C-N	5.25	124.70	119.24
1	A	358	PRO	C-N-CA	5.25	124.70	119.24
1	A	230	LYS	N-CA-C	-5.24	106.94	113.38
1	A	456	ALA	CA-C-N	5.24	131.55	121.54
1	A	456	ALA	C-N-CA	5.24	131.55	121.54
1	A	258	GLY	CA-C-N	5.21	127.53	120.65
1	A	258	GLY	C-N-CA	5.21	127.53	120.65
1	A	532	VAL	N-CA-C	-5.21	104.89	110.36
1	A	909	ALA	N-CA-C	5.18	119.45	113.18
1	A	339	GLN	N-CA-C	-5.18	105.81	111.82
1	A	755	LEU	CA-C-N	5.17	126.30	119.84
1	A	755	LEU	C-N-CA	5.17	126.30	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	728	HIS	N-CA-C	5.17	121.81	110.80
1	A	908	ILE	CB-CA-C	-5.16	105.26	112.02
1	A	677	LYS	N-CA-C	-5.15	104.93	111.11
1	A	1034	GLY	N-CA-C	5.13	125.34	113.18
1	A	639	ASN	N-CA-C	5.12	117.14	110.53
1	A	862	GLN	N-CA-C	-5.11	105.35	112.30
1	A	524	HIS	N-CA-C	5.11	118.39	112.97
2	B	12	DT	C4'-C3'-O3'	-5.10	102.35	110.00
1	A	357	LEU	N-CA-C	-5.09	103.35	109.72
1	A	822	LEU	N-CA-C	5.06	120.32	114.04
1	A	568	ILE	N-CA-C	-5.04	105.65	113.16
1	A	731	THR	CB-CA-C	-5.02	100.27	110.17
1	A	830	HIS	N-CA-C	-5.02	106.44	113.37
1	A	910	SER	N-CA-C	5.02	118.24	112.57
3	C	21	DG	C2'-C3'-O3'	5.02	119.03	111.50
1	A	868	PRO	N-CA-C	-5.01	106.88	113.65

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	Peptide,Mainchain
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	6244	718	0
2	B	764	0	427	51	0
3	C	788	0	432	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7103	803	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 55.

All (803) 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:200:PRO:HG3	1:A:222:HIS:CE1	1.83	1.13
1:A:697:THR:OG1	1:A:700:GLN:HB2	1.49	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: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
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:206:VAL:C	1:A:208:VAL:H	1.56	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:708:ILE:HB	1:A:742:ASP:CG	1.95	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
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:206:VAL:C	1:A:208:VAL:N	2.30	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
1:A:212:HIS:HA	1:A:213:ILE:C	2.03	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: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: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:287:LEU:O	1:A:288:ASN:HB2	1.81	0.79
1:A:1046:ASN:CB	1:A:1047:SER:CA	2.58	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:O	1:A:1040:VAL:CG1	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:729:GLY:C	1:A:730:LEU:HD23	2.11	0.75
1:A:861:CYS:CB	4:A:1168:HOH:O	2.32	0.75
1:A:718:GLN:NE2	1:A:718:GLN:HA	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:200:PRO:HG3	1:A:222:HIS:ND1	2.02	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:A:1232:HOH:O	3:C:19:DG:C2'	2.30	0.73
2:B:14:DC:H2''	2:B:15:DT:O5'	1.88	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:1045:SER:O	1:A:1046:ASN:C	2.24	0.72
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
1:A:829:ALA:C	1:A:831:GLY:H	1.96	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:9:DC:H2''	2:B:10:DC:O5'	1.89	0.71
2:B:11:DC:H2''	2:B:12:DT:O5'	1.90	0.71
1:A:650:GLN:CG	1:A:651:ARG:N	2.51	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:965:ASP:OD2	1:A:965:ASP:C	2.33	0.70
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
3:C:23:DG:N7	4:C:104:HOH:O	2.24	0.70
1:A:596:PRO:O	1:A:599:VAL:N	2.23	0.70
1:A:391:LEU:HD12	1:A:395:GLN:CB	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1045:SER:O	1:A:1046:ASN:CB	2.29	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:192:HIS:O	1:A:193:ILE:C	2.32	0.69
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: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: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: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
1:A:697:THR:HG1	1:A:700:GLN:HB2	1.58	0.66
2:B:-4:DG:H5'	4:B:72:HOH:O	1.96	0.66
1:A:686:LEU:CD2	1:A:718:GLN:HG2	2.23	0.66
1:A:1029:LEU:HD12	1:A:1040:VAL:CG2	2.25	0.66
1:A:721:LEU:HB3	1:A:722:PRO:CD	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:399:ILE:O	1:A:399:ILE:CG2	2.39	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:538:ASP:O	1:A:539:GLY:C	2.36	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: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:317:LEU:HD21	1:A:345:GLN:CD	2.23	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:CB	1:A:993:LEU:HD21	2.27	0.63
1:A:966:HIS:HB3	1:A:993:LEU:HD21	1.81	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:GLN:OE1	1:A:1017:GLN:N	2.23	0.62
1:A:192:HIS:C	1:A:193:ILE:O	2.36	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:953:GLU:CA	4:A:1154:HOH:O	2.39	0.62
1:A:1035:LEU:HD23	1:A:1036:THR:H	1.64	0.62
2:B:18:DA:H2''	2:B:19:DC:C5'	2.29	0.61
1:A:287:LEU:O	1:A:288:ASN:C	2.38	0.61
1:A:1041:VAL:HA	1:A:1042:ALA:C	2.25	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:302:GLY:O	1:A:303:GLY:C	2.41	0.60
1:A:391:LEU:CD2	1:A:396:VAL:HG22	2.29	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: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:381:LEU:HD11	1:A:413:GLN:HG3	1.83	0.60
1:A:392:THR:O	1:A:395:GLN:HB2	2.01	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:557:THR:HG22	1:A:558:HIS:N	2.16	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:543:ALA:O	1:A:544:LEU:C	2.45	0.59
1:A:912:ILE:CG2	4:A:1176:HOH:O	2.47	0.59
1:A:407:GLN:HB3	1:A:440:LYS:HZ3	1.68	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:293:GLN:CD	4:A:1217:HOH:O	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:O	1:A:253:LEU:HD22	2.02	0.59
1:A:299:SER:O	1:A:299:SER:OG	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
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: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:610:GLN:O	1:A:614:THR:OG1	2.22	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: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:662:LEU:O	1:A:663:THR:C	2.47	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:240:ALA:HB3	1:A:272:MET:HE3	1.87	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:O	1:A:399:ILE:HG23	2.04	0.57
1:A:598:GLN:HE22	1:A:634:VAL:HB	1.69	0.57
1:A:246:GLY:C	1:A:248:LEU:H	2.13	0.56
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:207:ALA:HB1	4:A:88:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:HIS:NE2	4:A:66:HOH:O	2.32	0.56
1:A:619:LEU:HD13	1:A:619:LEU:C	2.30	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
2:B:24:DC:H2''	2:B:25:DC:O5'	2.04	0.56
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:275:VAL:C	1:A:277:ALA:H	2.13	0.56
1:A:680:LEU:C	4:A:73:HOH:O	2.48	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:829:ALA:C	1:A:831:GLY:N	2.63	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:499:VAL:O	1:A:500:ALA:C	2.48	0.56
1:A:753:ARG:HG2	4:A:1156:HOH:O	2.05	0.56
1:A:1017:GLN:H	1:A:1017:GLN:CD	2.11	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:370:GLY:O	1:A:371:GLY:C	2.49	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:537:HIS:O	1:A:538:ASP:C	2.47	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:860:LEU:C	1:A:862:GLN:H	2.15	0.55
1:A:941:ALA:HA	1:A:944:SER:OG	2.06	0.55
1:A:207:ALA:O	1:A:208:VAL:C	2.50	0.55
1:A:288:ASN:HA	4:A:1201:HOH:O	2.06	0.55
1:A:648:THR:HG22	1:A:680:LEU:HD13	1.89	0.55
1:A:653:LEU:HD23	1:A:654:PRO:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:257:THR:C	1:A:259:GLN:N	2.62	0.55
1:A:571:HIS:O	1:A:572:ASP:C	2.46	0.55
1:A:588:LEU:O	1:A:592:HIS:CD2	2.57	0.55
1:A:694:HIS:O	1:A:695:GLY:C	2.49	0.55
2:B:-3:DA:H1'	2:B:-2:DT:H5'	1.88	0.55
2:B:22:DC:N4	4:B:178:HOH:O	2.23	0.55
1:A:350:VAL:O	1:A:355:HIS:CD2	2.60	0.55
1:A:632:GLN:HG2	1:A:668:VAL:HG21	1.88	0.55
1:A:318:CYS:HA	1:A:323:LEU:H	1.72	0.55
1:A:1044:ALA:O	1:A:1046:ASN:O	2.25	0.55
2:B:7:DC:N4	4:B:99:HOH:O	2.40	0.55
2:B:10:DC:H42	3:C:20:DG:H1	1.54	0.55
1:A:568:ILE:CG2	1:A:603:ALA:HB1	2.37	0.54
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: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:678:GLN:HG3	2:B:11:DC:O3'	2.07	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: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:213:ILE:C	1:A:214:ILE:HG13	2.33	0.54
1:A:348:LEU:HB3	1:A:349:PRO:CD	2.38	0.54
1:A:688:PRO:C	1:A:690:LEU:H	2.15	0.54
1:A:620:PRO:C	1:A:622:LEU:H	2.14	0.54
1:A:741:HIS:CD2	1:A:774:SER:C	2.85	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:C6	3:C:38:DC:OP2	2.61	0.54
1:A:771:ALA:C	1:A:773:ALA:H	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:294:VAL:O	1:A:295:VAL:C	2.51	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: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:674:GLY:C	1:A:676:GLY:H	2.17	0.53
1:A:305:GLN:O	1:A:306:ALA:C	2.52	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:664:PRO:O	1:A:665:ASP:C	2.51	0.53
1:A:674:GLY:O	1:A:676:GLY:N	2.34	0.53
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:875:ALA:C	1:A:877:ASN:H	2.16	0.52
1:A:925:LEU:O	1:A:926:PRO:C	2.51	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:826:LEU:C	1:A:828:GLN:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:VAL:C	1:A:771:ALA:H	2.16	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
1:A:417:PRO:O	1:A:418:VAL:C	2.53	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:OD2	1:A:965:ASP:O	2.28	0.51
1:A:237:ALA:O	1:A:272:MET:HE1	2.11	0.51
1:A:948:GLY:O	1:A:949:LYS:C	2.51	0.51
1:A:297:ILE:HG22	1:A:333:SER:HA	1.92	0.51
1:A:470:ASN:O	1:A:471:GLY:C	2.54	0.51
1:A:527:THR:O	1:A:531:VAL:HG23	2.11	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:880:GLY:O	1:A:881:LYS:C	2.54	0.51
3:C:38:DC:OP2	3:C:38:DC:H6	1.94	0.51
1:A:499:VAL:CG2	4:A:50:HOH:O	2.59	0.51
1:A:649:VAL:O	1:A:650:GLN:C	2.49	0.51
1:A:995:VAL:O	1:A:999:ASP:HB2	2.11	0.51
1:A:391:LEU:CD2	1:A:396:VAL:HG13	2.41	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:257:THR:C	1:A:259:GLN:H	2.18	0.50
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:955:VAL:O	1:A:956:GLN:C	2.54	0.50
1:A:192:HIS:O	1:A:193:ILE:O	2.29	0.50
1:A:212:HIS:CA	1:A:213:ILE:C	2.82	0.50
1:A:336:GLY:O	1:A:340:ALA:N	2.33	0.50
1:A:607:GLY:C	4:A:1153:HOH:O	2.50	0.50
1:A:853:VAL:O	1:A:857:LEU:N	2.44	0.50
1:A:866:LEU:HD12	1:A:870:GLN:OE1	2.11	0.50
1:A:813:LYS:C	1:A:815:ALA:H	2.18	0.50
1:A:834:PRO:O	1:A:838:VAL:HG23	2.12	0.50
1:A:670:ILE:CD1	1:A:702:VAL:HG23	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LEU:HB2	4:A:73:HOH:O	2.06	0.50
1:A:751:VAL:O	1:A:755:LEU:N	2.32	0.50
1:A:780:GLN:HE21	1:A:813:LYS:HZ2	1.59	0.50
1:A:895:CYS:HA	1:A:900:LEU:O	2.11	0.50
2:B:6:DT:H71	4:B:165:HOH:O	2.11	0.50
1:A:486:VAL:CG2	1:A:514:GLN:HE22	2.24	0.50
1:A:497:GLN:O	1:A:498:VAL:C	2.52	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:254:GLN:N	1:A:254:GLN:OE1	2.45	0.49
1:A:339:GLN:HE21	1:A:339:GLN:CA	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:982:GLY:C	1:A:984:GLN:H	2.20	0.49
1:A:689:VAL:HG12	1:A:689:VAL:O	2.13	0.49
1:A:803:VAL:O	1:A:804:VAL:C	2.54	0.49
1:A:210:TYR:O	1:A:211:GLN:C	2.55	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
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:347:LEU:O	1:A:348:LEU:C	2.56	0.49
1:A:629:THR:HB	1:A:630:PRO:HD2	1.95	0.49
1:A:997:CYS:HA	1:A:1002:LEU:H	1.76	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:O	1:A:912:ILE:HG22	2.10	0.49
1:A:391:LEU:O	1:A:391:LEU:HG	2.13	0.48
1:A:407:GLN:OE1	1:A:407:GLN:HA	2.14	0.48
1:A:634:VAL:C	1:A:636:ILE:H	2.20	0.48
1:A:328:VAL:C	1:A:330:ALA:H	2.22	0.48
1:A:850:LEU:HA	1:A:853:VAL:HG23	1.95	0.48
1:A:822:LEU:O	1:A:823:LEU:C	2.56	0.48
1:A:899:GLY:O	1:A:900:LEU:C	2.56	0.48
1:A:996:LEU:HD21	1:A:1023:GLN:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:DT:H2''	3:C:34:DC:C6	2.48	0.48
1:A:203:LEU:HA	1:A:204:GLY:C	2.38	0.48
1:A:660:HIS:O	1:A:698:GLN:OE1	2.32	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:477:LEU:O	1:A:478:GLU:C	2.57	0.48
1:A:690:LEU:HD23	1:A:694:HIS:HD2	1.78	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:718:GLN:NE2	1:A:718:GLN:CA	2.77	0.48
1:A:1013:ASN:OD1	1:A:1013:ASN:C	2.57	0.48
2:B:-1:DA:C2'	2:B:0:DT:H5''	2.43	0.48
1:A:532:VAL:O	1:A:533:ALA:C	2.54	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: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
1:A:860:LEU:HD23	1:A:888:GLN:HA	1.95	0.47
1:A:344:MET:O	1:A:348:LEU:HB2	2.14	0.47
1:A:547:VAL:O	1:A:548:GLN:C	2.57	0.47
1:A:698:GLN:O	1:A:699:VAL:C	2.56	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:463:GLN:O	1:A:464:VAL:C	2.57	0.47
1:A:639:ASN:CG	1:A:640:GLY:H	2.22	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:812:GLY:O	1:A:815:ALA:HB3	2.15	0.47
1:A:954:THR:HG23	1:A:958:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:301:ASN:C	1:A:303:GLY:H	2.23	0.47
1:A:639:ASN:CG	1:A:640:GLY:N	2.72	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:429:GLN:O	1:A:430:VAL:C	2.57	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:467:ILE:HG22	1:A:467:ILE:O	2.15	0.46
1:A:962:LEU:N	1:A:962:LEU:HD22	2.30	0.46
1:A:596:PRO:O	1:A:597:ASP:C	2.57	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:N	2.73	0.46
1:A:713:ALA:O	1:A:714:LEU:C	2.58	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:527:THR:C	1:A:529:ASP:H	2.23	0.46
1:A:581:VAL:CG1	1:A:582:GLN:N	2.78	0.46
1:A:741:HIS:O	1:A:742:ASP:C	2.59	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:552:PRO:O	1:A:553:VAL:C	2.58	0.46
1:A:324:THR:OG1	1:A:327:GLN:HG2	2.15	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:1032:ASP:CG	1:A:1033:HIS:H	2.23	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:717:VAL:O	1:A:718:GLN:C	2.57	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:275:VAL:C	1:A:277:ALA:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:HD21	1:A:396:VAL:CB	2.42	0.45
1:A:620:PRO:C	1:A:622:LEU:N	2.73	0.45
1:A:831:GLY:HA2	1:A:868:PRO:HB2	1.98	0.45
1:A:209:THR:C	1:A:210:TYR:CD1	2.94	0.45
1:A:510:LEU:O	1:A:511:GLU:C	2.57	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: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:1037:PRO:O	4:A:45:HOH:O	2.21	0.45
1:A:451:PRO:HG2	1:A:452:VAL:H	1.81	0.45
1:A:704:ILE:C	1:A:706:SER:H	2.25	0.45
1:A:821:ARG:HB3	1:A:822:LEU:HD23	1.98	0.45
1:A:1017:GLN:CB	4:B:129:HOH:O	2.65	0.45
1:A:391:LEU:CD1	1:A:396:VAL:HG13	2.46	0.45
1:A:918:LEU:C	1:A:920:THR:N	2.74	0.45
1:A:996:LEU:O	1:A:1002:LEU:HB2	2.16	0.45
1:A:848:GLN:NE2	1:A:848:GLN:CA	2.76	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:769:VAL:C	1:A:771:ALA:N	2.75	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:995:VAL:HG13	1:A:999:ASP:HB2	1.99	0.45
1:A:217:LEU:CD2	4:A:1187:HOH:O	2.63	0.45
1:A:294:VAL:C	1:A:296:ALA:N	2.73	0.45
1:A:701:VAL:C	1:A:703:ALA:N	2.73	0.44
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
1:A:476:ALA:O	1:A:477:LEU:C	2.59	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:980:ILE:O	1:A:981:GLY:C	2.60	0.44
1:A:339:GLN:N	1:A:339:GLN:NE2	2.54	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:342:GLU:C	1:A:344:MET:H	2.25	0.44
1:A:433:ILE:O	1:A:433:ILE:HG22	2.18	0.44
1:A:521:CYS:HA	1:A:526:LEU:HB2	1.99	0.44
1:A:738:ILE:HD13	1:A:773:ALA:O	2.17	0.44
1:A:1000:HIS:CD2	1:A:1026:LEU:HD22	2.53	0.44
1:A:499:VAL:O	1:A:502:ALA:N	2.50	0.44
1:A:785:VAL:O	1:A:786:GLN:C	2.61	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:242:LEU:HD22	1:A:242:LEU:C	2.43	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:610:GLN:HA	1:A:610:GLN:OE1	2.17	0.43
1:A:918:LEU:O	1:A:920:THR:N	2.50	0.43
1:A:392:THR:HA	1:A:393:PRO:HD2	1.66	0.43
1:A:513:VAL:HG23	1:A:544:LEU:CD1	2.48	0.43
1:A:688:PRO:C	1:A:690:LEU:N	2.76	0.43
1:A:758:LEU:O	1:A:762:HIS:C	2.61	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:996:LEU:HD21	1:A:1023:GLN:HB2	1.98	0.43
1:A:517:LEU:N	1:A:518:PRO:HD2	2.33	0.43
1:A:578:LEU:HD23	1:A:578:LEU:HA	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:1010:ILE:O	1:A:1015:GLY:N	2.49	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:334:HIS:HB3	1:A:369:ILE:HD12	2.00	0.43
1:A:430:VAL:O	1:A:431:VAL:C	2.60	0.43
1:A:921:VAL:HG12	1:A:922:GLN:N	2.34	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:674:GLY:C	1:A:676:GLY:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:852:THR:HG22	1:A:884:LEU:HD12	2.01	0.43
1:A:860:LEU:CD2	1:A:887:VAL:HG12	2.48	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: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:527:THR:C	1:A:529:ASP:N	2.76	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:788:LEU:O	1:A:789:LEU:C	2.61	0.42
1:A:887:VAL:O	1:A:891:LEU:HB2	2.20	0.42
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:860:LEU:C	1:A:862:GLN:N	2.75	0.42
1:A:912:ILE:HG13	4:A:1207:HOH:O	2.18	0.42
1:A:259:GLN:CD	1:A:295:VAL:HG21	2.44	0.42
1:A:334:HIS:HD2	1:A:368:ASN:HA	1.84	0.42
1:A:574:GLY:O	1:A:575:LYS:C	2.62	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:1023:GLN:CD	1:A:1024:ARG:HG2	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:GLN:O	1:A:701:VAL:N	2.48	0.42
1:A:964:GLN:HG2	1:A:964:GLN:H	1.33	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:921:VAL:HG13	1:A:922:GLN:N	2.33	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:O	1:A:316:VAL:HG12	2.18	0.42
1:A:343:THR:OG1	1:A:372:LYS:HG3	2.20	0.42
2:B:-5:DA:N1	3:C:35:DT:O4	2.53	0.42
2:B:1:DG:C2	3:C:30:DA:C2	3.08	0.42
1:A:288:ASN:HD22	1:A:288:ASN:H	1.67	0.42
1:A:710:GLY:O	1:A:711:LYS:C	2.62	0.42
1:A:909:ALA:HB2	1:A:918:LEU:HD11	2.00	0.42
1:A:328:VAL:C	1:A:330:ALA:N	2.77	0.42
1:A:405:GLY:O	1:A:406:LYS:C	2.63	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:741:HIS:HD2	1:A:774:SER:C	2.28	0.42
1:A:886:THR:O	1:A:887:VAL:C	2.60	0.42
1:A:902:LEU:O	1:A:903:ALA:C	2.62	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:536:SER:C	1:A:537:HIS:CG	2.98	0.41
1:A:558:HIS:HE1	1:A:586:PRO:HD3	1.85	0.41
1:A:1045:SER:C	1:A:1046:ASN:O	2.46	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:605:ASN:OD1	1:A:605:ASN:N	2.53	0.41
1:A:775:ASN:CG	1:A:808:SER:O	2.64	0.41
2:B:-5:DA:N3	4:B:170:HOH:O	2.53	0.41
1:A:996:LEU:HD21	1:A:1023:GLN:CB	2.50	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:755:LEU:C	1:A:755:LEU:HD23	2.45	0.41
1:A:231:GLN:O	1:A:232:TRP:C	2.64	0.41
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLY:O	1:A:407:GLN:N	2.54	0.41
1:A:419:LEU:H	1:A:419:LEU:HG	1.57	0.41
1:A:1036:THR:OG1	1:A:1037:PRO:HD2	2.21	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:588:LEU:HD21	1:A:615:VAL:HG13	1.95	0.41
1:A:982:GLY:C	1:A:984:GLN:N	2.78	0.41
1:A:339:GLN:O	1:A:343:THR:OG1	2.39	0.41
1:A:361:GLN:HG2	1:A:397:VAL:HG11	2.02	0.41
1:A:419:LEU:C	1:A:421:GLN:N	2.79	0.41
1:A:427:PRO:N	4:A:1209:HOH:O	2.53	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:HD13	1:A:890:LEU:O	2.21	0.41
1:A:1026:LEU:O	1:A:1027:PRO:C	2.62	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:701:VAL:O	1:A:702:VAL:C	2.62	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:775:ASN:HB3	4:A:1196:HOH:O	2.21	0.40
1:A:1043:ILE:O	1:A:1044:ALA:C	2.64	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: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
1:A:821:ARG:C	1:A:822:LEU:HD22	2.46	0.40
2:B:-5:DA:OP2	2:B:-5:DA:H8	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

5.3.1 Protein backbone

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%)	1 9

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
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

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Mol	Chain	Res	Type
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%)	465 (73%)	170 (27%)	0 2

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	HIS
1	A	221	THR
1	A	228	VAL
1	A	230	LYS
1	A	239	GLU
1	A	242	LEU
1	A	247	GLU
1	A	248	LEU
1	A	254	GLN
1	A	263	ILE

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Mol	Chain	Res	Type
1	A	265	LYS
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	304	LYS
1	A	307	LEU
1	A	310	VAL
1	A	325	PRO
1	A	338	LYS
1	A	339	GLN
1	A	343	THR
1	A	345	GLN
1	A	348	LEU
1	A	349	PRO
1	A	355	HIS
1	A	357	LEU
1	A	363	VAL
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	385	LEU
1	A	391	LEU
1	A	392	THR
1	A	396	VAL
1	A	399	ILE
1	A	406	LYS
1	A	409	LEU
1	A	411	THR
1	A	412	VAL
1	A	414	ARG
1	A	415	LEU
1	A	419	LEU
1	A	421	GLN

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Mol	Chain	Res	Type
1	A	435	SER
1	A	440	LYS
1	A	441	GLN
1	A	452	VAL
1	A	455	GLN
1	A	459	LEU
1	A	462	ASP
1	A	478	GLU
1	A	480	VAL
1	A	481	GLN
1	A	484	LEU
1	A	486	VAL
1	A	504	ASN
1	A	510	LEU
1	A	514	GLN
1	A	515	ARG
1	A	521	CYS
1	A	536	SER
1	A	542	GLN
1	A	547	VAL
1	A	551	LEU
1	A	561	THR
1	A	565	VAL
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	602	ILE
1	A	605	ASN
1	A	614	THR
1	A	615	VAL
1	A	631	ASP
1	A	634	VAL
1	A	649	VAL
1	A	650	GLN
1	A	653	LEU
1	A	683	VAL

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Mol	Chain	Res	Type
1	A	684	GLN
1	A	687	LEU
1	A	692	GLN
1	A	696	LEU
1	A	698	GLN
1	A	701	VAL
1	A	708	ILE
1	A	711	LYS
1	A	716	THR
1	A	718	GLN
1	A	719	ARG
1	A	725	CYS
1	A	732	PRO
1	A	738	ILE
1	A	750	THR
1	A	751	VAL
1	A	752	GLN
1	A	754	LEU
1	A	757	VAL
1	A	770	VAL
1	A	772	ILE
1	A	779	LYS
1	A	780	GLN
1	A	785	VAL
1	A	788	LEU
1	A	789	LEU
1	A	790	PRO
1	A	799	THR
1	A	801	GLU
1	A	817	GLU
1	A	819	VAL
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	859	VAL
1	A	860	LEU
1	A	864	HIS
1	A	866	LEU
1	A	867	THR

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Mol	Chain	Res	Type
1	A	871	VAL
1	A	878	ILE
1	A	887	VAL
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	927	VAL
1	A	930	GLN
1	A	934	LEU
1	A	936	GLN
1	A	937	ASP
1	A	939	VAL
1	A	944	SER
1	A	946	ILE
1	A	956	GLN
1	A	959	LEU
1	A	962	LEU
1	A	964	GLN
1	A	974	VAL
1	A	979	ASN
1	A	980	ILE
1	A	983	LYS
1	A	989	VAL
1	A	1000	HIS
1	A	1002	LEU
1	A	1012	SER
1	A	1026	LEU
1	A	1031	GLN
1	A	1035	LEU
1	A	1038	ASP
1	A	1039	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
1	A	231	GLN
1	A	288	ASN
1	A	311	GLN

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Mol	Chain	Res	Type
1	A	334	HIS
1	A	339	GLN
1	A	353	GLN
1	A	355	HIS
1	A	368	ASN
1	A	436	HIS
1	A	470	ASN
1	A	475	GLN
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	712	GLN
1	A	718	GLN
1	A	760	GLN
1	A	780	GLN
1	A	809	ASN
1	A	848	GLN
1	A	882	GLN
1	A	888	GLN
1	A	904	GLN
1	A	945	ASN
1	A	950	GLN
1	A	1023	GLN
1	A	1031	GLN
1	A	1039	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

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, 95th 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 ²)	Q<0.9
1	A	854/1047 (81%)	0.45	56 (6%) 24 12	27, 84, 153, 200	0
2	B	38/38 (100%)	0.37	3 (7%) 18 10	31, 46, 132, 137	0
3	C	38/38 (100%)	0.60	1 (2%) 57 34	43, 70, 129, 135	0
All	All	930/1123 (82%)	0.45	60 (6%) 25 13	27, 83, 153, 200	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1040	VAL	5.2
1	A	593	GLY	4.2
1	A	834	PRO	4.2
1	A	1042	ALA	3.9
1	A	830	HIS	3.8
1	A	627	GLY	3.7
1	A	457	HIS	3.7
1	A	199	HIS	3.5
1	A	645	ALA	3.4
1	A	831	GLY	3.3
1	A	215	THR	3.3
1	A	864	HIS	3.2
1	A	214	ILE	3.2
1	A	211	GLN	3.1
1	A	197	SER	3.0
1	A	398	ALA	2.9
1	A	389	HIS	2.9
1	A	622	LEU	2.8
1	A	769	VAL	2.8
1	A	865	GLY	2.8
1	A	832	LEU	2.8
1	A	829	ALA	2.7
1	A	217	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	732	PRO	2.7
1	A	655	VAL	2.7
1	A	672	SER	2.7
1	A	892	PRO	2.6
1	A	222	HIS	2.6
1	A	524	HIS	2.6
1	A	638	SER	2.6
1	A	661	GLY	2.6
1	A	216	ALA	2.6
1	A	797	GLY	2.5
1	A	1029	LEU	2.5
1	A	602	ILE	2.4
1	A	973	VAL	2.4
1	A	523	ALA	2.4
3	C	7	DT	2.4
1	A	213	ILE	2.3
2	B	-6	DT	2.3
1	A	1048	GLY	2.3
1	A	862	GLN	2.3
1	A	264	ALA	2.2
1	A	681	GLU	2.2
1	A	966	HIS	2.2
1	A	220	ALA	2.2
1	A	890	LEU	2.2
2	B	31	DT	2.2
1	A	728	HIS	2.2
1	A	1021	THR	2.1
1	A	902	LEU	2.1
1	A	861	CYS	2.1
1	A	988	THR	2.1
1	A	659	ALA	2.1
1	A	181	GLU	2.1
1	A	400	ALA	2.0
1	A	251	PRO	2.0
2	B	29	DA	2.0
1	A	825	VAL	2.0
1	A	928	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.