



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:10 AM UTC

PDB ID : 1J5S / pdb_00001j5s
Title : Crystal structure of uronate isomerase (TM0064) from *Thermotoga maritima* at 2.85 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2002-07-02
Resolution : 2.85 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

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

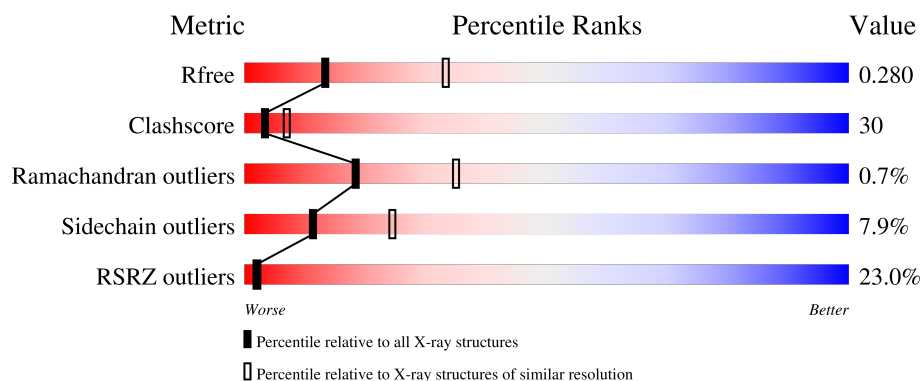
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	463	22% 52% 40% 6% .
1	B	463	22% 51% 39% 6% .
1	C	463	23% 53% 39% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11175 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 URONATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	81	0	0
			3696	2367	632	680	17			
1	B	450	Total	C	N	O	S	86	0	0
			3686	2361	629	679	17			
1	C	450	Total	C	N	O	S	83	0	0
			3686	2361	629	679	17			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q9WXR9
A	-10	GLY	-	expression tag	UNP Q9WXR9
A	-9	SER	-	expression tag	UNP Q9WXR9
A	-8	ASP	-	expression tag	UNP Q9WXR9
A	-7	LYS	-	expression tag	UNP Q9WXR9
A	-6	ILE	-	expression tag	UNP Q9WXR9
A	-5	HIS	-	expression tag	UNP Q9WXR9
A	-4	HIS	-	expression tag	UNP Q9WXR9
A	-3	HIS	-	expression tag	UNP Q9WXR9
A	-2	HIS	-	expression tag	UNP Q9WXR9
A	-1	HIS	-	expression tag	UNP Q9WXR9
A	0	HIS	-	expression tag	UNP Q9WXR9
B	-11	MET	-	expression tag	UNP Q9WXR9
B	-10	GLY	-	expression tag	UNP Q9WXR9
B	-9	SER	-	expression tag	UNP Q9WXR9
B	-8	ASP	-	expression tag	UNP Q9WXR9
B	-7	LYS	-	expression tag	UNP Q9WXR9
B	-6	ILE	-	expression tag	UNP Q9WXR9
B	-5	HIS	-	expression tag	UNP Q9WXR9
B	-4	HIS	-	expression tag	UNP Q9WXR9
B	-3	HIS	-	expression tag	UNP Q9WXR9
B	-2	HIS	-	expression tag	UNP Q9WXR9
B	-1	HIS	-	expression tag	UNP Q9WXR9

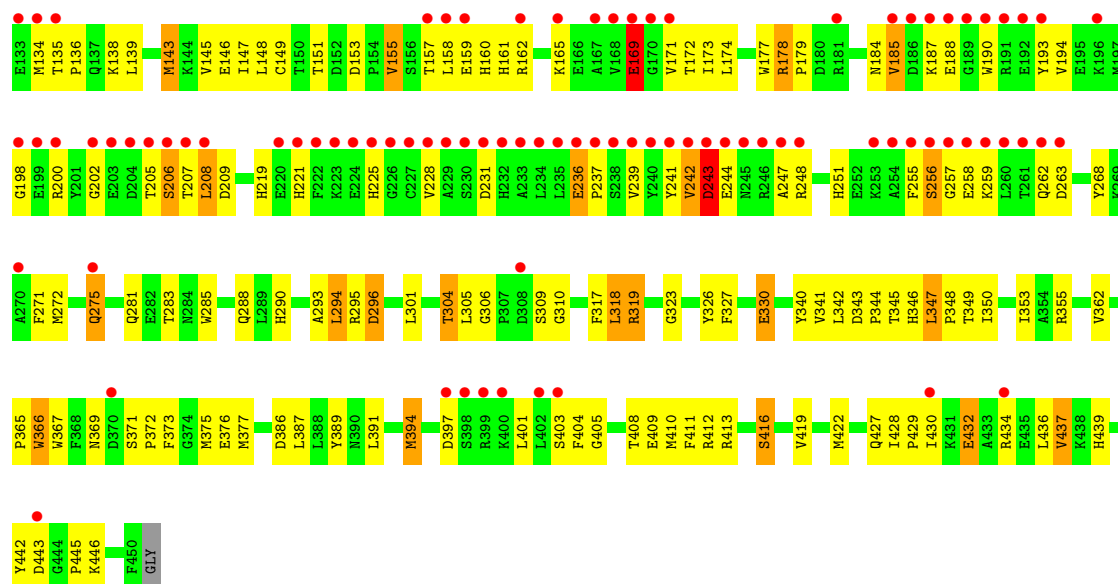
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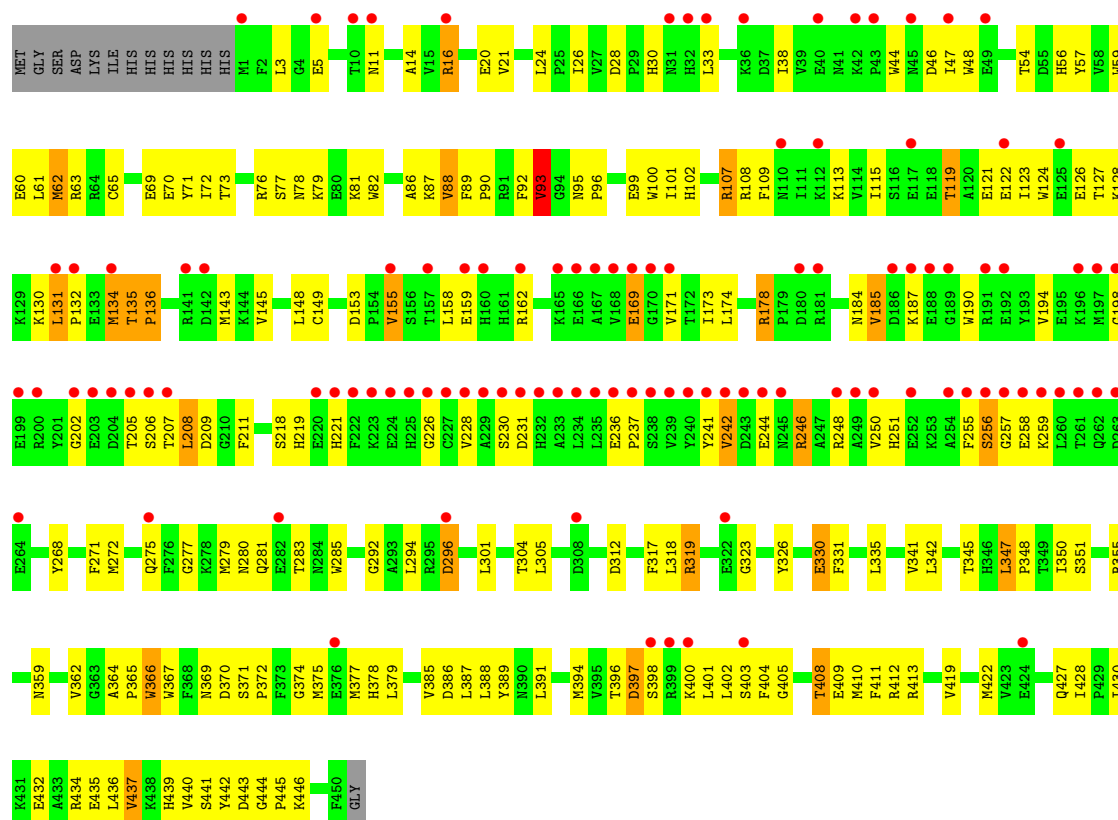
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP Q9WXR9
C	-11	MET	-	expression tag	UNP Q9WXR9
C	-10	GLY	-	expression tag	UNP Q9WXR9
C	-9	SER	-	expression tag	UNP Q9WXR9
C	-8	ASP	-	expression tag	UNP Q9WXR9
C	-7	LYS	-	expression tag	UNP Q9WXR9
C	-6	ILE	-	expression tag	UNP Q9WXR9
C	-5	HIS	-	expression tag	UNP Q9WXR9
C	-4	HIS	-	expression tag	UNP Q9WXR9
C	-3	HIS	-	expression tag	UNP Q9WXR9
C	-2	HIS	-	expression tag	UNP Q9WXR9
C	-1	HIS	-	expression tag	UNP Q9WXR9
C	0	HIS	-	expression tag	UNP Q9WXR9

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	40	Total O 40 40	0	0
2	B	33	Total O 33 33	0	0
2	C	34	Total O 34 34	0	0



• Molecule 1: URONATE ISOMERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.41Å 79.96Å 89.43Å 115.73° 97.57° 110.44°	Depositor
Resolution (Å)	24.99 – 2.85 24.99 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.6 (24.99-2.85) 96.5 (24.99-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.234 , 0.274 (Not available) , 0.280	Depositor DCC
R_{free} test set	4272 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for k,h,-h-k-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	11175	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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	0.69	4/3793 (0.1%)	1.08	12/5136 (0.2%)
1	B	0.70	1/3782 (0.0%)	1.10	14/5121 (0.3%)
1	C	0.70	1/3782 (0.0%)	1.09	11/5121 (0.2%)
All	All	0.70	6/11357 (0.1%)	1.09	37/15378 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	143	MET	SD-CE	-8.16	1.59	1.79
1	A	62	MET	SD-CE	-7.98	1.59	1.79
1	C	62	MET	SD-CE	-6.07	1.64	1.79
1	A	422	MET	SD-CE	-5.64	1.65	1.79
1	A	279	MET	SD-CE	-5.43	1.66	1.79
1	A	143	MET	SD-CE	-5.12	1.66	1.79

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	169	GLU	N-CA-C	10.57	122.76	111.03
1	B	243	ASP	N-CA-CB	-9.79	93.94	110.49
1	B	188	GLU	N-CA-C	-8.56	97.61	110.28
1	B	242	VAL	N-CA-C	8.43	119.16	106.42
1	C	242	VAL	N-CA-C	8.16	120.25	107.28
1	A	242	VAL	N-CA-C	7.38	119.02	107.28
1	A	132	PRO	CA-N-CD	-7.34	101.72	112.00
1	A	1	MET	N-CA-C	6.74	119.49	109.59
1	B	131	LEU	CA-C-N	6.35	125.57	118.97
1	B	131	LEU	C-N-CA	6.35	125.57	118.97
1	C	16	ARG	CB-CA-C	-6.13	100.61	110.79
1	C	366	TRP	N-CA-C	6.02	120.37	111.04
1	C	5	GLU	N-CA-C	5.94	118.52	111.33
1	A	259	LYS	N-CA-C	-5.80	100.79	109.15
1	B	366	TRP	N-CA-C	5.80	120.03	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	GLU	N-CA-C	5.64	118.15	111.33
1	B	178	ARG	CB-CA-C	-5.58	105.42	110.44
1	B	161	HIS	N-CA-C	-5.57	105.21	111.28
1	A	206	SER	N-CA-C	-5.49	106.65	113.19
1	C	259	LYS	N-CA-C	-5.44	101.32	109.15
1	B	169	GLU	N-CA-C	5.42	122.35	110.80
1	B	259	LYS	N-CA-C	-5.41	101.36	109.15
1	B	275	GLN	CA-CB-CG	-5.37	103.35	114.10
1	A	161	HIS	N-CA-C	-5.34	105.54	111.36
1	A	145	VAL	CB-CA-C	-5.33	104.84	111.08
1	B	206	SER	N-CA-C	-5.20	107.00	113.19
1	A	178	ARG	CB-CA-C	-5.17	105.78	110.44
1	A	115	ILE	CB-CA-C	-5.15	104.45	111.15
1	C	131	LEU	CA-C-N	5.13	124.30	118.97
1	C	131	LEU	C-N-CA	5.13	124.30	118.97
1	C	135	THR	O-C-N	5.12	125.52	121.88
1	A	366	TRP	N-CA-C	5.10	120.46	110.56
1	C	370	ASP	N-CA-CB	5.08	117.92	110.35
1	A	380	LYS	N-CA-C	-5.07	105.64	111.07
1	B	5	GLU	N-CA-C	5.07	116.81	111.28
1	C	292	GLY	N-CA-C	5.06	123.02	115.64
1	B	115	ILE	N-CA-C	5.04	115.54	108.89

There are no chirality outliers.

There are no planarity outliers.

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	3696	0	3621	229	7
1	B	3686	0	3614	216	11
1	C	3686	0	3614	240	4
2	A	40	0	0	3	0
2	B	33	0	0	4	0
2	C	34	0	0	5	0
All	All	11175	0	10849	644	11

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 30.

All (644) 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:194:VAL:HG12	1:A:205:THR:CG2	1.53	1.34
1:A:251:HIS:ND1	2:A:454:HOH:O	1.65	1.21
1:B:62:MET:CE	1:B:72:ILE:HG12	1.73	1.19
1:A:194:VAL:CG1	1:A:205:THR:CG2	2.22	1.17
1:C:400:LYS:HD3	2:C:458:HOH:O	1.40	1.17
1:A:41:ASN:CG	1:A:135:THR:HG21	1.71	1.14
1:B:62:MET:HE3	1:B:72:ILE:HG12	1.24	1.12
1:A:194:VAL:HG12	1:A:205:THR:HG21	1.12	1.10
1:A:194:VAL:CG1	1:A:205:THR:HG21	1.79	1.10
1:C:400:LYS:CD	2:C:458:HOH:O	1.96	1.04
1:C:47:ILE:HD11	1:C:82:TRP:CE2	1.92	1.03
1:A:424:GLU:HA	1:B:1:MET:SD	1.97	1.03
1:C:21:VAL:HG13	1:C:24:LEU:HD12	1.37	1.02
1:C:400:LYS:CE	2:C:458:HOH:O	2.03	1.02
1:A:194:VAL:HG12	1:A:205:THR:HG22	1.38	1.00
1:C:143:MET:HE1	1:C:404:PHE:HB2	1.43	0.99
1:C:47:ILE:HD11	1:C:82:TRP:CD2	1.98	0.98
1:C:219:HIS:CE1	1:C:285:TRP:CZ3	2.52	0.97
1:A:251:HIS:CE1	2:A:454:HOH:O	2.07	0.97
1:C:409:GLU:OE2	1:C:413:ARG:NH1	1.97	0.97
1:A:46:ASP:OD2	1:A:78:ASN:ND2	1.99	0.96
1:A:41:ASN:OD1	1:A:135:THR:CG2	2.13	0.96
1:C:194:VAL:CG1	1:C:205:THR:HG22	1.95	0.94
1:A:424:GLU:O	1:B:1:MET:SD	2.25	0.94
1:C:246:ARG:HG3	1:C:246:ARG:HH11	1.33	0.93
1:A:41:ASN:OD1	1:A:135:THR:HG21	1.67	0.92
1:C:209:ASP:OD1	1:C:248:ARG:NH2	2.04	0.90
1:C:143:MET:CE	1:C:404:PHE:HB2	2.02	0.89
1:A:105:LEU:CD1	1:A:123:ILE:HD11	2.01	0.89
1:C:256:SER:O	1:C:258:GLU:N	2.07	0.88
1:A:256:SER:O	1:A:258:GLU:N	2.07	0.88
1:C:119:THR:CG2	1:C:123:ILE:HD11	2.03	0.88
1:A:194:VAL:CG1	1:A:205:THR:HG22	1.99	0.87
1:B:109:PHE:CE2	1:B:134:MET:HE1	2.09	0.87
1:B:412:ARG:O	1:B:416:SER:OG	1.92	0.87
1:B:119:THR:CG2	1:B:123:ILE:HD11	2.05	0.86
1:A:135:THR:HG23	1:A:136:PRO:HD2	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:SER:O	1:B:258:GLU:N	2.07	0.86
1:A:20:GLU:OE2	1:A:434:ARG:HB3	1.77	0.85
1:A:389:TYR:CE2	1:A:439:HIS:CE1	2.65	0.85
1:C:194:VAL:HG12	1:C:205:THR:HG22	1.56	0.84
1:C:153:ASP:OD1	1:C:155:VAL:HG23	1.76	0.84
1:A:105:LEU:HD11	1:A:123:ILE:HD11	1.59	0.83
1:B:131:LEU:N	1:B:132:PRO:CD	2.40	0.83
1:C:244:GLU:O	1:C:248:ARG:HG3	1.77	0.83
1:B:135:THR:OG1	1:B:136:PRO:HD2	1.78	0.83
1:C:119:THR:CG2	1:C:123:ILE:CD1	2.57	0.83
1:C:145:VAL:HG11	1:C:148:LEU:HD21	1.61	0.83
1:C:241:TYR:HD1	1:C:326:TYR:OH	1.62	0.83
1:C:143:MET:HE3	1:C:405:GLY:H	1.42	0.82
1:B:165:LYS:O	2:B:466:HOH:O	1.95	0.82
1:C:241:TYR:HD1	1:C:326:TYR:HH	0.83	0.82
1:A:428:ILE:HG23	1:B:93:VAL:CG2	2.10	0.82
1:B:119:THR:CG2	1:B:123:ILE:CD1	2.58	0.81
1:A:241:TYR:HD1	1:A:326:TYR:OH	1.62	0.81
1:A:143:MET:CE	1:A:405:GLY:H	1.93	0.80
1:A:57:TYR:HH	1:A:367:TRP:CD1	1.99	0.80
1:B:71:TYR:CE2	1:B:76:ARG:HD3	2.17	0.80
1:C:159:GLU:OE1	1:C:159:GLU:HA	1.82	0.79
1:A:93:VAL:CG2	1:C:428:ILE:HG23	2.13	0.79
1:A:62:MET:HE3	1:A:72:ILE:HG12	1.65	0.79
1:A:241:TYR:HD1	1:A:326:TYR:HH	0.81	0.79
1:B:131:LEU:N	1:B:132:PRO:HD3	1.99	0.78
1:B:243:ASP:OD1	1:B:243:ASP:N	2.10	0.78
1:B:20:GLU:OE2	1:B:434:ARG:HB3	1.83	0.78
1:A:228:VAL:HG12	1:A:228:VAL:O	1.84	0.77
1:A:205:THR:HG22	1:A:205:THR:O	1.82	0.77
1:A:424:GLU:CA	1:B:1:MET:SD	2.72	0.77
1:B:146:GLU:OE1	1:B:446:LYS:NZ	2.18	0.77
1:B:21:VAL:HG12	1:B:412:ARG:HD3	1.66	0.77
1:A:71:TYR:CE2	1:A:76:ARG:HD3	2.20	0.77
1:A:244:GLU:O	1:A:248:ARG:HG3	1.84	0.77
1:C:219:HIS:CE1	1:C:285:TRP:CH2	2.73	0.77
1:B:58:VAL:O	1:B:62:MET:HG3	1.86	0.76
1:A:409:GLU:OE2	1:A:413:ARG:NH1	2.18	0.76
1:C:219:HIS:CE1	1:C:285:TRP:CE3	2.73	0.76
1:B:409:GLU:OE2	1:B:413:ARG:NH1	2.19	0.75
1:A:365:PRO:CD	1:A:378:HIS:HD2	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ASN:HB3	1:B:187:LYS:HG2	1.69	0.75
1:C:71:TYR:CE2	1:C:76:ARG:HD3	2.20	0.75
1:A:208:LEU:N	1:A:251:HIS:CD2	2.54	0.75
1:B:143:MET:CE	1:B:405:GLY:H	1.98	0.75
1:B:41:ASN:HD21	1:B:135:THR:HG21	1.50	0.75
1:B:21:VAL:HG21	1:B:437:VAL:HG13	1.67	0.75
1:C:21:VAL:HG21	1:C:437:VAL:HG13	1.69	0.74
1:C:347:LEU:HD23	1:C:350:ILE:HD11	1.68	0.74
1:B:153:ASP:OD1	1:B:155:VAL:HG23	1.87	0.74
1:A:442:TYR:HD2	1:A:443:ASP:OD1	1.71	0.73
1:A:347:LEU:HD11	1:A:378:HIS:ND1	2.04	0.73
1:C:16:ARG:HH11	1:C:430:ILE:CD1	2.01	0.73
1:B:185:VAL:HG21	1:B:268:TYR:CD2	2.23	0.73
1:B:228:VAL:HG12	1:B:228:VAL:O	1.87	0.73
1:C:47:ILE:CD1	1:C:82:TRP:CE2	2.72	0.73
1:A:153:ASP:OD1	1:A:193:TYR:OH	2.06	0.73
1:A:271:PHE:CZ	1:A:275:GLN:NE2	2.57	0.72
1:C:62:MET:HE3	1:C:72:ILE:HG12	1.71	0.72
1:A:41:ASN:OD1	1:A:135:THR:HG22	1.89	0.72
1:A:120:ALA:O	1:A:123:ILE:HG22	1.89	0.72
1:A:158:LEU:O	1:A:162:ARG:HG3	1.90	0.72
1:B:36:LYS:HB2	1:B:160:HIS:CD2	2.25	0.71
1:C:44:TRP:HH2	1:C:401:LEU:HD12	1.56	0.71
1:B:145:VAL:HG11	1:B:148:LEU:HD21	1.72	0.71
1:C:79:LYS:HE3	1:C:124:TRP:CD1	2.26	0.71
1:A:93:VAL:HG22	1:C:428:ILE:HG23	1.73	0.70
1:B:198:GLY:HA3	1:B:205:THR:HG23	1.72	0.70
1:B:430:ILE:O	1:B:434:ARG:HG3	1.92	0.70
1:A:424:GLU:C	1:B:1:MET:SD	2.75	0.70
1:B:62:MET:HE3	1:B:72:ILE:CG1	2.14	0.70
1:B:46:ASP:OD2	1:B:78:ASN:ND2	2.25	0.70
1:C:46:ASP:OD2	1:C:78:ASN:ND2	2.24	0.70
1:A:135:THR:HG23	1:A:136:PRO:CD	2.21	0.70
1:A:21:VAL:HG21	1:A:437:VAL:HG13	1.74	0.69
1:B:436:LEU:HD22	1:C:93:VAL:CG1	2.21	0.69
1:C:100:TRP:NE1	1:C:410:MET:HE3	2.07	0.69
1:C:283:THR:HG21	1:C:285:TRP:NE1	2.07	0.69
1:C:47:ILE:HD12	1:C:82:TRP:CH2	2.28	0.69
1:A:131:LEU:HA	1:A:134:MET:HG3	1.75	0.69
1:B:185:VAL:CG2	1:B:268:TYR:CD2	2.75	0.69
1:C:208:LEU:N	1:C:251:HIS:HD2	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:LYS:NZ	1:C:121:GLU:OE2	2.25	0.68
1:C:131:LEU:N	1:C:132:PRO:CD	2.56	0.68
1:B:32:HIS:NE2	2:B:452:HOH:O	1.78	0.68
1:B:271:PHE:CE2	1:B:275:GLN:OE1	2.45	0.68
1:C:21:VAL:HG12	1:C:412:ARG:HD3	1.76	0.68
1:C:228:VAL:HG12	1:C:228:VAL:O	1.92	0.68
1:C:271:PHE:CE2	1:C:275:GLN:OE1	2.47	0.68
1:A:44:TRP:HH2	1:A:401:LEU:HD12	1.59	0.68
1:A:153:ASP:OD1	1:A:155:VAL:HG23	1.93	0.68
1:A:436:LEU:HD22	1:B:93:VAL:CG1	2.24	0.68
1:B:155:VAL:O	1:B:200:ARG:NH1	2.25	0.68
1:A:271:PHE:CE2	1:A:275:GLN:NE2	2.61	0.67
1:A:145:VAL:HG11	1:A:148:LEU:HD21	1.77	0.67
1:A:322:GLU:OE1	1:B:294:LEU:HD11	1.94	0.67
1:A:190:TRP:O	1:A:194:VAL:HG23	1.94	0.67
1:B:71:TYR:CZ	1:B:76:ARG:HD3	2.28	0.67
1:A:194:VAL:HG13	1:A:205:THR:CG2	2.23	0.67
1:B:209:ASP:OD2	1:B:248:ARG:CZ	2.42	0.67
1:A:21:VAL:HG12	1:A:21:VAL:O	1.94	0.67
1:A:79:LYS:NZ	1:A:121:GLU:OE2	2.22	0.67
1:A:28:ASP:OD2	1:A:396:THR:OG1	2.10	0.67
1:A:208:LEU:N	1:A:251:HIS:HD2	1.93	0.67
1:C:56:HIS:HE1	1:C:57:TYR:CE2	2.12	0.67
1:A:366:TRP:CD1	1:A:366:TRP:C	2.73	0.67
1:C:246:ARG:HH11	1:C:246:ARG:CG	2.03	0.66
1:C:119:THR:HG21	1:C:123:ILE:HD11	1.78	0.66
1:C:283:THR:CG2	1:C:285:TRP:NE1	2.58	0.66
1:A:347:LEU:HD23	1:A:350:ILE:HD11	1.78	0.66
1:B:71:TYR:OH	1:B:76:ARG:NH1	2.29	0.66
1:C:194:VAL:HG13	1:C:205:THR:HG22	1.74	0.66
1:A:41:ASN:ND2	1:A:135:THR:HG21	2.10	0.65
1:C:208:LEU:N	1:C:251:HIS:CD2	2.64	0.65
1:A:212:LEU:HD21	1:A:275:GLN:OE1	1.95	0.65
1:C:143:MET:HE1	1:C:401:LEU:O	1.96	0.65
1:C:143:MET:CE	1:C:404:PHE:CB	2.75	0.65
1:A:135:THR:CG2	1:A:136:PRO:HD2	2.27	0.65
1:B:394:MET:HG2	2:B:458:HOH:O	1.97	0.65
1:C:145:VAL:HG11	1:C:148:LEU:CD2	2.26	0.65
1:C:219:HIS:CD2	1:C:279:MET:HB3	2.32	0.65
1:A:135:THR:CG2	1:A:136:PRO:CD	2.75	0.65
1:B:319:ARG:HG3	1:C:317:PHE:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:THR:HG22	1:A:136:PRO:N	2.10	0.64
1:C:16:ARG:NH1	1:C:430:ILE:CD1	2.60	0.64
1:C:131:LEU:O	1:C:134:MET:HB2	1.96	0.64
1:C:283:THR:HG22	1:C:285:TRP:CD1	2.31	0.64
1:A:430:ILE:O	1:A:434:ARG:HG3	1.97	0.64
1:B:63:ARG:NE	1:B:69:GLU:OE2	2.25	0.64
1:B:44:TRP:HH2	1:B:401:LEU:HD12	1.63	0.64
1:C:135:THR:HB	1:C:136:PRO:HD2	1.79	0.64
1:A:438:LYS:HE2	1:A:443:ASP:OD2	1.97	0.64
1:C:122:GLU:HG2	1:C:126:GLU:OE2	1.97	0.64
1:A:71:TYR:CZ	1:A:76:ARG:HD3	2.33	0.63
1:A:82:TRP:HZ2	1:A:123:ILE:HG21	1.63	0.63
1:C:178:ARG:HG3	1:C:231:ASP:HB3	1.79	0.63
1:C:47:ILE:CD1	1:C:82:TRP:CD2	2.77	0.63
1:B:198:GLY:CA	1:B:205:THR:CG2	2.76	0.63
1:C:16:ARG:HD3	1:C:430:ILE:HD11	1.81	0.63
1:A:30:HIS:C	1:A:30:HIS:CD2	2.76	0.63
1:C:21:VAL:HG12	1:C:21:VAL:O	1.98	0.63
1:C:47:ILE:HD12	1:C:82:TRP:CZ3	2.33	0.63
1:C:143:MET:HE3	1:C:405:GLY:N	2.13	0.63
1:A:21:VAL:HG13	1:A:24:LEU:HD12	1.79	0.62
1:B:442:TYR:HD2	1:B:443:ASP:OD1	1.81	0.62
1:A:365:PRO:CG	1:A:378:HIS:HD2	2.13	0.62
1:A:205:THR:CG2	1:A:205:THR:O	2.48	0.62
1:C:30:HIS:NE2	1:C:397:ASP:OD1	2.32	0.62
1:B:119:THR:HG23	1:B:123:ILE:CD1	2.30	0.62
1:B:198:GLY:N	1:B:205:THR:HG21	2.14	0.62
1:B:319:ARG:HG3	1:C:317:PHE:CE2	2.34	0.62
1:A:365:PRO:HG3	1:A:378:HIS:CD2	2.35	0.62
1:C:442:TYR:HD2	1:C:443:ASP:OD1	1.83	0.62
1:C:194:VAL:HG12	1:C:205:THR:CG2	2.30	0.62
1:A:419:VAL:HA	1:A:422:MET:CE	2.29	0.61
1:A:319:ARG:HG3	1:B:317:PHE:CD2	2.35	0.61
1:B:135:THR:HG23	1:B:138:LYS:H	1.65	0.61
1:B:242:VAL:O	1:B:271:PHE:HD1	1.82	0.61
1:C:119:THR:HG22	1:C:123:ILE:CD1	2.30	0.61
1:C:400:LYS:NZ	2:C:458:HOH:O	2.05	0.61
1:A:105:LEU:HD13	1:A:123:ILE:HD11	1.83	0.61
1:C:347:LEU:HD21	1:C:378:HIS:CE1	2.36	0.61
1:A:69:GLU:OE2	1:A:72:ILE:HD12	2.01	0.61
1:B:198:GLY:HA3	1:B:205:THR:CG2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:OG1	1:A:159:GLU:CG	2.49	0.60
1:B:88:VAL:CG1	1:B:88:VAL:O	2.49	0.60
1:B:65:CYS:SG	1:B:88:VAL:CG1	2.89	0.60
1:C:56:HIS:CE1	1:C:57:TYR:CE2	2.89	0.60
1:C:251:HIS:HB2	1:C:268:TYR:HE1	1.67	0.60
1:A:205:THR:C	1:A:207:THR:H	2.10	0.60
1:C:131:LEU:N	1:C:132:PRO:HD3	2.17	0.60
1:B:347:LEU:HD23	1:B:350:ILE:HD11	1.84	0.60
1:C:119:THR:HG22	1:C:123:ILE:HD12	1.84	0.60
1:A:143:MET:HE2	1:A:405:GLY:N	2.17	0.59
1:B:57:TYR:HH	1:B:367:TRP:CD1	2.20	0.59
1:B:428:ILE:HG23	1:C:93:VAL:CG2	2.32	0.59
1:C:57:TYR:HH	1:C:367:TRP:CD1	2.20	0.59
1:A:319:ARG:HG3	1:B:317:PHE:CE2	2.37	0.59
1:A:428:ILE:HG23	1:B:93:VAL:HG22	1.82	0.59
1:C:88:VAL:O	1:C:88:VAL:CG1	2.48	0.59
1:C:136:PRO:HA	1:C:401:LEU:CD1	2.33	0.59
1:C:219:HIS:ND1	1:C:285:TRP:CH2	2.70	0.59
1:A:347:LEU:HD21	1:A:378:HIS:CE1	2.36	0.59
1:B:158:LEU:O	1:B:162:ARG:HG3	2.03	0.59
1:B:365:PRO:HG2	1:B:375:MET:HG2	1.83	0.59
1:B:428:ILE:HG23	1:C:93:VAL:HG22	1.84	0.59
1:C:372:PRO:HD3	1:C:410:MET:SD	2.43	0.59
1:A:135:THR:CG2	1:A:136:PRO:N	2.65	0.59
1:A:143:MET:HE2	1:A:405:GLY:H	1.66	0.59
1:A:93:VAL:HG21	1:C:428:ILE:HG23	1.85	0.58
1:B:143:MET:HE2	1:B:405:GLY:N	2.18	0.58
1:C:47:ILE:CD1	1:C:82:TRP:CZ2	2.86	0.58
1:B:88:VAL:O	1:B:88:VAL:HG12	2.01	0.58
1:B:119:THR:HG22	1:B:123:ILE:HD12	1.85	0.58
1:C:100:TRP:NE1	1:C:410:MET:CE	2.66	0.58
1:C:109:PHE:CE2	1:C:134:MET:HE2	2.39	0.58
1:B:242:VAL:CG1	1:B:271:PHE:HB2	2.34	0.58
1:B:242:VAL:O	1:B:271:PHE:CD1	2.56	0.58
1:C:194:VAL:CG1	1:C:205:THR:CG2	2.78	0.58
1:A:71:TYR:OH	1:A:76:ARG:NH1	2.37	0.58
1:A:145:VAL:HG11	1:A:148:LEU:CD2	2.34	0.58
1:B:268:TYR:O	1:B:272:MET:HG2	2.04	0.58
1:C:95:ASN:OD1	1:C:96:PRO:HD2	2.04	0.58
1:A:194:VAL:HG13	1:A:205:THR:HG21	1.82	0.57
1:B:41:ASN:ND2	1:B:135:THR:HG21	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:GLU:OE2	2:C:474:HOH:O	2.17	0.57
1:C:158:LEU:O	1:C:162:ARG:HG3	2.04	0.57
1:C:11:ASN:OD1	1:C:14:ALA:N	2.30	0.57
1:C:143:MET:CE	1:C:405:GLY:H	2.14	0.57
1:C:30:HIS:C	1:C:30:HIS:CD2	2.83	0.57
1:C:47:ILE:CG2	1:C:127:THR:OG1	2.52	0.57
1:B:65:CYS:SG	1:B:88:VAL:HG11	2.45	0.57
1:A:365:PRO:HD3	1:A:378:HIS:HD2	1.68	0.57
1:B:377:MET:HE1	1:C:377:MET:CE	2.34	0.57
1:A:327:PHE:HE2	1:A:337:ILE:HD13	1.69	0.57
1:A:387:LEU:HD22	1:B:92:PHE:HA	1.86	0.57
1:B:135:THR:OG1	1:B:136:PRO:CD	2.52	0.57
1:B:198:GLY:CA	1:B:205:THR:HG21	2.35	0.57
1:A:149:CYS:HA	1:A:174:LEU:O	2.05	0.57
1:B:60:GLU:OE2	1:B:310:GLY:HA2	2.04	0.56
1:B:130:LYS:C	1:B:132:PRO:HD2	2.29	0.56
1:B:119:THR:HG23	1:B:123:ILE:HD11	1.84	0.56
1:B:65:CYS:CB	1:B:88:VAL:HG11	2.35	0.56
1:A:317:PHE:CD2	1:C:319:ARG:HG3	2.40	0.56
1:C:33:LEU:CD2	1:C:38:ILE:HD11	2.36	0.56
1:C:102:HIS:CE1	1:C:115:ILE:HD12	2.40	0.56
1:A:241:TYR:CD1	1:A:326:TYR:OH	2.45	0.56
1:A:246:ARG:HD3	1:A:267:ASP:OD2	2.05	0.56
1:A:283:THR:HG21	1:A:285:TRP:NE1	2.20	0.56
1:C:148:LEU:HD12	1:C:173:ILE:HG12	1.88	0.56
1:A:178:ARG:CG	1:A:231:ASP:HB3	2.36	0.56
1:A:209:ASP:OD1	1:A:248:ARG:NH2	2.38	0.56
1:A:327:PHE:HE2	1:A:337:ILE:CD1	2.17	0.56
1:A:185:VAL:HG21	1:A:268:TYR:CD2	2.39	0.56
1:B:242:VAL:HG11	1:B:271:PHE:HB2	1.88	0.56
1:B:389:TYR:CE2	1:B:439:HIS:CE1	2.93	0.56
1:A:386:ASP:CG	1:A:387:LEU:H	2.14	0.56
1:B:419:VAL:HA	1:B:422:MET:HE2	1.88	0.56
1:C:419:VAL:HA	1:C:422:MET:CE	2.35	0.56
1:B:326:TYR:O	1:B:330:GLU:HB2	2.05	0.55
1:C:159:GLU:OE1	1:C:159:GLU:CA	2.53	0.55
1:A:41:ASN:CG	1:A:135:THR:CG2	2.57	0.55
1:B:366:TRP:CD1	1:B:366:TRP:C	2.84	0.55
1:C:89:PHE:CZ	1:C:101:ILE:HD12	2.40	0.55
1:B:21:VAL:HG12	1:B:21:VAL:O	2.05	0.55
1:B:244:GLU:O	1:B:248:ARG:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:HA	1:A:401:LEU:HD13	1.89	0.55
1:A:136:PRO:HA	1:A:401:LEU:CD1	2.37	0.55
1:B:242:VAL:O	1:B:242:VAL:HG12	2.06	0.55
1:B:109:PHE:CZ	1:B:134:MET:HE1	2.42	0.55
1:C:184:ASN:HB3	1:C:187:LYS:HG2	1.88	0.55
1:A:93:VAL:HG22	1:C:428:ILE:HG12	1.88	0.54
1:C:136:PRO:HA	1:C:401:LEU:HD13	1.88	0.54
1:A:11:ASN:OD1	1:A:14:ALA:N	2.38	0.54
1:C:149:CYS:HA	1:C:174:LEU:O	2.08	0.54
1:B:136:PRO:HA	1:B:401:LEU:CD1	2.36	0.54
1:A:93:VAL:CG1	1:C:436:LEU:HD22	2.37	0.54
1:A:326:TYR:O	1:A:330:GLU:HB2	2.08	0.54
1:B:149:CYS:HA	1:B:174:LEU:O	2.08	0.54
1:B:283:THR:HG21	1:B:285:TRP:NE1	2.22	0.54
1:C:59:TRP:O	1:C:63:ARG:HG3	2.08	0.54
1:B:119:THR:HG21	1:B:123:ILE:HD11	1.88	0.54
1:B:241:TYR:CE2	1:B:243:ASP:OD1	2.61	0.54
1:C:366:TRP:CD1	1:C:366:TRP:C	2.86	0.53
1:A:205:THR:C	1:A:207:THR:N	2.63	0.53
1:B:119:THR:HG22	1:B:123:ILE:CD1	2.37	0.53
1:A:394:MET:HB2	1:A:411:PHE:CE2	2.43	0.53
1:C:3:LEU:O	1:C:107:ARG:NH2	2.41	0.53
1:C:100:TRP:CD1	1:C:410:MET:HE3	2.44	0.53
1:B:57:TYR:O	1:B:61:LEU:HG	2.09	0.53
1:B:442:TYR:O	1:B:445:PRO:HD2	2.08	0.53
1:A:418:VAL:O	1:A:422:MET:HE2	2.08	0.53
1:C:16:ARG:HH11	1:C:430:ILE:HD11	1.73	0.53
1:B:114:VAL:O	1:B:119:THR:HG21	2.09	0.53
1:C:394:MET:HB2	1:C:411:PHE:CE2	2.44	0.53
1:A:240:TYR:OH	1:A:266:ASN:HB3	2.09	0.53
1:A:283:THR:HG22	1:A:285:TRP:CD1	2.44	0.53
1:A:428:ILE:CG2	1:B:93:VAL:HG22	2.38	0.53
1:B:145:VAL:HG11	1:B:148:LEU:CD2	2.39	0.53
1:B:219:HIS:NE2	1:B:285:TRP:CZ3	2.77	0.53
1:A:48:TRP:CZ2	1:A:81:LYS:HD3	2.44	0.53
1:B:236:GLU:HG2	1:B:318:LEU:HD12	1.90	0.52
1:C:130:LYS:C	1:C:132:PRO:HD2	2.34	0.52
1:A:92:PHE:O	1:A:93:VAL:C	2.53	0.52
1:C:47:ILE:HG23	1:C:127:THR:OG1	2.09	0.52
1:C:219:HIS:HE1	1:C:285:TRP:CD2	2.27	0.52
1:A:178:ARG:HG2	1:A:231:ASP:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:THR:CG2	1:A:285:TRP:NE1	2.72	0.52
1:A:376:GLU:HG2	1:A:414:VAL:HG13	1.91	0.52
1:B:48:TRP:CE2	1:B:81:LYS:HD3	2.44	0.52
1:B:198:GLY:CA	1:B:205:THR:HG23	2.39	0.52
1:C:72:ILE:HG22	1:C:73:THR:HG23	1.91	0.52
1:B:109:PHE:CE2	1:B:134:MET:CE	2.89	0.52
1:B:237:PRO:O	1:B:323:GLY:HA3	2.09	0.52
1:C:205:THR:C	1:C:207:THR:H	2.17	0.52
1:B:209:ASP:OD1	1:B:248:ARG:NH2	2.43	0.52
1:A:207:THR:C	1:A:251:HIS:HE2	2.18	0.52
1:B:122:GLU:HG2	1:B:126:GLU:OE2	2.10	0.52
1:C:119:THR:HG23	1:C:123:ILE:HG13	1.91	0.52
1:A:21:VAL:HG13	1:A:24:LEU:CD1	2.40	0.51
1:A:317:PHE:CD2	1:C:319:ARG:CG	2.93	0.51
1:B:44:TRP:HZ3	1:B:139:LEU:CD1	2.23	0.51
1:C:119:THR:HG23	1:C:123:ILE:CD1	2.40	0.51
1:C:143:MET:HE2	1:C:404:PHE:CB	2.39	0.51
1:B:419:VAL:HA	1:B:422:MET:CE	2.41	0.51
1:C:56:HIS:CE1	1:C:57:TYR:CD2	2.98	0.51
1:C:242:VAL:O	1:C:271:PHE:CD1	2.63	0.51
1:C:44:TRP:CH2	1:C:401:LEU:HD12	2.42	0.51
1:A:105:LEU:HD11	1:A:123:ILE:CD1	2.37	0.51
1:B:178:ARG:HG2	1:B:231:ASP:HB3	1.92	0.51
1:B:283:THR:O	1:B:283:THR:HG22	2.09	0.51
1:C:89:PHE:HZ	1:C:101:ILE:HD12	1.75	0.51
1:C:347:LEU:CD2	1:C:350:ILE:HD11	2.36	0.51
1:A:228:VAL:O	1:A:228:VAL:CG1	2.55	0.51
1:A:365:PRO:CG	1:A:378:HIS:CD2	2.94	0.51
1:C:47:ILE:CD1	1:C:82:TRP:CE3	2.94	0.51
1:C:237:PRO:O	1:C:323:GLY:HA3	2.11	0.51
1:C:30:HIS:CD2	1:C:397:ASP:OD1	2.64	0.51
1:C:246:ARG:CG	1:C:246:ARG:NH1	2.68	0.51
1:C:283:THR:HG22	1:C:283:THR:O	2.10	0.51
1:B:219:HIS:NE2	1:B:285:TRP:CE3	2.79	0.51
1:C:21:VAL:HG11	1:C:441:SER:CB	2.41	0.51
1:A:319:ARG:CG	1:B:317:PHE:CD2	2.94	0.51
1:B:62:MET:HE2	1:B:72:ILE:HG12	1.81	0.50
1:B:345:THR:HG23	1:C:345:THR:CG2	2.41	0.50
1:C:70:GLU:OE1	1:C:76:ARG:NE	2.44	0.50
1:A:45:ASN:HB2	1:A:49:GLU:OE1	2.11	0.50
1:C:185:VAL:CG2	1:C:268:TYR:CD2	2.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ASP:OD2	1:C:248:ARG:CZ	2.59	0.50
1:A:375:MET:HE1	1:A:410:MET:SD	2.52	0.50
1:B:36:LYS:CB	1:B:160:HIS:CD2	2.94	0.50
1:C:16:ARG:HB3	1:C:434:ARG:HH21	1.75	0.50
1:A:21:VAL:HG11	1:A:441:SER:CB	2.41	0.50
1:A:89:PHE:CZ	1:A:101:ILE:HD12	2.46	0.50
1:C:130:LYS:O	1:C:134:MET:SD	2.69	0.50
1:B:345:THR:HG23	1:C:345:THR:HG23	1.94	0.50
1:C:326:TYR:O	1:C:330:GLU:HB2	2.11	0.50
1:A:60:GLU:HG2	2:A:476:HOH:O	2.11	0.50
1:B:21:VAL:O	1:B:21:VAL:CG1	2.60	0.50
1:C:123:ILE:O	1:C:127:THR:HG23	2.12	0.50
1:A:184:ASN:HB3	1:A:187:LYS:HG2	1.94	0.49
1:A:157:THR:OG1	1:A:159:GLU:HG3	2.12	0.49
1:B:198:GLY:O	1:B:202:GLY:N	2.45	0.49
1:B:157:THR:OG1	1:B:159:GLU:HG3	2.12	0.49
1:B:177:TRP:CZ3	1:B:179:PRO:HG3	2.47	0.49
1:C:92:PHE:O	1:C:93:VAL:C	2.55	0.49
1:A:237:PRO:O	1:A:323:GLY:HA3	2.13	0.49
1:A:345:THR:HG21	1:C:345:THR:CG2	2.43	0.49
1:A:428:ILE:HG12	1:B:93:VAL:HG22	1.94	0.49
1:B:48:TRP:CZ2	1:B:81:LYS:HD3	2.47	0.49
1:C:16:ARG:NH1	1:C:430:ILE:HD13	2.28	0.49
1:C:230:SER:OG	1:C:280:ASN:ND2	2.43	0.49
1:B:290:HIS:HB3	1:B:366:TRP:CH2	2.48	0.49
1:A:230:SER:OG	1:A:280:ASN:ND2	2.46	0.49
1:A:317:PHE:CE2	1:C:319:ARG:HG3	2.47	0.49
1:B:344:PRO:HD3	1:B:369:ASN:OD1	2.13	0.49
1:A:21:VAL:O	1:A:21:VAL:CG1	2.60	0.49
1:B:151:THR:HG23	1:B:178:ARG:HG3	1.94	0.49
1:A:72:ILE:HG22	1:A:73:THR:HG23	1.94	0.48
1:C:198:GLY:O	1:C:202:GLY:N	2.45	0.48
1:A:61:LEU:HB2	1:A:92:PHE:CE2	2.48	0.48
1:B:306:GLY:O	1:B:309:SER:OG	2.25	0.48
1:C:185:VAL:HG21	1:C:268:TYR:CD2	2.47	0.48
1:A:143:MET:HE1	1:A:401:LEU:O	2.13	0.48
1:A:219:HIS:CD2	1:A:279:MET:HB3	2.48	0.48
1:A:375:MET:O	1:A:379:LEU:HG	2.14	0.48
1:C:430:ILE:O	1:C:434:ARG:HG3	2.12	0.48
1:A:342:LEU:CD1	1:A:367:TRP:HB3	2.43	0.48
1:B:185:VAL:CG2	1:B:268:TYR:CE2	2.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TYR:OH	1:A:367:TRP:CD1	2.63	0.48
1:C:21:VAL:O	1:C:21:VAL:CG1	2.61	0.48
1:C:436:LEU:O	1:C:440:VAL:HG23	2.14	0.48
1:A:408:THR:O	1:A:412:ARG:HG3	2.14	0.48
1:B:21:VAL:CG1	1:B:412:ARG:HD3	2.40	0.48
1:B:143:MET:CE	1:B:405:GLY:N	2.70	0.48
1:A:428:ILE:CG2	1:B:93:VAL:CG2	2.86	0.48
1:B:178:ARG:CG	1:B:231:ASP:HB3	2.44	0.48
1:A:194:VAL:O	1:A:205:THR:HG21	2.14	0.48
1:C:33:LEU:HD23	1:C:38:ILE:HD11	1.96	0.48
1:C:283:THR:CG2	1:C:285:TRP:CD1	2.95	0.48
1:A:21:VAL:HG11	1:A:441:SER:OG	2.14	0.48
1:A:204:ASP:O	1:A:207:THR:OG1	2.32	0.48
1:B:219:HIS:CD2	1:B:285:TRP:CZ3	3.02	0.47
1:C:143:MET:CE	1:C:405:GLY:N	2.74	0.47
1:C:242:VAL:O	1:C:271:PHE:HD1	1.97	0.47
1:C:342:LEU:CD1	1:C:367:TRP:HB3	2.43	0.47
1:A:105:LEU:CD1	1:A:123:ILE:CD1	2.84	0.47
1:B:21:VAL:HG13	1:B:24:LEU:HD12	1.96	0.47
1:C:48:TRP:CZ2	1:C:81:LYS:HD3	2.50	0.47
1:A:89:PHE:N	1:A:90:PRO:CD	2.76	0.47
1:A:5:GLU:O	1:A:413:ARG:NH2	2.48	0.47
1:B:290:HIS:HD2	1:B:366:TRP:CE2	2.32	0.47
1:C:219:HIS:HD2	1:C:279:MET:HB3	1.80	0.47
1:C:364:ALA:HB1	1:C:365:PRO:HD2	1.97	0.47
1:A:365:PRO:HG3	1:A:378:HIS:HD2	1.70	0.47
1:A:436:LEU:HD22	1:B:93:VAL:HG13	1.96	0.47
1:C:379:LEU:HD22	1:C:388:LEU:HD11	1.96	0.47
1:B:7:TYR:OH	1:B:99:GLU:OE1	2.21	0.47
1:A:208:LEU:CA	1:A:251:HIS:CD2	2.98	0.47
1:A:327:PHE:CE2	1:A:337:ILE:HD13	2.49	0.47
1:A:349:THR:O	1:A:353:ILE:HG13	2.15	0.47
1:C:21:VAL:CG2	1:C:437:VAL:HG13	2.42	0.47
1:A:427:GLN:HG2	1:B:99:GLU:OE1	2.15	0.46
1:C:419:VAL:HA	1:C:422:MET:HE2	1.96	0.46
1:B:304:THR:HG22	1:B:305:LEU:HG	1.97	0.46
1:C:158:LEU:HD12	1:C:221:HIS:CD2	2.50	0.46
1:C:283:THR:HG22	1:C:285:TRP:NE1	2.27	0.46
1:B:394:MET:HB2	1:B:411:PHE:CE2	2.50	0.46
1:C:69:GLU:OE2	1:C:72:ILE:HD12	2.15	0.46
1:A:409:GLU:O	1:A:413:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:O	1:B:81:LYS:HE2	2.16	0.46
1:B:147:ILE:HG12	1:B:172:THR:HB	1.97	0.46
1:B:148:LEU:HD12	1:B:173:ILE:HG12	1.96	0.46
1:B:283:THR:HG22	1:B:285:TRP:CD1	2.51	0.46
1:C:113:LYS:CD	1:C:122:GLU:OE1	2.63	0.46
1:C:304:THR:HG22	1:C:305:LEU:HG	1.96	0.46
1:B:221:HIS:CE1	1:B:225:HIS:HE1	2.33	0.46
1:C:65:CYS:SG	1:C:88:VAL:CG1	3.04	0.46
1:C:194:VAL:HG13	1:C:205:THR:CG2	2.43	0.46
1:A:185:VAL:CG2	1:A:268:TYR:CD2	2.98	0.46
1:B:290:HIS:CD2	1:B:366:TRP:CE2	3.04	0.46
1:A:364:ALA:HB1	1:A:365:PRO:HD2	1.97	0.46
1:B:85:LEU:HD11	1:B:89:PHE:CD1	2.51	0.46
1:C:362:VAL:O	1:C:391:LEU:HD12	2.15	0.46
1:B:386:ASP:CG	1:B:387:LEU:H	2.24	0.46
1:C:208:LEU:CA	1:C:251:HIS:CD2	2.98	0.46
1:A:59:TRP:O	1:A:63:ARG:HG3	2.16	0.45
1:A:360:VAL:O	1:B:64:ARG:NH1	2.41	0.45
1:C:28:ASP:OD2	1:C:396:THR:OG1	2.31	0.45
1:C:88:VAL:O	1:C:88:VAL:HG13	2.14	0.45
1:C:219:HIS:HE1	1:C:285:TRP:CE3	2.23	0.45
1:B:130:LYS:C	1:B:132:PRO:CD	2.87	0.45
1:C:386:ASP:CG	1:C:387:LEU:H	2.25	0.45
1:B:26:ILE:HG12	1:B:408:THR:HG21	1.99	0.45
1:B:30:HIS:NE2	1:B:397:ASP:OD1	2.50	0.45
1:B:190:TRP:O	1:B:194:VAL:HG23	2.16	0.45
1:A:123:ILE:HG23	1:A:124:TRP:N	2.32	0.45
1:B:343:ASP:HB3	1:B:346:HIS:CE1	2.52	0.45
1:A:35:ALA:O	1:A:39:VAL:HG23	2.16	0.45
1:B:394:MET:HB2	1:B:411:PHE:CD2	2.52	0.45
1:B:92:PHE:O	1:B:93:VAL:C	2.58	0.45
1:A:50:VAL:HG11	1:A:402:LEU:HD12	1.98	0.45
1:A:82:TRP:CZ2	1:A:123:ILE:HG21	2.48	0.45
1:A:143:MET:CE	1:A:405:GLY:N	2.68	0.45
1:A:372:PRO:HD3	1:A:410:MET:SD	2.57	0.45
1:B:432:GLU:HB2	1:C:93:VAL:HG21	1.99	0.45
1:C:389:TYR:CE2	1:C:439:HIS:CD2	3.05	0.45
1:A:343:ASP:HB3	1:A:346:HIS:ND1	2.32	0.45
1:B:74:GLY:O	1:B:81:LYS:NZ	2.33	0.45
1:B:342:LEU:CD1	1:B:367:TRP:HB3	2.47	0.45
1:C:355:ARG:O	1:C:355:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LYS:HG3	1:A:403:SER:OG	2.18	0.44
1:B:288:GLN:NE2	1:B:340:TYR:OH	2.50	0.44
1:C:194:VAL:O	1:C:205:THR:HG21	2.17	0.44
1:A:65:CYS:SG	1:A:88:VAL:HG13	2.57	0.44
1:A:365:PRO:CD	1:A:378:HIS:CD2	2.90	0.44
1:B:427:GLN:HG2	1:C:99:GLU:OE1	2.17	0.44
1:C:148:LEU:HD22	1:C:404:PHE:CE2	2.53	0.44
1:C:296:ASP:OD1	1:C:296:ASP:N	2.47	0.44
1:A:148:LEU:HD22	1:A:404:PHE:CE2	2.52	0.44
1:A:157:THR:OG1	1:A:159:GLU:HG2	2.17	0.44
1:A:153:ASP:OD1	1:A:155:VAL:CG2	2.64	0.44
1:B:208:LEU:HD11	1:B:247:ALA:HB1	1.99	0.44
1:C:221:HIS:CD2	1:C:221:HIS:C	2.96	0.44
1:A:242:VAL:O	1:A:271:PHE:HD1	2.00	0.44
1:B:71:TYR:CZ	1:B:76:ARG:CD	3.00	0.44
1:C:89:PHE:N	1:C:90:PRO:CD	2.80	0.44
1:A:148:LEU:HD12	1:A:173:ILE:HG12	1.98	0.44
1:A:347:LEU:HD21	1:A:378:HIS:HE1	1.78	0.44
1:B:143:MET:HE2	1:B:405:GLY:H	1.72	0.44
1:B:46:ASP:HB2	1:B:49:GLU:H	1.83	0.44
1:B:239:VAL:HG11	1:B:327:PHE:HB2	2.00	0.44
1:B:375:MET:HE1	1:B:410:MET:HG2	2.00	0.44
1:C:268:TYR:O	1:C:272:MET:HG2	2.17	0.44
1:A:365:PRO:HG2	1:A:375:MET:HG2	2.00	0.44
1:A:419:VAL:HA	1:A:422:MET:HE3	2.00	0.44
1:A:422:MET:HE3	1:A:422:MET:HB2	1.77	0.44
1:B:109:PHE:O	1:B:130:LYS:NZ	2.43	0.44
1:B:293:ALA:HB3	1:B:295:ARG:HE	1.83	0.44
1:B:347:LEU:N	1:B:348:PRO:CD	2.81	0.44
1:B:349:THR:O	1:B:353:ILE:HG13	2.18	0.44
1:A:44:TRP:CH2	1:A:401:LEU:HD12	2.48	0.43
1:A:110:ASN:O	1:A:110:ASN:CG	2.60	0.43
1:B:157:THR:OG1	1:B:159:GLU:CG	2.66	0.43
1:B:319:ARG:CG	1:C:317:PHE:CD2	2.99	0.43
1:A:71:TYR:CZ	1:A:76:ARG:CD	3.01	0.43
1:A:216:TRP:HE3	1:A:279:MET:HG2	1.83	0.43
1:B:88:VAL:HG13	1:B:91:ARG:HD3	1.99	0.43
1:A:250:VAL:HG11	1:A:268:TYR:HB2	2.00	0.43
1:B:184:ASN:HB3	1:B:187:LYS:CG	2.42	0.43
1:C:119:THR:HG23	1:C:123:ILE:CG1	2.48	0.43
1:C:342:LEU:HB2	1:C:366:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:SER:HA	1:B:255:PHE:CE1	2.54	0.43
1:C:442:TYR:O	1:C:445:PRO:HD2	2.18	0.43
1:B:47:ILE:HD13	1:B:82:TRP:CH2	2.54	0.43
1:B:69:GLU:O	1:B:70:GLU:C	2.62	0.43
1:C:442:TYR:OH	1:C:446:LYS:NZ	2.49	0.43
1:A:198:GLY:O	1:A:202:GLY:N	2.48	0.43
1:A:244:GLU:O	1:A:248:ARG:N	2.44	0.43
1:C:26:ILE:HG12	1:C:408:THR:HG21	2.00	0.43
1:C:159:GLU:OE1	1:C:162:ARG:HD2	2.18	0.43
1:A:2:PHE:CE1	1:A:3:LEU:HD13	2.54	0.43
1:A:347:LEU:N	1:A:348:PRO:CD	2.81	0.43
1:A:0:HIS:CD2	1:A:1:MET:N	2.87	0.42
1:A:30:HIS:NE2	1:A:397:ASP:OD1	2.52	0.42
1:A:99:GLU:CD	1:C:427:GLN:HE21	2.26	0.42
1:A:242:VAL:O	1:A:271:PHE:CD1	2.71	0.42
1:B:290:HIS:HA	1:B:340:TYR:HB2	2.01	0.42
1:B:394:MET:HE3	1:B:394:MET:HB3	1.95	0.42
1:C:89:PHE:CE2	1:C:115:ILE:HD12	2.54	0.42
1:C:250:VAL:HG11	1:C:268:TYR:HB2	2.00	0.42
1:A:355:ARG:O	1:A:355:ARG:HG2	2.19	0.42
1:B:11:ASN:OD1	1:B:14:ALA:N	2.44	0.42
1:A:105:LEU:HD13	1:A:123:ILE:CD1	2.48	0.42
1:A:327:PHE:CE2	1:A:337:ILE:CD1	3.00	0.42
1:B:209:ASP:OD2	1:B:248:ARG:NH2	2.52	0.42
1:B:272:MET:HE3	1:B:272:MET:HA	2.01	0.42
1:A:147:ILE:HG12	1:A:172:THR:HB	2.01	0.42
1:B:55:ASP:CG	1:B:58:VAL:HG23	2.44	0.42
1:C:95:ASN:CG	1:C:96:PRO:HD2	2.45	0.42
1:C:190:TRP:O	1:C:194:VAL:HG23	2.18	0.42
1:C:244:GLU:O	1:C:248:ARG:N	2.43	0.42
1:C:312:ASP:HB2	1:C:367:TRP:HH2	1.84	0.42
1:A:57:TYR:HH	1:A:367:TRP:NE1	2.18	0.42
1:B:244:GLU:O	1:B:248:ARG:N	2.47	0.42
1:C:47:ILE:HD12	1:C:82:TRP:CZ2	2.54	0.42
1:C:277:GLY:HA3	1:C:331:PHE:CZ	2.53	0.42
1:C:205:THR:C	1:C:207:THR:N	2.75	0.42
1:A:386:ASP:CG	1:A:387:LEU:N	2.77	0.42
1:B:3:LEU:O	1:B:107:ARG:NH2	2.52	0.42
1:C:206:SER:HA	1:C:255:PHE:CE1	2.54	0.42
1:C:403:SER:O	1:C:404:PHE:C	2.63	0.42
1:A:51:GLU:OE1	1:A:400:LYS:NZ	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:THR:HG23	1:B:123:ILE:HG13	2.02	0.42
1:B:143:MET:HE1	1:B:401:LEU:O	2.20	0.42
1:B:296:ASP:N	1:B:296:ASP:OD1	2.53	0.42
1:B:283:THR:CG2	1:B:285:TRP:NE1	2.82	0.42
1:C:130:LYS:C	1:C:132:PRO:CD	2.91	0.42
1:C:335:LEU:O	1:C:359:ASN:HB2	2.19	0.42
1:A:93:VAL:HG22	1:C:428:ILE:CG2	2.45	0.42
1:A:283:THR:HG22	1:A:283:THR:O	2.20	0.42
1:A:288:GLN:NE2	1:A:340:TYR:OH	2.52	0.42
1:A:324:LEU:HB3	1:A:328:LEU:HD12	2.02	0.42
1:A:403:SER:O	1:A:404:PHE:C	2.63	0.42
1:B:113:LYS:HD2	1:B:122:GLU:OE1	2.20	0.42
1:A:189:GLY:O	1:A:190:TRP:C	2.63	0.41
1:A:271:PHE:CE2	1:A:275:GLN:CD	2.98	0.41
1:B:19:ASN:OD1	1:B:22:LYS:HE2	2.19	0.41
1:B:41:ASN:CG	1:B:135:THR:HG1	2.27	0.41
1:C:355:ARG:NE	1:C:385:VAL:O	2.44	0.41
1:A:18:PHE:CE1	1:A:413:ARG:HG2	2.55	0.41
1:A:88:VAL:HG13	1:A:88:VAL:O	2.21	0.41
1:A:135:THR:O	1:A:139:LEU:N	2.47	0.41
1:B:371:SER:O	1:B:372:PRO:C	2.62	0.41
1:C:350:ILE:HG13	1:C:351:SER:N	2.34	0.41
1:B:373:PHE:N	2:B:484:HOH:O	2.43	0.41
1:C:347:LEU:N	1:C:348:PRO:CD	2.84	0.41
1:A:135:THR:C	1:A:139:LEU:HD12	2.46	0.41
1:A:389:TYR:CD2	1:A:389:TYR:O	2.74	0.41
1:B:355:ARG:HD3	1:C:60:GLU:OE1	2.20	0.41
1:B:362:VAL:O	1:B:391:LEU:HD12	2.20	0.41
1:C:86:ALA:O	1:C:87:LYS:C	2.63	0.41
1:C:190:TRP:HH2	1:C:251:HIS:ND1	2.19	0.41
1:B:155:VAL:CG2	1:B:193:TYR:CE1	3.03	0.41
1:C:132:PRO:C	1:C:134:MET:H	2.27	0.41
1:C:246:ARG:HG3	1:C:246:ARG:NH1	2.14	0.41
1:A:47:ILE:HD13	1:A:82:TRP:CH2	2.56	0.41
1:B:136:PRO:HA	1:B:401:LEU:HD13	2.02	0.41
1:C:132:PRO:C	1:C:134:MET:N	2.79	0.41
1:C:218:SER:O	1:C:221:HIS:HB3	2.21	0.41
1:C:244:GLU:CD	1:C:248:ARG:HH21	2.26	0.41
1:B:122:GLU:O	1:B:126:GLU:HG3	2.21	0.41
1:A:155:VAL:CG2	1:A:193:TYR:CE1	3.04	0.41
1:A:283:THR:CG2	1:A:285:TRP:CD1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:HIS:CD2	1:A:340:TYR:CG	3.09	0.41
1:A:371:SER:O	1:A:372:PRO:C	2.64	0.41
1:A:428:ILE:HG22	1:A:429:PRO:O	2.21	0.41
1:B:283:THR:CG2	1:B:285:TRP:CD1	3.04	0.41
1:B:428:ILE:HG22	1:B:429:PRO:O	2.20	0.41
1:C:77:SER:O	1:C:78:ASN:C	2.64	0.41
1:C:365:PRO:HG3	1:C:378:HIS:CB	2.51	0.41
1:C:369:ASN:O	1:C:374:GLY:HA3	2.20	0.41
1:A:79:LYS:O	1:A:83:LEU:HG	2.21	0.41
1:A:207:THR:C	1:A:251:HIS:NE2	2.78	0.41
1:B:62:MET:HE3	1:B:62:MET:HB3	1.76	0.41
1:B:205:THR:C	1:B:207:THR:H	2.28	0.41
1:C:79:LYS:NZ	1:C:121:GLU:CD	2.78	0.41
1:C:394:MET:HB2	1:C:411:PHE:CD2	2.56	0.41
1:B:85:LEU:CD1	1:B:89:PHE:HD1	2.34	0.40
1:B:403:SER:O	1:B:404:PHE:C	2.64	0.40
1:C:71:TYR:CZ	1:C:76:ARG:HD3	2.54	0.40
1:C:219:HIS:HE1	1:C:285:TRP:CE2	2.39	0.40
1:C:365:PRO:HG3	1:C:378:HIS:CG	2.57	0.40
1:A:95:ASN:OD1	1:A:96:PRO:HD2	2.20	0.40
1:B:121:GLU:O	1:B:125:GLU:HG3	2.22	0.40
1:B:355:ARG:O	1:B:355:ARG:HG2	2.20	0.40
1:C:174:LEU:HD13	1:C:226:GLY:O	2.21	0.40
1:C:371:SER:O	1:C:372:PRO:C	2.64	0.40
1:C:375:MET:HE1	1:C:410:MET:HG2	2.03	0.40
1:B:89:PHE:N	1:B:90:PRO:CD	2.84	0.40
1:B:251:HIS:HB2	1:B:268:TYR:HE1	1.87	0.40
1:C:61:LEU:HB2	1:C:92:PHE:CE2	2.57	0.40
1:C:65:CYS:SG	1:C:88:VAL:HG13	2.62	0.40
1:C:205:THR:HG23	1:C:211:PHE:CD1	2.57	0.40
1:C:439:HIS:CE1	1:C:444:GLY:HA2	2.56	0.40
1:A:139:LEU:HD22	1:A:402:LEU:CD2	2.51	0.40
1:C:113:LYS:NZ	1:C:122:GLU:OE1	2.49	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ASP:OD2	1:B:112:LYS:NZ[1_655]	0.84	1.36
1:A:128:LYS:NZ	1:B:169:GLU:OE2[1_665]	1.20	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LYS:NZ	1:C:169:GLU:CD[1_556]	1.49	0.71
1:B:128:LYS:NZ	1:C:169:GLU:OE2[1_556]	1.51	0.69
1:A:255:PHE:O	1:B:5:GLU:OE2[1_655]	1.58	0.62
1:A:204:ASP:CG	1:B:112:LYS:NZ[1_655]	1.89	0.31
1:B:206:SER:O	1:C:16:ARG:NH2[1_545]	1.95	0.25
1:A:128:LYS:NZ	1:B:169:GLU:CD[1_665]	1.98	0.22
1:A:191:ARG:NH2	1:B:5:GLU:OE1[1_655]	2.03	0.17
1:A:255:PHE:C	1:B:5:GLU:OE2[1_655]	2.08	0.12
1:B:128:LYS:NZ	1:C:169:GLU:CG[1_556]	2.08	0.12

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	449/463 (97%)	425 (95%)	20 (4%)	4 (1%)	14	28
1	B	448/463 (97%)	420 (94%)	25 (6%)	3 (1%)	18	35
1	C	448/463 (97%)	422 (94%)	23 (5%)	3 (1%)	18	35
All	All	1345/1389 (97%)	1267 (94%)	68 (5%)	10 (1%)	18	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	257	GLY
1	B	257	GLY
1	C	257	GLY
1	B	169	GLU
1	B	243	ASP
1	A	29	PRO
1	A	136	PRO
1	A	93	VAL
1	C	93	VAL
1	C	136	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	399/409 (98%)	368 (92%)	31 (8%)	11	25
1	B	398/409 (97%)	366 (92%)	32 (8%)	11	24
1	C	398/409 (97%)	366 (92%)	32 (8%)	11	24
All	All	1195/1227 (97%)	1100 (92%)	95 (8%)	11	24

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	30	HIS
1	A	46	ASP
1	A	54	THR
1	A	56	HIS
1	A	88	VAL
1	A	93	VAL
1	A	107	ARG
1	A	119	THR
1	A	128	LYS
1	A	134	MET
1	A	155	VAL
1	A	171	VAL
1	A	208	LEU
1	A	236	GLU
1	A	256	SER
1	A	263	ASP
1	A	281	GLN
1	A	301	LEU
1	A	318	LEU
1	A	319	ARG
1	A	330	GLU
1	A	341	VAL
1	A	347	LEU
1	A	370	ASP
1	A	397	ASP

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Mol	Chain	Res	Type
1	A	398	SER
1	A	408	THR
1	A	421	GLU
1	A	432	GLU
1	A	437	VAL
1	B	3	LEU
1	B	20	GLU
1	B	54	THR
1	B	93	VAL
1	B	97	THR
1	B	113	LYS
1	B	119	THR
1	B	128	LYS
1	B	155	VAL
1	B	171	VAL
1	B	185	VAL
1	B	208	LEU
1	B	236	GLU
1	B	243	ASP
1	B	256	SER
1	B	262	GLN
1	B	263	ASP
1	B	281	GLN
1	B	294	LEU
1	B	296	ASP
1	B	301	LEU
1	B	304	THR
1	B	318	LEU
1	B	319	ARG
1	B	330	GLU
1	B	341	VAL
1	B	347	LEU
1	B	376	GLU
1	B	394	MET
1	B	416	SER
1	B	432	GLU
1	B	437	VAL
1	C	20	GLU
1	C	54	THR
1	C	88	VAL
1	C	93	VAL
1	C	107	ARG

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Mol	Chain	Res	Type
1	C	108	ARG
1	C	119	THR
1	C	128	LYS
1	C	134	MET
1	C	155	VAL
1	C	171	VAL
1	C	178	ARG
1	C	185	VAL
1	C	208	LEU
1	C	236	GLU
1	C	246	ARG
1	C	256	SER
1	C	281	GLN
1	C	294	LEU
1	C	296	ASP
1	C	301	LEU
1	C	318	LEU
1	C	319	ARG
1	C	330	GLU
1	C	341	VAL
1	C	347	LEU
1	C	397	ASP
1	C	398	SER
1	C	402	LEU
1	C	408	THR
1	C	432	GLU
1	C	437	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	HIS
1	A	221	HIS
1	A	232	HIS
1	A	288	GLN
1	A	439	HIS
1	B	45	ASN
1	B	221	HIS
1	B	232	HIS
1	B	288	GLN
1	B	378	HIS
1	B	439	HIS

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Mol	Chain	Res	Type
1	C	56	HIS
1	C	102	HIS
1	C	221	HIS
1	C	288	GLN
1	C	427	GLN
1	C	439	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](#)

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	451/463 (97%)	1.25	101 (22%) 2 2	8, 27, 80, 122	18 (3%)
1	B	450/463 (97%)	1.34	102 (22%) 2 2	4, 27, 80, 122	19 (4%)
1	C	450/463 (97%)	1.27	108 (24%) 2 2	8, 27, 80, 122	19 (4%)
All	All	1351/1389 (97%)	1.29	311 (23%) 2 2	4, 27, 80, 122	56 (4%)

All (311) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	241	TYR	10.2
1	B	259	LYS	9.5
1	C	226	GLY	8.9
1	A	257	GLY	8.9
1	A	228	VAL	8.6
1	C	228	VAL	8.3
1	C	227	CYS	7.8
1	C	229	ALA	7.7
1	B	233	ALA	7.6
1	A	226	GLY	7.6
1	A	233	ALA	7.6
1	A	229	ALA	7.5
1	A	231	ASP	7.5
1	A	256	SER	7.4
1	C	232	HIS	7.4
1	A	225	HIS	7.4
1	B	232	HIS	7.3
1	C	231	ASP	7.3
1	B	231	ASP	7.3
1	C	259	LYS	7.3
1	A	227	CYS	7.1
1	B	258	GLU	7.1
1	A	232	HIS	7.0

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Mol	Chain	Res	Type	RSRZ
1	C	233	ALA	7.0
1	B	243	ASP	6.9
1	C	243	ASP	6.9
1	B	228	VAL	6.8
1	B	229	ALA	6.8
1	B	257	GLY	6.8
1	B	230	SER	6.7
1	C	204	ASP	6.7
1	B	226	GLY	6.7
1	C	230	SER	6.6
1	B	255	PHE	6.6
1	B	244	GLU	6.6
1	B	204	ASP	6.6
1	B	225	HIS	6.5
1	A	230	SER	6.5
1	C	241	TYR	6.4
1	C	157	THR	6.4
1	B	260	LEU	6.3
1	A	260	LEU	6.3
1	B	227	CYS	6.3
1	C	225	HIS	6.1
1	C	263	ASP	6.1
1	A	236	GLU	6.1
1	B	234	LEU	6.0
1	C	235	LEU	5.9
1	B	224	GLU	5.9
1	B	235	LEU	5.9
1	C	234	LEU	5.8
1	A	235	LEU	5.7
1	A	45	ASN	5.7
1	A	240	TYR	5.6
1	B	240	TYR	5.5
1	B	242	VAL	5.5
1	A	238	SER	5.4
1	B	263	ASP	5.4
1	B	186	ASP	5.4
1	A	234	LEU	5.3
1	C	260	LEU	5.3
1	A	186	ASP	5.3
1	B	241	TYR	5.2
1	A	242	VAL	5.2
1	A	255	PHE	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	5.2
1	A	263	ASP	5.2
1	B	256	SER	5.2
1	A	261	THR	5.1
1	C	261	THR	5.0
1	C	238	SER	5.0
1	B	206	SER	4.9
1	B	238	SER	4.8
1	B	223	LYS	4.8
1	C	258	GLU	4.8
1	A	244	GLU	4.8
1	B	261	THR	4.7
1	C	236	GLU	4.7
1	B	162	ARG	4.6
1	B	245	ASN	4.6
1	C	255	PHE	4.6
1	C	244	GLU	4.6
1	C	242	VAL	4.6
1	A	199	GLU	4.5
1	A	169	GLU	4.5
1	B	5	GLU	4.5
1	C	206	SER	4.5
1	C	207	THR	4.4
1	B	200	ARG	4.4
1	C	189	GLY	4.3
1	B	203	GLU	4.3
1	C	239	VAL	4.3
1	C	257	GLY	4.3
1	C	134	MET	4.3
1	A	224	GLU	4.3
1	C	45	ASN	4.3
1	A	259	LYS	4.3
1	B	220	GLU	4.3
1	C	256	SER	4.2
1	A	254	ALA	4.2
1	B	237	PRO	4.2
1	B	254	ALA	4.2
1	A	246	ARG	4.2
1	B	239	VAL	4.2
1	B	236	GLU	4.1
1	C	169	GLU	4.1
1	C	188	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	258	GLU	4.1
1	C	240	TYR	4.0
1	B	188	GLU	4.0
1	A	237	PRO	3.9
1	A	187	LYS	3.9
1	B	262	GLN	3.9
1	A	134	MET	3.9
1	A	0	HIS	3.9
1	A	162	ARG	3.9
1	C	237	PRO	3.8
1	C	205	THR	3.8
1	C	220	GLU	3.8
1	A	262	GLN	3.8
1	A	123	ILE	3.7
1	A	239	VAL	3.7
1	B	246	ARG	3.7
1	A	223	LYS	3.6
1	B	45	ASN	3.6
1	B	169	GLU	3.6
1	B	192	GLU	3.6
1	C	223	LYS	3.6
1	C	162	ARG	3.6
1	C	200	ARG	3.5
1	A	168	VAL	3.5
1	C	254	ALA	3.5
1	C	224	GLU	3.5
1	A	200	ARG	3.5
1	A	282	GLU	3.5
1	C	1	MET	3.5
1	B	199	GLU	3.5
1	C	202	GLY	3.4
1	A	189	GLY	3.4
1	C	245	ASN	3.4
1	C	262	GLN	3.4
1	A	159	GLU	3.4
1	C	275	GLN	3.4
1	B	167	ALA	3.4
1	B	134	MET	3.4
1	A	245	ASN	3.3
1	A	202	GLY	3.3
1	A	42	LYS	3.3
1	A	205	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	308	ASP	3.3
1	B	133	GLU	3.3
1	C	248	ARG	3.3
1	B	187	LYS	3.2
1	A	125	GLU	3.2
1	A	252	GLU	3.2
1	C	186	ASP	3.2
1	A	167	ALA	3.2
1	C	187	LYS	3.2
1	A	188	GLU	3.2
1	B	398	SER	3.2
1	B	403	SER	3.2
1	C	141	ARG	3.2
1	A	192	GLU	3.2
1	A	220	GLU	3.2
1	B	159	GLU	3.2
1	C	181	ARG	3.1
1	B	253	LYS	3.1
1	A	370	ASP	3.1
1	B	190	TRP	3.1
1	C	5	GLU	3.1
1	C	198	GLY	3.1
1	C	199	GLU	3.1
1	B	205	THR	3.1
1	B	275	GLN	3.0
1	B	222	PHE	3.0
1	B	207	THR	3.0
1	B	221	HIS	3.0
1	B	248	ARG	3.0
1	B	202	GLY	3.0
1	B	247	ALA	2.9
1	B	157	THR	2.9
1	C	192	GLU	2.9
1	C	203	GLU	2.9
1	A	243	ASP	2.9
1	C	155	VAL	2.9
1	A	181	ARG	2.9
1	C	11	ASN	2.8
1	B	75	SER	2.8
1	A	275	GLN	2.8
1	B	36	LYS	2.8
1	A	34	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	34	ASP	2.8
1	A	398	SER	2.8
1	B	196	LYS	2.7
1	A	170	GLY	2.7
1	B	16	ARG	2.7
1	C	42	LYS	2.7
1	A	207	THR	2.7
1	C	49	GLU	2.7
1	B	185	VAL	2.7
1	A	196	LYS	2.7
1	A	330	GLU	2.7
1	C	167	ALA	2.7
1	B	117	GLU	2.7
1	C	165	LYS	2.6
1	A	43	PRO	2.6
1	C	221	HIS	2.6
1	B	135	THR	2.6
1	C	250	VAL	2.6
1	C	249	ALA	2.6
1	C	403	SER	2.6
1	A	248	ARG	2.6
1	C	170	GLY	2.6
1	B	33	LEU	2.6
1	A	47	ILE	2.6
1	B	370	ASP	2.6
1	A	185	VAL	2.6
1	B	430	ILE	2.6
1	C	168	VAL	2.6
1	B	443	ASP	2.6
1	B	434	ARG	2.5
1	A	131	LEU	2.5
1	B	170	GLY	2.5
1	C	160	HIS	2.5
1	A	190	TRP	2.5
1	C	222	PHE	2.5
1	A	376	GLU	2.5
1	B	189	GLY	2.4
1	A	206	SER	2.4
1	B	168	VAL	2.4
1	B	171	VAL	2.4
1	C	16	ARG	2.4
1	A	221	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	31	ASN	2.4
1	C	296	ASP	2.4
1	A	165	LYS	2.4
1	A	195	GLU	2.4
1	A	222	PHE	2.4
1	C	125	GLU	2.4
1	B	270	ALA	2.4
1	A	141	ARG	2.4
1	A	397	ASP	2.4
1	A	1	MET	2.4
1	B	402	LEU	2.4
1	C	196	LYS	2.3
1	A	247	ALA	2.3
1	C	117	GLU	2.3
1	C	252	GLU	2.3
1	B	158	LEU	2.3
1	C	131	LEU	2.3
1	B	129	LYS	2.3
1	B	41	ASN	2.3
1	C	424	GLU	2.3
1	A	158	LEU	2.3
1	B	208	LEU	2.3
1	B	399	ARG	2.3
1	B	39	VAL	2.3
1	C	10	THR	2.3
1	A	249	ALA	2.3
1	A	204	ASP	2.3
1	B	47	ILE	2.3
1	C	264	GLU	2.2
1	C	322	GLU	2.2
1	B	308	ASP	2.2
1	B	193	TYR	2.2
1	C	398	SER	2.2
1	B	198	GLY	2.2
1	C	159	GLU	2.2
1	C	282	GLU	2.2
1	C	197	MET	2.2
1	A	400	LYS	2.2
1	A	401	LEU	2.2
1	B	70	GLU	2.2
1	C	36	LYS	2.2
1	C	33	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	43	PRO	2.1
1	B	397	ASP	2.1
1	C	180	ASP	2.1
1	A	367	TRP	2.1
1	A	5	GLU	2.1
1	C	399	ARG	2.1
1	B	38	ILE	2.1
1	A	160	HIS	2.1
1	C	32	HIS	2.1
1	A	46	ASP	2.1
1	C	191	ARG	2.1
1	A	384	SER	2.1
1	C	112	LYS	2.1
1	C	132	PRO	2.1
1	C	142	ASP	2.1
1	A	44	TRP	2.1
1	B	400	LYS	2.1
1	C	171	VAL	2.1
1	A	16	ARG	2.1
1	A	203	GLU	2.1
1	C	40	GLU	2.1
1	C	110	ASN	2.0
1	A	399	ARG	2.0
1	B	191	ARG	2.0
1	A	299	ASP	2.0
1	C	122	GLU	2.0
1	C	376	GLU	2.0
1	C	400	LYS	2.0
1	A	41	ASN	2.0
1	B	181	ARG	2.0
1	C	31	ASN	2.0
1	C	47	ILE	2.0
1	A	296	ASP	2.0
1	A	36	LYS	2.0
1	B	165	LYS	2.0
1	C	166	GLU	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.