



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:07 PM UTC

PDB ID : 2AAF / pdb\_00002aaf  
Title : Structure of H278A arginine deiminase with L-arginine forming a S-alkylthiuronium reaction intermediate  
Authors : Galkin, A.; Lu, X.; Dunaway-Mariano, D.; Herzberg, O.  
Deposited on : 2005-07-13  
Resolution : 2.30 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.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
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

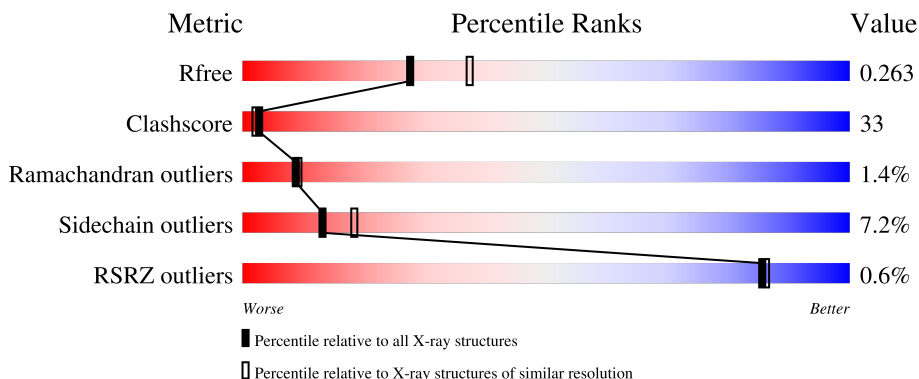
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	418	 46% 41% 8% ..
1	B	418	 56% 34% 7% ..
1	C	418	 50% 39% 8% ..
1	D	418	 2% 46% 42% 8% ..

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13542 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 Arginine deiminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	405	3170	2004	553	596	17	0	0	0
1	B	409	3202	2024	557	604	17	0	0	0
1	C	406	3185	2014	554	600	17	0	0	0
1	D	406	3183	2013	554	599	17	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	ALA	HIS	engineered mutation	UNP P13981
A	406	CYR	CYS	modified residue	UNP P13981
B	278	ALA	HIS	engineered mutation	UNP P13981
B	406	CYR	CYS	modified residue	UNP P13981
C	278	ALA	HIS	engineered mutation	UNP P13981
C	406	CYR	CYS	modified residue	UNP P13981
D	278	ALA	HIS	engineered mutation	UNP P13981
D	406	CYR	CYS	modified residue	UNP P13981

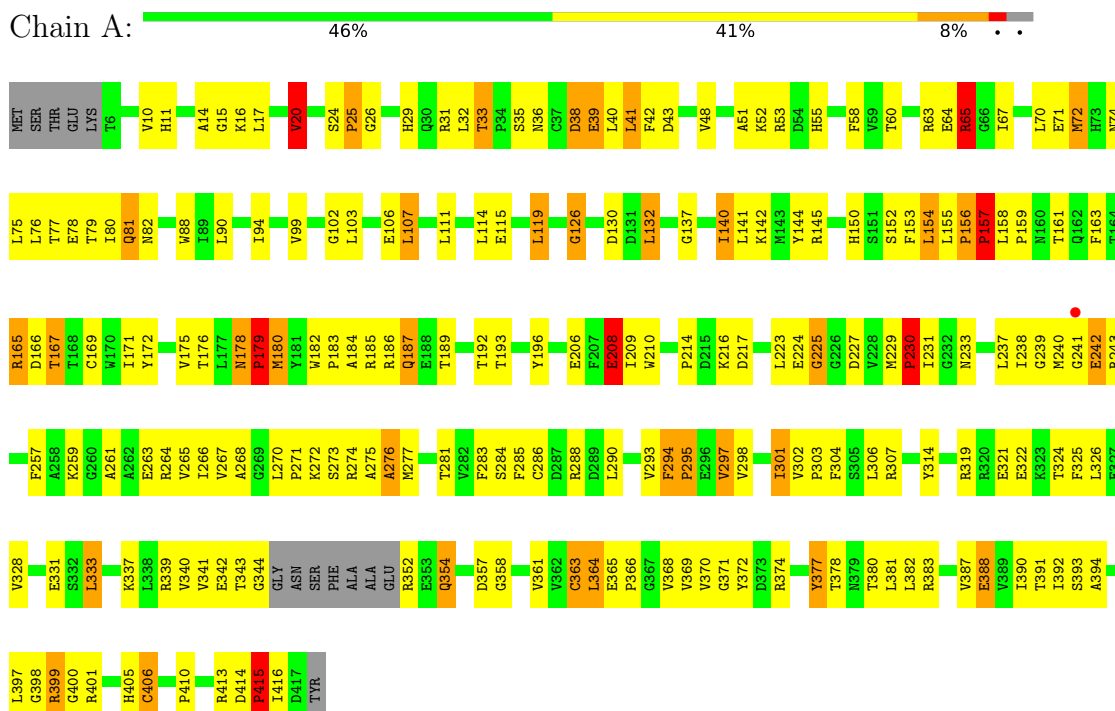
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	227	Total 227	O 227	0	0
2	B	209	Total 209	O 209	0	0
2	C	187	Total 187	O 187	0	0
2	D	179	Total 179	O 179	0	0

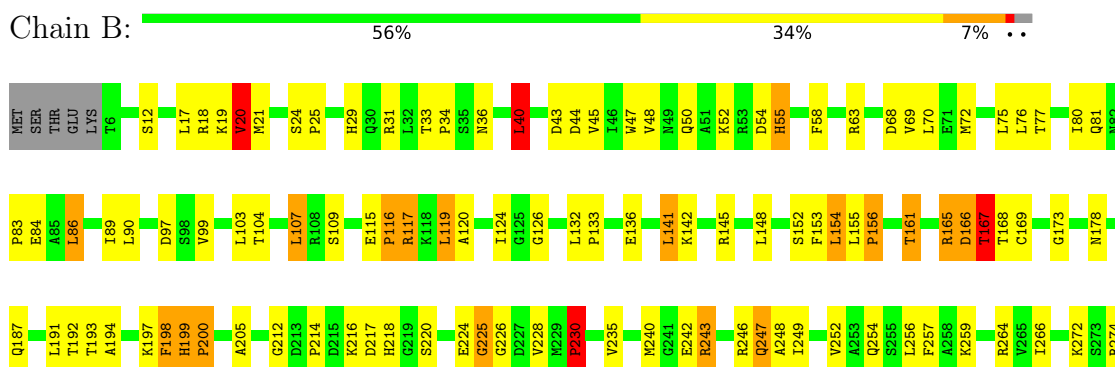
### 3 Residue-property plots

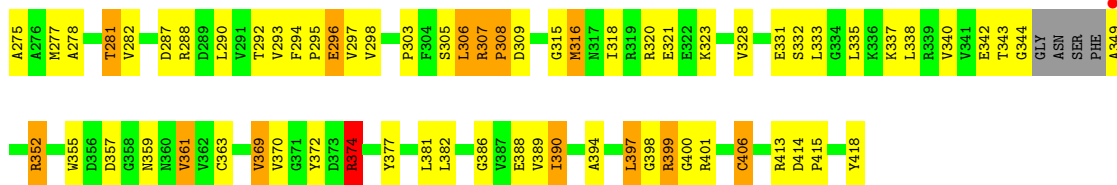
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

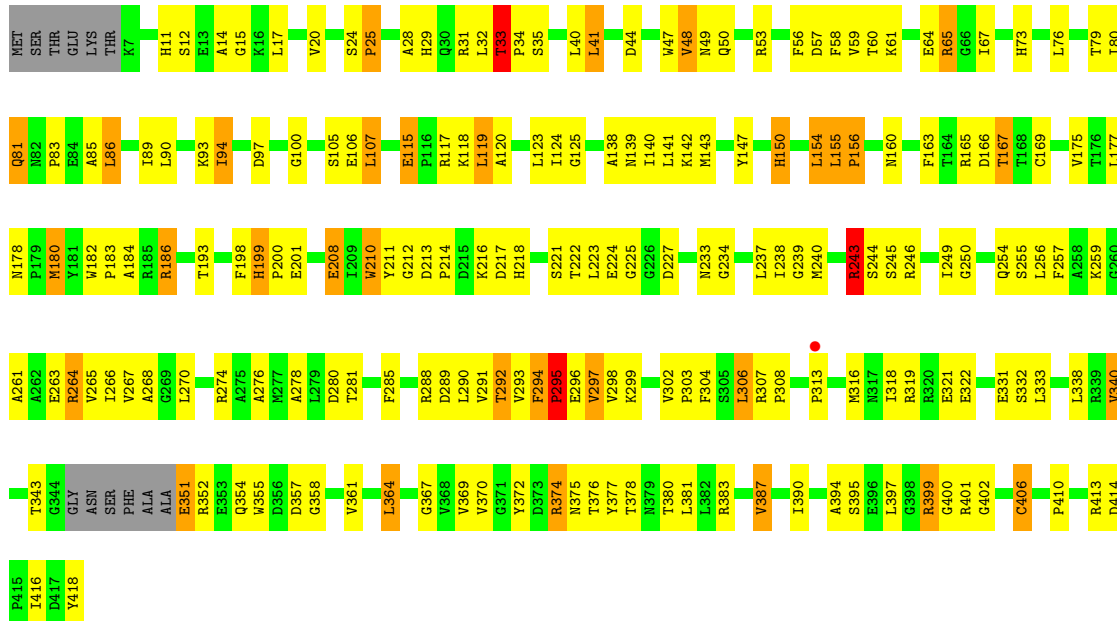


- Molecule 1: Arginine deiminase

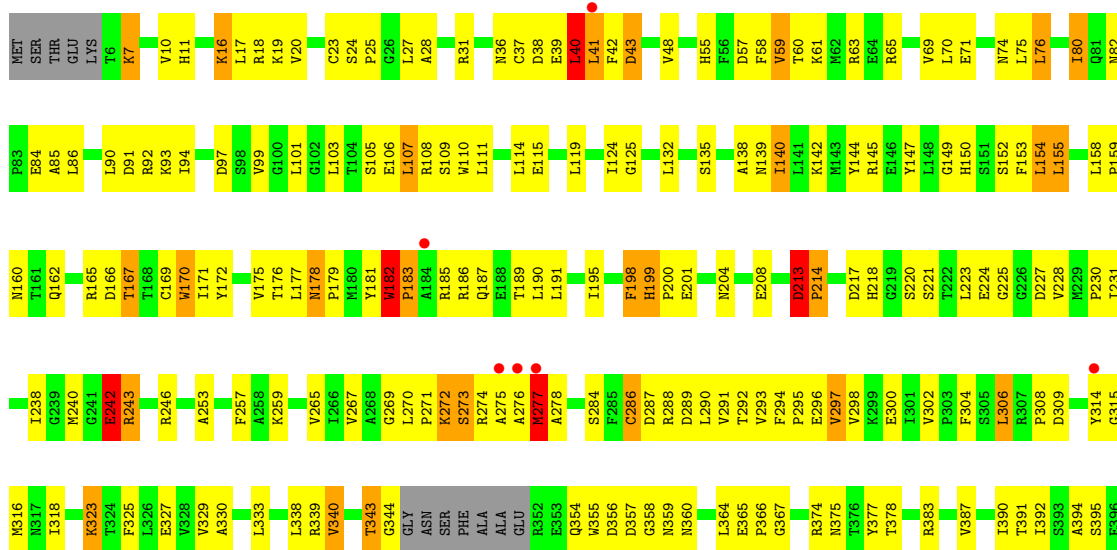




• Molecule 1: Arginine deiminase



• Molecule 1: Arginine deiminase



L397	G398	R399	G400	R401	G402	G403	G404	H405	C406	H407	T408	G409	P410	F411	V412	R413	D414	R415	L416	D417	Y418
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.80Å 121.20Å 151.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 98.6 (20.00-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.30Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.200 , 0.264 0.200 , 0.263	Depositor DCC
$R_{free}$ test set	3759 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtrriage
Anisotropy	0.290	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 56.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6062e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CYR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.90	2/3218 (0.1%)	1.41	54/4363 (1.2%)
1	B	0.96	1/3251 (0.0%)	1.33	38/4407 (0.9%)
1	C	0.86	0/3234	1.36	39/4383 (0.9%)
1	D	0.89	2/3232 (0.1%)	1.44	42/4381 (1.0%)
All	All	0.91	5/12935 (0.0%)	1.38	173/17534 (1.0%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	389	VAL	CA-CB	6.88	1.62	1.53
1	D	214	PRO	CA-C	-5.79	1.43	1.52
1	A	415	PRO	N-CD	5.18	1.55	1.47
1	A	284	SER	N-CA	5.12	1.52	1.45
1	D	390	ILE	CA-CB	5.08	1.61	1.54

All (173) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	277	MET	CA-C-N	22.12	152.68	121.05
1	D	277	MET	C-N-CA	22.12	152.68	121.05
1	C	166	ASP	N-CA-C	10.25	122.14	110.97
1	D	199	HIS	CA-C-N	10.01	129.65	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	HIS	C-N-CA	10.01	129.65	119.24
1	A	166	ASP	N-CA-C	10.00	121.94	111.14
1	A	294	PHE	CA-C-N	9.26	131.42	119.84
1	A	294	PHE	C-N-CA	9.26	131.42	119.84
1	C	154	LEU	N-CA-C	-9.26	101.27	111.36
1	D	364	LEU	N-CA-C	-9.25	101.56	113.12
1	B	230	PRO	CA-N-CD	-9.24	99.06	112.00
1	C	48	VAL	N-CA-C	9.13	119.16	110.30
1	A	156	PRO	O-C-N	9.11	132.21	121.46
1	A	354	GLN	OE1-CD-NE2	-8.99	113.61	122.60
1	B	178	ASN	N-CA-C	8.97	122.39	109.48
1	A	178	ASN	O-C-N	8.60	129.88	121.28
1	D	278	ALA	N-CA-CB	8.55	122.74	109.48
1	D	154	LEU	N-CA-C	-8.53	101.00	111.40
1	C	374	ARG	N-CA-C	8.44	121.61	111.82
1	B	167	THR	N-CA-C	8.41	120.45	111.28
1	D	166	ASP	N-CA-C	8.33	120.14	111.14
1	A	178	ASN	N-CA-C	8.29	121.69	109.50
1	D	340	VAL	N-CA-C	8.26	120.77	108.46
1	A	20	VAL	CB-CA-C	-8.24	97.50	110.69
1	C	292	THR	N-CA-C	-8.24	99.43	110.55
1	B	154	LEU	N-CA-C	-8.11	101.51	111.40
1	D	80	ILE	CB-CA-C	-8.02	101.31	112.14
1	A	157	PRO	CA-N-CD	-7.99	100.81	112.00
1	A	325	PHE	N-CA-C	-7.93	102.59	111.07
1	C	33	THR	CA-C-N	-7.89	111.66	119.87
1	C	33	THR	C-N-CA	-7.89	111.66	119.87
1	D	297	VAL	N-CA-C	7.59	118.51	111.45
1	A	179	PRO	CA-N-CD	-7.53	101.46	112.00
1	A	225	GLY	N-CA-C	7.50	121.98	112.83
1	A	81	GLN	N-CA-C	-7.41	103.70	112.89
1	D	198	PHE	N-CA-C	7.39	122.72	112.45
1	C	399	ARG	N-CA-C	-7.36	103.29	111.82
1	B	156	PRO	N-CA-C	7.34	117.51	110.47
1	A	230	PRO	CA-N-CD	-7.33	101.73	112.00
1	C	387	VAL	N-CA-C	7.33	118.43	108.17
1	C	340	VAL	N-CA-C	7.23	118.53	108.12
1	C	24	SER	CA-C-N	-7.18	112.92	120.03
1	C	24	SER	C-N-CA	-7.18	112.92	120.03
1	C	139	ASN	N-CA-C	7.03	118.95	111.28
1	A	414	ASP	CA-C-N	7.03	128.62	119.84
1	A	414	ASP	C-N-CA	7.03	128.62	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	115	GLU	CA-C-N	6.99	128.57	119.84
1	C	115	GLU	C-N-CA	6.99	128.57	119.84
1	B	20	VAL	CB-CA-C	-6.96	98.66	110.71
1	C	81	GLN	N-CA-C	-6.86	104.38	112.89
1	C	65	ARG	N-CA-C	-6.84	104.51	112.92
1	C	390	ILE	N-CA-C	-6.83	100.77	109.58
1	A	230	PRO	CA-C-N	-6.80	109.88	121.09
1	A	230	PRO	C-N-CA	-6.80	109.88	121.09
1	B	40	LEU	N-CA-C	-6.76	103.10	112.30
1	A	166	ASP	CB-CA-C	-6.75	100.23	110.90
1	D	11	HIS	N-CA-C	6.71	121.54	112.88
1	B	359	ASN	N-CA-C	-6.70	100.61	110.52
1	D	178	ASN	N-CA-C	6.67	121.52	109.44
1	B	166	ASP	N-CA-C	6.62	118.18	110.97
1	C	294	PHE	CA-C-N	6.61	128.10	119.84
1	C	294	PHE	C-N-CA	6.61	128.10	119.84
1	A	153	PHE	N-CA-C	6.59	119.02	108.41
1	A	187	GLN	N-CA-C	-6.53	104.24	111.36
1	C	11	HIS	N-CA-C	6.52	120.94	112.92
1	C	210	TRP	N-CA-C	6.49	118.44	111.36
1	A	38	ASP	N-CA-C	-6.46	105.42	113.55
1	B	212	GLY	N-CA-C	6.45	120.83	112.18
1	A	297	VAL	N-CA-C	6.44	116.58	110.53
1	B	191	LEU	N-CA-C	6.42	118.28	111.28
1	B	340	VAL	N-CA-C	6.39	117.99	108.46
1	B	55	HIS	N-CA-C	-6.39	103.83	111.69
1	A	354	GLN	CG-CD-NE2	6.34	125.92	116.40
1	B	361	VAL	N-CA-C	-6.33	103.15	110.05
1	C	178	ASN	N-CA-C	6.33	120.66	109.58
1	C	297	VAL	N-CA-C	6.30	116.45	110.53
1	C	186	ARG	N-CA-C	-6.26	105.60	113.18
1	A	167	THR	N-CA-C	6.24	120.63	112.89
1	C	243	ARG	N-CA-C	6.22	121.03	113.38
1	B	275	ALA	N-CA-C	6.20	120.57	113.19
1	D	399	ARG	N-CA-C	-6.20	105.68	113.18
1	B	199	HIS	CA-C-N	6.19	126.65	119.47
1	B	199	HIS	C-N-CA	6.19	126.65	119.47
1	B	307	ARG	O-C-N	6.11	125.62	121.71
1	A	302	VAL	N-CA-C	6.09	113.10	107.56
1	C	89	ILE	N-CA-C	6.09	116.14	110.42
1	B	374	ARG	N-CA-C	6.07	119.78	112.38
1	A	25	PRO	N-CA-C	-6.06	101.57	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	ARG	CA-C-N	6.05	126.07	119.90
1	B	307	ARG	C-N-CA	6.05	126.07	119.90
1	B	133	PRO	N-CA-C	-6.04	102.39	111.57
1	B	161	THR	N-CA-C	-6.04	104.77	111.71
1	D	153	PHE	N-CA-C	6.04	118.48	109.25
1	C	199	HIS	CA-C-N	5.98	125.69	119.05
1	C	199	HIS	C-N-CA	5.98	125.69	119.05
1	A	364	LEU	N-CA-C	-5.98	105.07	112.90
1	C	147	TYR	N-CA-C	5.97	120.73	112.90
1	D	41	LEU	N-CA-C	5.95	119.45	111.24
1	A	142	LYS	N-CA-C	-5.88	104.87	111.28
1	D	408	THR	N-CA-C	5.83	118.96	109.06
1	A	82	ASN	CA-C-N	5.82	126.22	119.47
1	A	82	ASN	C-N-CA	5.82	126.22	119.47
1	C	167	THR	N-CA-C	5.80	120.08	112.89
1	B	136	GLU	N-CA-C	-5.78	104.58	111.69
1	D	167	THR	N-CA-C	5.77	119.58	112.54
1	A	154	LEU	N-CA-C	-5.75	104.70	110.97
1	B	352	ARG	N-CA-C	-5.75	101.78	110.28
1	A	380	THR	N-CA-C	-5.72	105.12	111.36
1	B	386	GLY	N-CA-C	5.72	123.50	115.43
1	A	217	ASP	N-CA-C	-5.69	99.96	109.24
1	A	161	THR	N-CA-C	-5.68	105.18	111.71
1	D	170	TRP	N-CA-C	-5.64	100.05	109.24
1	D	155	LEU	N-CA-C	-5.63	101.82	110.32
1	C	94	ILE	N-CA-C	5.62	114.46	106.53
1	A	90	LEU	N-CA-C	5.58	117.80	111.11
1	A	11	HIS	CA-CB-CG	-5.57	108.23	113.80
1	B	388	GLU	N-CA-C	-5.51	101.00	109.76
1	D	343	THR	N-CA-C	5.50	117.37	108.34
1	C	94	ILE	CB-CA-C	-5.50	105.21	111.59
1	D	106	GLU	N-CA-C	5.43	116.89	110.97
1	D	140	ILE	N-CA-C	-5.43	104.30	111.09
1	D	48	VAL	N-CA-C	5.42	115.62	110.42
1	A	393	SER	N-CA-C	5.39	118.33	109.76
1	A	72	MET	N-CA-C	5.38	117.56	111.11
1	A	79	THR	N-CA-C	5.37	116.81	111.07
1	A	326	LEU	N-CA-C	5.36	117.12	111.28
1	B	198	PHE	N-CA-C	5.35	120.29	113.55
1	B	242	GLU	N-CA-C	5.35	116.79	111.07
1	D	302	VAL	CA-C-N	5.34	125.10	119.76
1	D	302	VAL	C-N-CA	5.34	125.10	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	N-CA-C	-5.33	106.55	113.16
1	D	228	VAL	N-CA-C	5.33	115.97	108.36
1	B	33	THR	N-CA-C	-5.32	100.88	109.82
1	D	242	GLU	N-CA-C	5.32	118.93	112.23
1	A	165	ARG	CA-C-N	5.31	127.67	120.44
1	A	165	ARG	C-N-CA	5.31	127.67	120.44
1	A	341	VAL	N-CA-C	-5.30	99.52	107.37
1	D	359	ASN	N-CA-C	-5.30	103.62	110.19
1	C	364	LEU	N-CA-C	-5.30	106.83	113.72
1	B	230	PRO	CA-C-N	-5.29	113.03	121.34
1	B	230	PRO	C-N-CA	-5.29	113.03	121.34
1	D	147	TYR	N-CA-C	5.28	119.81	112.90
1	D	259	LYS	N-CA-C	-5.27	106.71	112.72
1	A	186	ARG	N-CA-C	-5.26	106.82	113.18
1	D	182	TRP	CA-C-N	5.24	126.39	119.84
1	D	182	TRP	C-N-CA	5.24	126.39	119.84
1	B	390	ILE	CB-CA-C	-5.23	104.43	110.91
1	D	214	PRO	O-C-N	5.21	128.48	122.23
1	D	204	ASN	N-CA-C	5.20	119.60	113.16
1	B	308	PRO	CA-N-CD	-5.19	104.74	112.00
1	D	213	ASP	CA-CB-CG	-5.18	107.42	112.60
1	D	187	GLN	N-CA-C	5.18	118.70	112.38
1	A	157	PRO	CA-C-N	-5.17	116.67	123.34
1	A	157	PRO	C-N-CA	-5.17	116.67	123.34
1	B	292	THR	N-CA-C	-5.17	101.84	110.17
1	A	126	GLY	N-CA-C	-5.16	105.17	112.81
1	B	228	VAL	N-CA-C	5.14	116.69	108.87
1	C	198	PHE	N-CA-C	5.14	119.44	112.04
1	A	208	GLU	N-CA-C	5.13	118.05	110.46
1	B	225	GLY	N-CA-C	5.12	118.83	112.64
1	D	286	CYS	N-CA-C	-5.11	107.71	114.31
1	B	316	MET	N-CA-C	5.10	117.00	108.99
1	C	264	ARG	N-CA-C	5.07	116.76	108.55
1	C	150	HIS	N-CA-C	5.06	117.23	110.35
1	A	115	GLU	CA-C-N	5.05	126.16	119.84
1	A	115	GLU	C-N-CA	5.05	126.16	119.84
1	D	59	VAL	CA-C-N	5.05	127.05	120.28
1	D	59	VAL	C-N-CA	5.05	127.05	120.28
1	A	399	ARG	N-CA-C	-5.05	106.41	113.37
1	A	361	VAL	N-CA-C	-5.04	104.55	110.05
1	D	391	THR	N-CA-C	5.04	117.78	109.72
1	C	270	LEU	CA-C-N	5.01	124.91	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed( <sup>o</sup> )	Ideal( <sup>o</sup> )
1	C	270	LEU	C-N-CA	5.01	124.91	119.85

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3170	0	3160	233	0
1	B	3202	0	3185	192	0
1	C	3185	0	3168	216	0
1	D	3183	0	3169	234	0
2	A	227	0	0	82	0
2	B	209	0	0	54	0
2	C	187	0	0	79	0
2	D	179	0	0	74	0
All	All	13542	0	12682	847	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 33.

All (847) 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:C:364:LEU:HG	2:C:604:HOH:O	1.29	1.27
1:A:364:LEU:HB3	2:A:634:HOH:O	1.30	1.27
1:B:187:GLN:HG2	2:B:423:HOH:O	1.33	1.26
1:A:192:THR:HB	2:A:623:HOH:O	1.26	1.24
1:A:74:ASN:HB3	2:A:620:HOH:O	1.36	1.22
1:C:44:ASP:HB2	2:C:586:HOH:O	1.41	1.20
1:D:253:ALA:HB3	2:D:586:HOH:O	1.40	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:THR:HB	2:D:571:HOH:O	1.37	1.20
1:A:114:LEU:HB2	2:A:622:HOH:O	1.41	1.19
1:C:333:LEU:HA	2:C:597:HOH:O	1.40	1.18
1:B:357:ASP:HB3	2:B:614:HOH:O	1.45	1.17
1:A:14:ALA:HB2	2:A:621:HOH:O	1.43	1.15
1:A:140:ILE:HB	2:A:626:HOH:O	1.46	1.14
1:C:100:GLY:HA3	2:C:602:HOH:O	1.46	1.13
1:C:418:TYR:HD1	2:C:598:HOH:O	1.31	1.13
1:D:60:THR:HA	2:D:588:HOH:O	1.50	1.11
1:C:33:THR:HG22	1:C:35:SER:H	1.15	1.10
1:B:167:THR:HG22	1:B:168:THR:HG23	1.35	1.09
1:D:7:LYS:H	1:D:7:LYS:HD2	1.05	1.09
1:B:153:PHE:HD2	2:B:625:HOH:O	1.37	1.08
1:A:180:MET:HE2	2:A:481:HOH:O	1.54	1.08
1:D:343:THR:HG21	1:D:358:GLY:H	1.11	1.07
1:A:322:GLU:HG3	2:A:630:HOH:O	1.53	1.07
1:D:43:ASP:CG	1:D:401:ARG:HH12	1.60	1.07
1:B:277:MET:HE1	1:B:297:VAL:HG21	1.30	1.06
1:C:150:HIS:HD2	2:C:590:HOH:O	1.37	1.06
1:D:344:GLY:HA2	2:D:580:HOH:O	1.56	1.05
1:A:344:GLY:HA2	2:A:607:HOH:O	1.56	1.05
1:D:76:LEU:HG	2:D:583:HOH:O	1.54	1.04
1:B:257:PHE:CE2	1:B:308:PRO:HD3	1.92	1.03
1:B:352:ARG:HD2	2:B:620:HOH:O	1.58	1.03
1:B:397:LEU:HD22	2:B:622:HOH:O	1.57	1.02
1:B:145:ARG:HD3	1:B:152:SER:HB3	1.40	1.02
1:C:76:LEU:HD12	1:C:120:ALA:CB	1.91	1.00
1:D:293:VAL:HB	2:D:582:HOH:O	1.59	1.00
1:A:179:PRO:HD3	2:A:602:HOH:O	1.61	1.00
1:A:343:THR:HB	2:A:608:HOH:O	1.61	0.99
1:A:377:TYR:HD2	2:A:625:HOH:O	1.45	0.99
1:B:274:ARG:HB3	1:B:277:MET:HE2	1.40	0.99
1:D:276:ALA:HB1	2:D:577:HOH:O	1.61	0.98
1:B:99:VAL:HB	2:B:612:HOH:O	1.63	0.98
1:B:369:VAL:HG13	2:B:623:HOH:O	1.62	0.97
1:B:361:VAL:HB	2:B:623:HOH:O	1.64	0.97
1:D:69:VAL:HG21	2:D:570:HOH:O	1.65	0.96
1:D:124:ILE:HA	2:D:584:HOH:O	1.64	0.96
1:D:190:LEU:HD21	2:D:576:HOH:O	1.66	0.95
1:D:177:LEU:HB3	2:D:574:HOH:O	1.67	0.95
1:A:171:ILE:HG23	1:A:230:PRO:HG3	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:PHE:CE1	1:B:344:GLY:HA3	2.02	0.93
1:D:288:ARG:HD2	2:D:466:HOH:O	1.66	0.93
1:B:294:PHE:HE1	1:B:344:GLY:HA3	1.33	0.93
1:C:213:ASP:HB3	2:C:595:HOH:O	1.67	0.92
1:B:323:LYS:HB2	2:B:605:HOH:O	1.71	0.91
1:B:217:ASP:HA	2:C:582:HOH:O	1.68	0.91
1:C:274:ARG:HG2	1:C:297:VAL:HG22	1.51	0.91
1:A:38:ASP:HA	2:A:604:HOH:O	1.69	0.91
1:A:241:GLY:HA3	2:A:603:HOH:O	1.71	0.91
1:A:400:GLY:HA2	2:A:629:HOH:O	1.71	0.91
1:C:288:ARG:HB2	2:C:600:HOH:O	1.69	0.91
1:A:67:ILE:HD11	2:A:634:HOH:O	1.70	0.90
1:B:257:PHE:CD2	1:B:308:PRO:HD3	2.07	0.90
1:C:278:ALA:O	1:C:281:THR:HG22	1.71	0.90
1:D:7:LYS:H	1:D:7:LYS:CD	1.84	0.90
1:D:43:ASP:CG	1:D:401:ARG:NH1	2.28	0.90
1:C:31:ARG:HA	2:C:546:HOH:O	1.72	0.89
1:D:183:PRO:HA	1:D:186:ARG:NE	1.88	0.89
1:A:224:GLU:OE2	1:A:243:ARG:HD3	1.71	0.89
1:B:303:PRO:HG2	1:B:321:GLU:HB2	1.54	0.89
1:C:33:THR:HG22	1:C:35:SER:N	1.87	0.89
1:C:65:ARG:HB2	2:C:538:HOH:O	1.73	0.87
1:A:259:LYS:HD3	2:A:638:HOH:O	1.75	0.87
1:D:293:VAL:HG13	1:D:298:VAL:HG21	1.53	0.87
1:C:184:ALA:HB3	2:C:570:HOH:O	1.75	0.86
1:D:340:VAL:HB	2:D:582:HOH:O	1.75	0.86
1:A:274:ARG:HA	1:A:277:MET:HE3	1.57	0.86
1:A:274:ARG:HD2	1:A:277:MET:HE1	1.58	0.86
2:C:583:HOH:O	1:D:399:ARG:HG3	1.74	0.86
1:D:103:LEU:HD13	1:D:154:LEU:HD21	1.56	0.86
1:A:180:MET:SD	2:A:627:HOH:O	2.33	0.86
1:A:102:GLY:HA3	2:A:624:HOH:O	1.75	0.86
1:C:183:PRO:HA	1:C:186:ARG:HH11	1.37	0.86
1:A:293:VAL:O	1:A:295:PRO:HD3	1.76	0.86
1:A:286:CYS:HB2	1:A:290:LEU:HD12	1.58	0.85
1:C:374:ARG:NH2	1:D:399:ARG:HH21	1.73	0.85
1:D:7:LYS:HD2	1:D:7:LYS:N	1.89	0.85
1:D:186:ARG:HA	2:D:595:HOH:O	1.76	0.84
1:C:240:MET:HE2	1:C:246:ARG:HB3	1.60	0.84
1:D:59:VAL:HG13	2:D:570:HOH:O	1.76	0.84
1:B:17:LEU:HB2	2:B:601:HOH:O	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:ALA:HB2	2:D:581:HOH:O	1.78	0.83
1:C:180:MET:HA	1:C:180:MET:CE	2.09	0.83
1:B:25:PRO:HA	1:B:29:HIS:CE1	2.13	0.83
1:C:216:LYS:HB3	2:C:595:HOH:O	1.79	0.82
1:D:23:CYS:SG	2:D:593:HOH:O	2.35	0.82
1:C:76:LEU:HD12	1:C:120:ALA:HB1	1.60	0.82
1:A:259:LYS:CD	2:A:638:HOH:O	2.26	0.82
1:C:107:LEU:HD11	1:C:155:LEU:HD22	1.60	0.82
1:D:343:THR:HG21	1:D:358:GLY:N	1.92	0.82
1:A:17:LEU:HD21	1:A:20:VAL:HG13	1.61	0.82
1:C:156:PRO:HG2	2:C:594:HOH:O	1.79	0.81
2:C:583:HOH:O	1:D:399:ARG:CG	2.29	0.81
1:A:358:GLY:HA3	1:A:378:THR:HG21	1.62	0.81
1:B:306:LEU:HD11	1:B:316:MET:SD	2.20	0.81
1:C:180:MET:SD	2:C:588:HOH:O	2.39	0.81
1:C:67:ILE:HG22	2:C:540:HOH:O	1.80	0.80
1:D:99:VAL:HG13	1:D:154:LEU:HD22	1.62	0.80
1:D:124:ILE:HD13	2:D:593:HOH:O	1.81	0.80
1:A:25:PRO:HA	1:A:29:HIS:CE1	2.16	0.80
1:B:272:LYS:HD3	2:C:507:HOH:O	1.80	0.80
1:A:240:MET:HE3	1:A:267:VAL:CG1	2.12	0.80
1:B:413:ARG:CZ	2:B:601:HOH:O	2.29	0.80
1:A:337:LYS:HE3	2:A:473:HOH:O	1.81	0.80
1:A:377:TYR:CD2	2:A:625:HOH:O	2.23	0.80
1:B:72:MET:CE	2:B:421:HOH:O	2.30	0.80
1:B:274:ARG:HB3	1:B:277:MET:CE	2.12	0.80
1:A:240:MET:HE3	1:A:267:VAL:HG11	1.63	0.79
1:C:165:ARG:O	1:C:225:GLY:HA3	1.83	0.79
1:D:150:HIS:CE1	2:D:597:HOH:O	2.35	0.79
1:A:265:VAL:HG12	2:A:591:HOH:O	1.80	0.79
1:B:254:GLN:HB2	1:B:316:MET:HE2	1.62	0.79
1:D:416:ILE:HG13	1:D:417:ASP:H	1.48	0.79
1:C:180:MET:HA	1:C:180:MET:HE2	1.66	0.78
1:A:119:LEU:HB2	2:A:622:HOH:O	1.84	0.77
1:B:277:MET:HE1	1:B:297:VAL:CG2	2.14	0.77
1:B:349:ALA:HB2	2:B:487:HOH:O	1.84	0.77
1:C:33:THR:CG2	1:C:35:SER:H	1.94	0.77
1:D:401:ARG:HG2	1:D:401:ARG:HH11	1.50	0.77
1:D:191:LEU:CD1	2:D:584:HOH:O	2.33	0.77
1:D:76:LEU:CG	2:D:583:HOH:O	2.22	0.76
1:C:140:ILE:HA	1:C:143:MET:HE2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:LEU:HD11	1:C:20:VAL:HG13	1.68	0.76
1:B:72:MET:HE2	2:B:421:HOH:O	1.85	0.76
1:C:183:PRO:HA	1:C:186:ARG:NH1	2.00	0.76
1:D:107:LEU:HG	1:D:154:LEU:HD13	1.67	0.76
1:A:119:LEU:HG	2:A:622:HOH:O	1.86	0.75
1:D:189:THR:HA	2:D:571:HOH:O	1.85	0.75
1:D:214:PRO:HD3	2:D:574:HOH:O	1.86	0.75
1:C:374:ARG:NH2	1:D:399:ARG:NH2	2.34	0.75
1:C:224:GLU:HG3	2:C:543:HOH:O	1.85	0.75
1:C:14:ALA:HB2	2:C:541:HOH:O	1.86	0.75
1:B:257:PHE:CZ	1:B:308:PRO:HD3	2.21	0.75
1:C:218:HIS:ND1	2:C:593:HOH:O	2.20	0.75
1:D:63:ARG:HB3	2:D:588:HOH:O	1.87	0.75
1:D:277:MET:HB3	2:D:572:HOH:O	1.86	0.74
1:A:169:CYS:SG	1:A:225:GLY:HA2	2.27	0.74
1:A:119:LEU:CB	2:A:622:HOH:O	2.36	0.74
1:C:17:LEU:HD11	1:C:20:VAL:CG1	2.18	0.74
1:D:84:GLU:HG3	2:D:591:HOH:O	1.87	0.74
1:B:141:LEU:HB2	2:B:607:HOH:O	1.88	0.73
1:C:107:LEU:HD11	1:C:155:LEU:CD2	2.19	0.73
1:C:238:ILE:HB	2:C:571:HOH:O	1.89	0.73
1:A:99:VAL:HG21	1:A:107:LEU:HD12	1.72	0.72
1:B:166:ASP:OD1	1:B:406:CYS:H51	1.89	0.72
1:C:180:MET:HE2	2:C:543:HOH:O	1.89	0.72
1:A:43:ASP:HB3	1:A:399:ARG:O	1.88	0.72
1:B:337:LYS:CE	2:B:624:HOH:O	2.38	0.72
1:B:337:LYS:HE2	2:B:624:HOH:O	1.88	0.72
1:C:150:HIS:HA	2:C:507:HOH:O	1.88	0.72
1:D:330:ALA:HB2	1:D:338:LEU:HG	1.71	0.72
1:A:337:LYS:CE	2:A:473:HOH:O	2.37	0.71
1:C:17:LEU:HD21	1:C:20:VAL:HG11	1.72	0.71
1:B:217:ASP:CA	2:C:582:HOH:O	2.31	0.71
1:C:47:TRP:CZ2	2:C:587:HOH:O	2.42	0.71
1:D:223:LEU:HD23	1:D:224:GLU:N	2.06	0.71
1:A:182:TRP:HE1	1:A:243:ARG:HH21	1.37	0.71
1:A:267:VAL:HG23	2:A:591:HOH:O	1.89	0.71
1:D:316:MET:HE1	2:D:586:HOH:O	1.90	0.71
1:A:272:LYS:HG3	1:A:273:SER:H	1.56	0.71
1:C:199:HIS:HE1	1:C:201:GLU:HG3	1.55	0.71
1:C:216:LYS:CB	2:C:595:HOH:O	2.37	0.71
1:D:70:LEU:HD22	1:D:75:LEU:HD21	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ASP:OD1	1:C:61:LYS:HE3	1.90	0.71
1:C:93:LYS:HA	2:C:579:HOH:O	1.89	0.70
1:B:80:ILE:HG23	1:B:86:LEU:HG	1.73	0.70
1:C:240:MET:CE	1:C:246:ARG:HB3	2.20	0.70
1:A:107:LEU:HA	1:A:132:LEU:HD11	1.73	0.70
1:C:199:HIS:CE1	1:C:201:GLU:HG3	2.27	0.70
1:C:160:ASN:HD21	1:C:406:CYR:C1	2.05	0.69
1:D:242:GLU:HB3	2:D:471:HOH:O	1.92	0.69
1:B:274:ARG:CB	1:B:277:MET:HE2	2.19	0.69
1:D:290:LEU:O	1:D:291:VAL:HG13	1.92	0.69
1:A:102:GLY:CA	2:A:624:HOH:O	2.36	0.69
1:C:307:ARG:HD2	2:C:485:HOH:O	1.92	0.69
1:D:93:LYS:HB2	2:D:576:HOH:O	1.92	0.69
1:A:102:GLY:N	2:A:624:HOH:O	2.25	0.69
1:B:274:ARG:HG3	1:B:297:VAL:HG22	1.75	0.69
1:C:293:VAL:HG13	1:C:298:VAL:HG21	1.75	0.69
1:D:186:ARG:HA	2:D:569:HOH:O	1.91	0.69
1:C:303:PRO:HG2	1:C:321:GLU:HB2	1.75	0.69
1:D:360:ASN:HB3	2:D:482:HOH:O	1.93	0.69
1:B:372:TYR:CG	1:B:394:ALA:HB2	2.28	0.68
1:C:115:GLU:H	1:C:118:LYS:HZ2	1.41	0.68
1:A:324:THR:O	1:A:328:VAL:HG23	1.93	0.68
1:B:109:SER:HB2	2:B:528:HOH:O	1.94	0.68
1:B:217:ASP:CB	2:C:582:HOH:O	2.41	0.68
1:A:363:CYS:O	1:A:413:ARG:NH2	2.26	0.68
1:C:186:ARG:HG2	2:C:545:HOH:O	1.91	0.68
1:A:33:THR:HG23	1:A:35:SER:H	1.59	0.68
1:C:182:TRP:HB3	2:C:570:HOH:O	1.93	0.68
1:A:372:TYR:CG	1:A:394:ALA:HB2	2.30	0.67
1:B:349:ALA:N	1:B:352:ARG:HE	1.92	0.67
2:A:471:HOH:O	1:B:45:VAL:HG12	1.93	0.67
1:C:120:ALA:O	1:C:124:ILE:HD12	1.95	0.67
1:B:369:VAL:HG22	2:B:623:HOH:O	1.95	0.67
1:C:289:ASP:HB2	2:C:504:HOH:O	1.94	0.67
1:C:50:GLN:HB2	2:C:587:HOH:O	1.95	0.67
1:A:80:ILE:HD12	1:A:119:LEU:HD13	1.77	0.67
1:A:17:LEU:HD21	1:A:20:VAL:CG1	2.25	0.66
1:B:145:ARG:CD	1:B:152:SER:HB3	2.23	0.66
1:C:254:GLN:HB2	1:C:316:MET:HE2	1.77	0.66
1:D:76:LEU:HA	2:D:583:HOH:O	1.96	0.66
1:B:398:GLY:C	1:B:400:GLY:H	2.03	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ARG:HD3	2:A:616:HOH:O	1.95	0.66
1:A:231:ILE:HD12	1:A:333:LEU:HD13	1.77	0.66
1:C:211:TYR:CD1	2:C:585:HOH:O	2.47	0.66
1:C:376:THR:O	1:C:380:THR:HG23	1.96	0.66
1:C:296:GLU:HB2	2:C:503:HOH:O	1.96	0.66
1:B:397:LEU:HD13	2:B:622:HOH:O	1.96	0.65
1:B:331:GLU:HG2	2:B:608:HOH:O	1.95	0.65
1:D:276:ALA:O	1:D:277:MET:HB3	1.96	0.65
1:B:17:LEU:HD11	1:B:20:VAL:HG13	1.78	0.65
1:A:343:THR:HG21	1:A:378:THR:HG23	1.78	0.65
1:D:276:ALA:O	1:D:277:MET:CB	2.44	0.65
1:B:355:TRP:CH2	1:B:357:ASP:HB2	2.31	0.65
1:A:337:LYS:NZ	2:A:473:HOH:O	2.29	0.65
1:B:257:PHE:CG	1:B:308:PRO:HG3	2.32	0.64
1:B:374:ARG:NH1	2:B:603:HOH:O	2.29	0.64
1:A:267:VAL:CG2	2:A:591:HOH:O	2.45	0.64
1:A:71:GLU:HG3	1:A:74:ASN:H	1.63	0.64
1:B:132:LEU:HD11	1:B:154:LEU:HD11	1.80	0.64
1:A:274:ARG:HD2	1:A:277:MET:CE	2.28	0.64
1:C:254:GLN:HB2	1:C:316:MET:CE	2.28	0.64
1:A:240:MET:CE	1:A:267:VAL:HG11	2.28	0.64
1:A:267:VAL:N	2:A:591:HOH:O	2.30	0.63
1:A:286:CYS:HB2	1:A:290:LEU:CD1	2.26	0.63
1:C:193:THR:HG21	1:C:214:PRO:HG3	1.80	0.63
1:C:267:VAL:HB	1:C:304:PHE:HB2	1.80	0.63
1:A:88:TRP:HB2	2:A:577:HOH:O	1.98	0.63
1:B:303:PRO:CD	2:B:613:HOH:O	2.46	0.63
1:A:126:GLY:HA2	1:A:156:PRO:O	1.99	0.63
1:C:20:VAL:HG22	2:C:540:HOH:O	1.99	0.63
1:A:42:PHE:CD2	1:A:159:PRO:HB2	2.33	0.63
1:A:103:LEU:HD22	1:A:154:LEU:HD11	1.80	0.63
1:D:84:GLU:CG	2:D:591:HOH:O	2.44	0.63
1:A:119:LEU:CG	2:A:622:HOH:O	2.44	0.63
1:B:352:ARG:HG2	1:B:377:TYR:CE2	2.34	0.63
1:A:343:THR:HG21	1:A:378:THR:CG2	2.28	0.62
1:A:189:THR:HA	2:A:623:HOH:O	1.99	0.62
1:D:93:LYS:N	2:D:576:HOH:O	2.31	0.62
1:A:126:GLY:CA	1:A:156:PRO:O	2.48	0.62
1:A:398:GLY:C	1:A:400:GLY:H	2.07	0.62
1:C:115:GLU:H	1:C:118:LYS:NZ	1.97	0.62
1:D:191:LEU:HD11	2:D:584:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLU:HB3	2:B:605:HOH:O	1.99	0.62
1:D:343:THR:HB	2:D:544:HOH:O	1.99	0.62
1:D:416:ILE:HG23	1:D:417:ASP:N	2.14	0.62
1:C:274:ARG:HG2	1:C:297:VAL:CG2	2.27	0.62
1:C:313:PRO:HD2	2:C:510:HOH:O	1.99	0.62
1:B:272:LYS:NZ	2:B:618:HOH:O	2.31	0.62
1:D:43:ASP:CB	1:D:401:ARG:HH12	2.13	0.62
1:B:103:LEU:HD11	2:B:607:HOH:O	2.00	0.62
1:B:153:PHE:CD2	2:B:625:HOH:O	2.23	0.62
1:A:182:TRP:HD1	2:A:498:HOH:O	1.82	0.61
1:B:303:PRO:HD2	2:B:613:HOH:O	1.98	0.61
1:A:185:ARG:N	2:A:420:HOH:O	2.32	0.61
1:D:140:ILE:HG13	2:D:550:HOH:O	1.98	0.61
1:B:217:ASP:HB2	2:C:582:HOH:O	1.98	0.61
1:A:337:LYS:HD2	1:A:337:LYS:O	2.01	0.61
1:D:69:VAL:HG11	2:D:570:HOH:O	2.00	0.61
1:C:25:PRO:HA	1:C:29:HIS:CE1	2.36	0.61
1:A:43:ASP:HB2	1:A:401:ARG:HE	1.66	0.61
1:A:285:PHE:HB3	2:A:621:HOH:O	2.00	0.61
1:B:278:ALA:O	1:B:281:THR:HB	2.01	0.61
1:D:39:GLU:C	1:D:41:LEU:H	2.09	0.61
1:B:257:PHE:HB3	1:B:308:PRO:HG3	1.82	0.60
1:B:320:ARG:HD3	1:C:143:MET:HG2	1.83	0.60
1:B:320:ARG:HH11	1:B:320:ARG:HG2	1.66	0.60
1:C:265:VAL:HG12	2:C:571:HOH:O	2.02	0.60
1:C:401:ARG:HB2	1:C:406:CYR:HN22	1.66	0.60
1:A:208:GLU:OE1	1:A:259:LYS:HE2	2.01	0.60
1:B:318:ILE:HG21	1:C:140:ILE:HD13	1.82	0.60
1:D:416:ILE:HG13	1:D:417:ASP:N	2.16	0.60
1:D:132:LEU:HD11	1:D:154:LEU:HD11	1.84	0.60
1:A:39:GLU:OE2	1:A:39:GLU:O	2.19	0.60
2:A:448:HOH:O	1:D:150:HIS:HE1	1.82	0.60
1:A:41:LEU:HD12	2:A:441:HOH:O	2.02	0.59
1:D:242:GLU:HG3	1:D:243:ARG:HG2	1.82	0.59
1:A:288:ARG:HG3	1:A:288:ARG:HH11	1.67	0.59
1:D:132:LEU:HD11	1:D:154:LEU:CD1	2.33	0.59
1:D:182:TRP:HE3	1:D:183:PRO:HD3	1.68	0.59
1:A:99:VAL:HG12	1:A:103:LEU:HB2	1.85	0.59
1:D:343:THR:HG23	1:D:378:THR:OG1	2.03	0.59
1:A:368:VAL:HG13	1:A:388:GLU:HG2	1.85	0.59
1:C:81:GLN:O	1:C:83:PRO:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ARG:HA	1:D:387:VAL:O	2.02	0.59
1:A:399:ARG:HH12	1:B:399:ARG:HG2	1.68	0.59
1:B:401:ARG:HB3	2:B:572:HOH:O	2.02	0.59
1:D:36:ASN:O	1:D:38:ASP:N	2.36	0.59
1:D:314:TYR:O	1:D:316:MET:HG2	2.03	0.59
1:B:165:ARG:O	1:B:225:GLY:HA3	2.03	0.58
1:D:267:VAL:HB	1:D:304:PHE:HB2	1.85	0.58
1:D:291:VAL:HG23	1:D:340:VAL:HG12	1.85	0.58
1:A:145:ARG:HB2	1:A:152:SER:HB3	1.85	0.58
1:A:239:GLY:HA2	1:A:268:ALA:HB3	1.84	0.58
1:A:33:THR:HG23	1:A:35:SER:N	2.18	0.58
1:A:400:GLY:O	1:A:401:ARG:HB2	2.04	0.58
1:C:94:ILE:O	1:C:94:ILE:HG22	2.03	0.58
1:C:182:TRP:HE1	1:C:243:ARG:NH1	2.01	0.58
1:D:140:ILE:CG1	2:D:550:HOH:O	2.52	0.58
1:A:41:LEU:C	1:A:41:LEU:HD23	2.28	0.58
1:A:242:GLU:HB2	2:A:597:HOH:O	2.02	0.58
1:A:243:ARG:HB2	2:A:636:HOH:O	2.02	0.58
1:A:264:ARG:HD3	1:A:307:ARG:CZ	2.33	0.58
1:A:94:ILE:HD13	1:A:107:LEU:HD13	1.85	0.58
1:D:213:ASP:C	1:D:213:ASP:OD1	2.44	0.58
1:B:72:MET:HE1	2:B:458:HOH:O	2.01	0.58
1:B:254:GLN:HB2	1:B:316:MET:CE	2.32	0.58
1:A:274:ARG:CA	1:A:277:MET:HE3	2.31	0.57
1:C:169:CYS:O	1:C:175:VAL:HA	2.04	0.57
1:B:293:VAL:O	1:B:295:PRO:HD3	2.04	0.57
1:C:76:LEU:HD12	1:C:120:ALA:CA	2.34	0.57
1:C:156:PRO:CG	2:C:594:HOH:O	2.47	0.57
1:A:294:PHE:CD1	1:A:344:GLY:HA3	2.40	0.57
1:A:182:TRP:HE1	1:A:243:ARG:NH2	2.02	0.57
1:C:180:MET:HA	1:C:180:MET:HE3	1.84	0.57
1:D:323:LYS:HB3	1:D:327:GLU:OE1	2.04	0.57
1:B:169:CYS:SG	1:B:225:GLY:HA2	2.44	0.57
1:A:42:PHE:CE1	2:A:629:HOH:O	2.53	0.57
1:D:186:ARG:CA	2:D:569:HOH:O	2.51	0.57
1:A:65:ARG:HH11	1:A:65:ARG:HB3	1.70	0.57
1:B:318:ILE:CG2	1:C:140:ILE:HD13	2.35	0.57
1:D:158:LEU:HD12	2:D:584:HOH:O	2.04	0.57
1:A:77:THR:O	1:A:81:GLN:HG3	2.04	0.56
1:A:272:LYS:HG3	1:A:273:SER:N	2.20	0.56
1:A:295:PRO:CG	1:A:342:GLU:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:THR:O	1:C:293:VAL:HG23	2.06	0.56
1:C:295:PRO:O	1:C:299:LYS:HG2	2.06	0.56
1:C:338:LEU:O	1:C:340:VAL:HG23	2.06	0.56
1:C:394:ALA:HB3	2:C:566:HOH:O	2.05	0.56
1:B:145:ARG:HH11	1:B:152:SER:CB	2.17	0.56
1:D:7:LYS:CD	1:D:7:LYS:N	2.58	0.56
1:B:107:LEU:HD23	1:B:132:LEU:HD21	1.85	0.56
1:D:186:ARG:HB3	2:D:433:HOH:O	2.04	0.56
1:A:63:ARG:HD2	2:A:570:HOH:O	2.05	0.56
1:A:107:LEU:HD11	1:A:155:LEU:HD21	1.87	0.56
1:D:124:ILE:HG21	2:D:593:HOH:O	2.05	0.56
1:D:223:LEU:HD23	1:D:223:LEU:C	2.31	0.56
1:A:58:PHE:HE1	1:A:370:VAL:HG11	1.71	0.56
1:B:295:PRO:HB2	1:B:296:GLU:OE1	2.05	0.56
1:D:39:GLU:O	1:D:41:LEU:N	2.38	0.56
1:D:17:LEU:HD11	1:D:20:VAL:CG1	2.36	0.55
1:A:274:ARG:O	1:A:276:ALA:N	2.40	0.55
1:C:76:LEU:HD11	1:C:123:LEU:HD12	1.87	0.55
1:A:295:PRO:HG2	1:A:342:GLU:HB3	1.89	0.55
1:B:107:LEU:HD11	1:B:155:LEU:HD11	1.89	0.55
1:C:307:ARG:HB3	2:C:523:HOH:O	2.06	0.55
1:A:58:PHE:CE1	1:A:370:VAL:HG11	2.41	0.55
1:C:243:ARG:CZ	2:C:439:HOH:O	2.54	0.55
1:B:399:ARG:NE	2:B:453:HOH:O	2.38	0.55
1:D:183:PRO:O	1:D:186:ARG:HG3	2.07	0.55
1:C:160:ASN:ND2	1:C:406:CYR:C1	2.70	0.55
1:B:43:ASP:HB3	1:B:399:ARG:O	2.06	0.55
1:B:335:LEU:HD12	1:B:338:LEU:HD23	1.89	0.55
1:A:42:PHE:CE2	1:A:159:PRO:HB2	2.42	0.55
1:B:217:ASP:O	1:B:218:HIS:HB2	2.06	0.55
1:C:76:LEU:HD12	1:C:120:ALA:HB2	1.84	0.55
1:C:367:GLY:O	1:C:387:VAL:HG13	2.07	0.55
1:A:399:ARG:NH1	2:A:639:HOH:O	2.40	0.55
1:B:264:ARG:HD3	1:B:307:ARG:CZ	2.37	0.55
1:A:103:LEU:HD11	1:A:141:LEU:HD11	1.88	0.54
1:D:55:HIS:O	1:D:58:PHE:HB3	2.07	0.54
1:D:293:VAL:HG13	1:D:298:VAL:CG2	2.32	0.54
1:B:19:LYS:NZ	1:B:68:ASP:OD2	2.40	0.54
1:C:138:ALA:O	1:C:142:LYS:HG3	2.06	0.54
1:B:318:ILE:CG2	1:C:140:ILE:CD1	2.86	0.54
1:B:363:CYS:O	1:B:413:ARG:NH2	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ASN:C	1:D:38:ASP:H	2.16	0.54
1:D:183:PRO:HA	1:D:186:ARG:HE	1.68	0.54
1:D:165:ARG:CZ	1:D:405:HIS:CE1	2.91	0.54
1:A:102:GLY:C	1:A:103:LEU:HG	2.33	0.54
1:C:400:GLY:O	1:C:401:ARG:HB2	2.07	0.54
1:D:242:GLU:CB	2:D:471:HOH:O	2.54	0.54
1:B:197:LYS:HD3	1:B:198:PHE:CE2	2.43	0.54
1:C:296:GLU:HA	1:C:299:LYS:HE2	1.89	0.54
1:D:28:ALA:HB2	1:D:125:GLY:HA2	1.89	0.54
1:D:182:TRP:HB3	1:D:183:PRO:CD	2.38	0.54
1:B:119:LEU:HB3	2:B:619:HOH:O	2.08	0.53
1:B:240:MET:HE3	1:C:150:HIS:CD2	2.43	0.53
1:D:140:ILE:C	2:D:550:HOH:O	2.50	0.53
1:A:357:ASP:CB	2:A:607:HOH:O	2.56	0.53
1:B:81:GLN:O	1:B:83:PRO:HD3	2.09	0.53
1:C:306:LEU:HD21	1:C:318:ILE:HD12	1.90	0.53
1:D:288:ARG:HH22	1:D:417:ASP:HA	1.72	0.53
1:A:42:PHE:CZ	2:A:629:HOH:O	2.62	0.53
1:B:156:PRO:HG2	2:B:519:HOH:O	2.08	0.53
1:C:47:TRP:CE2	2:C:587:HOH:O	2.59	0.53
1:D:214:PRO:CD	2:D:574:HOH:O	2.51	0.53
1:B:398:GLY:C	1:B:400:GLY:N	2.66	0.53
1:C:211:TYR:CG	2:C:585:HOH:O	2.62	0.53
1:D:186:ARG:CA	2:D:595:HOH:O	2.46	0.53
1:A:72:MET:CE	2:A:546:HOH:O	2.57	0.53
1:B:274:ARG:N	1:B:274:ARG:HD2	2.23	0.53
1:B:397:LEU:CD2	2:B:622:HOH:O	2.33	0.53
1:C:233:ASN:CG	2:C:597:HOH:O	2.52	0.53
1:C:76:LEU:CD1	1:C:120:ALA:CB	2.76	0.53
1:D:325:PHE:O	1:D:329:VAL:HG23	2.09	0.53
1:B:333:LEU:HD22	1:B:418:TYR:CE1	2.44	0.53
1:B:397:LEU:CG	2:B:622:HOH:O	2.55	0.53
1:C:41:LEU:HD11	2:C:570:HOH:O	2.08	0.53
1:C:211:TYR:CE1	2:C:585:HOH:O	2.62	0.53
1:A:231:ILE:HD12	1:A:333:LEU:CD1	2.38	0.52
1:B:294:PHE:CD1	1:B:344:GLY:HA3	2.41	0.52
1:A:36:ASN:C	1:A:36:ASN:OD1	2.52	0.52
1:D:40:LEU:N	1:D:40:LEU:CD1	2.72	0.52
1:D:295:PRO:O	1:D:296:GLU:C	2.53	0.52
1:A:171:ILE:CG2	1:A:230:PRO:HG3	2.31	0.52
1:A:259:LYS:HD2	2:A:638:HOH:O	2.01	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASP:OD2	1:C:218:HIS:HA	2.09	0.52
1:B:187:GLN:N	2:B:423:HOH:O	2.41	0.52
1:B:370:VAL:HA	1:B:390:ILE:O	2.10	0.52
1:C:177:LEU:O	1:C:212:GLY:HA3	2.08	0.52
1:A:400:GLY:O	1:A:401:ARG:CB	2.55	0.52
1:B:397:LEU:N	2:B:622:HOH:O	2.42	0.52
1:C:20:VAL:HG12	1:C:410:PRO:HA	1.92	0.52
1:C:41:LEU:HD21	2:C:570:HOH:O	2.08	0.52
1:C:67:ILE:HD11	1:C:364:LEU:HB3	1.91	0.52
1:C:211:TYR:OH	1:C:221:SER:HB3	2.10	0.52
1:D:257:PHE:HZ	1:D:306:LEU:O	1.91	0.52
1:B:44:ASP:CG	1:B:45:VAL:H	2.16	0.52
1:D:85:ALA:HB2	1:D:198:PHE:CG	2.44	0.52
1:D:23:CYS:HA	1:D:71:GLU:OE2	2.09	0.52
1:C:257:PHE:CG	1:C:308:PRO:HG3	2.45	0.52
1:C:343:THR:HG22	1:C:378:THR:OG1	2.10	0.52
1:D:16:LYS:HB3	1:D:18:ARG:HH12	1.74	0.52
1:D:101:LEU:HA	2:D:578:HOH:O	2.10	0.52
1:A:94:ILE:HD11	1:A:111:LEU:HD12	1.92	0.52
1:D:140:ILE:CB	2:D:550:HOH:O	2.57	0.52
1:D:288:ARG:NH2	1:D:417:ASP:HA	2.25	0.52
1:B:17:LEU:HD21	1:B:20:VAL:CG1	2.40	0.52
1:D:186:ARG:HB3	2:D:569:HOH:O	2.10	0.52
1:A:43:ASP:HA	1:A:401:ARG:HH21	1.75	0.51
1:A:294:PHE:CE1	1:A:344:GLY:HA3	2.45	0.51
1:B:288:ARG:HD2	2:B:439:HOH:O	2.10	0.51
1:C:160:ASN:HB2	2:C:480:HOH:O	2.10	0.51
1:D:182:TRP:O	1:D:186:ARG:CZ	2.58	0.51
1:A:140:ILE:HD12	1:D:318:ILE:HG21	1.92	0.51
1:D:195:ILE:HG13	2:D:583:HOH:O	2.09	0.51
1:A:227:ASP:O	1:A:238:ILE:HA	2.10	0.51
1:B:145:ARG:HD3	1:B:152:SER:CB	2.26	0.51
1:B:318:ILE:HG23	1:C:140:ILE:HD11	1.91	0.51
1:A:268:ALA:HB1	1:A:301:ILE:CD1	2.40	0.51
1:C:224:GLU:OE1	1:C:243:ARG:NE	2.44	0.51
1:D:63:ARG:HG2	1:D:63:ARG:HH11	1.75	0.51
1:B:43:ASP:HB2	1:B:401:ARG:HE	1.75	0.51
1:B:86:LEU:HD22	1:B:90:LEU:HG	1.93	0.51
1:C:180:MET:CE	1:C:180:MET:CA	2.84	0.51
1:D:63:ARG:HG2	1:D:63:ARG:NH1	2.25	0.51
1:D:107:LEU:HD11	1:D:155:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:HD3	2:C:595:HOH:O	2.10	0.51
1:D:92:ARG:HG3	1:D:92:ARG:HH11	1.76	0.51
1:D:231:ILE:HD12	1:D:333:LEU:HD21	1.92	0.51
1:A:165:ARG:O	1:A:225:GLY:HA3	2.11	0.51
1:C:238:ILE:CB	2:C:571:HOH:O	2.52	0.51
1:C:239:GLY:HA2	1:C:268:ALA:HB3	1.93	0.51
1:A:144:TYR:CZ	1:D:240:MET:HE1	2.46	0.50
1:A:398:GLY:C	1:A:400:GLY:N	2.68	0.50
1:D:76:LEU:O	1:D:80:ILE:HG13	2.11	0.50
1:A:33:THR:HG22	1:A:36:ASN:CG	2.37	0.50
1:A:171:ILE:O	1:A:172:TYR:C	2.53	0.50
1:D:140:ILE:HB	2:D:550:HOH:O	2.11	0.50
1:D:199:HIS:CG	1:D:200:PRO:HD2	2.46	0.50
1:B:257:PHE:CG	1:B:308:PRO:HD3	2.46	0.50
1:B:309:ASP:O	1:B:315:GLY:HA2	2.11	0.50
1:C:93:LYS:HE3	1:C:155:LEU:HG	1.93	0.50
1:D:36:ASN:C	1:D:38:ASP:N	2.69	0.50
1:D:199:HIS:HD2	1:D:201:GLU:H	1.58	0.50
1:D:243:ARG:NH2	1:D:406:CYR:O1	2.44	0.50
1:D:292:THR:HG21	2:D:493:HOH:O	2.12	0.50
1:A:180:MET:CE	2:A:627:HOH:O	2.59	0.50
1:A:374:ARG:NH1	1:B:47:TRP:HB2	2.26	0.50
1:C:73:HIS:HB3	1:C:117:ARG:NH1	2.27	0.50
1:A:103:LEU:HD13	1:A:154:LEU:CD1	2.41	0.50
1:C:199:HIS:ND1	1:C:201:GLU:HB2	2.26	0.50
1:C:238:ILE:N	2:C:571:HOH:O	2.45	0.50
1:B:70:LEU:HD22	1:B:75:LEU:HD21	1.93	0.50
1:B:257:PHE:CB	1:B:308:PRO:HG3	2.42	0.50
1:B:398:GLY:O	1:B:400:GLY:N	2.44	0.50
1:C:322:GLU:HG2	2:C:498:HOH:O	2.12	0.50
1:D:57:ASP:O	1:D:61:LYS:HG3	2.11	0.50
1:A:163:PHE:HZ	1:A:400:GLY:HA3	1.77	0.49
1:A:399:ARG:CZ	2:A:584:HOH:O	2.60	0.49
1:D:16:LYS:HB3	1:D:18:ARG:NH1	2.26	0.49
1:C:117:ARG:HD3	2:C:513:HOH:O	2.11	0.49
1:B:48:VAL:O	1:B:52:LYS:HG3	2.12	0.49
1:D:59:VAL:HA	2:D:570:HOH:O	2.11	0.49
1:B:318:ILE:HG23	1:C:140:ILE:CD1	2.43	0.49
1:C:240:MET:HE2	1:C:246:ARG:CB	2.39	0.49
1:A:70:LEU:HB3	1:A:75:LEU:HD11	1.93	0.49
1:B:44:ASP:OD2	1:B:45:VAL:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ARG:HG2	1:C:319:ARG:HH11	1.77	0.49
1:C:375:ASN:ND2	2:C:433:HOH:O	2.37	0.49
1:D:271:PRO:HG3	1:D:300:GLU:CB	2.43	0.49
1:A:229:MET:HE1	1:A:283:PHE:HD2	1.78	0.49
1:B:36:ASN:OD1	1:B:36:ASN:C	2.55	0.49
1:B:374:ARG:HD2	2:B:493:HOH:O	2.13	0.49
1:D:289:ASP:CG	1:D:339:ARG:HE	2.19	0.49
1:B:295:PRO:HG3	1:B:342:GLU:HG2	1.94	0.49
1:C:17:LEU:HD21	1:C:20:VAL:CG1	2.40	0.49
1:D:377:TYR:HB2	2:D:558:HOH:O	2.11	0.49
1:B:320:ARG:HG2	1:B:320:ARG:NH1	2.26	0.49
1:C:208:GLU:HG2	1:C:210:TRP:CZ3	2.47	0.49
1:A:185:ARG:HD3	2:A:498:HOH:O	2.13	0.49
1:A:288:ARG:HG3	1:A:288:ARG:NH1	2.28	0.49
1:A:314:TYR:HD2	2:A:554:HOH:O	1.95	0.49
1:D:31:ARG:HG2	1:D:31:ARG:HH11	1.77	0.49
1:A:17:LEU:HB2	1:A:413:ARG:HH21	1.76	0.49
1:A:183:PRO:HD2	2:A:453:HOH:O	2.12	0.49
1:A:74:ASN:O	1:A:78:GLU:HG3	2.13	0.48
1:A:240:MET:HE3	1:A:267:VAL:HG13	1.94	0.48
1:D:199:HIS:CD2	1:D:201:GLU:H	2.31	0.48
1:D:401:ARG:NH1	1:D:401:ARG:HG2	2.22	0.48
1:A:184:ALA:C	2:A:420:HOH:O	2.55	0.48
1:B:43:ASP:HA	1:B:401:ARG:HH21	1.79	0.48
1:B:224:GLU:HG3	1:B:243:ARG:HB3	1.95	0.48
1:B:333:LEU:HD22	1:B:418:TYR:CZ	2.48	0.48
1:A:297:VAL:O	1:A:301:ILE:HG22	2.13	0.48
1:B:287:ASP:O	1:B:288:ARG:C	2.56	0.48
1:C:32:LEU:HD23	1:C:40:LEU:HD23	1.96	0.48
1:D:150:HIS:ND1	2:D:597:HOH:O	2.35	0.48
1:D:175:VAL:HG22	1:D:176:THR:N	2.27	0.48
1:C:28:ALA:HB2	1:C:125:GLY:HA2	1.95	0.48
1:A:31:ARG:HG2	1:A:31:ARG:HH11	1.78	0.48
1:D:10:VAL:CG2	1:D:170:TRP:HB2	2.44	0.48
1:D:308:PRO:HG2	2:D:549:HOH:O	2.13	0.48
1:A:209:ILE:O	1:A:209:ILE:HG22	2.14	0.48
1:B:12:SER:HA	1:B:230:PRO:O	2.14	0.48
1:B:116:PRO:O	2:B:619:HOH:O	2.20	0.48
1:D:57:ASP:HB2	2:D:484:HOH:O	2.13	0.48
1:D:416:ILE:HG23	1:D:417:ASP:H	1.78	0.48
1:A:169:CYS:HB2	1:A:176:THR:OG1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:ARG:CB	2:C:600:HOH:O	2.45	0.48
1:C:255:SER:O	1:C:256:LEU:C	2.55	0.48
1:A:72:MET:HE1	2:A:582:HOH:O	2.14	0.48
1:A:187:GLN:CG	2:A:613:HOH:O	2.62	0.48
1:C:374:ARG:HH22	1:D:399:ARG:HH21	1.56	0.48
1:A:167:THR:HG23	2:A:595:HOH:O	2.13	0.47
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.79	0.47
1:B:18:ARG:HD2	1:B:414:ASP:OD2	2.14	0.47
1:C:243:ARG:NE	2:C:439:HOH:O	2.46	0.47
1:D:17:LEU:HD21	1:D:20:VAL:HG11	1.95	0.47
1:A:31:ARG:HD2	1:A:157:PRO:HG3	1.95	0.47
1:B:337:LYS:HE3	2:B:624:HOH:O	2.09	0.47
1:C:216:LYS:HG2	1:C:217:ASP:N	2.28	0.47
1:C:222:THR:O	1:C:244:SER:HA	2.14	0.47
1:C:254:GLN:CB	1:C:316:MET:HE2	2.43	0.47
1:D:374:ARG:HD2	1:D:394:ALA:HB3	1.96	0.47
1:A:224:GLU:O	1:A:227:ASP:HB2	2.14	0.47
1:B:372:TYR:CD2	1:B:394:ALA:HB2	2.49	0.47
1:D:185:ARG:N	2:D:489:HOH:O	2.46	0.47
1:D:199:HIS:CD2	1:D:200:PRO:HD2	2.49	0.47
1:A:141:LEU:HD21	1:D:246:ARG:NE	2.30	0.47
1:B:17:LEU:CA	2:B:601:HOH:O	2.61	0.47
1:C:186:ARG:HA	2:C:545:HOH:O	2.14	0.47
1:D:19:LYS:HB3	1:D:412:VAL:HG23	1.95	0.47
1:D:40:LEU:HD13	1:D:40:LEU:H	1.79	0.47
1:D:165:ARG:O	1:D:225:GLY:HA3	2.14	0.47
1:A:60:THR:O	1:A:64:GLU:HG2	2.15	0.47
1:A:58:PHE:CD1	1:A:392:ILE:HD13	2.49	0.47
1:A:257:PHE:HZ	1:A:306:LEU:O	1.98	0.47
1:A:267:VAL:HB	1:A:304:PHE:HB2	1.97	0.47
1:B:43:ASP:HB2	1:B:401:ARG:HG3	1.97	0.47
1:B:84:GLU:HG2	1:B:198:PHE:CE1	2.50	0.47
1:C:358:GLY:HA3	1:C:378:THR:HG21	1.97	0.47
1:D:10:VAL:HG23	1:D:170:TRP:HB2	1.96	0.47
1:D:41:LEU:HD13	1:D:406:CYR:O2	2.15	0.47
1:A:99:VAL:CG1	1:A:103:LEU:HB2	2.43	0.47
1:B:99:VAL:HG12	1:B:99:VAL:O	2.13	0.47
1:C:15:GLY:HA3	1:C:414:ASP:O	2.14	0.47
1:C:90:LEU:HD22	1:C:94:ILE:CD1	2.45	0.47
1:D:23:CYS:HB3	1:D:162:GLN:HA	1.97	0.47
1:D:39:GLU:C	1:D:41:LEU:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:CD1	1:A:107:LEU:HD13	2.45	0.47
1:A:263:GLU:HG2	2:A:572:HOH:O	2.14	0.47
1:B:43:ASP:HB2	1:B:401:ARG:NE	2.30	0.47
1:C:150:HIS:CD2	2:C:590:HOH:O	2.26	0.47
1:C:276:ALA:CB	2:C:572:HOH:O	2.62	0.47
1:D:108:ARG:O	1:D:109:SER:C	2.56	0.47
1:A:72:MET:HE1	2:A:546:HOH:O	2.13	0.47
1:B:370:VAL:N	2:B:623:HOH:O	2.48	0.47
1:C:245:SER:O	1:C:249:ILE:HG13	2.15	0.47
1:D:110:TRP:O	1:D:111:LEU:C	2.58	0.47
1:D:144:TYR:HE2	2:D:542:HOH:O	1.96	0.47
1:D:394:ALA:O	1:D:395:SER:C	2.57	0.47
1:A:357:ASP:CA	2:A:607:HOH:O	2.63	0.47
1:B:247:GLN:HG3	1:C:97:ASP:O	2.15	0.47
1:D:145:ARG:HD3	1:D:152:SER:HB2	1.97	0.47
1:B:36:ASN:O	1:B:40:LEU:HB2	2.15	0.46
1:C:383:ARG:HG3	1:C:383:ARG:HH11	1.81	0.46
1:D:40:LEU:CD1	1:D:40:LEU:H	2.27	0.46
1:A:241:GLY:N	2:A:549:HOH:O	2.35	0.46
1:B:397:LEU:CD1	2:B:622:HOH:O	2.61	0.46
1:C:100:GLY:CA	2:C:602:HOH:O	2.27	0.46
1:C:374:ARG:HH21	1:D:399:ARG:HH21	1.58	0.46
2:C:583:HOH:O	1:D:399:ARG:HG2	2.05	0.46
1:D:59:VAL:CA	2:D:570:HOH:O	2.62	0.46
1:D:272:LYS:O	1:D:273:SER:HB3	2.14	0.46
1:A:303:PRO:HG2	1:A:321:GLU:HB2	1.96	0.46
1:B:254:GLN:CB	1:B:316:MET:HE2	2.38	0.46
1:C:76:LEU:HD12	1:C:120:ALA:HA	1.98	0.46
1:C:293:VAL:CG1	1:C:294:PHE:N	2.79	0.46
1:A:36:ASN:O	1:A:40:LEU:HB2	2.16	0.46
1:B:50:GLN:NE2	1:B:54:ASP:OD1	2.48	0.46
1:C:57:ASP:O	1:C:61:LYS:HG3	2.15	0.46
1:C:60:THR:O	1:C:64:GLU:HG3	2.15	0.46
1:D:135:SER:O	1:D:139:ASN:ND2	2.48	0.46
1:C:313:PRO:HD3	2:C:502:HOH:O	2.15	0.46
1:D:177:LEU:CB	2:D:574:HOH:O	2.44	0.46
1:A:185:ARG:CZ	2:A:627:HOH:O	2.63	0.46
1:D:355:TRP:CZ2	1:D:357:ASP:HB2	2.50	0.46
1:C:163:PHE:CE2	1:C:406:CYP:HC2	2.51	0.46
1:C:180:MET:HE1	1:C:224:GLU:HG2	1.96	0.46
1:C:210:TRP:CH2	1:C:261:ALA:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:CYS:O	1:D:175:VAL:HG23	2.16	0.46
1:A:272:LYS:HE2	1:D:149:GLY:HA3	1.98	0.46
1:A:337:LYS:HD2	1:A:337:LYS:C	2.41	0.46
1:B:246:ARG:HG2	1:B:247:GLN:OE1	2.16	0.46
1:C:14:ALA:HB3	1:C:416:ILE:CD1	2.46	0.46
1:A:94:ILE:HG23	1:A:99:VAL:HG21	1.97	0.46
1:B:104:THR:N	2:B:612:HOH:O	2.48	0.46
1:C:49:ASN:HB3	1:C:53:ARG:NH2	2.30	0.46
1:C:276:ALA:HB3	2:C:572:HOH:O	2.16	0.46
1:D:217:ASP:O	1:D:218:HIS:HB2	2.16	0.46
1:C:355:TRP:CH2	1:C:357:ASP:HB2	2.50	0.45
1:C:399:ARG:NH2	2:C:583:HOH:O	2.49	0.45
1:D:172:TYR:HB3	2:D:449:HOH:O	2.15	0.45
1:C:48:VAL:HG23	1:D:354:GLN:OE1	2.16	0.45
1:C:374:ARG:HH21	1:D:399:ARG:NH2	2.14	0.45
1:A:339:ARG:C	1:A:340:VAL:HG23	2.42	0.45
1:A:339:ARG:HA	2:A:467:HOH:O	2.16	0.45
1:B:343:THR:O	1:B:344:GLY:C	2.59	0.45
1:A:10:VAL:HG21	1:A:410:PRO:HB2	1.99	0.45
1:A:106:GLU:HG3	2:A:576:HOH:O	2.16	0.45
1:A:237:LEU:HD23	1:A:266:ILE:HB	1.99	0.45
1:A:363:CYS:HA	1:A:369:VAL:HG23	1.98	0.45
1:C:76:LEU:CD1	1:C:120:ALA:HB2	2.43	0.45
1:D:284:SER:O	1:D:291:VAL:HA	2.16	0.45
1:A:94:ILE:HD11	1:A:111:LEU:CD1	2.47	0.45
1:A:399:ARG:NE	2:A:584:HOH:O	2.50	0.45
1:A:26:GLY:HA2	1:A:52:LYS:HE2	1.99	0.45
1:A:29:HIS:HA	1:A:32:LEU:HG	1.99	0.45
1:A:242:GLU:N	2:A:603:HOH:O	2.46	0.45
1:A:392:ILE:HB	2:A:575:HOH:O	2.17	0.45
1:C:397:LEU:HD13	2:C:427:HOH:O	2.17	0.45
1:A:175:VAL:HG22	1:A:176:THR:N	2.32	0.45
1:A:206:GLU:HG3	2:A:525:HOH:O	2.16	0.45
1:B:43:ASP:CB	1:B:401:ARG:HE	2.30	0.45
1:C:33:THR:HG23	1:C:34:PRO:CD	2.47	0.45
1:C:167:THR:HG23	2:C:425:HOH:O	2.16	0.45
1:A:268:ALA:HB1	1:A:301:ILE:HD12	1.98	0.45
1:B:17:LEU:HD21	1:B:20:VAL:HG13	1.98	0.45
1:D:65:ARG:HD2	2:D:442:HOH:O	2.17	0.44
1:D:186:ARG:C	2:D:595:HOH:O	2.60	0.44
1:D:286:CYS:SG	1:D:292:THR:HG23	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:VAL:CG2	2:D:582:HOH:O	2.65	0.44
1:A:210:TRP:HZ3	1:A:259:LYS:HG2	1.82	0.44
1:A:259:LYS:C	1:A:261:ALA:H	2.25	0.44
1:B:374:ARG:NE	2:B:456:HOH:O	2.45	0.44
1:A:210:TRP:CH2	1:A:261:ALA:HB2	2.53	0.44
1:C:295:PRO:O	1:C:296:GLU:C	2.60	0.44
1:B:77:THR:HG23	1:B:117:ARG:N	2.33	0.44
1:C:180:MET:HG2	2:C:545:HOH:O	2.18	0.44
1:D:246:ARG:HD2	2:D:562:HOH:O	2.17	0.44
1:D:270:LEU:HD22	1:D:277:MET:O	2.18	0.44
1:B:257:PHE:CD2	1:B:308:PRO:CD	2.93	0.44
1:C:56:PHE:HA	2:C:539:HOH:O	2.17	0.44
1:D:287:ASP:HB3	1:D:290:LEU:HB2	1.99	0.44
1:A:298:VAL:HA	1:A:301:ILE:CG2	2.47	0.44
1:B:235:VAL:HG21	1:B:332:SER:HB2	1.99	0.44
1:D:272:LYS:HD3	1:D:273:SER:H	1.83	0.44
1:D:274:ARG:C	1:D:276:ALA:H	2.26	0.44
1:A:357:ASP:HA	2:A:608:HOH:O	2.17	0.44
1:B:89:ILE:HD11	1:B:194:ALA:HB1	2.00	0.44
1:C:40:LEU:C	1:C:41:LEU:HD12	2.42	0.44
1:C:361:VAL:HG22	2:C:544:HOH:O	2.17	0.44
1:A:293:VAL:HB	1:A:298:VAL:HG21	2.00	0.44
1:B:381:LEU:HA	1:B:381:LEU:HD23	1.78	0.44
1:D:82:ASN:OD1	1:D:82:ASN:C	2.60	0.44
1:A:399:ARG:HG2	1:B:399:ARG:HH12	1.83	0.43
1:B:148:LEU:HD21	1:C:302:VAL:HB	2.01	0.43
1:B:252:VAL:O	1:B:256:LEU:HG	2.18	0.43
1:B:320:ARG:HD3	1:C:143:MET:CG	2.48	0.43
1:C:293:VAL:HG13	1:C:298:VAL:CG2	2.46	0.43
1:D:189:THR:CB	2:D:571:HOH:O	2.65	0.43
1:D:227:ASP:O	1:D:238:ILE:HA	2.18	0.43
1:B:126:GLY:HA2	1:B:155:LEU:O	2.18	0.43
1:C:150:HIS:CE1	2:C:517:HOH:O	2.70	0.43
1:D:43:ASP:OD1	1:D:401:ARG:NH1	2.44	0.43
1:D:189:THR:HG23	2:D:571:HOH:O	2.17	0.43
1:A:163:PHE:CD2	1:A:406:CYR:HC2	2.53	0.43
1:C:399:ARG:NH1	1:D:374:ARG:NH2	2.66	0.43
1:D:80:ILE:HD13	1:D:80:ILE:HG21	1.78	0.43
1:D:101:LEU:HA	1:D:101:LEU:HD23	1.75	0.43
1:D:213:ASP:OD1	1:D:214:PRO:N	2.50	0.43
1:A:51:ALA:HB1	1:A:397:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:CD1	1:A:141:LEU:HD11	2.48	0.43
1:B:86:LEU:HD22	1:B:90:LEU:CD1	2.48	0.43
1:B:103:LEU:HD13	1:B:154:LEU:CD2	2.48	0.43
1:D:177:LEU:HD13	2:D:574:HOH:O	2.17	0.43
1:B:126:GLY:CA	1:B:155:LEU:O	2.66	0.43
1:C:167:THR:H	1:C:167:THR:HG22	1.47	0.43
1:C:186:ARG:NH2	2:C:437:HOH:O	2.50	0.43
1:D:277:MET:HG2	2:D:572:HOH:O	2.18	0.43
1:A:165:ARG:CZ	1:A:405:HIS:CE1	3.02	0.43
1:B:266:ILE:HD13	1:B:328:VAL:CG1	2.48	0.43
1:A:180:MET:CE	2:A:481:HOH:O	2.36	0.43
1:B:17:LEU:HD13	1:B:413:ARG:NH1	2.33	0.43
1:B:193:THR:HG21	1:B:214:PRO:HG3	1.99	0.43
1:D:138:ALA:O	1:D:142:LYS:HG3	2.18	0.43
1:D:171:ILE:HG23	1:D:230:PRO:HB3	2.01	0.43
1:D:356:ASP:OD2	1:D:375:ASN:HA	2.19	0.43
1:A:178:ASN:HA	1:A:179:PRO:HD2	1.96	0.43
1:A:51:ALA:O	1:A:397:LEU:HD11	2.19	0.43
1:B:63:ARG:HE	1:B:69:VAL:HB	1.84	0.43
1:D:271:PRO:HG3	1:D:300:GLU:HB3	1.99	0.43
1:D:367:GLY:O	1:D:387:VAL:HG13	2.18	0.43
1:C:58:PHE:CE1	1:C:370:VAL:HG11	2.53	0.42
1:C:79:THR:HG22	1:C:85:ALA:HB1	2.01	0.42
1:C:259:LYS:C	1:C:261:ALA:H	2.26	0.42
1:D:290:LEU:HD23	1:D:290:LEU:HA	1.68	0.42
1:A:65:ARG:HH11	1:A:65:ARG:CG	2.32	0.42
1:C:265:VAL:CG1	2:C:571:HOH:O	2.65	0.42
1:D:240:MET:HB3	1:D:269:GLY:HA2	2.02	0.42
1:D:374:ARG:HD3	2:D:548:HOH:O	2.18	0.42
1:A:383:ARG:HA	1:A:387:VAL:O	2.19	0.42
1:B:31:ARG:HG2	1:B:31:ARG:HH11	1.84	0.42
1:B:303:PRO:HD3	2:B:613:HOH:O	2.17	0.42
1:C:280:ASP:HB3	2:C:435:HOH:O	2.18	0.42
1:C:372:TYR:CD2	1:C:394:ALA:HB2	2.54	0.42
1:A:15:GLY:O	1:A:16:LYS:C	2.59	0.42
1:A:103:LEU:HD13	1:A:154:LEU:HD13	2.00	0.42
1:A:370:VAL:HA	1:A:390:ILE:O	2.20	0.42
1:B:413:ARG:HG3	2:B:601:HOH:O	2.18	0.42
1:A:314:TYR:HB3	2:A:554:HOH:O	2.19	0.42
1:A:415:PRO:O	1:A:416:ILE:HG13	2.19	0.42
1:C:12:SER:O	1:C:413:ARG:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:GLY:HA3	1:C:263:GLU:OE1	2.19	0.42
1:C:285:PHE:HA	1:C:291:VAL:HG12	2.01	0.42
1:C:418:TYR:CD1	2:C:598:HOH:O	2.24	0.42
1:A:365:GLU:O	1:A:366:PRO:C	2.62	0.42
1:B:58:PHE:CE1	1:B:370:VAL:HG11	2.55	0.42
1:B:246:ARG:CZ	1:C:141:LEU:HD11	2.50	0.42
1:C:218:HIS:HB3	1:C:221:SER:HB2	2.01	0.42
1:D:218:HIS:O	1:D:221:SER:HB2	2.20	0.42
1:A:24:SER:HA	1:A:55:HIS:CE1	2.54	0.42
1:A:106:GLU:O	1:A:107:LEU:C	2.62	0.42
1:A:331:GLU:HB2	2:A:531:HOH:O	2.20	0.42
1:B:21:MET:HE1	1:B:192:THR:CG2	2.50	0.42
1:B:99:VAL:HA	2:B:461:HOH:O	2.19	0.42
1:B:266:ILE:HD13	1:B:328:VAL:HG12	2.02	0.42
1:D:27:LEU:HD12	1:D:27:LEU:O	2.20	0.42
1:D:403:GLY:O	1:D:404:GLY:C	2.61	0.42
1:A:65:ARG:HD3	2:A:433:HOH:O	2.20	0.42
1:A:354:GLN:HB2	2:B:520:HOH:O	2.20	0.42
1:B:24:SER:HB2	1:B:55:HIS:ND1	2.34	0.42
1:B:397:LEU:CB	2:B:622:HOH:O	2.67	0.42
1:C:33:THR:HG23	1:C:34:PRO:HD2	2.02	0.42
1:A:107:LEU:O	1:A:107:LEU:HD22	2.19	0.42
1:A:216:LYS:HE2	1:D:97:ASP:OD2	2.19	0.42
1:B:120:ALA:N	2:B:619:HOH:O	2.52	0.42
1:C:240:MET:HG3	1:C:249:ILE:HD12	2.02	0.42
1:D:365:GLU:HB2	1:D:366:PRO:CD	2.50	0.42
1:B:199:HIS:HA	1:B:200:PRO:HD3	1.85	0.41
1:B:226:GLY:HA3	2:B:602:HOH:O	2.20	0.41
1:D:91:ASP:OD1	1:D:108:ARG:NH2	2.45	0.41
1:C:288:ARG:HB2	1:C:288:ARG:HE	1.75	0.41
1:C:351:GLU:HB2	1:C:352:ARG:H	1.53	0.41
1:D:20:VAL:HG12	1:D:410:PRO:HA	2.02	0.41
1:B:294:PHE:HE1	1:B:344:GLY:CA	2.18	0.41
1:C:29:HIS:ND1	1:C:29:HIS:N	2.68	0.41
1:C:259:LYS:C	1:C:261:ALA:N	2.78	0.41
1:C:377:TYR:CE2	1:C:381:LEU:HD11	2.55	0.41
1:D:16:LYS:HD2	1:D:18:ARG:NH1	2.36	0.41
1:D:97:ASP:N	2:D:445:HOH:O	2.34	0.41
1:A:43:ASP:CB	1:A:401:ARG:HE	2.30	0.41
1:A:150:HIS:ND1	2:A:543:HOH:O	2.37	0.41
1:A:381:LEU:HD23	1:A:381:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LYS:HG2	1:B:217:ASP:H	1.85	0.41
1:B:277:MET:HE3	1:B:282:VAL:HG11	2.01	0.41
1:C:76:LEU:CD1	1:C:120:ALA:HA	2.50	0.41
1:D:90:LEU:HD13	1:D:108:ARG:HG3	2.03	0.41
1:A:39:GLU:CB	1:D:274:ARG:HH22	2.34	0.41
1:B:166:ASP:CG	1:B:406:CYR:H51	2.46	0.41
1:A:48:VAL:HG12	1:A:52:LYS:HE3	2.02	0.41
1:A:185:ARG:NH1	2:A:627:HOH:O	2.54	0.41
1:A:371:GLY:O	1:A:391:THR:HA	2.20	0.41
1:A:372:TYR:CD2	1:A:394:ALA:HB2	2.55	0.41
1:B:89:ILE:HD11	1:B:194:ALA:CB	2.50	0.41
1:B:248:ALA:O	1:B:249:ILE:C	2.62	0.41
1:B:349:ALA:CB	2:B:487:HOH:O	2.56	0.41
1:B:406:CYR:HN6	1:B:406:CYR:HB2	1.73	0.41
1:C:249:ILE:O	1:C:250:GLY:C	2.63	0.41
1:D:183:PRO:C	1:D:185:ARG:H	2.28	0.41
1:D:58:PHE:HB2	1:D:392:ILE:HG21	2.03	0.41
1:D:401:ARG:NH1	1:D:401:ARG:CG	2.81	0.41
1:B:124:ILE:HG23	1:B:161:THR:HG21	2.02	0.41
1:C:86:LEU:HD22	1:C:90:LEU:HG	2.01	0.41
1:C:237:LEU:HD23	1:C:266:ILE:HB	2.03	0.41
1:C:383:ARG:HG3	1:C:383:ARG:NH1	2.36	0.41
1:D:18:ARG:NH1	1:D:414:ASP:CG	2.78	0.41
1:D:294:PHE:CE2	1:D:297:VAL:HG23	2.56	0.41
1:A:187:GLN:HG2	2:A:613:HOH:O	2.20	0.41
1:D:40:LEU:N	1:D:40:LEU:HD12	2.36	0.41
1:D:42:PHE:CE2	1:D:159:PRO:HB2	2.56	0.41
1:D:114:LEU:HD12	1:D:119:LEU:HD13	2.03	0.41
1:D:309:ASP:O	1:D:315:GLY:HA2	2.21	0.41
1:A:331:GLU:O	1:A:331:GLU:HG2	2.20	0.40
1:A:400:GLY:C	1:A:401:ARG:HG3	2.46	0.40
1:B:115:GLU:O	1:B:116:PRO:C	2.64	0.40
1:D:94:ILE:HD11	1:D:111:LEU:CD1	2.51	0.40
1:D:160:ASN:HB3	1:D:185:ARG:CZ	2.51	0.40
1:D:354:GLN:HG3	1:D:355:TRP:O	2.22	0.40
1:A:14:ALA:CB	2:A:621:HOH:O	2.27	0.40
1:A:241:GLY:CA	2:A:603:HOH:O	2.50	0.40
1:A:270:LEU:HA	1:A:271:PRO:HD3	1.87	0.40
1:B:305:SER:O	1:B:318:ILE:HA	2.20	0.40
1:C:141:LEU:HG	1:C:154:LEU:HD21	2.03	0.40
1:C:372:TYR:CG	1:C:394:ALA:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ASN:HA	1:D:179:PRO:HD3	1.80	0.40
1:D:287:ASP:CB	1:D:290:LEU:HB2	2.52	0.40
1:A:40:LEU:HD12	1:A:40:LEU:HA	1.87	0.40
1:A:193:THR:HG21	1:A:214:PRO:HG2	2.02	0.40
1:B:240:MET:HE3	2:C:590:HOH:O	2.21	0.40
1:C:80:ILE:CD1	1:C:119:LEU:HB3	2.51	0.40
1:C:372:TYR:OH	1:C:402:GLY:O	2.33	0.40
1:D:17:LEU:HD11	1:D:20:VAL:HG13	2.03	0.40
1:C:227:ASP:O	1:C:238:ILE:HA	2.21	0.40
1:D:265:VAL:O	1:D:306:LEU:HB2	2.22	0.40
1:A:137:GLY:O	1:A:140:ILE:HG12	2.21	0.40
1:B:25:PRO:CA	1:B:29:HIS:CE1	2.96	0.40
1:B:145:ARG:NH1	1:B:152:SER:CB	2.85	0.40
1:C:186:ARG:HH11	1:C:186:ARG:HG3	1.86	0.40
1:C:199:HIS:HA	1:C:200:PRO:HD3	1.87	0.40
1:C:293:VAL:O	1:C:295:PRO:HD3	2.22	0.40
1:C:331:GLU:HG3	1:C:332:SER:N	2.36	0.40
1:D:24:SER:HB3	1:D:55:HIS:ND1	2.37	0.40
1:D:189:THR:CA	2:D:571:HOH:O	2.55	0.40
1:D:343:THR:HG22	1:D:357:ASP:HA	2.02	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	400/418 (96%)	363 (91%)	32 (8%)	5 (1%)	9 10
1	B	404/418 (97%)	374 (93%)	26 (6%)	4 (1%)	12 15
1	C	401/418 (96%)	371 (92%)	28 (7%)	2 (0%)	24 31
1	D	401/418 (96%)	349 (87%)	41 (10%)	11 (3%)	4 3
All	All	1606/1672 (96%)	1457 (91%)	127 (8%)	22 (1%)	9 9

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	ALA
1	D	277	MET
1	B	399	ARG
1	D	40	LEU
1	D	273	SER
1	D	416	ILE
1	A	41	LEU
1	A	276	ALA
1	B	173	GLY
1	B	205	ALA
1	D	37	CYS
1	D	183	PRO
1	D	275	ALA
1	D	181	TYR
1	B	116	PRO
1	D	43	ASP
1	D	182	TRP
1	A	377	TYR
1	C	395	SER
1	D	213	ASP
1	C	295	PRO
1	A	415	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	343/353 (97%)	315 (92%)	28 (8%)	10	14
1	B	345/353 (98%)	317 (92%)	28 (8%)	11	14
1	C	344/353 (98%)	322 (94%)	22 (6%)	16	23
1	D	344/353 (98%)	323 (94%)	21 (6%)	17	24
All	All	1376/1412 (98%)	1277 (93%)	99 (7%)	13	18

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	33	THR
1	A	39	GLU
1	A	65	ARG
1	A	76	LEU
1	A	107	LEU
1	A	119	LEU
1	A	130	ASP
1	A	132	LEU
1	A	140	ILE
1	A	157	PRO
1	A	158	LEU
1	A	179	PRO
1	A	180	MET
1	A	208	GLU
1	A	223	LEU
1	A	230	PRO
1	A	233	ASN
1	A	242	GLU
1	A	281	THR
1	A	295	PRO
1	A	301	ILE
1	A	319	ARG
1	A	333	LEU
1	A	352	ARG
1	A	363	CYS
1	A	382	LEU
1	A	388	GLU
1	B	20	VAL
1	B	34	PRO
1	B	40	LEU
1	B	76	LEU
1	B	86	LEU
1	B	107	LEU
1	B	117	ARG
1	B	119	LEU
1	B	141	LEU
1	B	142	LYS
1	B	165	ARG
1	B	167	THR
1	B	200	PRO
1	B	220	SER
1	B	230	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	243	ARG
1	B	247	GLN
1	B	259	LYS
1	B	281	THR
1	B	290	LEU
1	B	296	GLU
1	B	298	VAL
1	B	306	LEU
1	B	369	VAL
1	B	374	ARG
1	B	382	LEU
1	B	397	LEU
1	B	415	PRO
1	C	25	PRO
1	C	33	THR
1	C	41	LEU
1	C	59	VAL
1	C	86	LEU
1	C	105	SER
1	C	106	GLU
1	C	107	LEU
1	C	119	LEU
1	C	155	LEU
1	C	156	PRO
1	C	180	MET
1	C	208	GLU
1	C	223	LEU
1	C	243	ARG
1	C	264	ARG
1	C	290	LEU
1	C	295	PRO
1	C	306	LEU
1	C	351	GLU
1	C	354	GLN
1	C	369	VAL
1	D	7	LYS
1	D	16	LYS
1	D	25	PRO
1	D	40	LEU
1	D	74	ASN
1	D	76	LEU
1	D	86	LEU

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Mol	Chain	Res	Type
1	D	105	SER
1	D	107	LEU
1	D	115	GLU
1	D	208	GLU
1	D	220	SER
1	D	242	GLU
1	D	243	ARG
1	D	272	LYS
1	D	306	LEU
1	D	323	LYS
1	D	397	LEU
1	D	401	ARG
1	D	410	PRO
1	D	418	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	B	11	HIS
1	B	139	ASN
1	B	317	ASN
1	C	49	ASN
1	C	74	ASN
1	C	150	HIS
1	C	160	ASN
1	C	187	GLN
1	C	199	HIS
1	D	29	HIS
1	D	160	ASN
1	D	199	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CYR	D	406	1	14,16,17	3.03	4 (28%)	11,19,21	2.68	2 (18%)
1	CYR	B	406	1	14,16,17	2.99	3 (21%)	11,19,21	2.42	4 (36%)
1	CYR	A	406	1	14,16,17	3.09	4 (28%)	11,19,21	2.78	4 (36%)
1	CYR	C	406	1	14,16,17	3.01	4 (28%)	11,19,21	2.99	3 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CYR	D	406	1	-	2/15/18/20	-
1	CYR	B	406	1	-	3/15/18/20	-
1	CYR	A	406	1	-	3/15/18/20	-
1	CYR	C	406	1	-	3/15/18/20	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	406	CYR	C7-SG	7.53	1.83	1.76
1	D	406	CYR	C7-SG	7.47	1.83	1.76
1	C	406	CYR	C7-SG	7.30	1.83	1.76
1	B	406	CYR	C7-SG	7.26	1.83	1.76
1	D	406	CYR	C7-N6	6.44	1.47	1.35
1	A	406	CYR	C7-N6	6.38	1.47	1.35
1	C	406	CYR	C7-N6	6.37	1.47	1.35
1	B	406	CYR	C7-N6	6.36	1.47	1.35
1	A	406	CYR	C7-N7	5.39	1.47	1.28
1	B	406	CYR	C7-N7	5.12	1.46	1.28
1	C	406	CYR	C7-N7	5.02	1.46	1.28
1	D	406	CYR	C7-N7	4.79	1.45	1.28
1	D	406	CYR	O1-C1	-2.35	1.23	1.30
1	C	406	CYR	O1-C1	-2.24	1.23	1.30
1	A	406	CYR	O1-C1	-2.12	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	406	CYR	C5-N6-C7	-9.01	107.44	123.55
1	D	406	CYR	C5-N6-C7	-8.06	109.14	123.55
1	A	406	CYR	C5-N6-C7	-7.43	110.26	123.55
1	B	406	CYR	C5-N6-C7	-6.49	111.94	123.55
1	A	406	CYR	N6-C7-N7	-3.79	109.51	120.61
1	B	406	CYR	O1-C1-O2	-2.49	118.43	124.08
1	A	406	CYR	CB-SG-C7	2.39	105.33	102.56
1	B	406	CYR	N6-C7-N7	-2.28	113.93	120.61
1	B	406	CYR	SG-C7-N6	-2.25	110.68	117.20
1	C	406	CYR	N6-C7-N7	-2.20	114.18	120.61
1	D	406	CYR	O1-C1-O2	-2.19	119.10	124.08
1	C	406	CYR	O1-C1-O2	-2.05	119.42	124.08
1	A	406	CYR	O1-C1-O2	-2.03	119.47	124.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	406	CYR	SG-C7-N6-C5
1	A	406	CYR	N7-C7-SG-CB
1	B	406	CYR	N7-C7-SG-CB
1	C	406	CYR	SG-C7-N6-C5
1	C	406	CYR	N7-C7-SG-CB
1	D	406	CYR	SG-C7-N6-C5
1	B	406	CYR	O1-C1-C2-N2
1	B	406	CYR	O2-C1-C2-N2
1	A	406	CYR	N6-C7-SG-CB
1	C	406	CYR	N6-C7-SG-CB
1	D	406	CYR	N7-C7-SG-CB

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	406	CYR	2	0
1	B	406	CYR	3	0
1	A	406	CYR	1	0
1	C	406	CYR	4	0

## 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 [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	404/418 (96%)	-0.55	1 (0%) 91 91	14, 31, 57, 74	0
1	B	408/418 (97%)	-0.64	1 (0%) 91 91	12, 26, 55, 77	0
1	C	405/418 (96%)	-0.54	1 (0%) 91 91	13, 34, 59, 76	0
1	D	405/418 (96%)	-0.45	7 (1%) 69 70	16, 34, 63, 79	0
All	All	1622/1672 (97%)	-0.54	10 (0%) 85 86	12, 31, 59, 79	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	277	MET	4.0
1	D	184	ALA	3.5
1	D	275	ALA	3.3
1	D	400	GLY	3.2
1	D	314	TYR	3.1
1	B	349	ALA	2.5
1	D	276	ALA	2.5
1	A	241	GLY	2.3
1	D	41	LEU	2.2
1	C	313	PRO	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	CYR	C	406	17/18	0.93	0.10	18,51,67,68	0
1	CYR	B	406	17/18	0.95	0.08	18,34,61,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CYR	A	406	17/18	0.95	0.09	15,37,68,68	0
1	CYR	D	406	17/18	0.96	0.07	20,36,65,68	0

### 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.