



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:16 am GMT

PDB ID : 1J5S
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

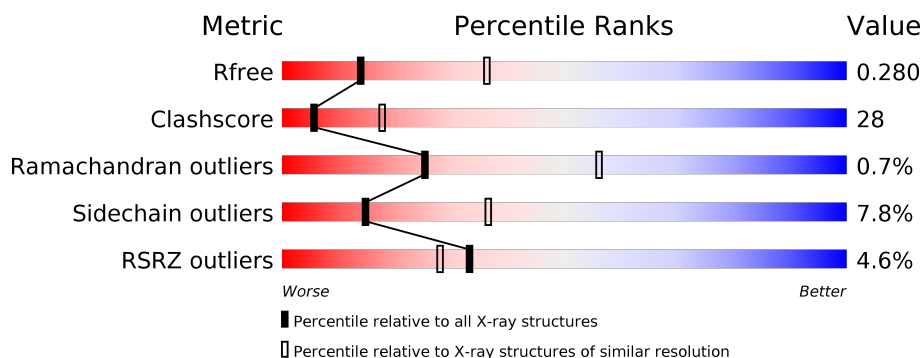
1 Overall quality at a glance ⓘ

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}	100719	2469 (2.90-2.82)
Clashscore	112137	2749 (2.90-2.82)
Ramachandran outliers	110173	2687 (2.90-2.82)
Sidechain outliers	110143	2690 (2.90-2.82)
RSRZ outliers	101464	2487 (2.90-2.82)

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

Mol	Chain	Length	Quality of chain
1	A	463	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div>5%</div> </div> </div>
1	B	463	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>40%</div> <div>5%</div> </div> </div>
1	C	463	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>37%</div> <div>5%</div> </div> </div>

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	-	LEADER SEQUENCE	UNP Q9WXR9
A	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXR9
A	-9	SER	-	LEADER SEQUENCE	UNP Q9WXR9
A	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXR9
A	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXR9
A	-6	ILE	-	LEADER SEQUENCE	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	-	LEADER SEQUENCE	UNP Q9WXR9
B	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXR9
B	-9	SER	-	LEADER SEQUENCE	UNP Q9WXR9
B	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXR9
B	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXR9
B	-6	ILE	-	LEADER SEQUENCE	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	-	LEADER SEQUENCE	UNP Q9WXR9
C	-10	GLY	-	LEADER SEQUENCE	UNP Q9WXR9
C	-9	SER	-	LEADER SEQUENCE	UNP Q9WXR9
C	-8	ASP	-	LEADER SEQUENCE	UNP Q9WXR9
C	-7	LYS	-	LEADER SEQUENCE	UNP Q9WXR9
C	-6	ILE	-	LEADER SEQUENCE	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

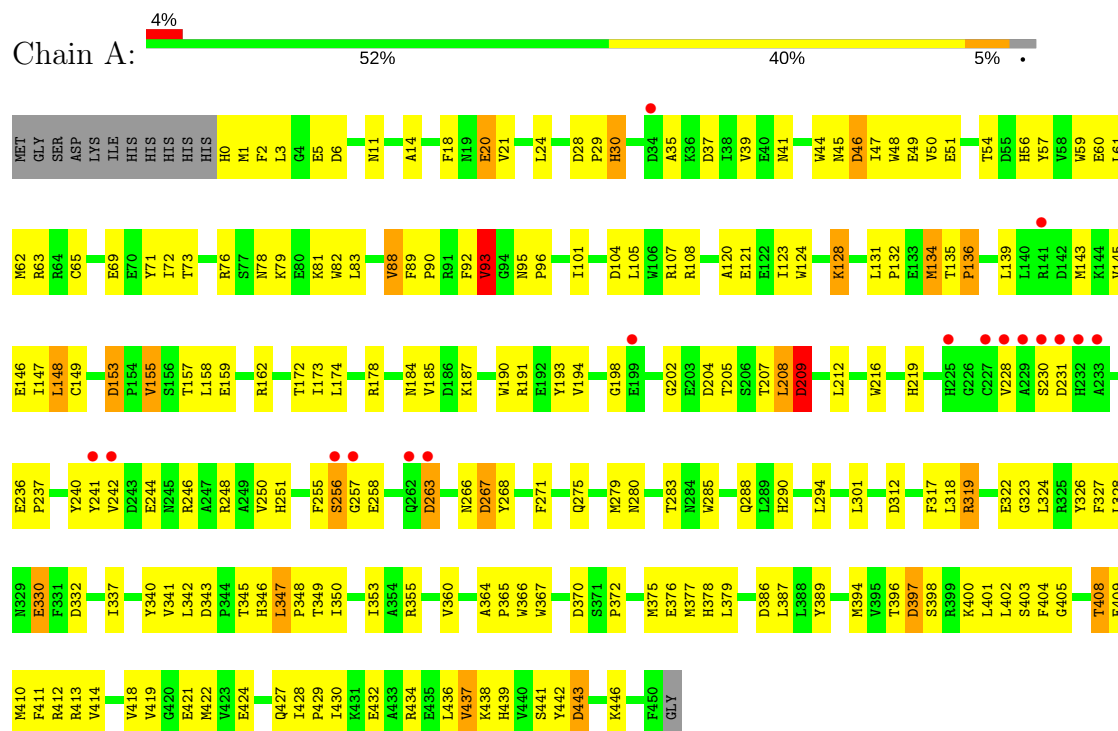
- Molecule 2 is water.

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

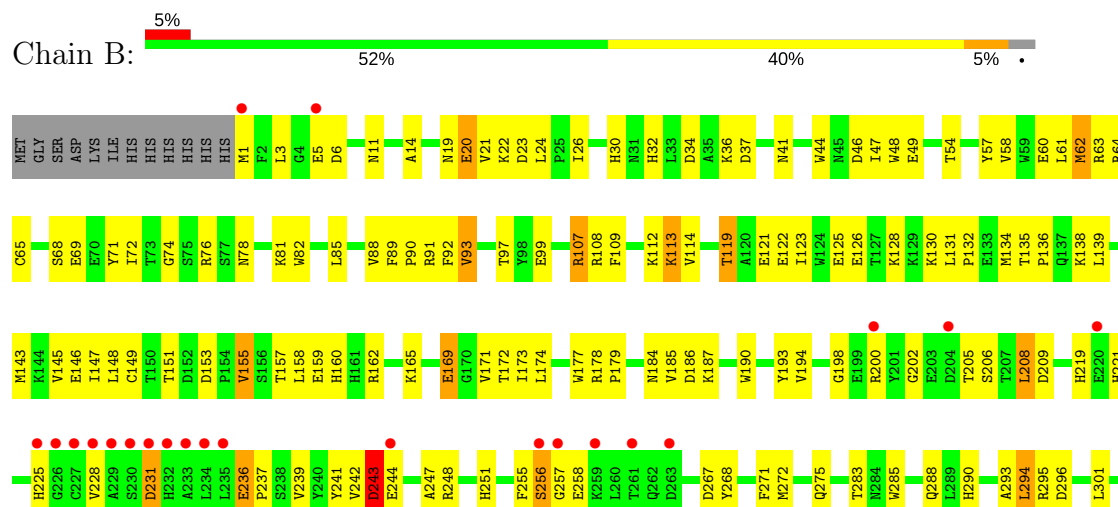
3 Residue-property plots

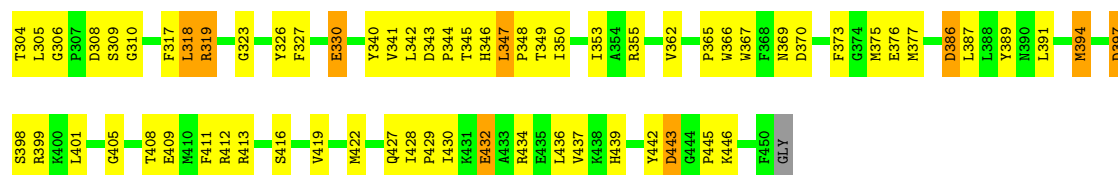
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: URONATE ISOMERASE

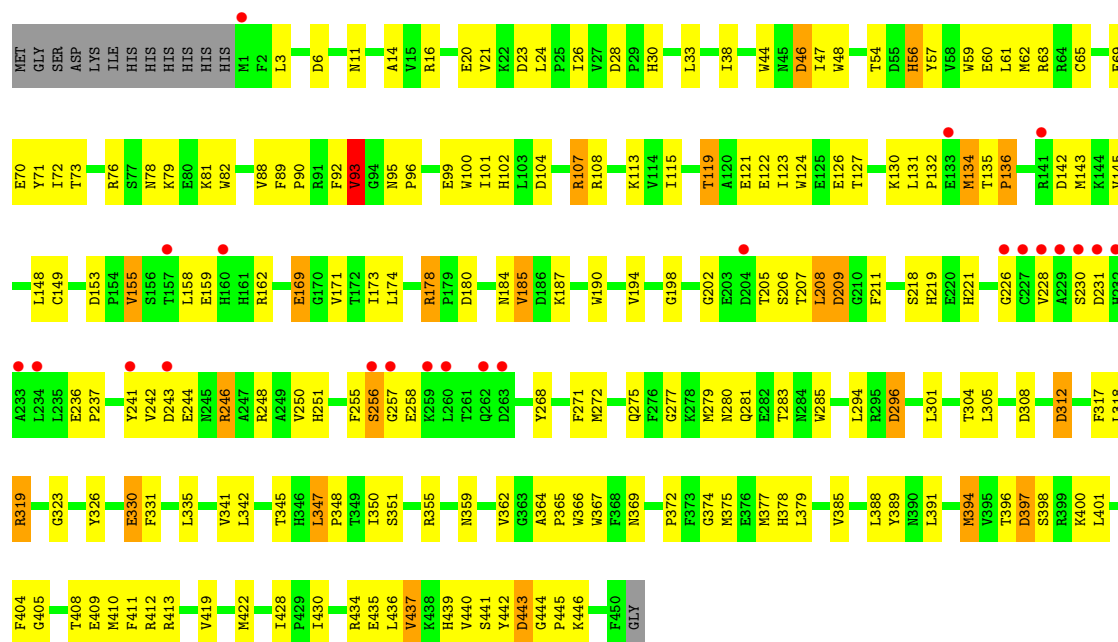


• Molecule 1: URONATE ISOMERASE





• 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 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.6 (24.99-2.85) 77.0 (24.99-2.75)	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	Depositor
R, R_{free}	0.234 , 0.274 0.248 , 0.280	Depositor DCC
R_{free} test set	1941 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 58.7	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	0.86	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 [i](#)

5.1 Standard geometry [i](#)

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	0.52	0/3793	0.88	12/5136 (0.2%)
1	B	0.54	0/3782	0.90	12/5121 (0.2%)
1	C	0.54	0/3782	0.89	12/5121 (0.2%)
All	All	0.54	0/11357	0.89	36/15378 (0.2%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ASP	N-CA-CB	-9.25	93.94	110.60
1	B	243	ASP	CB-CG-OD2	8.96	126.37	118.30
1	A	104	ASP	CB-CG-OD2	7.03	124.62	118.30
1	A	132	PRO	CA-N-CD	-6.98	101.72	111.50
1	B	23	ASP	CB-CG-OD2	6.65	124.29	118.30
1	B	34	ASP	CB-CG-OD2	6.15	123.84	118.30
1	C	443	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	46	ASP	CB-CG-OD2	6.07	123.77	118.30
1	C	6	ASP	CB-CG-OD2	6.03	123.72	118.30
1	C	104	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	332	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	23	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	6	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	443	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	142	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	308	ASP	CB-CG-OD2	5.65	123.39	118.30
1	B	267	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	186	ASP	CB-CG-OD2	5.33	123.09	118.30
1	C	209	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	267	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	6	ASP	CB-CG-OD2	5.28	123.06	118.30
1	C	312	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	231	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	263	ASP	CB-CG-OD2	5.18	122.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	308	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	312	ASP	CB-CG-OD2	5.14	122.92	118.30
1	C	243	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	153	ASP	CB-CG-OD2	5.13	122.91	118.30
1	C	169	GLU	CA-C-N	5.11	126.42	116.20
1	A	443	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	386	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	148	LEU	CB-CA-C	-5.09	100.53	110.20
1	A	209	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	37	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	37	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	180	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3696	0	3621	217	7
1	B	3686	0	3614	202	11
1	C	3686	0	3614	223	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	603	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 28.

All (603) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:143:MET:HE1	1:C:404:PHE:HB2	1.22	1.16
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:A:41:ASN:CG	1:A:135:THR:HG21	1.71	1.09
1:C:400:LYS:CD	2:C:458:HOH:O	1.96	1.04
1:B:62:MET:HE3	1:B:72:ILE:HG12	1.33	1.03
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: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:HH11	1:C:246:ARG:HG3	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: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
1:B:256:SER:O	1:B:258:GLU:N	2.07	0.86
1:C:143:MET:HE1	1:C:404:PHE:CB	2.06	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:71:TYR:CE2	1:B:76:ARG:HD3	2.17	0.80
1:C:159:GLU:HA	1:C:159:GLU:OE1	1.82	0.79
1:A:93:VAL:CG2	1:C:428:ILE:HG23	2.13	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:N	1:B:243:ASP:OD1	2.10	0.78
1:B:20:GLU:OE2	1:B:434:ARG:HB3	1.83	0.78
1:A:228:VAL:O	1:A:228:VAL:HG12	1.84	0.77
1:A:205:THR:O	1:A:205:THR:HG22	1.82	0.77
1:A:62:MET:HE3	1:A:72:ILE:HG12	1.67	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:244:GLU:O	1:A:248:ARG:HG3	1.84	0.77
1:A:71:TYR:CE2	1:A:76:ARG:HD3	2.20	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
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:B:62:MET:HE2	1:B:72:ILE:HG12	1.66	0.74
1:C:21:VAL:HG21	1:C:437:VAL:HG13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:228:VAL:HG12	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: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:A:41:ASN:OD1	1:A:135:THR:HG22	1.89	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:A:79:LYS:NZ	1:A:121:GLU:OE2	2.22	0.70
1:B:430:ILE:O	1:B:434:ARG:HG3	1.92	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: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
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:A:28:ASP:OD2	1:A:396:THR:OG1	2.10	0.68
1:B:271:PHE:CE2	1:B:275:GLN:OE1	2.45	0.68
1:B:32:HIS:NE2	2:B:452:HOH:O	1.78	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:153:ASP:OD1	1:A:155:VAL:HG23	1.93	0.68
1:A:44:TRP:HH2	1:A:401:LEU:HD12	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:419:VAL:HA	1:C:422:MET:HE2	1.77	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:424:GLU:C	1:B:1:MET:SD	2.75	0.65
1:A:212:LEU:HD21	1:A:275:GLN:OE1	1.95	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
1:B:62:MET:HE3	1:B:72:ILE:CG1	2.19	0.65
1:A:135:THR:HG22	1:A:136:PRO:N	2.10	0.64
1:C:131:LEU:O	1:C:134:MET:HB2	1.96	0.64
1:C:16:ARG:NH1	1:C:430:ILE:CD1	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:O	1:A:205:THR:CG2	2.48	0.62
1:C:30:HIS:NE2	1:C:397:ASP:OD1	2.32	0.62
1:A:366:TRP:CD1	1:A:366:TRP:C	2.73	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:B:109:PHE:CE2	1:B:134:MET:HE1	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
1:C:143:MET:CE	1:C:405:GLY:H	2.14	0.61
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:251:HIS:HB2	1:C:268:TYR:HE1	1.67	0.60
1:C:56:HIS:CE1	1:C:57:TYR:CE2	2.89	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:428:ILE:HG23	1:C:93:VAL:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ILE:HG23	1:B:93:VAL:HG22	1.82	0.59
1:A:319:ARG:HG3	1:B:317:PHE:CE2	2.37	0.59
1:C:219:HIS:ND1	1:C:285:TRP:CH2	2.70	0.59
1:C:136:PRO:HA	1:C:401:LEU:CD1	2.33	0.59
1:C:88:VAL:CG1	1:C:88:VAL:O	2.48	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:143:MET:CE	1:C:404:PHE:CB	2.75	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:C:47:ILE:CD1	1:C:82:TRP:CZ2	2.86	0.58
1:B:88:VAL:HG12	1:B:88:VAL:O	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:B:242:VAL:CG1	1:B:271:PHE:HB2	2.34	0.58
1:A:30:HIS:C	1:A:30:HIS:CD2	2.76	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:145:VAL:HG11	1:A:148:LEU:CD2	2.34	0.58
1:A:71:TYR:OH	1:A:76:ARG:NH1	2.37	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
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:65:CYS:HG	1:C:92:PHE:HE1	1.52	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:A:327:PHE:HE2	1:A:337:ILE:HD13	1.69	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:387:LEU:HD22	1:B:92:PHE:HA	1.86	0.57
1:C:143:MET:HE3	1:C:405:GLY:H	1.69	0.57
1:A:149:CYS:HA	1:A:174:LEU:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:MET:HE2	1:B:405:GLY:N	2.20	0.56
1:B:60:GLU:OE2	1:B:310:GLY:HA2	2.04	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:C:102:HIS:CE1	1:C:115:ILE:HD12	2.40	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: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:B:419:VAL:HA	1:B:422:MET:HE2	1.88	0.56
1:B:109:PHE:CE2	1:B:134:MET:CE	2.89	0.55
1:B:326:TYR:O	1:B:330:GLU:HB2	2.05	0.55
1:C:159:GLU:CA	1:C:159:GLU:OE1	2.53	0.55
1:A:205:THR:C	1:A:207:THR:H	2.10	0.55
1:C:89:PHE:CZ	1:C:101:ILE:HD12	2.40	0.55
1:B:21:VAL:O	1:B:21:VAL:HG12	2.05	0.55
1:B:244:GLU:O	1:B:248:ARG:HG3	2.07	0.55
1:C:419:VAL:HA	1:C:422:MET:CE	2.35	0.55
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: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:326:TYR:O	1:A:330:GLU:HB2	2.08	0.54
1:A:93:VAL:CG1	1:C:436:LEU:HD22	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:TYR:CE2	1:B:243:ASP:OD1	2.61	0.54
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:B:442:TYR:O	1:B:445:PRO:HD2	2.08	0.53
1:B:57:TYR:O	1:B:61:LEU:HG	2.09	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:B:130:LYS:C	1:B:132:PRO:HD2	2.29	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: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:428:ILE:CG2	1:B:93:VAL:HG22	2.38	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: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:C:30:HIS:C	1:C:30:HIS:CD2	2.83	0.52
1:A:178:ARG:HG2	1:A:231:ASP:HB3	1.91	0.52
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:198:GLY:CA	1:B:205:THR:HG23	2.39	0.52
1:B:48:TRP:CE2	1:B:81:LYS:HD3	2.44	0.52
1:C:72:ILE:HG22	1:C:73:THR:HG23	1.91	0.52
1:B:237:PRO:O	1:B:323:GLY:HA3	2.09	0.52
1:B:209:ASP:OD1	1:B:248:ARG:NH2	2.43	0.52
1:A:418:VAL:O	1:A:422:MET:HE2	2.09	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:C:100:TRP:NE1	1:C:410:MET:HE3	2.25	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:B:419:VAL:HA	1:B:422:MET:CE	2.41	0.51
1:C:242:VAL:O	1:C:271:PHE:CD1	2.63	0.51
1:C:56:HIS:CE1	1:C:57:TYR:CD2	2.98	0.51
1:B:283:THR:HG22	1:B:283:THR:O	2.09	0.51
1:C:44:TRP:CH2	1:C:401:LEU:HD12	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:347:LEU:CD2	1:C:350:ILE:HD11	2.36	0.51
1:C:89:PHE:HZ	1:C:101:ILE:HD12	1.75	0.51
1:A:228:VAL:CG1	1:A:228:VAL:O	2.55	0.51
1:A:365:PRO:CG	1:A:378:HIS:CD2	2.94	0.51
1:C:237:PRO:O	1:C:323:GLY:HA3	2.11	0.51
1:C:47:ILE:CD1	1:C:82:TRP:CE3	2.94	0.51
1:A:386:ASP:CG	1:A:387:LEU:H	2.14	0.51
1:C:246:ARG:CG	1:C:246:ARG:NH1	2.68	0.51
1:C:30:HIS:CD2	1:C:397:ASP:OD1	2.64	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:205:THR:C	1:A:207:THR:N	2.63	0.51
1:A:319:ARG:CG	1:B:317:PHE:CD2	2.94	0.51
1:B:366:TRP:C	1:B:366:TRP:CD1	2.84	0.51
1:C:143:MET:HE2	1:C:405:GLY:N	2.26	0.51
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:209:ASP:OD2	1:C:248:ARG:CZ	2.59	0.50
1:C:185:VAL:CG2	1:C:268:TYR:CD2	2.95	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:89:PHE:CZ	1:A:101:ILE:HD12	2.46	0.50
1:A:21:VAL:HG11	1:A:441:SER:CB	2.41	0.50
1:C:130:LYS:O	1:C:134:MET:SD	2.69	0.50
1:C:143:MET:CE	1:C:405:GLY:N	2.74	0.50
1:C:326:TYR:O	1:C:330:GLU:HB2	2.11	0.50
1:B:345:THR:HG23	1:C:345:THR:HG23	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TRP:CZ2	1:B:81:LYS:HD3	2.47	0.49
1:A:428:ILE:HG12	1:B:93:VAL:HG22	1.94	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:C:366:TRP:C	1:C:366:TRP:CD1	2.86	0.49
1:A:21:VAL:CG1	1:A:21:VAL:O	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: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:A:143:MET:HE1	1:A:401:LEU:O	2.13	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
1:A:57:TYR:OH	1:A:367:TRP:CD1	2.63	0.48
1:C:21:VAL:CG1	1:C:21:VAL:O	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:143:MET:CE	1:B:405:GLY:N	2.70	0.48
1:B:21:VAL:CG1	1:B:412:ARG:HD3	2.40	0.48
1:B:178:ARG:CG	1:B:231:ASP:HB3	2.44	0.48
1:A:428:ILE:CG2	1:B:93:VAL:CG2	2.86	0.48
1:A:194:VAL:O	1:A:205:THR:HG21	2.14	0.48
1:C:130:LYS:C	1:C:132:PRO:HD2	2.34	0.48
1:C:283:THR:CG2	1:C:285:TRP:CD1	2.95	0.48
1:C:33:LEU:HD23	1:C:38:ILE:HD11	1.96	0.48
1:A:21:VAL:HG11	1:A:441:SER:OG	2.14	0.48
1:A:92:PHE:O	1:A:93:VAL:C	2.53	0.48
1:B:219:HIS:CD2	1:B:285:TRP:CZ3	3.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:THR:C	1:C:207:THR:H	2.17	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:143:MET:HE2	1:B:405:GLY:H	1.73	0.47
1:A:207:THR:C	1:A:251:HIS:HE2	2.18	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:A:146:GLU:OE1	1:A:446:LYS:NZ	2.37	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: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
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:B:72:ILE:O	1:B:81:LYS:HE2	2.16	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:A:204:ASP:O	1:A:207:THR:OG1	2.32	0.46
1:B:109:PHE:CD2	1:B:134:MET:HE1	2.50	0.46
1:C:194:VAL:HG13	1:C:205:THR:CG2	2.43	0.46
1:C:65:CYS:SG	1:C:88:VAL:CG1	3.04	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:C:208:LEU:CA	1:C:251:HIS:CD2	2.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:219:HIS:HE1	1:C:285:TRP:CE3	2.23	0.45
1:C:88:VAL:O	1:C:88:VAL:HG13	2.14	0.45
1:A:419:VAL:HA	1:A:422:MET:HE2	1.96	0.45
1:B:190:TRP:O	1:B:194:VAL:HG23	2.16	0.45
1:B:30:HIS:NE2	1:B:397:ASP:OD1	2.50	0.45
1:B:26:ILE:HG12	1:B:408:THR:HG21	1.99	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: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:A:50:VAL:HG11	1:A:402:LEU:HD12	1.98	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:342:LEU:CD1	1:B:367:TRP:HB3	2.47	0.45
1:B:74:GLY:O	1:B:81:LYS:NZ	2.33	0.45
1:C:355:ARG:HG2	1:C:355:ARG:O	2.16	0.45
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:C:92:PHE:O	1:C:93:VAL:C	2.55	0.44
1:A:365:PRO:CD	1:A:378:HIS:CD2	2.90	0.44
1:A:65:CYS:SG	1:A:88:VAL:HG13	2.57	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:157:THR:OG1	1:A:159:GLU:HG2	2.17	0.44
1:A:148:LEU:HD22	1:A:404:PHE:CE2	2.52	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: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:239:VAL:HG11	1:B:327:PHE:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ASP:HB2	1:B:49:GLU:H	1.83	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: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:B:131:LEU:N	1:B:132:PRO:HD2	2.29	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:216:TRP:HE3	1:A:279:MET:HG2	1.83	0.43
1:A:71:TYR:CZ	1:A:76:ARG:CD	3.01	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
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: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:159:GLU:OE1	1:C:162:ARG:HD2	2.18	0.43
1:C:26:ILE:HG12	1:C:408:THR:HG21	2.00	0.43
1:A:347:LEU:N	1:A:348:PRO:CD	2.81	0.43
1:A:2:PHE:CE1	1:A:3:LEU:HD13	2.54	0.43
1:A:0:HIS:CD2	1:A:1:MET:N	2.87	0.42
1:A:242:VAL:O	1:A:271:PHE:CD1	2.71	0.42
1:A:30:HIS:NE2	1:A:397:ASP:OD1	2.52	0.42
1:B:290:HIS:HA	1:B:340:TYR:HB2	2.01	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:A:147:ILE:HG12	1:A:172:THR:HB	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:312:ASP:HB2	1:C:367:TRP:HH2	1.84	0.42
1:B:244:GLU:O	1:B:248:ARG:N	2.47	0.42
1:C:277:GLY:HA3	1:C:331:PHE:CZ	2.53	0.42
1:C:47:ILE:HD12	1:C:82:TRP:CZ2	2.54	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:A:51:GLU:OE1	1:A:400:LYS:NZ	2.31	0.42
1:B:119:THR:HG23	1:B:123:ILE:HG13	2.02	0.42
1:B:296:ASP:OD1	1:B:296:ASP:N	2.53	0.42
1:B:283:THR:CG2	1:B:285:TRP:NE1	2.82	0.42
1:C:335:LEU:O	1:C:359:ASN:HB2	2.19	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:93:VAL:HG22	1:C:428:ILE:CG2	2.45	0.42
1:B:113:LYS:HD2	1:B:122:GLU:OE1	2.20	0.42
1:A:62:MET:CE	1:A:72:ILE:HG12	2.45	0.41
1:B:19:ASN:OD1	1:B:22:LYS:HE2	2.19	0.41
1:C:28:ASP:OD2	1:C:396:THR:OG1	2.31	0.41
1:C:355:ARG:NE	1:C:385:VAL:O	2.44	0.41
1:C:62:MET:HB2	1:C:62:MET:HE2	1.82	0.41
1:A:135:THR:O	1:A:139:LEU:N	2.47	0.41
1:A:18:PHE:CE1	1:A:413:ARG:HG2	2.55	0.41
1:A:88:VAL:O	1:A:88:VAL:HG13	2.21	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:389:TYR:O	1:A:389:TYR:CD2	2.74	0.41
1:B:362:VAL:O	1:B:391:LEU:HD12	2.20	0.41
1:C:190:TRP:HH2	1:C:251:HIS:ND1	2.19	0.41
1:B:355:ARG:HD3	1:C:60:GLU:OE1	2.20	0.41
1:B:155:VAL:CG2	1:B:193:TYR:CE1	3.03	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:218:SER:O	1:C:221:HIS:HB3	2.21	0.41
1:B:122:GLU:O	1:B:126:GLU:HG3	2.21	0.41
1:A:283:THR:CG2	1:A:285:TRP:CD1	3.04	0.41
1:A:290:HIS:CD2	1:A:340:TYR:CG	3.09	0.41
1:B:428:ILE:HG22	1:B:429:PRO:O	2.20	0.41
1:C:365:PRO:HG3	1:C:378:HIS:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:CG2	1:A:193:TYR:CE1	3.04	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: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:B:130:LYS:C	1:B:132:PRO:CD	2.87	0.41
1:C:394:MET:HB2	1:C:411:PHE:CD2	2.56	0.41
1:B:386:ASP:CG	1:B:387:LEU:H	2.24	0.40
1:B:85:LEU:CD1	1:B:89:PHE:HD1	2.34	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:C:71:TYR:CZ	1:C:76:ARG:HD3	2.54	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:B:251:HIS:HB2	1:B:268:TYR:HE1	1.87	0.40
1:B:89:PHE:N	1:B:90:PRO:CD	2.84	0.40
1:C:100:TRP:CD1	1:C:410:MET:HE3	2.56	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:C:65:CYS:SG	1:C:88:VAL:HG13	2.62	0.40
1:C:61:LEU:HB2	1:C:92:PHE:CE2	2.57	0.40
1:A:139:LEU:HD22	1:A:402:LEU:CD2	2.51	0.40
1:B:92:PHE:O	1:B:93:VAL:C	2.58	0.40
1:C:113:LYS:NZ	1:C:122:GLU:OE1	2.49	0.40
1:C:375:MET:HE1	1:C:410:MET:HG2	2.03	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	20	49
1	B	448/463 (97%)	420 (94%)	25 (6%)	3 (1%)	25	56
1	C	448/463 (97%)	422 (94%)	23 (5%)	3 (1%)	25	56
All	All	1345/1389 (97%)	1267 (94%)	68 (5%)	10 (1%)	25	56

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 [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	399/409 (98%)	367 (92%)	32 (8%)	14	35
1	B	398/409 (97%)	367 (92%)	31 (8%)	15	36
1	C	398/409 (97%)	368 (92%)	30 (8%)	16	39
All	All	1195/1227 (97%)	1102 (92%)	93 (8%)	15	36

All (93) 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	108	ARG
1	A	128	LYS
1	A	134	MET
1	A	155	VAL
1	A	208	LEU
1	A	209	ASP
1	A	236	GLU
1	A	256	SER
1	A	263	ASP
1	A	294	LEU
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	377	MET
1	A	397	ASP
1	A	398	SER
1	A	408	THR
1	A	421	GLU
1	A	432	GLU

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Mol	Chain	Res	Type
1	A	437	VAL
1	B	20	GLU
1	B	54	THR
1	B	62	MET
1	B	68	SER
1	B	93	VAL
1	B	97	THR
1	B	107	ARG
1	B	108	ARG
1	B	113	LYS
1	B	119	THR
1	B	155	VAL
1	B	171	VAL
1	B	208	LEU
1	B	236	GLU
1	B	243	ASP
1	B	256	SER
1	B	294	LEU
1	B	301	LEU
1	B	318	LEU
1	B	319	ARG
1	B	330	GLU
1	B	341	VAL
1	B	347	LEU
1	B	370	ASP
1	B	376	GLU
1	B	377	MET
1	B	394	MET
1	B	397	ASP
1	B	398	SER
1	B	399	ARG
1	B	432	GLU
1	C	20	GLU
1	C	54	THR
1	C	56	HIS
1	C	93	VAL
1	C	107	ARG
1	C	108	ARG
1	C	119	THR
1	C	134	MET
1	C	155	VAL
1	C	171	VAL

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Mol	Chain	Res	Type
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	377	MET
1	C	394	MET
1	C	397	ASP
1	C	398	SER
1	C	437	VAL

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

Mol	Chain	Res	Type
1	A	56	HIS
1	A	221	HIS
1	A	280	ASN
1	A	288	GLN
1	A	439	HIS
1	B	45	ASN
1	B	221	HIS
1	B	288	GLN
1	C	56	HIS
1	C	213	ASN
1	C	219	HIS
1	C	221	HIS
1	C	232	HIS
1	C	251	HIS
1	C	288	GLN
1	C	290	HIS
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.06	17 (3%)	41 35	8, 28, 84, 122	18 (3%)
1	B	450/463 (97%)	-0.07	22 (4%)	30 26	4, 27, 83, 122	19 (4%)
1	C	450/463 (97%)	-0.04	23 (5%)	29 24	8, 28, 83, 122	19 (4%)
All	All	1351/1389 (97%)	-0.05	62 (4%)	33 28	4, 28, 84, 122	56 (4%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	HIS	5.4
1	C	259	LYS	5.1
1	B	259	LYS	4.9
1	C	232	HIS	4.8
1	A	227	CYS	4.6
1	C	229	ALA	4.6
1	B	229	ALA	4.6
1	A	232	HIS	4.5
1	C	257	GLY	4.3
1	C	204	ASP	4.2
1	C	230	SER	4.1
1	B	256	SER	4.1
1	A	229	ALA	4.0
1	B	230	SER	3.9
1	B	227	CYS	3.8
1	B	231	ASP	3.8
1	C	227	CYS	3.8
1	A	228	VAL	3.8
1	A	230	SER	3.6
1	C	157	THR	3.6
1	A	231	ASP	3.6
1	B	233	ALA	3.5
1	B	204	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	241	TYR	3.4
1	C	243	ASP	3.4
1	C	256	SER	3.4
1	C	231	ASP	3.4
1	A	257	GLY	3.2
1	B	1	MET	3.0
1	C	263	ASP	2.9
1	A	233	ALA	2.8
1	C	226	GLY	2.7
1	A	225	HIS	2.7
1	C	141	ARG	2.7
1	C	160	HIS	2.6
1	C	241	TYR	2.6
1	C	1	MET	2.6
1	B	226	GLY	2.6
1	B	257	GLY	2.6
1	C	233	ALA	2.6
1	B	5	GLU	2.5
1	B	234	LEU	2.5
1	C	228	VAL	2.5
1	A	199	GLU	2.5
1	B	244	GLU	2.4
1	A	256	SER	2.4
1	C	133	GLU	2.4
1	B	228	VAL	2.3
1	A	34	ASP	2.3
1	C	260	LEU	2.3
1	B	225	HIS	2.2
1	B	200	ARG	2.2
1	A	263	ASP	2.2
1	B	235	LEU	2.2
1	B	220	GLU	2.2
1	B	263	ASP	2.2
1	C	234	LEU	2.2
1	C	262	GLN	2.2
1	A	141	ARG	2.2
1	B	261	THR	2.1
1	A	242	VAL	2.0
1	A	262	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.