Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:59 AM GMT

PDB ID	:	2Z1B
Title	:	Crystal Structure of 5-aminolevulinic acid dehydratase (ALAD) from Mus musculs
Authors	:	Xie, Y.; Wang, H.; Kawazoe, M.; Kishishita, S.; Murayama, K.; Takemoto, C.; Terada, T.; Shirozu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-05-08
Resolution	:	3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

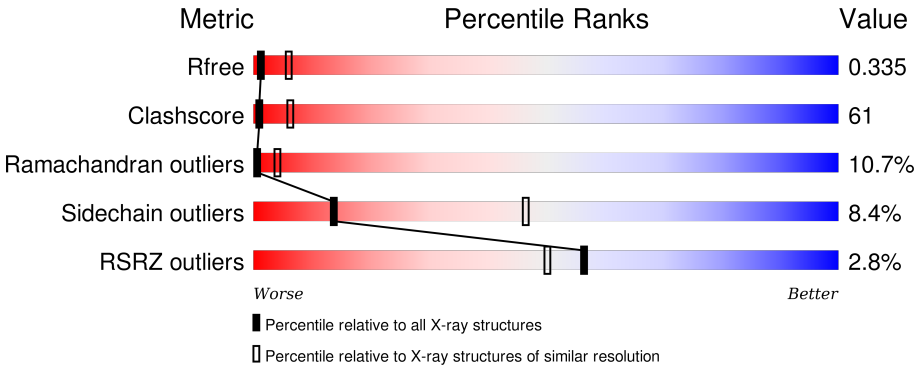
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 <=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	330	% 29% 49% 10% 12%
1	B	330	% 27% 56% 14% •
1	C	330	5% 20% 54% 13% • 13%
1	D	330	3% 22% 55% 12% • 10%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9223 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 Delta-aminolevulinic acid dehydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2230	1428	387	400	15			
1	B	320	Total	C	N	O	S	0	0	0
			2445	1557	426	445	17			
1	C	288	Total	C	N	O	S	0	0	0
			2217	1420	385	398	14			
1	D	296	Total	C	N	O	S	0	0	0
			2274	1454	397	408	15			

- Molecule 2 is water.

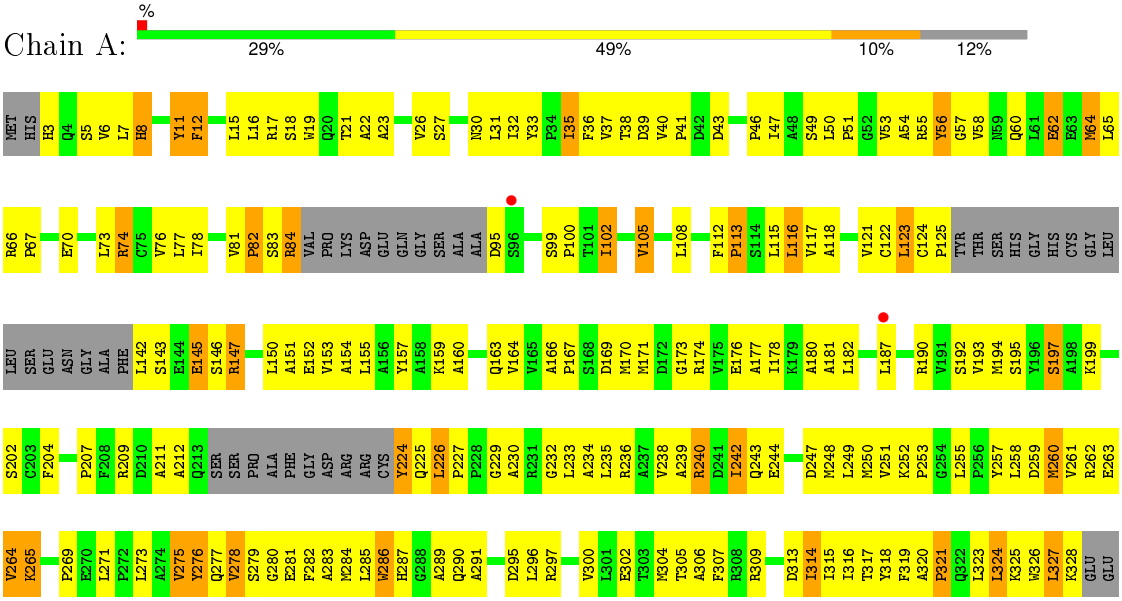
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	20	Total	O	0	0
			20	20		
2	C	15	Total	O	0	0
			15	15		
2	D	10	Total	O	0	0
			10	10		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

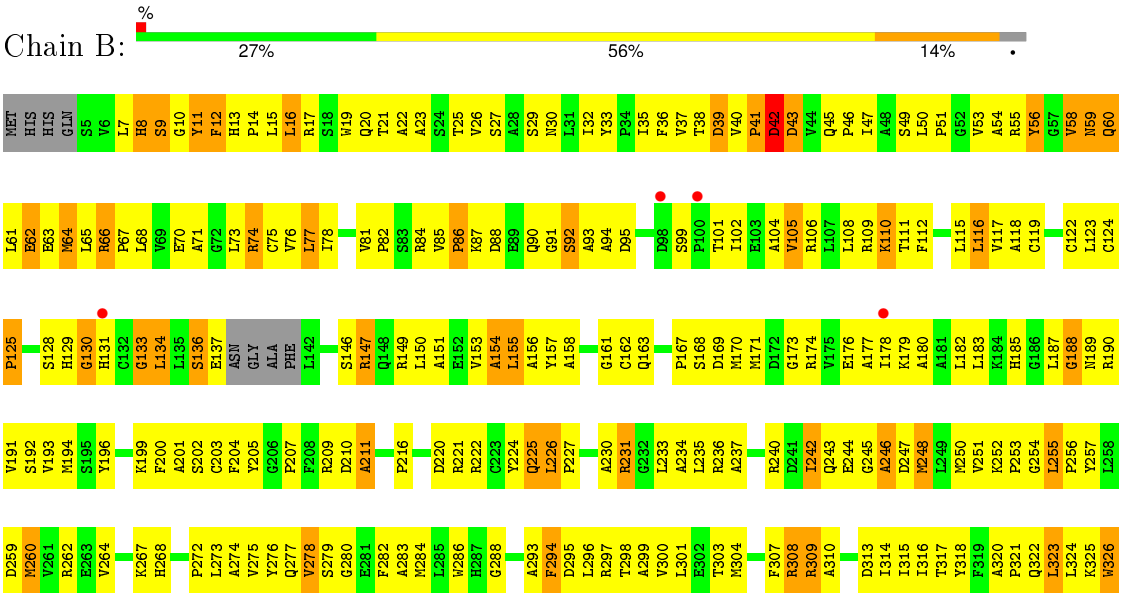
- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain A:



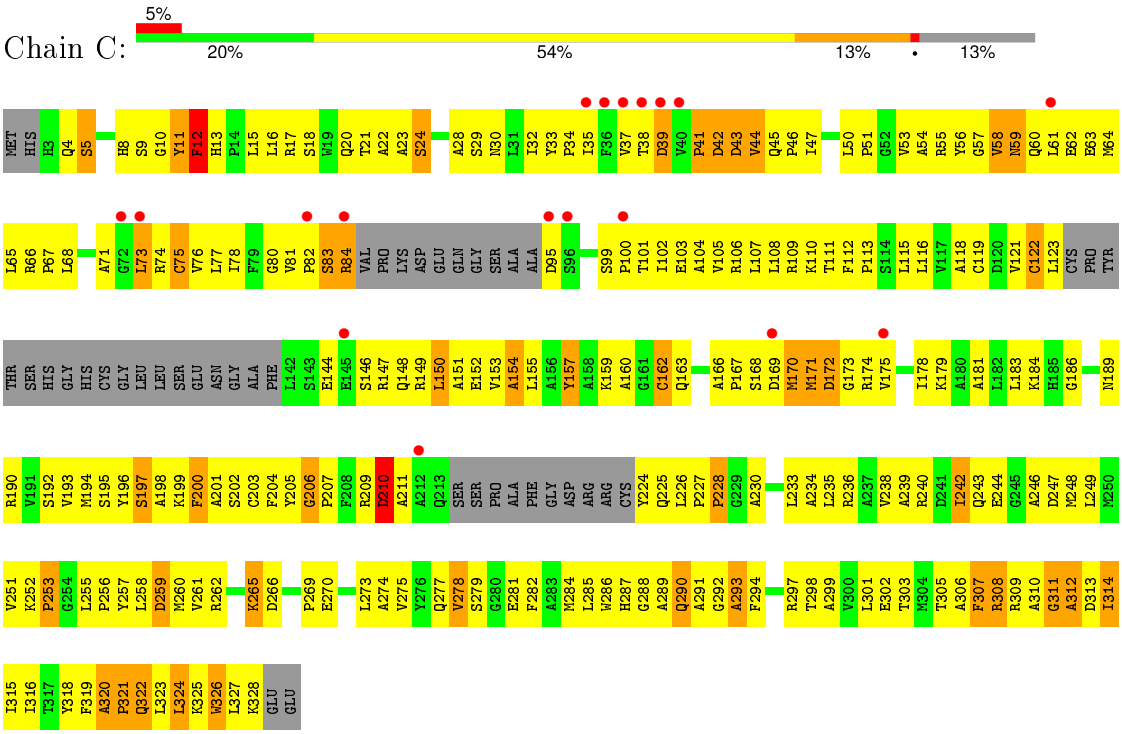
- Molecule 1: Delta-aminolevulinic acid dehydratase

Chain B:



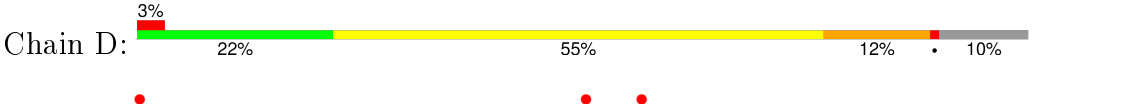
• Molecule 1: Delta-aminolevulinic acid dehydratase

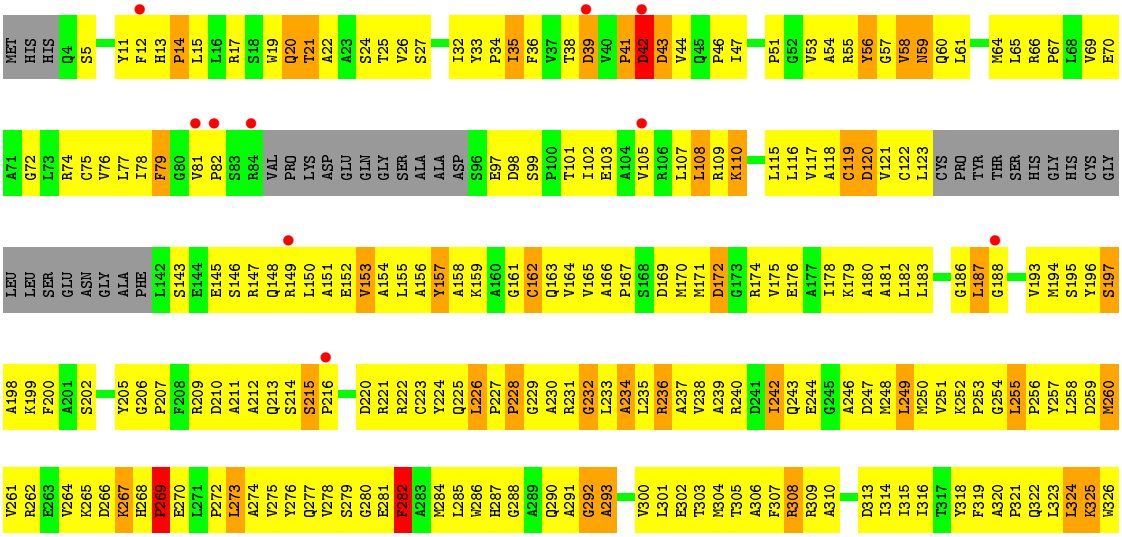
Chain C:



• Molecule 1: Delta-aminolevulinic acid dehydratase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	240.92Å 240.92Å 103.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.40 – 3.30 47.72 – 3.29	Depositor EDS
% Data completeness (in resolution range)	88.7 (43.40-3.30) 95.4 (47.72-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.79 (at 3.33Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.278 , 0.353 0.266 , 0.335	Depositor DCC
R_{free} test set	2400 reflections (9.94%)	DCC
Wilson B-factor (Å^2)	98.3	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 89.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 27430 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9223	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.33	0/2278	0.57	0/3091
1	B	0.34	0/2500	0.61	0/3394
1	C	0.31	0/2264	0.57	0/3071
1	D	0.32	0/2323	0.56	0/3151
All	All	0.32	0/9365	0.58	0/12707

There are no bond length outliers.

There are no bond angle outliers.

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	2230	0	2252	229	0
1	B	2445	0	2452	303	0
1	C	2217	0	2240	352	0
1	D	2274	0	2297	324	0
2	A	12	0	0	3	0
2	B	20	0	0	5	0
2	C	15	0	0	4	0
2	D	10	0	0	5	0
All	All	9223	0	9241	1127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

All (1127) 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:227:PRO:HG2	1:A:230:ALA:HB2	1.35	1.09
1:A:5:SER:HB2	1:B:240:ARG:HG3	1.39	1.03
1:A:242:ILE:HD13	1:A:271:LEU:HD11	1.40	1.03
1:C:227:PRO:HG2	1:C:230:ALA:HB2	1.40	1.03
1:C:255:LEU:HD11	1:D:256:PRO:HA	1.40	1.02
1:C:84:ARG:HB2	1:C:84:ARG:HH21	1.24	1.00
1:A:255:LEU:HD11	1:B:256:PRO:HA	1.42	0.99
1:C:262:ARG:NH2	1:C:310:ALA:HA	1.81	0.96
1:D:227:PRO:HG2	1:D:230:ALA:HB2	1.45	0.94
1:C:233:LEU:HD12	1:D:20:GLN:HG2	1.51	0.93
1:C:201:ALA:HB2	1:C:225:GLN:HB3	1.50	0.92
1:D:77:LEU:HA	1:D:118:ALA:HB3	1.50	0.92
1:C:32:ILE:HD11	1:C:314:ILE:HG23	1.54	0.89
1:C:149:ARG:HB3	1:C:149:ARG:HH11	1.33	0.89
1:A:99:SER:HB2	1:A:100:PRO:HD2	1.54	0.87
1:D:145:GLU:HA	1:D:148:GLN:HE21	1.38	0.87
1:B:45:GLN:HB2	1:B:55:ARG:HB2	1.57	0.87
1:A:224:TYR:HA	1:B:11:TYR:HE2	1.38	0.86
1:B:273:LEU:H	1:B:313:ASP:HB2	1.39	0.86
1:B:226:LEU:H	1:B:226:LEU:HD12	1.40	0.86
1:D:39:ASP:O	1:D:41:PRO:HD3	1.75	0.86
1:B:35:ILE:HD11	1:B:78:ILE:HG13	1.57	0.85
1:B:116:LEU:HD23	1:C:15:LEU:HB3	1.59	0.85
1:B:39:ASP:O	1:B:41:PRO:HD3	1.76	0.84
1:D:199:LYS:HD2	1:D:205:TYR:OH	1.78	0.84
1:C:47:ILE:HG22	1:C:50:LEU:H	1.40	0.83
1:A:84:ARG:HB2	1:A:84:ARG:HH21	1.40	0.83
1:C:253:PRO:HD2	1:C:257:TYR:CE2	2.14	0.82
1:A:260:MET:O	1:A:264:VAL:HG22	1.79	0.82
1:B:47:ILE:HD11	1:B:55:ARG:HG3	1.59	0.82
1:C:265:LYS:HA	1:C:265:LYS:HE3	1.62	0.82
1:C:259:ASP:HA	1:D:259:ASP:HA	1.62	0.81
1:D:207:PRO:HB2	1:D:279:SER:HB2	1.59	0.81
1:B:27:SER:H	1:B:30:ASN:ND2	1.79	0.81
1:A:123:LEU:HD21	1:A:150:LEU:HD13	1.60	0.81
1:D:306:ALA:HA	1:D:309:ARG:NH1	1.96	0.81
1:D:66:ARG:O	1:D:70:GLU:HG2	1.82	0.80
1:C:168:SER:HB2	1:C:199:LYS:HE3	1.62	0.80
1:C:84:ARG:HB2	1:C:84:ARG:NH2	1.97	0.80
1:D:221:ARG:HB2	1:D:222:ARG:HH11	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:HH21	1:B:7:LEU:HD12	1.45	0.79
1:D:216:PRO:HD3	1:D:221:ARG:HH21	1.46	0.79
1:C:265:LYS:HE2	1:C:269:PRO:HA	1.65	0.79
1:B:27:SER:H	1:B:30:ASN:HD21	1.29	0.79
1:D:117:VAL:HG11	1:D:162:CYS:HA	1.65	0.79
1:A:32:ILE:HD13	1:A:314:ILE:HG22	1.65	0.79
1:C:33:TYR:HB3	1:C:76:VAL:HG12	1.64	0.79
1:D:279:SER:HA	1:D:318:TYR:HE2	1.48	0.78
1:C:11:TYR:O	1:C:13:HIS:N	2.16	0.78
1:B:39:ASP:OD1	1:B:82:PRO:HA	1.84	0.78
1:C:297:ARG:HA	2:C:332:HOH:O	1.83	0.78
1:B:8:HIS:HB3	1:C:189:ASN:HB2	1.66	0.77
1:D:170:MET:HA	1:D:174:ARG:NH1	1.98	0.77
1:C:149:ARG:HB3	1:C:149:ARG:NH1	1.98	0.77
1:A:102:ILE:O	1:A:105:VAL:HG12	1.84	0.77
1:C:106:ARG:NH1	1:C:160:ALA:HA	2.00	0.77
1:B:105:VAL:HG13	1:B:106:ARG:H	1.49	0.77
1:D:110:LYS:HE2	1:D:110:LYS:HA	1.67	0.77
1:B:250:MET:HA	1:B:274:ALA:O	1.86	0.76
1:A:95:ASP:HA	1:A:99:SER:HB3	1.67	0.76
1:A:262:ARG:O	1:A:265:LYS:HB3	1.85	0.76
1:C:260:MET:HE3	1:D:309:ARG:HE	1.51	0.76
1:C:167:PRO:HB2	1:C:174:ARG:HD2	1.67	0.76
1:B:207:PRO:HB2	1:B:279:SER:HB2	1.68	0.76
1:D:277:GLN:NE2	1:D:303:THR:HG21	2.01	0.75
1:A:323:LEU:O	1:A:327:LEU:HD13	1.85	0.75
1:C:29:SER:HA	1:C:74:ARG:HG3	1.69	0.75
1:B:320:ALA:HB3	1:B:321:PRO:HD3	1.69	0.74
1:C:77:LEU:HD23	1:C:118:ALA:O	1.87	0.74
1:D:77:LEU:HA	1:D:118:ALA:CB	2.16	0.74
1:A:5:SER:HB2	1:B:240:ARG:CG	2.15	0.74
1:C:205:TYR:CE1	1:C:252:LYS:HE2	2.22	0.74
1:A:227:PRO:CG	1:A:230:ALA:HB2	2.17	0.73
1:D:154:ALA:HB1	1:D:165:VAL:HG11	1.69	0.73
1:C:73:LEU:H	1:C:324:LEU:HD13	1.53	0.73
1:D:117:VAL:HG12	1:D:119:CYS:SG	2.28	0.73
1:B:101:THR:HG23	1:B:102:ILE:H	1.54	0.73
1:C:259:ASP:HB2	1:D:262:ARG:HB2	1.71	0.73
1:B:151:ALA:HA	1:B:178:ILE:HD13	1.70	0.73
1:C:201:ALA:HB2	1:C:225:GLN:CB	2.19	0.73
1:A:74:ARG:NH1	1:A:74:ARG:HB3	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LEU:HB3	1:D:258:LEU:HB3	1.70	0.73
1:A:239:ALA:O	1:A:243:GLN:HG3	1.88	0.73
1:D:157:TYR:HB3	1:D:162:CYS:HB2	1.70	0.73
1:D:33:TYR:HB3	1:D:76:VAL:HG12	1.70	0.72
1:B:179:LYS:O	1:B:183:LEU:HD23	1.90	0.72
1:D:205:TYR:CE1	1:D:252:LYS:HE2	2.23	0.72
1:B:154:ALA:HB2	1:B:178:ILE:HD12	1.71	0.72
1:A:146:SER:HB2	1:A:147:ARG:NH2	2.04	0.72
1:C:320:ALA:HB3	1:C:321:PRO:HD3	1.71	0.72
1:D:75:CYS:HB2	1:D:116:LEU:HB3	1.72	0.71
1:D:255:LEU:HD23	1:D:303:THR:HG23	1.72	0.71
1:D:275:VAL:HG12	1:D:315:ILE:HG12	1.72	0.71
1:C:275:VAL:HG12	1:C:315:ILE:HA	1.72	0.71
1:D:250:MET:HG2	1:D:251:VAL:H	1.55	0.71
1:C:193:VAL:H	1:C:247:ASP:HB2	1.55	0.71
1:C:32:ILE:HD13	1:C:316:ILE:HG12	1.72	0.71
1:A:76:VAL:HG13	1:A:115:LEU:HD11	1.72	0.71
1:C:99:SER:HB2	1:C:100:PRO:HD2	1.73	0.71
1:A:46:PRO:C	1:A:47:ILE:HD12	2.11	0.71
1:C:306:ALA:HA	1:C:309:ARG:CZ	2.20	0.71
1:B:53:VAL:HG12	1:B:54:ALA:N	2.07	0.70
1:B:233:LEU:HA	1:B:236:ARG:HB2	1.74	0.70
1:A:199:LYS:HE2	1:A:252:LYS:HZ3	1.57	0.70
1:A:253:PRO:HD2	1:A:257:TYR:CE2	2.27	0.70
1:A:166:ALA:HB2	1:A:194:MET:HB3	1.72	0.70
1:C:227:PRO:HG2	1:C:230:ALA:CB	2.21	0.70
1:D:76:VAL:O	1:D:118:ALA:HB3	1.92	0.69
1:B:40:VAL:HG12	1:B:43:ASP:HB3	1.74	0.69
1:B:267:LYS:HE2	1:B:268:HIS:HE1	1.57	0.69
1:B:182:LEU:HD13	1:B:191:VAL:HB	1.74	0.69
1:C:255:LEU:HD23	1:D:255:LEU:HD12	1.74	0.69
1:C:284:MET:HB3	1:D:284:MET:HB3	1.74	0.69
1:D:155:LEU:O	1:D:155:LEU:HD23	1.92	0.69
1:A:233:LEU:HD23	1:A:233:LEU:O	1.93	0.69
1:A:289:ALA:C	1:A:291:ALA:H	1.96	0.69
1:C:32:ILE:N	1:C:32:ILE:HD12	2.08	0.69
1:C:105:VAL:HG13	1:C:106:ARG:N	2.08	0.69
1:D:222:ARG:N	1:D:222:ARG:HD2	2.08	0.69
1:B:17:ARG:O	1:B:21:THR:HG22	1.92	0.69
1:D:279:SER:HA	1:D:318:TYR:CE2	2.28	0.69
1:B:231:ARG:HG3	1:B:260:MET:HE1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:HD12	1:B:20:GLN:CG	2.22	0.68
1:C:260:MET:HE1	1:D:309:ARG:HG2	1.74	0.68
1:A:224:TYR:HA	1:B:11:TYR:CE2	2.24	0.68
1:B:174:ARG:O	1:B:178:ILE:HG12	1.92	0.68
1:D:77:LEU:HD23	1:D:118:ALA:HB1	1.75	0.68
1:D:205:TYR:HE1	1:D:252:LYS:HE2	1.57	0.68
1:B:38:THR:HG21	1:B:45:GLN:HE22	1.58	0.68
1:C:54:ALA:HB3	1:C:56:TYR:CZ	2.29	0.68
1:B:288:GLY:O	1:B:293:ALA:HB3	1.92	0.68
1:C:44:VAL:O	1:C:46:PRO:HD3	1.93	0.68
1:A:320:ALA:HB3	1:A:321:PRO:HD3	1.73	0.68
1:D:33:TYR:H	1:D:76:VAL:HA	1.60	0.67
1:C:11:TYR:CD1	1:C:11:TYR:N	2.61	0.67
1:A:278:VAL:HG22	1:A:281:GLU:OE2	1.94	0.67
1:C:50:LEU:HB3	1:C:53:VAL:HG21	1.76	0.67
1:D:250:MET:HA	1:D:274:ALA:O	1.94	0.67
1:C:106:ARG:HH11	1:C:160:ALA:HA	1.56	0.67
1:B:53:VAL:HG12	1:B:54:ALA:H	1.59	0.67
1:D:149:ARG:HA	1:D:152:GLU:HB2	1.77	0.67
1:D:107:LEU:O	1:D:110:LYS:N	2.27	0.67
1:C:226:LEU:H	1:C:226:LEU:HD12	1.60	0.67
1:D:176:GLU:HB2	1:D:244:GLU:HG2	1.76	0.67
1:A:35:ILE:HD12	1:A:76:VAL:HB	1.77	0.67
1:A:33:TYR:HB2	1:A:320:ALA:CB	2.24	0.67
1:D:250:MET:HG2	1:D:251:VAL:N	2.09	0.67
1:C:289:ALA:C	1:C:291:ALA:H	1.97	0.67
1:B:267:LYS:HE2	1:B:268:HIS:CE1	2.29	0.67
1:C:239:ALA:O	1:C:242:ILE:HG22	1.94	0.66
1:B:38:THR:HG21	1:B:45:GLN:NE2	2.09	0.66
1:C:155:LEU:HD23	1:C:155:LEU:O	1.96	0.66
1:D:155:LEU:HD21	1:D:159:LYS:HE3	1.77	0.66
1:D:35:ILE:HD11	1:D:78:ILE:HA	1.77	0.66
1:B:308:ARG:NH2	1:B:313:ASP:HA	2.11	0.66
1:B:105:VAL:HG13	1:B:106:ARG:N	2.09	0.66
1:B:303:THR:HG22	1:B:307:PHE:HE2	1.60	0.66
1:C:11:TYR:HD1	1:C:11:TYR:N	1.94	0.66
1:A:289:ALA:O	1:A:291:ALA:N	2.28	0.66
1:A:249:LEU:HB2	1:A:273:LEU:HD23	1.78	0.66
1:C:273:LEU:HD22	1:C:274:ALA:H	1.61	0.66
1:B:61:LEU:HD23	1:B:108:LEU:HD21	1.77	0.66
1:D:228:PRO:O	1:D:230:ALA:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:MET:SD	1:B:315:ILE:HG21	2.36	0.66
1:A:47:ILE:HG22	1:A:49:SER:H	1.59	0.65
1:A:159:LYS:HG2	1:A:187:LEU:HD11	1.78	0.65
1:B:15:LEU:HD11	1:B:19:TRP:HE1	1.61	0.65
1:D:306:ALA:HA	1:D:309:ARG:HH12	1.59	0.65
1:B:92:SER:HA	1:B:95:ASP:HB2	1.78	0.65
1:D:66:ARG:N	1:D:67:PRO:HD2	2.12	0.65
1:A:49:SER:O	1:A:51:PRO:HD3	1.96	0.65
1:C:233:LEU:HD12	1:D:20:GLN:CG	2.23	0.65
1:B:185:HIS:O	1:B:187:LEU:HG	1.96	0.65
1:D:242:ILE:C	1:D:242:ILE:HD13	2.17	0.65
1:B:50:LEU:HB3	1:B:53:VAL:HG21	1.78	0.65
1:D:13:HIS:HE1	1:D:15:LEU:HB3	1.61	0.64
1:B:43:ASP:N	1:B:60:GLN:HE21	1.95	0.64
1:D:280:GLY:O	1:D:284:MET:HG3	1.96	0.64
1:D:276:TYR:HE1	1:D:278:VAL:HA	1.62	0.64
1:B:50:LEU:HB3	1:B:53:VAL:CG2	2.28	0.64
1:C:11:TYR:HB2	1:C:17:ARG:HG2	1.79	0.64
1:C:174:ARG:O	1:C:178:ILE:HG13	1.97	0.64
1:C:105:VAL:HG13	1:C:106:ARG:H	1.61	0.64
1:B:235:LEU:HD13	1:B:267:LYS:HD3	1.79	0.64
1:C:282:PHE:HD2	1:C:318:TYR:HB2	1.64	0.63
1:A:47:ILE:HG21	1:A:211:ALA:HB2	1.80	0.63
1:B:58:VAL:O	1:B:61:LEU:HB2	1.97	0.63
1:A:233:LEU:HD12	1:B:20:GLN:HG2	1.79	0.63
1:B:173:GLY:O	1:B:176:GLU:HB3	1.99	0.63
1:C:192:SER:HA	1:C:247:ASP:OD2	1.98	0.63
1:C:150:LEU:HD21	1:C:169:ASP:OD2	1.98	0.63
1:B:308:ARG:HE	1:B:308:ARG:HA	1.64	0.63
1:B:43:ASP:H	1:B:60:GLN:HE21	1.47	0.63
1:B:66:ARG:HD2	2:B:347:HOH:O	1.99	0.63
1:D:216:PRO:HD3	1:D:221:ARG:NH2	2.14	0.62
1:A:173:GLY:HA2	1:A:244:GLU:OE1	1.99	0.62
1:A:49:SER:HB3	1:A:207:PRO:HA	1.80	0.62
1:B:46:PRO:HA	1:B:54:ALA:CB	2.29	0.62
1:D:176:GLU:O	1:D:180:ALA:HB2	1.99	0.62
1:B:66:ARG:O	1:B:70:GLU:HG2	2.00	0.62
1:C:282:PHE:CD2	1:C:318:TYR:HB2	2.35	0.62
1:B:296:LEU:HG	1:B:300:VAL:CG2	2.30	0.62
1:A:74:ARG:HH11	1:A:74:ARG:HB3	1.64	0.62
1:B:274:ALA:HB2	1:B:314:ILE:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:GLN:HB2	1:C:326:TRP:CH2	2.35	0.62
1:B:194:MET:HA	1:B:248:MET:HG2	1.82	0.62
1:B:123:LEU:HD23	1:B:130:GLY:H	1.62	0.62
1:B:133:GLY:O	1:B:134:LEU:HB2	1.99	0.62
1:A:50:LEU:HD21	1:A:279:SER:HB2	1.82	0.62
1:D:277:GLN:HG3	1:D:281:GLU:OE1	1.99	0.62
1:D:320:ALA:O	1:D:324:LEU:HG	1.99	0.62
1:C:301:LEU:HD11	1:C:326:TRP:HB3	1.82	0.62
1:A:278:VAL:CG2	1:A:281:GLU:HG3	2.30	0.62
1:C:313:ASP:O	1:C:314:ILE:HD12	1.99	0.62
1:B:101:THR:HG23	1:B:102:ILE:N	2.15	0.62
1:C:266:ASP:O	1:C:269:PRO:HD3	1.99	0.62
1:A:95:ASP:CG	1:A:153:VAL:HG13	2.20	0.62
1:B:227:PRO:HG2	1:B:230:ALA:CB	2.30	0.62
1:D:221:ARG:HB2	1:D:222:ARG:NH1	2.14	0.62
1:D:47:ILE:HD12	1:D:210:ASP:O	2.00	0.62
1:D:99:SER:OG	1:D:101:THR:HG22	2.00	0.61
1:C:256:PRO:HA	1:D:255:LEU:HD11	1.82	0.61
1:D:99:SER:HB3	1:D:102:ILE:HG12	1.82	0.61
1:D:81:VAL:HG11	1:D:212:ALA:HA	1.82	0.61
1:C:306:ALA:HA	1:C:309:ARG:NH1	2.15	0.61
1:B:54:ALA:HB3	1:B:56:TYR:CE1	2.36	0.61
1:B:11:TYR:O	1:B:13:HIS:N	2.32	0.61
1:B:7:LEU:O	1:B:10:GLY:N	2.34	0.61
1:C:77:LEU:HA	1:C:118:ALA:HB3	1.82	0.61
1:D:19:TRP:C	1:D:21:THR:H	2.04	0.61
1:B:224:TYR:O	1:B:225:GLN:HB2	2.00	0.61
1:A:55:ARG:HH21	1:A:212:ALA:N	1.98	0.61
1:D:153:VAL:HG12	1:D:157:TYR:HE1	1.65	0.61
1:C:297:ARG:HG3	1:C:326:TRP:CD1	2.36	0.61
1:D:110:LYS:HA	1:D:110:LYS:CE	2.30	0.61
1:B:122:CYS:SG	1:B:129:HIS:CE1	2.94	0.61
1:C:111:THR:HG22	1:C:112:PHE:CE1	2.36	0.61
1:B:99:SER:OG	1:B:101:THR:HG22	2.00	0.61
1:A:73:LEU:HD12	2:A:341:HOH:O	2.00	0.61
1:A:56:TYR:HD1	1:A:56:TYR:H	1.47	0.61
1:B:26:VAL:HG22	1:B:308:ARG:HG3	1.81	0.61
1:C:170:MET:HE1	1:C:174:ARG:HH21	1.64	0.61
1:D:242:ILE:O	1:D:242:ILE:HD13	2.00	0.61
1:A:116:LEU:HD13	1:A:163:GLN:HB2	1.83	0.61
1:C:32:ILE:CD1	1:C:314:ILE:HG23	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ILE:CD1	1:D:78:ILE:HA	2.31	0.60
1:C:102:ILE:HA	1:C:105:VAL:HG12	1.83	0.60
1:B:41:PRO:O	1:B:43:ASP:N	2.34	0.60
1:C:226:LEU:N	1:C:226:LEU:HD12	2.16	0.60
1:C:292:GLY:O	1:C:294:PHE:N	2.34	0.60
1:B:273:LEU:O	1:B:314:ILE:N	2.34	0.60
1:D:60:GLN:O	1:D:60:GLN:HG3	2.01	0.60
1:C:17:ARG:O	1:C:21:THR:HG22	2.01	0.60
1:C:54:ALA:HB3	1:C:56:TYR:CE1	2.37	0.60
1:C:20:GLN:NE2	1:D:233:LEU:HG	2.17	0.60
1:B:101:THR:HG21	1:B:157:TYR:CZ	2.37	0.60
1:D:51:PRO:O	1:D:53:VAL:HG23	2.01	0.60
1:D:75:CYS:CB	1:D:116:LEU:HB3	2.31	0.60
1:A:278:VAL:HG22	1:A:281:GLU:HG3	1.83	0.60
1:B:282:PHE:CD2	1:B:318:TYR:HB2	2.37	0.60
1:C:314:ILE:C	1:C:315:ILE:HD12	2.22	0.59
1:B:227:PRO:HG2	1:B:230:ALA:HB2	1.82	0.59
1:C:33:TYR:CD1	1:C:320:ALA:HB3	2.37	0.59
1:A:78:ILE:HD11	1:A:108:LEU:HD12	1.82	0.59
1:D:65:LEU:O	1:D:69:VAL:HG23	2.02	0.59
1:C:306:ALA:HA	1:C:309:ARG:NH2	2.17	0.59
1:D:145:GLU:HA	1:D:148:GLN:NE2	2.14	0.59
1:B:273:LEU:N	1:B:313:ASP:HB2	2.16	0.59
1:C:281:GLU:HA	1:C:284:MET:CE	2.31	0.59
1:A:280:GLY:O	1:A:284:MET:HB2	2.02	0.59
1:B:91:GLY:C	1:B:93:ALA:H	2.05	0.59
1:D:221:ARG:HA	1:D:224:TYR:CZ	2.37	0.59
1:A:240:ARG:NH2	1:B:7:LEU:HD12	2.16	0.59
1:C:287:HIS:ND1	1:D:291:ALA:HB1	2.18	0.59
1:D:22:ALA:O	1:D:24:SER:N	2.32	0.59
1:C:323:LEU:O	1:C:327:LEU:HD13	2.02	0.59
1:C:200:PHE:HD1	1:C:200:PHE:N	1.98	0.59
1:B:64:MET:HG3	1:B:65:LEU:HD23	1.84	0.59
1:C:273:LEU:HD13	1:C:274:ALA:N	2.17	0.59
1:D:277:GLN:HE21	1:D:303:THR:HG21	1.68	0.59
1:B:296:LEU:HG	1:B:300:VAL:HG23	1.85	0.59
1:B:110:LYS:NZ	1:B:110:LYS:HA	2.17	0.59
1:C:251:VAL:HG12	1:C:252:LYS:N	2.18	0.59
1:D:236:ARG:HG3	1:D:236:ARG:HH11	1.67	0.59
1:C:38:THR:HG23	1:C:55:ARG:HB3	1.84	0.59
1:C:32:ILE:HB	1:C:316:ILE:HG23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:TYR:CD1	1:B:309:ARG:NH1	2.70	0.59
1:D:153:VAL:HG12	1:D:157:TYR:CE1	2.38	0.59
1:D:105:VAL:HG21	1:D:162:CYS:H	1.65	0.59
1:D:39:ASP:OD1	1:D:82:PRO:HA	2.02	0.59
1:B:25:THR:O	1:B:308:ARG:HD2	2.02	0.59
1:C:111:THR:HG22	1:C:112:PHE:CD1	2.38	0.58
1:C:75:CYS:HB2	1:C:116:LEU:O	2.04	0.58
1:C:301:LEU:HD11	1:C:326:TRP:CB	2.33	0.58
1:C:32:ILE:HG23	1:C:75:CYS:SG	2.43	0.58
1:B:47:ILE:HD12	1:B:211:ALA:HA	1.85	0.58
1:D:38:THR:HG23	1:D:55:ARG:HB3	1.86	0.58
1:C:149:ARG:CB	1:C:149:ARG:HH11	2.10	0.58
1:C:41:PRO:O	1:C:43:ASP:N	2.36	0.58
1:C:257:TYR:O	1:C:261:VAL:HG23	2.04	0.58
1:D:56:TYR:N	1:D:56:TYR:CD1	2.71	0.58
1:A:56:TYR:N	1:A:56:TYR:CD1	2.70	0.58
1:C:200:PHE:N	1:C:200:PHE:CD1	2.67	0.58
1:D:307:PHE:CB	1:D:315:ILE:HD11	2.34	0.58
1:B:75:CYS:SG	1:B:116:LEU:HB3	2.43	0.58
1:D:169:ASP:O	1:D:170:MET:HB2	2.04	0.58
1:D:22:ALA:C	1:D:24:SER:H	2.07	0.58
1:A:174:ARG:O	1:A:178:ILE:HD13	2.03	0.58
1:C:41:PRO:HB3	1:C:59:ASN:H	1.68	0.58
1:B:122:CYS:C	1:B:123:LEU:HD22	2.24	0.58
1:B:201:ALA:HB2	1:B:225:GLN:O	2.03	0.58
1:A:173:GLY:HA2	1:A:244:GLU:CD	2.24	0.57
1:C:321:PRO:HB2	1:C:322:GLN:OE1	2.04	0.57
1:C:226:LEU:H	1:C:226:LEU:CD1	2.15	0.57
1:C:207:PRO:HG3	1:D:293:ALA:HB1	1.85	0.57
1:C:255:LEU:CD1	1:D:256:PRO:HA	2.25	0.57
1:D:278:VAL:O	1:D:281:GLU:HB2	2.04	0.57
1:C:116:LEU:HD22	1:C:163:GLN:OE1	2.04	0.57
1:C:209:ARG:HH11	1:C:209:ARG:HG2	1.69	0.57
1:B:226:LEU:CD1	1:B:226:LEU:H	2.15	0.57
1:A:182:LEU:HD22	1:A:187:LEU:O	2.04	0.57
1:C:28:ALA:O	1:C:74:ARG:HG2	2.04	0.57
1:B:77:LEU:HA	1:B:118:ALA:O	2.05	0.57
1:B:22:ALA:O	1:B:23:ALA:HB3	2.05	0.57
1:D:157:TYR:HD1	1:D:157:TYR:H	1.52	0.57
1:C:84:ARG:HH21	1:C:84:ARG:CB	2.09	0.57
1:B:15:LEU:HD11	1:B:19:TRP:NE1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ARG:NH1	1:C:163:GLN:NE2	2.52	0.57
1:C:23:ALA:O	1:C:24:SER:HB3	2.05	0.57
1:D:167:PRO:HB2	1:D:174:ARG:HE	1.69	0.57
1:C:236:ARG:HG3	1:C:236:ARG:HH11	1.69	0.57
1:A:233:LEU:HD12	1:B:20:GLN:CD	2.25	0.57
1:C:253:PRO:HB3	1:C:278:VAL:HG22	1.86	0.57
1:D:281:GLU:HB3	2:D:340:HOH:O	2.04	0.57
1:B:95:ASP:OD1	1:B:153:VAL:HG22	2.05	0.57
1:A:116:LEU:HD11	1:A:164:VAL:HG23	1.86	0.57
1:C:24:SER:HA	1:C:308:ARG:HB3	1.86	0.57
1:D:14:PRO:HA	1:D:17:ARG:CZ	2.35	0.56
1:A:55:ARG:HH21	1:A:211:ALA:C	2.08	0.56
1:C:198:ALA:HB1	1:C:200:PHE:HE1	1.70	0.56
1:C:205:TYR:HB3	1:C:209:ARG:NH1	2.21	0.56
1:B:91:GLY:O	1:B:93:ALA:N	2.38	0.56
1:B:255:LEU:HB3	1:B:256:PRO:HD3	1.86	0.56
1:A:95:ASP:OD2	1:A:153:VAL:HG13	2.04	0.56
1:A:259:ASP:OD1	1:A:260:MET:N	2.38	0.56
1:B:194:MET:HG2	1:B:194:MET:O	2.05	0.56
1:C:207:PRO:CG	1:D:293:ALA:HB1	2.35	0.56
1:C:166:ALA:O	1:C:196:TYR:HE1	1.87	0.56
1:A:235:LEU:HD21	1:A:263:GLU:HB3	1.87	0.56
1:C:240:ARG:O	1:C:244:GLU:HG3	2.05	0.56
1:A:155:LEU:HD12	1:A:181:ALA:HB1	1.87	0.56
1:A:27:SER:H	1:A:30:ASN:HD22	1.53	0.56
1:B:196:TYR:CD2	1:B:250:MET:SD	2.98	0.56
1:A:240:ARG:HD3	1:A:244:GLU:OE2	2.05	0.56
1:B:43:ASP:N	1:B:60:GLN:NE2	2.54	0.56
1:C:226:LEU:HD23	1:C:234:ALA:HA	1.88	0.56
1:D:242:ILE:HA	1:D:246:ALA:HB3	1.87	0.56
1:D:233:LEU:O	1:D:236:ARG:HB2	2.06	0.56
1:C:257:TYR:HA	1:D:309:ARG:HH21	1.70	0.56
1:D:11:TYR:C	1:D:13:HIS:H	2.09	0.56
1:D:287:HIS:O	1:D:291:ALA:HB2	2.05	0.56
1:D:13:HIS:CE1	1:D:15:LEU:HB3	2.40	0.56
1:B:35:ILE:CD1	1:B:78:ILE:HG13	2.32	0.56
1:C:47:ILE:N	1:C:47:ILE:HD12	2.21	0.56
1:C:265:LYS:O	1:C:269:PRO:HD3	2.05	0.56
1:B:296:LEU:O	1:B:300:VAL:HG23	2.05	0.56
1:C:286:TRP:O	1:C:289:ALA:N	2.35	0.56
1:A:66:ARG:HH11	1:A:66:ARG:HG2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:HIS:HD2	1:B:146:SER:HA	1.71	0.56
1:D:314:ILE:HG22	1:D:315:ILE:N	2.21	0.55
1:C:149:ARG:O	1:C:153:VAL:HG23	2.06	0.55
1:A:26:VAL:HG22	1:A:27:SER:N	2.22	0.55
1:B:136:SER:O	1:B:137:GLU:HB2	2.06	0.55
1:D:260:MET:O	1:D:264:VAL:HG22	2.07	0.55
1:C:154:ALA:HA	1:C:157:TYR:CD1	2.42	0.55
1:B:85:VAL:O	1:B:86:PRO:O	2.24	0.55
1:C:255:LEU:HG	1:D:255:LEU:O	2.06	0.55
1:B:303:THR:HG22	1:B:307:PHE:CE2	2.41	0.55
1:A:36:PHE:N	1:A:36:PHE:CD2	2.74	0.55
1:B:221:ARG:HG2	1:B:221:ARG:O	2.06	0.55
1:B:19:TRP:CD1	1:C:314:ILE:HD11	2.41	0.55
1:D:282:PHE:CD2	1:D:318:TYR:HB2	2.41	0.55
1:B:231:ARG:HB3	1:B:231:ARG:HH11	1.70	0.55
1:B:199:LYS:NZ	1:B:252:LYS:NZ	2.55	0.55
1:A:3:HIS:C	1:A:5:SER:H	2.11	0.55
1:D:276:TYR:CE1	1:D:278:VAL:HA	2.41	0.55
1:C:197:SER:HB3	1:C:238:VAL:HG22	1.89	0.55
1:C:252:LYS:HA	1:C:253:PRO:O	2.06	0.55
1:C:47:ILE:HD13	1:C:53:VAL:HG12	1.89	0.55
1:C:322:GLN:HB2	1:C:326:TRP:CZ3	2.42	0.55
1:A:142:LEU:HD13	1:A:145:GLU:HG2	1.87	0.55
1:A:17:ARG:O	1:A:21:THR:HG22	2.07	0.55
1:C:265:LYS:HA	1:C:265:LYS:CE	2.34	0.54
1:A:35:ILE:CD1	1:A:76:VAL:HB	2.37	0.54
1:C:116:LEU:HA	1:C:163:GLN:OE1	2.07	0.54
2:C:333:HOH:O	1:D:262:ARG:HD2	2.07	0.54
1:D:254:GLY:O	1:D:257:TYR:N	2.37	0.54
1:B:274:ALA:HA	1:B:314:ILE:O	2.07	0.54
1:D:323:LEU:O	1:D:325:LYS:N	2.40	0.54
1:C:170:MET:HE1	1:C:174:ARG:NH2	2.22	0.54
1:B:169:ASP:HB3	1:B:171:MET:HG2	1.88	0.54
1:A:307:PHE:HD2	1:A:315:ILE:HD13	1.71	0.54
1:B:13:HIS:CE1	1:B:15:LEU:H	2.24	0.54
1:C:277:GLN:HE22	1:C:285:LEU:HD11	1.72	0.54
1:A:54:ALA:HB3	1:A:56:TYR:CE1	2.42	0.54
1:A:40:VAL:HB	1:A:43:ASP:HB2	1.89	0.54
1:C:305:THR:HG21	1:D:228:PRO:CB	2.38	0.54
1:C:273:LEU:HD12	1:C:312:ALA:HA	1.89	0.54
1:C:32:ILE:HD11	1:C:314:ILE:CG2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ASP:OD2	1:B:85:VAL:HG23	2.08	0.54
1:B:85:VAL:HG13	1:B:86:PRO:HD2	1.90	0.54
1:A:123:LEU:HD22	1:A:123:LEU:N	2.22	0.54
1:C:275:VAL:CG1	1:C:315:ILE:HG13	2.38	0.54
1:A:316:ILE:N	1:A:316:ILE:HD12	2.23	0.54
1:D:102:ILE:HG22	1:D:102:ILE:O	2.07	0.54
1:C:11:TYR:O	1:C:16:LEU:HB3	2.08	0.54
1:C:58:VAL:C	1:C:60:GLN:H	2.10	0.54
1:D:149:ARG:O	1:D:153:VAL:HG23	2.07	0.54
1:A:257:TYR:HD1	1:B:309:ARG:NH1	2.06	0.54
1:B:105:VAL:HG23	1:B:117:VAL:HG11	1.90	0.54
1:C:99:SER:O	1:C:103:GLU:HG3	2.07	0.54
1:D:11:TYR:O	1:D:13:HIS:N	2.41	0.53
1:C:174:ARG:HG2	1:C:174:ARG:HH11	1.71	0.53
1:D:286:TRP:C	1:D:288:GLY:H	2.11	0.53
1:D:158:ALA:HB1	1:D:187:LEU:HD13	1.90	0.53
1:D:42:ASP:HA	1:D:60:GLN:HE21	1.73	0.53
1:B:108:LEU:HD23	1:B:108:LEU:N	2.23	0.53
1:A:300:VAL:C	1:A:302:GLU:H	2.11	0.53
1:C:157:TYR:H	1:C:157:TYR:HD1	1.57	0.53
1:C:51:PRO:O	1:C:53:VAL:HG23	2.07	0.53
1:B:183:LEU:HD13	1:B:188:GLY:HA3	1.91	0.53
1:D:301:LEU:O	1:D:304:MET:HB2	2.09	0.53
1:B:59:ASN:O	1:B:61:LEU:N	2.41	0.53
1:D:238:VAL:CG1	1:D:249:LEU:HD13	2.39	0.53
1:A:304:MET:C	1:A:306:ALA:H	2.11	0.53
1:C:253:PRO:HG3	1:C:278:VAL:HG11	1.90	0.53
1:C:22:ALA:O	1:C:23:ALA:HB3	2.08	0.53
1:B:233:LEU:HD23	1:B:236:ARG:HG3	1.89	0.53
1:D:78:ILE:HB	1:D:118:ALA:O	2.09	0.53
1:B:8:HIS:CB	1:C:189:ASN:HB2	2.35	0.53
1:B:123:LEU:HB3	1:B:125:PRO:HD3	1.91	0.53
1:A:305:THR:O	1:A:305:THR:HG22	2.09	0.53
1:D:58:VAL:HG12	1:D:59:ASN:N	2.24	0.53
1:C:147:ARG:HE	1:C:173:GLY:HA3	1.74	0.53
1:A:105:VAL:HG23	1:A:117:VAL:CG1	2.39	0.53
1:C:18:SER:HA	1:C:21:THR:CG2	2.39	0.53
1:C:35:ILE:O	1:C:35:ILE:HG13	2.08	0.53
1:B:209:ARG:HH12	1:B:221:ARG:NH2	2.07	0.53
1:D:202:SER:HB3	2:D:337:HOH:O	2.09	0.53
1:D:281:GLU:O	1:D:282:PHE:C	2.47	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG23	1:A:117:VAL:HG11	1.91	0.53
1:D:231:ARG:O	1:D:234:ALA:HB3	2.10	0.53
1:C:287:HIS:H	1:C:287:HIS:CD2	2.27	0.53
1:D:266:ASP:O	1:D:268:HIS:N	2.42	0.53
1:A:6:VAL:O	1:A:7:LEU:HD23	2.09	0.52
1:C:281:GLU:HA	1:C:284:MET:HE2	1.90	0.52
1:B:260:MET:O	1:B:264:VAL:HG22	2.08	0.52
1:C:242:ILE:HG23	1:C:243:GLN:N	2.24	0.52
1:A:11:TYR:CD1	1:A:11:TYR:N	2.77	0.52
1:A:11:TYR:O	1:A:12:PHE:CG	2.63	0.52
1:B:170:MET:CG	1:B:199:LYS:HB3	2.39	0.52
1:B:204:PHE:HB3	1:B:280:GLY:HA3	1.90	0.52
1:A:260:MET:HE3	1:B:309:ARG:HD2	1.90	0.52
1:D:275:VAL:CG1	1:D:315:ILE:HG12	2.39	0.52
1:A:173:GLY:HA2	1:A:244:GLU:OE2	2.09	0.52
1:C:58:VAL:O	1:C:60:GLN:N	2.43	0.52
1:A:11:TYR:HA	1:A:16:LEU:HB3	1.90	0.52
1:D:209:ARG:HG2	1:D:209:ARG:HH11	1.75	0.52
1:A:255:LEU:HD11	1:B:256:PRO:CA	2.30	0.52
1:C:149:ARG:C	1:C:151:ALA:H	2.12	0.52
1:C:73:LEU:H	1:C:324:LEU:CD1	2.19	0.52
1:B:317:THR:HG23	1:B:320:ALA:N	2.25	0.52
1:A:35:ILE:HD13	1:A:35:ILE:N	2.24	0.52
1:B:147:ARG:O	1:B:150:LEU:HB3	2.08	0.52
1:D:320:ALA:HB3	1:D:321:PRO:HD3	1.92	0.52
1:B:207:PRO:O	1:B:210:ASP:HB2	2.10	0.52
1:A:47:ILE:HD12	1:A:47:ILE:N	2.24	0.52
1:A:326:TRP:C	1:A:328:LYS:H	2.13	0.52
1:B:32:ILE:HB	1:B:316:ILE:HG12	1.92	0.52
1:B:176:GLU:N	1:B:244:GLU:OE1	2.43	0.52
1:B:47:ILE:HD11	1:B:55:ARG:CG	2.34	0.52
1:A:199:LYS:HZ3	1:A:252:LYS:HE2	1.74	0.52
1:C:178:ILE:O	1:C:181:ALA:HB3	2.09	0.52
1:C:77:LEU:HA	1:C:118:ALA:O	2.10	0.52
1:B:280:GLY:O	1:B:284:MET:HG3	2.09	0.52
1:C:275:VAL:HG11	1:C:315:ILE:HG13	1.92	0.51
1:B:273:LEU:O	1:B:313:ASP:N	2.43	0.51
1:C:12:PHE:CD1	1:C:12:PHE:C	2.84	0.51
1:B:162:CYS:SG	1:B:163:GLN:N	2.83	0.51
1:B:73:LEU:HA	1:B:324:LEU:HD11	1.91	0.51
1:B:133:GLY:O	1:B:134:LEU:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:TYR:HD1	1:D:56:TYR:N	2.08	0.51
1:D:186:GLY:C	1:D:188:GLY:H	2.13	0.51
1:C:293:ALA:O	1:D:206:GLY:HA3	2.10	0.51
1:C:227:PRO:HA	2:C:340:HOH:O	2.11	0.51
1:C:151:ALA:C	1:C:153:VAL:N	2.64	0.51
1:A:265:LYS:HE2	1:A:269:PRO:HA	1.93	0.51
1:D:197:SER:HB3	1:D:238:VAL:HA	1.92	0.51
1:A:39:ASP:OD2	1:A:82:PRO:HA	2.11	0.51
1:B:245:GLY:O	1:B:246:ALA:O	2.27	0.51
1:A:242:ILE:HD13	1:A:271:LEU:CD1	2.27	0.51
1:C:233:LEU:HD23	1:C:233:LEU:O	2.11	0.51
1:B:296:LEU:HD23	1:B:326:TRP:HH2	1.76	0.51
1:A:78:ILE:HD11	1:A:108:LEU:CD1	2.41	0.51
1:A:66:ARG:N	1:A:67:PRO:HD2	2.26	0.51
1:C:174:ARG:HH12	1:C:240:ARG:HH22	1.59	0.51
1:B:53:VAL:CG1	1:B:54:ALA:N	2.74	0.51
1:A:164:VAL:HG22	1:A:192:SER:HB2	1.92	0.51
1:D:282:PHE:HD2	1:D:318:TYR:HD2	1.58	0.51
1:A:199:LYS:O	1:A:225:GLN:HG2	2.11	0.51
1:A:122:CYS:SG	1:A:123:LEU:N	2.83	0.51
1:B:68:LEU:O	1:B:71:ALA:N	2.43	0.51
1:D:78:ILE:N	1:D:118:ALA:O	2.39	0.51
1:D:242:ILE:HG23	1:D:243:GLN:N	2.26	0.51
1:B:122:CYS:SG	1:B:129:HIS:CG	3.04	0.51
1:D:97:GLU:HG2	1:D:98:ASP:N	2.26	0.51
1:B:122:CYS:SG	1:B:129:HIS:CD2	3.04	0.51
1:D:272:PRO:HA	1:D:313:ASP:OD2	2.10	0.51
1:C:4:GLN:O	1:C:5:SER:HB3	2.11	0.51
1:C:281:GLU:HA	1:C:284:MET:HE3	1.94	0.50
1:B:327:LEU:O	1:B:328:LYS:HD2	2.11	0.50
1:B:11:TYR:C	1:B:13:HIS:H	2.15	0.50
1:B:272:PRO:HG3	1:C:20:GLN:OE1	2.12	0.50
1:D:58:VAL:HG21	1:D:103:GLU:CD	2.31	0.50
1:D:25:THR:O	1:D:25:THR:HG23	2.10	0.50
1:A:95:ASP:OD1	1:A:153:VAL:HG13	2.12	0.50
1:A:257:TYR:HD1	1:B:309:ARG:NH2	2.10	0.50
1:A:323:LEU:C	1:A:325:LYS:N	2.64	0.50
1:D:64:MET:C	1:D:64:MET:SD	2.89	0.50
1:B:260:MET:HE2	1:B:260:MET:HA	1.93	0.50
1:C:66:ARG:N	1:C:67:PRO:HD2	2.26	0.50
1:A:7:LEU:HD12	1:B:240:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:GLN:HG2	1:C:149:ARG:N	2.26	0.50
1:D:41:PRO:O	1:D:43:ASP:N	2.45	0.50
1:D:107:LEU:O	1:D:108:LEU:C	2.50	0.50
1:B:90:GLN:HA	1:B:131:HIS:HE1	1.77	0.50
1:C:310:ALA:O	1:C:312:ALA:N	2.45	0.50
1:C:11:TYR:HA	1:C:16:LEU:O	2.12	0.50
1:C:12:PHE:HD1	1:C:12:PHE:O	1.95	0.50
1:D:236:ARG:NH1	1:D:236:ARG:HG3	2.26	0.50
1:D:251:VAL:O	1:D:253:PRO:O	2.29	0.50
1:A:38:THR:HG22	1:A:81:VAL:O	2.11	0.50
1:C:105:VAL:HA	1:C:108:LEU:HD12	1.94	0.50
1:B:314:ILE:C	1:B:315:ILE:HD12	2.31	0.50
1:D:323:LEU:C	1:D:325:LYS:N	2.66	0.50
1:C:18:SER:HA	1:C:21:THR:HG22	1.94	0.50
1:B:151:ALA:HA	1:B:178:ILE:CD1	2.40	0.50
1:B:199:LYS:HZ2	1:B:252:LYS:HZ3	1.60	0.50
1:A:22:ALA:O	1:A:23:ALA:HB3	2.12	0.50
1:C:50:LEU:HB3	1:C:53:VAL:CG2	2.41	0.49
1:B:105:VAL:CG1	1:B:106:ARG:H	2.22	0.49
1:C:308:ARG:O	1:C:309:ARG:C	2.50	0.49
1:D:282:PHE:HD2	1:D:318:TYR:HB2	1.75	0.49
1:D:70:GLU:C	1:D:72:GLY:H	2.15	0.49
1:C:319:PHE:O	1:C:320:ALA:C	2.50	0.49
1:A:277:GLN:HG2	1:A:277:GLN:O	2.12	0.49
1:B:104:ALA:O	1:B:108:LEU:HG	2.11	0.49
1:D:146:SER:O	1:D:150:LEU:HB2	2.11	0.49
1:D:279:SER:CA	1:D:318:TYR:HE2	2.21	0.49
1:B:262:ARG:O	1:B:262:ARG:HD3	2.12	0.49
1:A:263:GLU:C	1:A:265:LYS:H	2.15	0.49
1:D:196:TYR:O	1:D:198:ALA:N	2.45	0.49
1:D:282:PHE:HD2	1:D:318:TYR:CD2	2.30	0.49
1:C:327:LEU:O	1:C:328:LYS:C	2.50	0.49
1:C:20:GLN:HG2	1:D:233:LEU:HD12	1.93	0.49
1:C:197:SER:CB	1:C:238:VAL:HG22	2.43	0.49
1:C:205:TYR:CZ	1:C:252:LYS:HE2	2.48	0.49
1:D:258:LEU:O	1:D:261:VAL:N	2.40	0.49
1:A:147:ARG:O	1:A:150:LEU:N	2.43	0.49
1:D:226:LEU:H	1:D:226:LEU:HD12	1.77	0.49
1:C:307:PHE:HD2	1:C:315:ILE:CG1	2.26	0.49
1:C:84:ARG:HD3	1:C:84:ARG:N	2.28	0.49
1:D:72:GLY:O	1:D:324:LEU:HD22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:PRO:C	1:B:323:LEU:H	2.15	0.49
1:C:289:ALA:C	1:C:291:ALA:N	2.65	0.49
1:B:199:LYS:HZ2	1:B:252:LYS:NZ	2.10	0.49
1:B:94:ALA:HB2	1:B:124:CYS:SG	2.52	0.49
1:C:198:ALA:HB1	1:C:200:PHE:CE1	2.47	0.49
1:D:228:PRO:C	1:D:230:ALA:H	2.13	0.49
1:D:275:VAL:HG11	1:D:307:PHE:CD1	2.48	0.49
1:B:154:ALA:HB1	1:B:178:ILE:HG23	1.95	0.49
1:B:315:ILE:N	1:B:315:ILE:HD12	2.27	0.49
1:C:56:TYR:CD1	1:C:56:TYR:N	2.80	0.49
1:D:323:LEU:C	1:D:325:LYS:H	2.15	0.49
1:D:155:LEU:HD12	1:D:181:ALA:HB1	1.94	0.49
1:B:61:LEU:C	1:B:63:GLU:H	2.16	0.49
1:D:239:ALA:O	1:D:242:ILE:HG22	2.13	0.49
1:C:122:CYS:O	1:C:122:CYS:SG	2.70	0.49
1:A:238:VAL:O	1:A:242:ILE:HG22	2.12	0.49
1:B:301:LEU:O	1:B:304:MET:N	2.46	0.49
1:A:240:ARG:HH21	1:B:7:LEU:CD1	2.22	0.49
1:D:36:PHE:O	1:D:56:TYR:N	2.46	0.49
1:A:157:TYR:O	1:A:160:ALA:HB3	2.13	0.49
1:C:205:TYR:HE1	1:C:252:LYS:HE2	1.76	0.49
1:C:119:CYS:HB3	1:C:157:TYR:CD2	2.48	0.49
1:A:204:PHE:HB3	1:A:280:GLY:HA3	1.95	0.49
1:A:121:VAL:HG11	1:A:154:ALA:HB2	1.94	0.49
1:D:258:LEU:HA	1:D:261:VAL:HG23	1.95	0.48
1:D:33:TYR:O	1:D:77:LEU:N	2.46	0.48
1:C:325:LYS:C	1:C:327:LEU:H	2.16	0.48
1:C:258:LEU:CB	1:D:258:LEU:HB3	2.42	0.48
1:D:307:PHE:HB3	1:D:315:ILE:HD11	1.93	0.48
1:C:242:ILE:CG2	1:C:243:GLN:N	2.76	0.48
1:C:258:LEU:HG	1:D:259:ASP:HB3	1.95	0.48
1:D:314:ILE:HG22	1:D:315:ILE:H	1.78	0.48
1:D:11:TYR:CB	1:D:17:ARG:HG2	2.43	0.48
1:A:99:SER:HB2	1:A:100:PRO:CD	2.36	0.48
1:C:175:VAL:HG11	1:C:246:ALA:HB2	1.95	0.48
1:B:53:VAL:CG1	1:B:54:ALA:H	2.24	0.48
1:B:91:GLY:C	1:B:93:ALA:N	2.67	0.48
1:C:104:ALA:O	1:C:107:LEU:HB3	2.13	0.48
1:D:77:LEU:CD1	1:D:316:ILE:HD13	2.42	0.48
1:C:155:LEU:CD2	1:C:159:LYS:HE3	2.43	0.48
1:B:275:VAL:HG11	1:B:307:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:GLU:HA	2:A:339:HOH:O	2.13	0.48
1:C:162:CYS:SG	1:C:163:GLN:N	2.86	0.48
1:C:259:ASP:CA	1:D:259:ASP:HA	2.39	0.48
1:D:282:PHE:CD1	1:D:282:PHE:C	2.87	0.48
1:A:283:ALA:HB1	1:A:287:HIS:CE1	2.49	0.48
1:C:259:ASP:HB2	1:D:262:ARG:CB	2.42	0.48
1:C:149:ARG:HA	1:C:152:GLU:HG2	1.94	0.48
1:B:274:ALA:CB	1:B:314:ILE:HB	2.42	0.48
1:D:58:VAL:O	1:D:59:ASN:C	2.51	0.48
1:A:37:VAL:HG12	1:A:38:THR:N	2.29	0.48
1:D:199:LYS:HA	1:D:252:LYS:O	2.14	0.48
1:C:45:GLN:O	1:C:54:ALA:HA	2.14	0.48
1:D:225:GLN:O	1:D:226:LEU:C	2.52	0.48
1:D:231:ARG:HG2	1:D:231:ARG:HH11	1.78	0.48
1:C:110:LYS:O	1:C:110:LYS:HG2	2.14	0.48
1:A:234:ALA:O	1:A:238:VAL:HG23	2.12	0.48
1:B:182:LEU:O	1:B:188:GLY:N	2.45	0.48
1:B:66:ARG:HB3	1:B:67:PRO:CD	2.44	0.48
1:A:54:ALA:HB3	1:A:56:TYR:CZ	2.49	0.48
1:D:308:ARG:C	1:D:310:ALA:H	2.18	0.48
1:B:8:HIS:C	1:B:10:GLY:H	2.18	0.48
1:A:169:ASP:OD1	1:A:174:ARG:HD2	2.13	0.48
1:D:179:LYS:HA	1:D:182:LEU:HD12	1.96	0.48
1:B:76:VAL:HG21	1:B:115:LEU:HD21	1.96	0.47
1:A:277:GLN:NE2	1:A:317:THR:OG1	2.47	0.47
1:A:306:ALA:HA	1:A:309:ARG:NH1	2.29	0.47
1:D:116:LEU:HD22	1:D:163:GLN:OE1	2.14	0.47
1:C:170:MET:HA	1:C:174:ARG:CZ	2.43	0.47
1:C:42:ASP:HA	1:C:60:GLN:HG2	1.96	0.47
1:A:282:PHE:O	1:A:285:LEU:HB2	2.14	0.47
1:C:64:MET:SD	1:C:65:LEU:HG	2.54	0.47
1:C:312:ALA:HB1	1:C:315:ILE:HD11	1.95	0.47
1:D:258:LEU:O	1:D:261:VAL:HG23	2.14	0.47
1:C:255:LEU:HD11	1:D:256:PRO:CA	2.28	0.47
1:B:154:ALA:CB	1:B:178:ILE:HG23	2.44	0.47
1:B:183:LEU:HD22	1:B:188:GLY:HA3	1.96	0.47
1:A:40:VAL:HB	1:A:43:ASP:CB	2.44	0.47
1:A:304:MET:C	1:A:306:ALA:N	2.68	0.47
1:D:322:GLN:O	1:D:326:TRP:HB2	2.14	0.47
1:C:251:VAL:CG1	1:C:252:LYS:N	2.77	0.47
1:B:43:ASP:H	1:B:60:GLN:NE2	2.10	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASP:OD2	1:B:310:ALA:HB2	2.15	0.47
1:B:7:LEU:O	1:B:8:HIS:C	2.52	0.47
1:C:34:PRO:HG2	1:C:318:TYR:CE1	2.49	0.47
1:B:293:ALA:O	1:B:294:PHE:HB3	2.14	0.47
1:C:287:HIS:CD2	1:C:287:HIS:N	2.82	0.47
1:B:109:ARG:HG3	1:B:161:GLY:O	2.14	0.47
1:D:158:ALA:CB	1:D:187:LEU:HD13	2.43	0.47
1:B:86:PRO:C	1:B:87:LYS:HG3	2.35	0.47
1:A:253:PRO:HD2	1:A:257:TYR:CD2	2.49	0.47
1:C:311:GLY:O	1:C:312:ALA:C	2.52	0.47
1:A:66:ARG:O	1:A:70:GLU:HG3	2.14	0.47
1:C:144:GLU:C	1:C:146:SER:H	2.16	0.47
1:C:299:ALA:O	1:C:302:GLU:N	2.43	0.47
1:B:128:SER:OG	1:B:216:PRO:HB3	2.14	0.47
1:D:153:VAL:CG1	1:D:157:TYR:HE1	2.27	0.47
1:D:35:ILE:HD13	1:D:35:ILE:H	1.80	0.47
1:D:252:LYS:HA	1:D:253:PRO:O	2.15	0.47
1:A:99:SER:OG	1:A:102:ILE:HG12	2.15	0.47
1:B:99:SER:HB3	1:B:102:ILE:HG12	1.97	0.47
1:C:20:GLN:HG2	1:D:233:LEU:CD1	2.43	0.47
1:A:285:LEU:HD13	1:A:300:VAL:HG22	1.97	0.47
1:C:153:VAL:O	1:C:155:LEU:N	2.48	0.47
1:C:202:SER:HB2	1:C:257:TYR:OH	2.15	0.47
1:C:24:SER:HA	1:C:308:ARG:HD3	1.95	0.47
1:D:196:TYR:HA	1:D:250:MET:HB3	1.97	0.47
1:A:19:TRP:O	1:A:22:ALA:HB2	2.15	0.47
1:A:190:ARG:HG3	1:A:190:ARG:HH11	1.80	0.47
1:C:253:PRO:HA	1:C:278:VAL:HG13	1.97	0.47
1:D:277:GLN:NE2	1:D:303:THR:CG2	2.76	0.47
1:D:32:ILE:HG12	1:D:75:CYS:SG	2.55	0.47
1:C:105:VAL:CG1	1:C:106:ARG:H	2.27	0.47
1:C:281:GLU:O	1:C:282:PHE:C	2.54	0.47
1:C:11:TYR:C	1:C:13:HIS:N	2.68	0.47
1:B:105:VAL:CG1	1:B:106:ARG:N	2.78	0.47
1:C:35:ILE:HG12	1:C:77:LEU:O	2.15	0.47
1:B:295:ASP:OD2	1:B:297:ARG:N	2.41	0.47
1:C:205:TYR:HB3	1:C:209:ARG:HH12	1.80	0.46
1:C:253:PRO:HB3	1:C:278:VAL:CG2	2.45	0.46
1:C:275:VAL:HG11	1:C:307:PHE:CD2	2.50	0.46
1:D:13:HIS:HE1	1:D:15:LEU:CB	2.27	0.46
1:B:260:MET:CE	1:B:260:MET:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ALA:O	1:A:324:LEU:HG	2.15	0.46
1:D:81:VAL:CG1	1:D:212:ALA:HA	2.45	0.46
1:A:169:ASP:O	1:A:170:MET:HB2	2.16	0.46
1:C:205:TYR:CB	1:C:209:ARG:HH12	2.27	0.46
1:C:32:ILE:HD13	1:C:316:ILE:CG1	2.43	0.46
1:D:258:LEU:O	1:D:259:ASP:C	2.54	0.46
1:A:258:LEU:O	1:A:261:VAL:HB	2.15	0.46
1:C:279:SER:O	1:C:282:PHE:HB3	2.15	0.46
1:D:122:CYS:HA	1:D:169:ASP:OD2	2.14	0.46
1:B:66:ARG:HB3	1:B:67:PRO:HD3	1.98	0.46
1:C:20:GLN:HE21	1:D:233:LEU:HD11	1.80	0.46
1:D:262:ARG:HD3	1:D:262:ARG:C	2.35	0.46
1:D:75:CYS:HB2	1:D:116:LEU:CB	2.43	0.46
1:C:170:MET:HA	1:C:174:ARG:NH2	2.30	0.46
1:C:68:LEU:O	1:C:71:ALA:HB3	2.15	0.46
1:D:253:PRO:HD2	1:D:257:TYR:CD2	2.50	0.46
1:D:66:ARG:N	1:D:67:PRO:CD	2.77	0.46
1:B:155:LEU:O	1:B:158:ALA:HB3	2.16	0.46
1:B:92:SER:HA	1:B:95:ASP:OD2	2.16	0.46
1:C:242:ILE:HD13	1:C:242:ILE:O	2.16	0.46
1:A:306:ALA:HA	1:A:309:ARG:HH12	1.80	0.46
1:A:12:PHE:C	1:A:12:PHE:CD1	2.88	0.46
1:B:19:TRP:CG	1:C:314:ILE:HD11	2.51	0.46
1:A:239:ALA:O	1:A:242:ILE:HG23	2.16	0.46
1:A:31:LEU:C	1:A:32:ILE:HD12	2.35	0.46
1:C:78:ILE:N	1:C:78:ILE:HD12	2.31	0.46
1:B:149:ARG:HB3	2:B:350:HOH:O	2.14	0.46
1:D:200:PHE:C	1:D:202:SER:H	2.17	0.46
1:C:84:ARG:HD3	1:C:84:ARG:H	1.79	0.46
1:A:229:GLY:HA2	1:B:309:ARG:HD3	1.97	0.46
1:B:283:ALA:O	1:B:286:TRP:N	2.48	0.46
1:A:151:ALA:O	1:A:155:LEU:N	2.47	0.46
1:B:131:HIS:CD2	1:B:146:SER:HA	2.49	0.46
1:C:147:ARG:NE	1:C:173:GLY:HA3	2.30	0.46
1:B:200:PHE:HB2	1:B:253:PRO:HD2	1.97	0.46
1:B:240:ARG:HD3	1:B:244:GLU:OE2	2.16	0.46
1:B:308:ARG:HH22	1:B:313:ASP:HA	1.80	0.46
1:B:68:LEU:CD2	1:B:321:PRO:HB3	2.46	0.46
1:C:123:LEU:HD22	1:C:123:LEU:N	2.31	0.46
1:C:109:ARG:C	1:C:111:THR:H	2.18	0.46
1:D:307:PHE:HB2	1:D:315:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:TYR:CE2	1:B:250:MET:SD	3.09	0.46
1:A:313:ASP:C	1:A:314:ILE:HD13	2.35	0.46
1:D:235:LEU:O	1:D:236:ARG:C	2.54	0.46
1:C:55:ARG:NH2	1:C:210:ASP:O	2.49	0.46
1:B:200:PHE:HB2	1:B:253:PRO:CD	2.45	0.46
1:C:323:LEU:O	1:C:325:LYS:N	2.48	0.46
1:C:284:MET:SD	1:D:285:LEU:HD23	2.56	0.46
1:D:238:VAL:HG13	1:D:249:LEU:HD13	1.97	0.46
1:C:24:SER:HA	1:C:308:ARG:CB	2.46	0.46
1:D:253:PRO:HG3	2:D:337:HOH:O	2.15	0.46
1:C:105:VAL:CG1	1:C:106:ARG:N	2.76	0.46
1:D:319:PHE:O	1:D:323:LEU:HG	2.16	0.46
1:A:55:ARG:NH2	1:A:211:ALA:C	2.69	0.46
1:A:50:LEU:O	1:A:53:VAL:HB	2.16	0.46
1:A:297:ARG:HG3	1:A:326:TRP:CD1	2.51	0.46
1:C:190:ARG:HG2	1:C:190:ARG:O	2.15	0.46
1:D:183:LEU:HD13	1:D:183:LEU:C	2.36	0.46
1:D:193:VAL:H	1:D:247:ASP:HB2	1.81	0.46
1:A:230:ALA:HB1	1:A:233:LEU:HB3	1.98	0.45
1:B:13:HIS:NE2	1:C:116:LEU:HD23	2.32	0.45
1:A:7:LEU:HD22	1:B:236:ARG:NH2	2.31	0.45
1:C:83:SER:OG	1:C:84:ARG:HD3	2.15	0.45
1:C:47:ILE:HG21	1:C:50:LEU:HB2	1.98	0.45
1:A:26:VAL:HG22	1:A:27:SER:H	1.81	0.45
1:A:326:TRP:C	1:A:328:LYS:N	2.70	0.45
1:C:298:THR:O	1:C:302:GLU:HB2	2.16	0.45
1:C:265:LYS:O	1:C:269:PRO:CD	2.64	0.45
1:C:273:LEU:HD12	1:C:312:ALA:N	2.31	0.45
1:A:255:LEU:CD1	1:A:258:LEU:HD22	2.46	0.45
1:B:167:PRO:HB2	1:B:174:ARG:HE	1.81	0.45
1:B:9:SER:HB3	1:C:189:ASN:HA	1.98	0.45
1:C:235:LEU:N	1:C:235:LEU:HD23	2.30	0.45
1:B:15:LEU:HD21	1:B:19:TRP:CZ2	2.51	0.45
1:C:265:LYS:CE	1:C:269:PRO:HA	2.41	0.45
1:C:273:LEU:HD22	1:C:274:ALA:N	2.29	0.45
1:D:149:ARG:C	1:D:151:ALA:H	2.20	0.45
1:C:279:SER:N	1:C:318:TYR:HE2	2.14	0.45
1:D:266:ASP:O	1:D:269:PRO:HD3	2.16	0.45
1:B:13:HIS:HA	1:B:14:PRO:HD2	1.73	0.45
1:C:209:ARG:C	1:C:211:ALA:H	2.19	0.45
1:D:32:ILE:HD11	1:D:314:ILE:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LYS:HD3	1:B:193:VAL:CG2	2.47	0.45
1:D:226:LEU:CD2	1:D:234:ALA:HA	2.47	0.45
1:D:300:VAL:O	1:D:304:MET:HG2	2.17	0.45
1:B:242:ILE:HG23	1:B:243:GLN:N	2.30	0.45
1:A:6:VAL:C	1:A:7:LEU:HD23	2.37	0.45
1:B:40:VAL:HG11	1:B:43:ASP:OD2	2.16	0.45
1:B:327:LEU:N	1:B:327:LEU:HD12	2.31	0.45
1:C:37:VAL:HG12	1:C:100:PRO:HB2	1.99	0.45
1:C:258:LEU:O	1:C:261:VAL:N	2.48	0.45
1:D:222:ARG:N	1:D:222:ARG:CD	2.79	0.45
1:D:61:LEU:HD23	1:D:107:LEU:HD23	1.97	0.45
1:B:129:HIS:CE1	2:B:334:HOH:O	2.69	0.45
1:D:22:ALA:C	1:D:24:SER:N	2.70	0.45
1:C:262:ARG:O	1:C:265:LYS:HB3	2.16	0.45
1:C:151:ALA:C	1:C:153:VAL:H	2.19	0.45
1:C:240:ARG:HD2	1:C:240:ARG:C	2.36	0.45
1:B:317:THR:HG23	1:B:320:ALA:H	1.81	0.45
1:C:58:VAL:C	1:C:60:GLN:N	2.70	0.45
1:B:202:SER:OG	1:B:203:CYS:N	2.48	0.45
1:D:282:PHE:HD1	1:D:282:PHE:C	2.19	0.45
1:B:151:ALA:O	1:B:154:ALA:HB3	2.17	0.45
1:B:167:PRO:O	1:B:196:TYR:HD1	2.00	0.45
1:C:170:MET:CE	1:C:170:MET:H	2.30	0.45
1:A:121:VAL:O	1:A:167:PRO:HA	2.17	0.45
1:C:299:ALA:O	1:C:303:THR:HG23	2.17	0.45
1:D:259:ASP:CG	1:D:260:MET:N	2.71	0.45
1:A:49:SER:C	1:A:51:PRO:HD3	2.38	0.45
1:D:235:LEU:O	1:D:238:VAL:N	2.50	0.45
1:C:179:LYS:HG3	1:C:183:LEU:HG	1.99	0.45
1:C:255:LEU:N	1:C:256:PRO:CD	2.80	0.45
1:D:147:ARG:HA	2:D:338:HOH:O	2.17	0.45
1:A:202:SER:HB3	1:A:253:PRO:HG2	1.99	0.45
1:D:242:ILE:C	1:D:242:ILE:CD1	2.85	0.45
1:C:20:GLN:HE21	1:D:233:LEU:CG	2.30	0.45
1:D:233:LEU:O	1:D:234:ALA:C	2.56	0.45
1:A:64:MET:O	1:A:64:MET:SD	2.75	0.45
1:C:305:THR:HG21	1:D:228:PRO:HB2	1.98	0.44
1:B:227:PRO:HG2	1:B:230:ALA:HB3	1.99	0.44
1:C:305:THR:HG21	1:D:228:PRO:HB3	1.99	0.44
1:A:262:ARG:O	1:A:265:LYS:N	2.50	0.44
1:D:44:VAL:HG23	1:D:44:VAL:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:TYR:C	1:D:162:CYS:HB3	2.38	0.44
1:D:255:LEU:CD2	1:D:303:THR:HG23	2.42	0.44
1:A:257:TYR:HD1	1:B:309:ARG:HH22	1.64	0.44
1:C:285:LEU:HD12	1:C:319:PHE:HE2	1.82	0.44
1:C:11:TYR:O	1:C:12:PHE:C	2.56	0.44
1:C:12:PHE:HD1	1:C:12:PHE:C	2.18	0.44
1:A:193:VAL:O	1:A:247:ASP:HB2	2.16	0.44
1:C:201:ALA:HA	1:C:225:GLN:OE1	2.18	0.44
1:C:153:VAL:HG12	1:C:157:TYR:HE1	1.82	0.44
1:B:38:THR:HG22	1:B:81:VAL:O	2.17	0.44
1:B:33:TYR:CD1	1:B:320:ALA:HB3	2.53	0.44
1:C:37:VAL:HG13	1:C:57:GLY:HA2	1.99	0.44
1:A:73:LEU:HA	2:A:341:HOH:O	2.17	0.44
1:B:149:ARG:NE	2:B:350:HOH:O	2.50	0.44
1:D:237:ALA:O	1:D:240:ARG:N	2.49	0.44
1:D:26:VAL:HG12	1:D:27:SER:N	2.33	0.44
1:B:13:HIS:CE1	1:C:116:LEU:HD23	2.52	0.44
1:D:105:VAL:CG2	1:D:162:CYS:H	2.31	0.44
1:D:254:GLY:O	1:D:255:LEU:C	2.56	0.44
1:B:26:VAL:HG22	1:B:308:ARG:CG	2.47	0.44
1:D:42:ASP:O	1:D:43:ASP:HB2	2.18	0.44
1:B:267:LYS:HB3	1:B:268:HIS:ND1	2.32	0.44
1:A:276:TYR:O	1:A:278:VAL:N	2.50	0.44
1:D:24:SER:OG	1:D:305:THR:HG23	2.18	0.44
1:C:258:LEU:C	1:C:260:MET:N	2.71	0.44
1:D:119:CYS:O	1:D:165:VAL:HA	2.18	0.44
1:C:255:LEU:HD21	1:D:256:PRO:HA	1.99	0.44
1:C:170:MET:O	1:C:172:ASP:N	2.49	0.44
1:B:153:VAL:O	1:B:156:ALA:HB3	2.18	0.44
1:B:90:GLN:HG2	1:B:131:HIS:CE1	2.52	0.44
1:B:252:LYS:HG3	1:B:278:VAL:CG1	2.47	0.44
1:C:33:TYR:HE1	1:C:318:TYR:O	2.01	0.44
1:B:119:CYS:HB3	1:B:157:TYR:CD2	2.53	0.44
1:A:284:MET:HG3	1:B:294:PHE:HZ	1.82	0.44
1:A:233:LEU:HD11	1:B:11:TYR:CD1	2.52	0.44
1:C:260:MET:HE3	1:D:309:ARG:NE	2.26	0.44
1:A:259:ASP:HA	1:B:259:ASP:HA	1.99	0.44
1:D:155:LEU:C	1:D:155:LEU:HD23	2.38	0.44
1:A:8:HIS:CE1	1:B:171:MET:HA	2.53	0.44
1:D:290:GLN:C	1:D:292:GLY:H	2.21	0.44
1:D:251:VAL:HG23	1:D:273:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:TYR:HA	1:A:316:ILE:HB	2.00	0.44
1:D:47:ILE:HD11	1:D:55:ARG:HG3	1.99	0.44
1:D:74:ARG:O	1:D:116:LEU:N	2.50	0.43
1:A:242:ILE:HD12	1:A:242:ILE:O	2.18	0.43
1:D:199:LYS:HD3	1:D:252:LYS:HD3	1.99	0.43
1:B:40:VAL:O	1:B:41:PRO:O	2.36	0.43
1:B:42:ASP:HA	1:B:60:GLN:HE21	1.83	0.43
1:A:286:TRP:O	1:A:289:ALA:N	2.52	0.43
1:D:46:PRO:HA	1:D:54:ALA:CB	2.48	0.43
1:B:65:LEU:HD12	1:B:112:PHE:CE2	2.53	0.43
1:C:258:LEU:O	1:C:260:MET:N	2.52	0.43
1:B:40:VAL:CG1	1:B:43:ASP:HB3	2.45	0.43
1:B:85:VAL:CG1	1:B:86:PRO:HD2	2.48	0.43
1:B:49:SER:O	1:B:51:PRO:HD3	2.17	0.43
1:B:36:PHE:HB2	1:B:55:ARG:HA	2.01	0.43
1:A:55:ARG:NH2	1:A:211:ALA:HA	2.33	0.43
1:B:64:MET:HG3	1:B:65:LEU:CD2	2.49	0.43
1:C:305:THR:O	1:C:306:ALA:C	2.57	0.43
1:D:260:MET:O	1:D:264:VAL:HG13	2.19	0.43
1:C:202:SER:OG	1:D:302:GLU:OE1	2.32	0.43
1:A:257:TYR:HD1	1:B:309:ARG:CZ	2.31	0.43
1:C:325:LYS:C	1:C:327:LEU:N	2.72	0.43
1:B:155:LEU:HD23	1:B:156:ALA:N	2.34	0.43
1:B:231:ARG:O	1:B:234:ALA:HB3	2.18	0.43
1:B:294:PHE:CD1	1:B:299:ALA:HB2	2.54	0.43
1:D:209:ARG:C	1:D:211:ALA:H	2.21	0.43
1:B:168:SER:HB3	1:B:196:TYR:CD1	2.54	0.43
1:C:74:ARG:NH1	1:C:74:ARG:HB3	2.34	0.43
1:C:203:CYS:O	1:C:205:TYR:N	2.51	0.43
1:D:11:TYR:C	1:D:13:HIS:N	2.71	0.43
1:C:61:LEU:O	1:C:63:GLU:N	2.39	0.43
1:B:250:MET:HG2	1:B:251:VAL:H	1.84	0.43
1:B:301:LEU:O	1:B:304:MET:HB2	2.19	0.43
1:A:147:ARG:HD3	1:A:147:ARG:HA	1.82	0.43
1:D:167:PRO:HG2	1:D:178:ILE:HG13	1.99	0.43
1:A:265:LYS:CE	1:A:269:PRO:HA	2.49	0.43
1:A:279:SER:N	1:A:318:TYR:HE2	2.17	0.43
1:D:54:ALA:HB3	1:D:56:TYR:CE1	2.54	0.43
1:D:235:LEU:HD13	1:D:267:LYS:HD3	2.00	0.43
1:A:40:VAL:CG1	1:A:43:ASP:HB2	2.49	0.43
1:B:277:GLN:O	1:B:277:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ILE:CD1	1:C:316:ILE:HG12	2.47	0.43
1:A:55:ARG:NH2	1:A:212:ALA:N	2.65	0.43
1:A:249:LEU:CB	1:A:273:LEU:HD23	2.48	0.43
1:D:21:THR:O	1:D:21:THR:HG23	2.19	0.43
1:C:64:MET:C	1:C:64:MET:SD	2.97	0.43
1:B:55:ARG:HD3	1:B:211:ALA:O	2.19	0.43
1:A:118:ALA:HA	1:A:164:VAL:O	2.19	0.43
1:C:207:PRO:HG3	1:D:293:ALA:CB	2.47	0.43
1:B:254:GLY:O	1:B:257:TYR:N	2.41	0.43
1:A:289:ALA:C	1:A:291:ALA:N	2.63	0.43
1:C:81:VAL:HG21	1:C:211:ALA:O	2.19	0.42
1:D:158:ALA:N	1:D:162:CYS:HB3	2.34	0.42
1:A:255:LEU:HD12	1:A:258:LEU:HD22	2.00	0.42
1:C:11:TYR:C	1:C:13:HIS:H	2.22	0.42
1:C:170:MET:SD	1:C:174:ARG:NH2	2.92	0.42
1:B:295:ASP:OD2	1:B:295:ASP:C	2.58	0.42
1:A:62:GLU:O	1:A:62:GLU:HG3	2.19	0.42
1:B:12:PHE:CE2	1:B:16:LEU:HD23	2.53	0.42
1:B:176:GLU:O	1:B:180:ALA:HB2	2.19	0.42
1:B:47:ILE:HD11	1:B:55:ARG:NE	2.34	0.42
1:C:73:LEU:HD21	1:C:76:VAL:CG1	2.49	0.42
1:D:122:CYS:C	1:D:123:LEU:HG	2.40	0.42
1:D:19:TRP:C	1:D:21:THR:N	2.71	0.42
1:A:300:VAL:C	1:A:302:GLU:N	2.72	0.42
1:A:11:TYR:O	1:A:12:PHE:CD2	2.72	0.42
1:C:257:TYR:CD1	1:D:309:ARG:NH2	2.87	0.42
1:D:117:VAL:HB	1:D:163:GLN:H	1.84	0.42
1:D:276:TYR:CD2	1:D:316:ILE:HG21	2.55	0.42
1:D:35:ILE:HD13	1:D:77:LEU:O	2.19	0.42
1:B:250:MET:HG2	1:B:251:VAL:N	2.34	0.42
1:C:41:PRO:O	1:C:57:GLY:HA3	2.18	0.42
1:A:50:LEU:HB3	1:A:53:VAL:HB	2.00	0.42
1:A:65:LEU:C	1:A:67:PRO:HD2	2.38	0.42
1:A:251:VAL:O	1:A:275:VAL:HA	2.19	0.42
1:A:232:GLY:C	1:A:234:ALA:N	2.73	0.42
1:D:276:TYR:CD1	1:D:276:TYR:C	2.92	0.42
1:B:309:ARG:O	1:B:309:ARG:HG2	2.18	0.42
1:A:176:GLU:HB2	1:A:244:GLU:HB3	2.02	0.42
1:D:99:SER:HB3	1:D:102:ILE:CG1	2.48	0.42
1:D:286:TRP:C	1:D:288:GLY:N	2.72	0.42
1:D:58:VAL:HG21	1:D:103:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:PRO:O	1:D:228:PRO:O	2.38	0.42
1:D:259:ASP:CG	1:D:260:MET:H	2.23	0.42
1:B:177:ALA:HA	1:B:180:ALA:HB3	2.00	0.42
1:A:255:LEU:HG	1:B:255:LEU:CD1	2.49	0.42
1:C:102:ILE:HA	1:C:105:VAL:CG1	2.49	0.42
1:C:286:TRP:C	1:C:288:GLY:N	2.73	0.42
1:B:123:LEU:HD23	1:B:130:GLY:N	2.31	0.42
1:C:265:LYS:HD2	1:C:311:GLY:HA2	2.02	0.42
1:B:41:PRO:O	1:B:42:ASP:C	2.55	0.42
1:C:33:TYR:CD1	1:C:321:PRO:HD3	2.55	0.42
1:B:50:LEU:O	1:B:51:PRO:C	2.57	0.42
1:A:277:GLN:HE22	1:A:319:PHE:HD2	1.67	0.42
1:D:232:GLY:O	1:D:233:LEU:C	2.57	0.42
1:A:174:ARG:HG2	1:A:174:ARG:HH11	1.85	0.42
1:D:116:LEU:HD11	1:D:164:VAL:HG21	2.00	0.42
1:B:38:THR:OG1	1:B:45:GLN:NE2	2.53	0.42
1:B:262:ARG:NH2	1:B:309:ARG:O	2.52	0.42
1:C:74:ARG:O	1:C:115:LEU:HD12	2.20	0.42
1:D:167:PRO:HB3	1:D:174:ARG:HD2	2.01	0.42
1:B:33:TYR:CD1	1:B:321:PRO:HD3	2.55	0.42
1:B:46:PRO:HA	1:B:54:ALA:HB2	1.99	0.42
1:D:155:LEU:HD23	1:D:159:LYS:HG3	2.01	0.42
1:C:38:THR:HG23	1:C:55:ARG:CB	2.48	0.42
1:A:170:MET:HE3	1:A:174:ARG:NH2	2.34	0.42
1:D:120:ASP:OD1	1:D:121:VAL:N	2.53	0.42
1:A:226:LEU:N	1:A:226:LEU:HD12	2.35	0.42
1:B:237:ALA:O	1:B:240:ARG:N	2.52	0.42
1:C:149:ARG:C	1:C:151:ALA:N	2.73	0.42
1:C:282:PHE:CD1	1:C:282:PHE:C	2.93	0.42
1:C:8:HIS:C	1:C:10:GLY:H	2.23	0.42
1:D:176:GLU:HB2	1:D:244:GLU:CG	2.47	0.42
1:C:207:PRO:HD3	1:D:293:ALA:O	2.20	0.42
1:C:147:ARG:HE	1:C:173:GLY:CA	2.32	0.42
1:A:197:SER:HB3	1:A:238:VAL:HG22	2.02	0.42
1:C:61:LEU:HD23	1:C:108:LEU:HD21	2.02	0.42
1:A:147:ARG:CA	1:A:147:ARG:NE	2.83	0.42
1:D:19:TRP:O	1:D:21:THR:N	2.52	0.42
1:A:193:VAL:N	1:A:247:ASP:OD2	2.45	0.42
1:C:255:LEU:CD2	1:D:255:LEU:HD12	2.47	0.42
1:D:13:HIS:O	1:D:17:ARG:HG3	2.20	0.42
1:D:266:ASP:C	1:D:268:HIS:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LEU:HD12	1:B:324:LEU:HD11	2.02	0.42
1:B:200:PHE:HE1	1:B:257:TYR:HB3	1.85	0.42
1:C:258:LEU:C	1:C:260:MET:H	2.22	0.41
1:D:166:ALA:O	1:D:196:TYR:CE1	2.73	0.41
1:D:78:ILE:CG2	1:D:79:PHE:N	2.83	0.41
1:C:151:ALA:O	1:C:153:VAL:N	2.52	0.41
1:C:121:VAL:HB	1:C:167:PRO:HA	2.00	0.41
1:C:289:ALA:O	1:C:291:ALA:N	2.46	0.41
1:D:44:VAL:O	1:D:46:PRO:HD3	2.20	0.41
1:B:209:ARG:HH12	1:B:221:ARG:HH22	1.68	0.41
1:B:16:LEU:HD12	1:B:16:LEU:HA	1.91	0.41
1:C:258:LEU:HB3	1:D:259:ASP:H	1.85	0.41
1:A:195:SER:O	1:A:197:SER:N	2.53	0.41
1:D:253:PRO:HA	1:D:278:VAL:HG13	2.01	0.41
1:D:77:LEU:HD12	1:D:316:ILE:HD13	2.02	0.41
1:B:226:LEU:HA	1:B:227:PRO:HD2	1.93	0.41
1:B:74:ARG:HB3	1:C:15:LEU:HD22	2.02	0.41
1:C:175:VAL:HG22	1:C:195:SER:HB2	2.02	0.41
1:A:47:ILE:C	1:A:49:SER:H	2.23	0.41
1:A:151:ALA:HB2	1:A:178:ILE:HD12	2.02	0.41
1:B:77:LEU:HD23	1:B:118:ALA:O	2.20	0.41
1:B:90:GLN:HA	1:B:131:HIS:CE1	2.55	0.41
1:A:295:ASP:OD2	1:A:296:LEU:N	2.53	0.41
1:D:33:TYR:HA	1:D:34:PRO:HD3	1.75	0.41
1:C:233:LEU:HD11	1:D:11:TYR:CD1	2.55	0.41
1:A:252:LYS:HA	1:A:253:PRO:C	2.40	0.41
1:C:34:PRO:HG2	1:C:318:TYR:CD1	2.55	0.41
1:D:36:PHE:HB2	1:D:55:ARG:HA	2.02	0.41
1:D:120:ASP:CG	1:D:121:VAL:N	2.73	0.41
1:D:70:GLU:C	1:D:72:GLY:N	2.74	0.41
1:B:296:LEU:HG	1:B:300:VAL:HG21	2.02	0.41
1:A:35:ILE:H	1:A:35:ILE:HD13	1.83	0.41
1:C:20:GLN:HE21	1:D:233:LEU:CD1	2.34	0.41
1:D:171:MET:O	1:D:172:ASP:C	2.57	0.41
1:C:80:GLY:HA3	1:C:101:THR:HG23	2.02	0.41
1:C:228:PRO:HD3	2:C:340:HOH:O	2.20	0.41
1:C:44:VAL:HG12	1:C:44:VAL:O	2.20	0.41
1:B:199:LYS:HZ1	1:B:252:LYS:HZ1	1.67	0.41
1:A:326:TRP:O	1:A:328:LYS:N	2.53	0.41
1:D:75:CYS:SG	1:D:76:VAL:N	2.94	0.41
1:B:255:LEU:O	1:B:255:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:PRO:N	1:D:17:ARG:NH1	2.68	0.41
1:C:33:TYR:CE1	1:C:318:TYR:O	2.73	0.41
1:C:323:LEU:C	1:C:325:LYS:N	2.72	0.41
1:A:143:SER:C	1:A:145:GLU:H	2.22	0.41
1:D:270:GLU:HG2	1:D:270:GLU:H	1.69	0.41
1:B:62:GLU:HB2	1:B:111:THR:HG21	2.01	0.41
1:D:117:VAL:HB	1:D:163:GLN:HB2	2.02	0.41
1:D:39:ASP:OD1	1:D:39:ASP:N	2.53	0.41
1:B:42:ASP:O	1:B:43:ASP:HB2	2.21	0.41
1:C:73:LEU:HD21	1:C:76:VAL:HG13	2.03	0.41
1:B:323:LEU:O	1:B:326:TRP:N	2.52	0.41
1:B:231:ARG:HG3	1:B:260:MET:CE	2.48	0.41
1:D:308:ARG:C	1:D:310:ALA:N	2.72	0.41
1:C:262:ARG:NH2	1:C:309:ARG:O	2.53	0.41
1:C:157:TYR:O	1:C:160:ALA:HB3	2.20	0.41
1:A:102:ILE:O	1:A:105:VAL:N	2.54	0.41
1:A:152:GLU:HG3	1:A:153:VAL:N	2.35	0.41
1:A:199:LYS:HE2	1:A:252:LYS:NZ	2.32	0.41
1:D:221:ARG:C	1:D:223:CYS:H	2.24	0.41
1:B:129:HIS:CE1	2:B:342:HOH:O	2.74	0.41
1:C:197:SER:HB2	1:C:198:ALA:H	1.58	0.41
1:A:17:ARG:HD3	1:B:222:ARG:O	2.21	0.41
1:A:15:LEU:O	1:A:18:SER:N	2.54	0.41
1:A:112:PHE:HA	1:A:113:PRO:HD2	1.95	0.41
1:A:77:LEU:HD23	1:A:77:LEU:C	2.41	0.41
1:C:112:PHE:HA	1:C:113:PRO:HD2	1.88	0.41
1:C:205:TYR:O	1:C:206:GLY:C	2.59	0.41
1:C:273:LEU:HD12	1:C:312:ALA:CA	2.51	0.41
1:C:315:ILE:HD12	1:C:315:ILE:N	2.36	0.41
1:A:197:SER:HB2	1:A:250:MET:O	2.21	0.41
1:D:255:LEU:N	1:D:256:PRO:CD	2.84	0.41
1:D:20:GLN:HA	1:D:20:GLN:OE1	2.21	0.41
1:B:308:ARG:NE	1:B:308:ARG:HA	2.33	0.41
1:A:147:ARG:NH1	1:A:171:MET:HB2	2.36	0.41
1:C:319:PHE:O	1:C:322:GLN:HG2	2.21	0.41
1:C:325:LYS:O	1:C:327:LEU:N	2.53	0.41
1:C:73:LEU:HD12	1:C:74:ARG:H	1.85	0.41
1:C:8:HIS:HA	1:C:11:TYR:CE1	2.56	0.41
1:C:171:MET:O	1:C:172:ASP:C	2.59	0.41
1:C:174:ARG:HG3	1:C:175:VAL:H	1.86	0.41
1:B:207:PRO:HB2	1:B:279:SER:CB	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:LEU:HD23	1:B:326:TRP:CH2	2.54	0.41
1:A:33:TYR:HB2	1:A:320:ALA:HB2	2.00	0.41
1:B:122:CYS:O	1:B:123:LEU:HD13	2.21	0.41
1:A:15:LEU:O	1:A:16:LEU:C	2.59	0.41
1:D:175:VAL:HG23	2:D:336:HOH:O	2.20	0.41
1:D:156:ALA:O	1:D:157:TYR:C	2.59	0.41
1:D:161:GLY:O	1:D:162:CYS:C	2.58	0.41
1:D:13:HIS:CE1	1:D:15:LEU:H	2.38	0.41
1:A:84:ARG:HH21	1:A:84:ARG:CB	2.23	0.41
1:A:32:ILE:HD13	1:A:314:ILE:CG2	2.45	0.41
1:D:57:GLY:O	1:D:61:LEU:HB2	2.21	0.41
1:C:238:VAL:CG1	1:C:249:LEU:HD13	2.51	0.41
1:D:97:GLU:HG2	1:D:98:ASP:OD2	2.21	0.41
1:D:193:VAL:O	1:D:195:SER:N	2.49	0.41
1:C:273:LEU:HD13	1:C:273:LEU:C	2.42	0.40
1:D:264:VAL:HG23	1:D:265:LYS:N	2.37	0.40
1:D:32:ILE:HB	1:D:316:ILE:HG12	2.01	0.40
1:B:38:THR:HG22	1:B:81:VAL:HB	2.02	0.40
1:B:38:THR:CG2	1:B:45:GLN:HE22	2.29	0.40
1:A:319:PHE:O	1:A:320:ALA:C	2.59	0.40
1:B:192:SER:HA	1:B:247:ASP:OD2	2.21	0.40
1:B:13:HIS:CD2	1:C:116:LEU:HD23	2.57	0.40
1:D:205:TYR:HE1	1:D:252:LYS:CE	2.30	0.40
1:D:221:ARG:HA	1:D:224:TYR:OH	2.21	0.40
1:C:322:GLN:O	1:C:325:LYS:HB3	2.21	0.40
1:D:325:LYS:NZ	1:D:325:LYS:HB2	2.36	0.40
1:B:323:LEU:O	1:B:327:LEU:HD13	2.20	0.40
1:A:166:ALA:CB	1:A:194:MET:O	2.69	0.40
1:B:205:TYR:OH	1:B:253:PRO:HD3	2.22	0.40
1:A:57:GLY:O	1:A:60:GLN:N	2.55	0.40
1:A:124:CYS:HA	1:A:125:PRO:HD2	1.98	0.40
1:C:261:VAL:HG13	1:C:273:LEU:HD11	2.03	0.40
1:D:149:ARG:C	1:D:151:ALA:N	2.74	0.40
1:D:33:TYR:HE1	1:D:318:TYR:O	2.04	0.40
1:C:47:ILE:CD1	1:C:54:ALA:HA	2.52	0.40
1:C:323:LEU:HA	1:C:326:TRP:HE3	1.86	0.40
1:B:179:LYS:HD3	1:B:193:VAL:HG21	2.02	0.40
1:D:225:GLN:O	1:D:226:LEU:O	2.39	0.40
1:D:214:SER:O	1:D:215:SER:HB3	2.20	0.40
1:C:194:MET:HG3	1:C:248:MET:HG3	2.03	0.40
1:B:15:LEU:O	1:B:16:LEU:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:VAL:O	1:D:109:ARG:HB2	2.22	0.40
1:C:95:ASP:HB3	1:C:153:VAL:HA	2.04	0.40
1:D:147:ARG:O	1:D:148:GLN:C	2.60	0.40
1:D:285:LEU:HD12	1:D:319:PHE:HE2	1.86	0.40
1:D:122:CYS:SG	1:D:123:LEU:N	2.93	0.40
1:B:153:VAL:HG12	1:B:157:TYR:CE1	2.57	0.40
1:C:238:VAL:HG11	1:C:249:LEU:HD13	2.02	0.40
1:A:66:ARG:NH1	1:A:66:ARG:HG2	2.35	0.40
1:A:304:MET:O	1:A:306:ALA:N	2.54	0.40
1:D:186:GLY:O	1:D:188:GLY:N	2.54	0.40
1:B:84:ARG:HG3	1:B:84:ARG:O	2.21	0.40
1:C:306:ALA:CB	1:C:309:ARG:HH22	2.35	0.40
1:A:234:ALA:C	1:A:236:ARG:N	2.75	0.40
1:D:166:ALA:O	1:D:196:TYR:HE1	2.04	0.40
1:B:75:CYS:SG	1:B:76:VAL:N	2.95	0.40
1:B:27:SER:C	1:B:29:SER:H	2.24	0.40
1:D:110:LYS:CA	1:D:110:LYS:CE	2.99	0.40
1:C:43:ASP:O	1:C:44:VAL:HG23	2.22	0.40
1:B:37:VAL:HA	1:B:56:TYR:O	2.21	0.40
1:B:282:PHE:O	1:B:283:ALA:C	2.60	0.40
1:A:177:ALA:O	1:A:180:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	282/330 (86%)	196 (70%)	68 (24%)	18 (6%)	2 13
1	B	316/330 (96%)	203 (64%)	80 (25%)	33 (10%)	1 4
1	C	280/330 (85%)	179 (64%)	60 (21%)	41 (15%)	0 1
1	D	290/330 (88%)	178 (61%)	79 (27%)	33 (11%)	0 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1168/1320 (88%)	756 (65%)	287 (25%)	125 (11%)	0 4

All (125) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	VAL
1	A	226	LEU
1	A	278	VAL
1	A	290	GLN
1	B	12	PHE
1	B	41	PRO
1	B	42	ASP
1	B	58	VAL
1	B	59	ASN
1	B	86	PRO
1	B	92	SER
1	B	134	LEU
1	B	220	ASP
1	B	225	GLN
1	B	226	LEU
1	B	246	ALA
1	B	298	THR
1	C	5	SER
1	C	12	PHE
1	C	24	SER
1	C	39	ASP
1	C	42	ASP
1	C	58	VAL
1	C	73	LEU
1	C	82	PRO
1	C	122	CYS
1	C	206	GLY
1	C	293	ALA
1	C	311	GLY
1	C	312	ALA
1	D	12	PHE
1	D	41	PRO
1	D	42	ASP
1	D	58	VAL
1	D	115	LEU
1	D	228	PRO
1	A	82	PRO

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Mol	Chain	Res	Type
1	A	197	SER
1	A	264	VAL
1	A	275	VAL
1	B	43	ASP
1	B	88	ASP
1	B	147	ARG
1	B	211	ALA
1	C	41	PRO
1	C	44	VAL
1	C	59	ASN
1	C	83	SER
1	C	154	ALA
1	C	172	ASP
1	C	186	GLY
1	C	204	PHE
1	C	278	VAL
1	D	5	SER
1	D	20	GLN
1	D	21	THR
1	D	59	ASN
1	D	143	SER
1	D	162	CYS
1	D	187	LEU
1	D	197	SER
1	D	226	LEU
1	D	229	GLY
1	D	232	GLY
1	D	267	LYS
1	D	293	ALA
1	D	324	LEU
1	A	209	ARG
1	B	8	HIS
1	B	56	TYR
1	B	60	GLN
1	B	130	GLY
1	B	133	GLY
1	B	136	SER
1	B	278	VAL
1	B	294	PHE
1	B	309	ARG
1	C	9	SER
1	C	150	LEU

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Mol	Chain	Res	Type
1	C	170	MET
1	C	184	LYS
1	C	228	PRO
1	C	324	LEU
1	D	194	MET
1	D	234	ALA
1	A	8	HIS
1	B	9	SER
1	B	154	ALA
1	C	30	ASN
1	C	270	GLU
1	C	290	GLN
1	C	307	PHE
1	C	320	ALA
1	C	321	PRO
1	D	213	GLN
1	D	292	GLY
1	A	41	PRO
1	A	83	SER
1	A	286	TRP
1	A	327	LEU
1	B	105	VAL
1	B	322	GLN
1	C	62	GLU
1	C	259	ASP
1	C	326	TRP
1	D	43	ASP
1	D	108	LEU
1	D	172	ASP
1	D	236	ARG
1	D	282	PHE
1	A	12	PHE
1	B	125	PRO
1	C	162	CYS
1	C	171	MET
1	C	210	ASP
1	D	269	PRO
1	A	113	PRO
1	B	188	GLY
1	A	102	ILE
1	D	153	VAL
1	B	242	ILE

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Mol	Chain	Res	Type
1	D	14	PRO
1	A	321	PRO
1	D	215	SER
1	C	253	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	235/267 (88%)	214 (91%)	21 (9%)	12	43
1	B	258/267 (97%)	235 (91%)	23 (9%)	12	43
1	C	233/267 (87%)	216 (93%)	17 (7%)	17	53
1	D	239/267 (90%)	219 (92%)	20 (8%)	14	46
All	All	965/1068 (90%)	884 (92%)	81 (8%)	14	46

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	35	ILE
1	A	56	TYR
1	A	62	GLU
1	A	64	MET
1	A	74	ARG
1	A	84	ARG
1	A	105	VAL
1	A	116	LEU
1	A	123	LEU
1	A	145	GLU
1	A	147	ARG
1	A	224	TYR
1	A	240	ARG
1	A	242	ILE
1	A	248	MET
1	A	260	MET

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Mol	Chain	Res	Type
1	A	265	LYS
1	A	276	TYR
1	A	314	ILE
1	A	324	LEU
1	B	11	TYR
1	B	16	LEU
1	B	39	ASP
1	B	42	ASP
1	B	62	GLU
1	B	64	MET
1	B	66	ARG
1	B	74	ARG
1	B	77	LEU
1	B	110	LYS
1	B	116	LEU
1	B	155	LEU
1	B	189	ASN
1	B	190	ARG
1	B	231	ARG
1	B	248	MET
1	B	255	LEU
1	B	260	MET
1	B	276	TYR
1	B	308	ARG
1	B	323	LEU
1	B	325	LYS
1	B	326	TRP
1	C	11	TYR
1	C	12	PHE
1	C	39	ASP
1	C	43	ASP
1	C	75	CYS
1	C	84	ARG
1	C	157	TYR
1	C	197	SER
1	C	200	PHE
1	C	210	ASP
1	C	224	TYR
1	C	242	ILE
1	C	265	LYS
1	C	290	GLN
1	C	308	ARG

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Mol	Chain	Res	Type
1	C	314	ILE
1	C	322	GLN
1	D	35	ILE
1	D	39	ASP
1	D	42	ASP
1	D	56	TYR
1	D	79	PHE
1	D	110	LYS
1	D	119	CYS
1	D	120	ASP
1	D	157	TYR
1	D	220	ASP
1	D	242	ILE
1	D	248	MET
1	D	249	LEU
1	D	255	LEU
1	D	260	MET
1	D	269	PRO
1	D	273	LEU
1	D	282	PHE
1	D	308	ARG
1	D	325	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	60	GLN
1	A	277	GLN
1	B	8	HIS
1	B	30	ASN
1	B	45	GLN
1	B	59	ASN
1	B	60	GLN
1	B	131	HIS
1	C	60	GLN
1	C	277	GLN
1	D	59	ASN
1	D	60	GLN
1	D	148	GLN
1	D	185	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	290/330 (87%)	-0.06	2 (0%)	89	86	25, 54, 106, 135	0
1	B	320/330 (96%)	-0.06	4 (1%)	79	74	24, 56, 101, 127	0
1	C	288/330 (87%)	0.22	18 (6%)	23	19	36, 80, 126, 148	0
1	D	296/330 (89%)	0.21	10 (3%)	49	42	34, 83, 130, 143	0
All	All	1194/1320 (90%)	0.07	34 (2%)	56	50	24, 66, 120, 148	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	96	SER	6.3
1	C	95	ASP	5.2
1	C	38	THR	4.6
1	B	131	HIS	4.0
1	C	169	ASP	3.9
1	D	42	ASP	3.7
1	C	61	LEU	3.7
1	A	96	SER	3.5
1	D	82	PRO	3.1
1	C	37	VAL	3.1
1	C	73	LEU	3.0
1	A	187	LEU	3.0
1	C	100	PRO	2.9
1	C	40	VAL	2.8
1	B	178	ILE	2.8
1	B	98	ASP	2.7
1	D	84	ARG	2.6
1	D	39	ASP	2.5
1	C	82	PRO	2.4
1	C	36	PHE	2.4
1	B	100	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	12	PHE	2.3
1	C	175	VAL	2.3
1	C	212	ALA	2.3
1	D	216	PRO	2.3
1	D	188	GLY	2.3
1	C	35	ILE	2.2
1	C	145	GLU	2.2
1	D	105	VAL	2.2
1	C	84	ARG	2.2
1	C	72	GLY	2.1
1	D	149	ARG	2.1
1	D	81	VAL	2.1
1	C	39	ASP	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.