Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:11 AM GMT

PDB ID	:	2ZV6
Title	:	Crystal structure of human squamous cell carcinoma antigen 1
Authors	:	Zheng, B.; Matoba, Y.; Katagiri, C.; Hibino, T.; Sugiyama, M.
Deposited on	:	2008-11-01
Resolution	:	2.70 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:

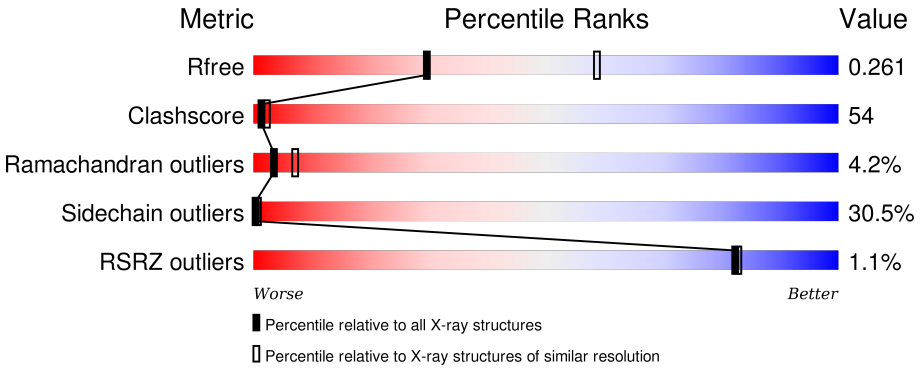
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	401	% 21% 48% 17% • 13%
1	B	401	19% 49% 22% • 7%
1	C	401	% 19% 51% 17% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9041 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 Serpin B3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2866	1838	476	541	11			
1	B	371	Total	C	N	O	S	0	0	0
			2999	1918	497	573	11			
1	C	350	Total	C	N	O	S	0	0	0
			2864	1837	475	541	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	INITIATING METHIONINE	UNP P29508
A	-9	ARG	-	EXPRESSION TAG	UNP P29508
A	-8	GLY	-	EXPRESSION TAG	UNP P29508
A	-7	SER	-	EXPRESSION TAG	UNP P29508
A	-6	HIS	-	EXPRESSION TAG	UNP P29508
A	-5	HIS	-	EXPRESSION TAG	UNP P29508
A	-4	HIS	-	EXPRESSION TAG	UNP P29508
A	-3	HIS	-	EXPRESSION TAG	UNP P29508
A	-2	HIS	-	EXPRESSION TAG	UNP P29508
A	-1	HIS	-	EXPRESSION TAG	UNP P29508
A	0	GLY	-	EXPRESSION TAG	UNP P29508
A	1	SER	-	EXPRESSION TAG	UNP P29508
B	-10	MET	-	INITIATING METHIONINE	UNP P29508
B	-9	ARG	-	EXPRESSION TAG	UNP P29508
B	-8	GLY	-	EXPRESSION TAG	UNP P29508
B	-7	SER	-	EXPRESSION TAG	UNP P29508
B	-6	HIS	-	EXPRESSION TAG	UNP P29508
B	-5	HIS	-	EXPRESSION TAG	UNP P29508
B	-4	HIS	-	EXPRESSION TAG	UNP P29508
B	-3	HIS	-	EXPRESSION TAG	UNP P29508
B	-2	HIS	-	EXPRESSION TAG	UNP P29508
B	-1	HIS	-	EXPRESSION TAG	UNP P29508
B	0	GLY	-	EXPRESSION TAG	UNP P29508

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1	SER	-	EXPRESSION TAG	UNP P29508
C	-10	MET	-	INITIATING METHIONINE	UNP P29508
C	-9	ARG	-	EXPRESSION TAG	UNP P29508
C	-8	GLY	-	EXPRESSION TAG	UNP P29508
C	-7	SER	-	EXPRESSION TAG	UNP P29508
C	-6	HIS	-	EXPRESSION TAG	UNP P29508
C	-5	HIS	-	EXPRESSION TAG	UNP P29508
C	-4	HIS	-	EXPRESSION TAG	UNP P29508
C	-3	HIS	-	EXPRESSION TAG	UNP P29508
C	-2	HIS	-	EXPRESSION TAG	UNP P29508
C	-1	HIS	-	EXPRESSION TAG	UNP P29508
C	0	GLY	-	EXPRESSION TAG	UNP P29508
C	1	SER	-	EXPRESSION TAG	UNP P29508

- Molecule 2 is water.

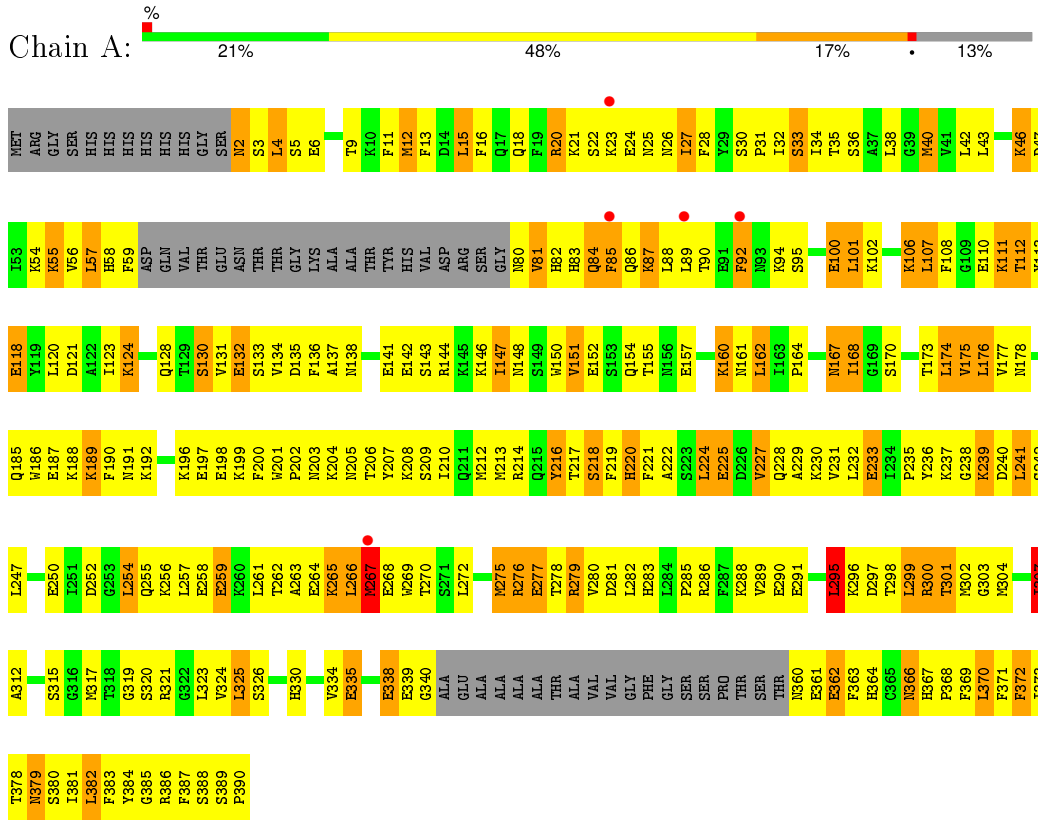
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	124	Total O 124 124	0	0
2	B	107	Total O 107 107	0	0
2	C	81	Total O 81 81	0	0

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.

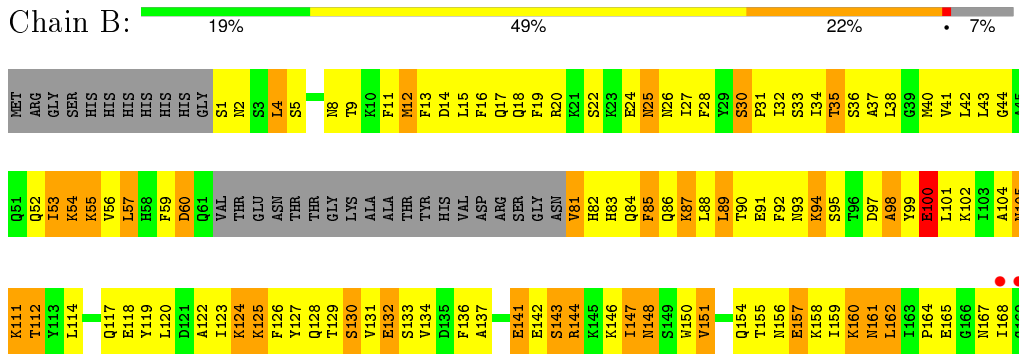
- Molecule 1: Serpin B3

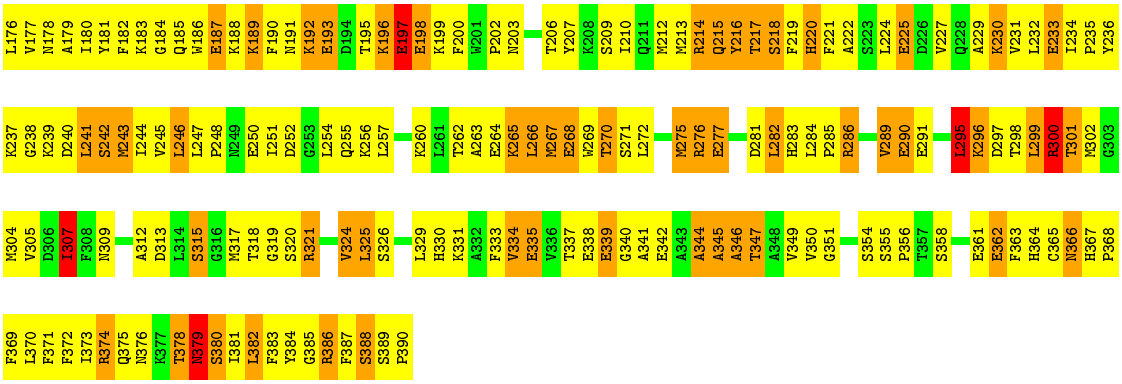
Chain A:



- Molecule 1: Serpin B3

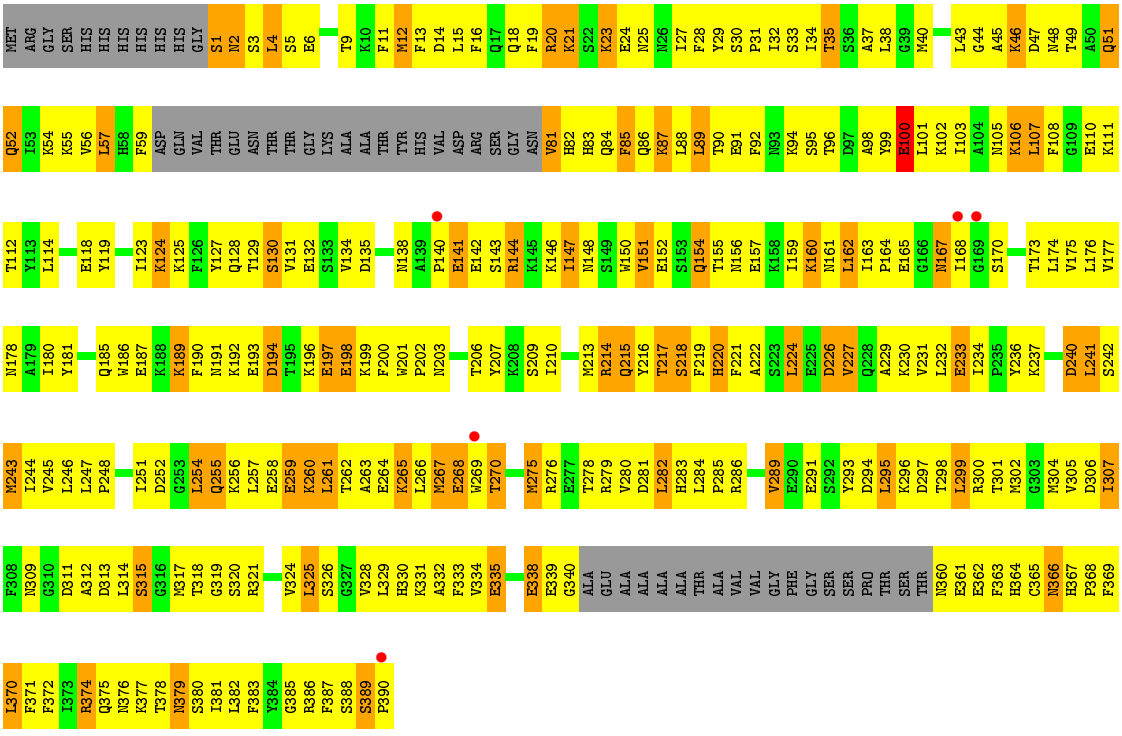
Chain B:





• Molecule 1: Serpin B3

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	263.48Å 263.48Å 48.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.70 49.79 – 2.70	Depositor EDS
% Data completeness (in resolution range)	76.3 (30.00-2.70) 84.5 (49.79-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.190 , 0.270 0.201 , 0.261	Depositor DCC
R_{free} test set	1431 reflections (4.90%)	DCC
Wilson B-factor (Å^2)	54.4	Xtriage
Anisotropy	0.625	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 100.3	EDS
Estimated twinning fraction	0.013 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 29220 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9041	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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	0.41	0/2925	0.60	0/3931
1	B	0.41	0/3061	0.61	0/4120
1	C	0.40	0/2923	0.57	0/3928
All	All	0.41	0/8909	0.59	0/11979

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	2866	0	2844	297	0
1	B	2999	0	2971	340	0
1	C	2864	0	2846	303	0
2	A	124	0	0	6	0
2	B	107	0	0	1	0
2	C	81	0	0	2	0
All	All	9041	0	8661	937	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 54.

All (937) 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:B:307:ILE:H	1:B:307:ILE:HD12	1.06	1.18
1:A:222:ALA:HB2	1:A:275:MET:HG3	1.40	1.04
1:C:38:LEU:HD12	1:C:57:LEU:HD11	1.39	1.01
1:C:16:PHE:HE1	1:C:27:ILE:HD11	1.19	1.01
1:B:222:ALA:HB2	1:B:275:MET:HG3	1.43	0.99
1:C:312:ALA:HB3	1:C:324:VAL:HG12	1.45	0.99
1:C:307:ILE:HD13	1:C:307:ILE:H	1.27	0.98
1:B:366:ASN:HD22	1:B:366:ASN:N	1.60	0.97
1:B:222:ALA:HB3	1:B:231:VAL:HG13	1.47	0.96
1:B:244:ILE:HD11	1:B:374:ARG:CZ	1.95	0.95
1:C:92:PHE:HB3	1:C:101:LEU:HD21	1.43	0.95
1:B:366:ASN:H	1:B:366:ASN:ND2	1.59	0.94
1:A:15:LEU:HA	1:A:302:MET:HE1	1.49	0.94
1:B:298:THR:O	1:B:302:MET:HG3	1.68	0.93
1:A:110:GLU:HG2	1:A:136:PHE:HB2	1.49	0.93
1:B:307:ILE:H	1:B:307:ILE:CD1	1.82	0.91
1:C:102:LYS:HB3	1:C:155:THR:HA	1.53	0.90
1:C:282:LEU:HD11	1:C:284:LEU:HB2	1.54	0.90
1:B:289:VAL:HG23	1:B:334:VAL:HG12	1.55	0.88
1:B:92:PHE:HB3	1:B:101:LEU:HD21	1.56	0.87
1:C:298:THR:O	1:C:302:MET:HG3	1.75	0.87
1:C:222:ALA:HB2	1:C:275:MET:HG3	1.56	0.87
1:B:100:GLU:O	1:B:100:GLU:HG3	1.75	0.86
1:A:381:ILE:H	1:A:381:ILE:HD12	1.40	0.86
1:C:28:PHE:H	1:C:291:GLU:HG3	1.40	0.86
1:C:264:GLU:H	1:C:264:GLU:CD	1.79	0.86
1:C:196:LYS:H	1:C:214:ARG:HH22	1.24	0.86
1:A:81:VAL:HG13	1:A:82:HIS:H	1.40	0.85
1:B:222:ALA:HB3	1:B:231:VAL:CG1	2.06	0.85
1:B:104:ALA:HB3	1:B:179:ALA:HB3	1.58	0.85
1:A:204:LYS:HE2	1:C:55:LYS:HD2	1.59	0.85
1:C:84:GLN:HG3	1:C:87:LYS:NZ	1.91	0.85
1:B:307:ILE:N	1:B:307:ILE:HD12	1.92	0.84
1:B:367:HIS:HB2	1:B:368:PRO:HD2	1.58	0.84
1:A:244:ILE:HG21	1:A:270:THR:HG22	1.59	0.84
1:A:5:SER:O	1:A:9:THR:HG23	1.79	0.82
1:C:381:ILE:HD12	1:C:381:ILE:H	1.43	0.82
1:B:27:ILE:HG12	1:B:386:ARG:HG2	1.62	0.82
1:C:240:ASP:HB3	2:C:426:HOH:O	1.77	0.82
1:C:366:ASN:ND2	1:C:366:ASN:H	1.77	0.82
1:C:196:LYS:H	1:C:214:ARG:NH2	1.76	0.82
1:C:44:GLY:HA3	1:C:317:MET:HG3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:CD1	1:B:130:SER:HA	2.10	0.82
1:C:366:ASN:H	1:C:366:ASN:HD22	1.26	0.81
1:A:307:ILE:HD13	1:A:307:ILE:H	1.43	0.81
1:A:280:VAL:HA	1:A:361:GLU:O	1.79	0.81
1:C:16:PHE:CE1	1:C:27:ILE:HD11	2.10	0.81
1:C:387:PHE:HZ	1:C:390:PRO:HB3	1.45	0.81
1:B:35:THR:HB	1:B:85:PHE:HZ	1.44	0.81
1:C:5:SER:O	1:C:9:THR:HG23	1.81	0.81
1:B:37:ALA:HB1	1:B:176:LEU:HD11	1.62	0.80
1:B:196:LYS:H	1:B:196:LYS:HD3	1.45	0.80
1:C:100:GLU:HG3	1:C:100:GLU:O	1.78	0.80
1:C:106:LYS:HB3	1:C:108:PHE:HE1	1.46	0.80
1:B:295:LEU:O	1:B:299:LEU:HB2	1.82	0.79
1:C:2:ASN:H	1:C:2:ASN:ND2	1.76	0.79
1:C:210:ILE:HD12	1:C:285:PRO:HB3	1.61	0.79
1:C:91:GLU:O	1:C:94:LYS:HB3	1.83	0.79
1:A:282:LEU:HD12	1:A:283:HIS:N	1.97	0.79
1:C:34:ILE:HA	1:C:178:ASN:ND2	1.98	0.78
1:B:123:ILE:HD11	1:B:130:SER:HA	1.66	0.78
1:C:20:ARG:CZ	1:C:258:GLU:HB3	2.13	0.78
1:A:312:ALA:HB3	1:A:324:VAL:HG22	1.65	0.77
1:C:106:LYS:HB3	1:C:108:PHE:CE1	2.19	0.77
1:B:220:HIS:HA	1:B:276:ARG:O	1.83	0.77
1:A:9:THR:HG22	1:A:381:ILE:HD13	1.64	0.77
1:A:198:GLU:HG3	1:A:199:LYS:H	1.48	0.77
1:B:386:ARG:HG3	1:B:386:ARG:O	1.84	0.77
1:B:1:SER:OG	1:B:88:LEU:HD21	1.84	0.77
1:B:189:LYS:HG2	1:B:190:PHE:H	1.48	0.77
1:B:289:VAL:HG23	1:B:334:VAL:CG1	2.13	0.77
1:C:84:GLN:HG3	1:C:87:LYS:HZ2	1.50	0.77
1:A:247:LEU:HD21	1:A:364:HIS:O	1.85	0.76
1:A:186:TRP:HH2	1:A:243:MET:HG2	1.50	0.76
1:A:80:ASN:ND2	1:A:81:VAL:HG12	2.00	0.76
1:A:57:LEU:HB3	1:A:59:PHE:CZ	2.21	0.75
1:B:43:LEU:HD12	1:B:123:ILE:HG22	1.67	0.75
1:A:102:LYS:HB3	1:A:155:THR:HA	1.66	0.75
1:C:87:LYS:HG2	1:C:88:LEU:HD22	1.66	0.75
1:A:92:PHE:HB3	1:A:101:LEU:HD21	1.68	0.75
1:B:307:ILE:HG22	1:B:325:LEU:HB2	1.68	0.74
1:B:297:ASP:O	1:B:301:THR:HG23	1.87	0.74
1:C:368:PRO:HG3	1:C:388:SER:O	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:THR:HG23	1:B:339:GLU:HB2	1.69	0.74
1:B:233:GLU:HG3	1:B:233:GLU:O	1.86	0.74
1:C:297:ASP:O	1:C:301:THR:HG23	1.88	0.74
1:B:198:GLU:HG3	1:B:199:LYS:H	1.53	0.73
1:C:220:HIS:HD2	1:C:275:MET:HB3	1.53	0.73
1:A:233:GLU:HG3	1:A:233:GLU:O	1.87	0.73
1:A:276:ARG:O	1:A:278:THR:HG23	1.88	0.73
1:B:374:ARG:HG2	1:B:375:GLN:N	2.03	0.72
1:B:315:SER:HA	1:B:320:SER:O	1.90	0.72
1:C:30:SER:H	1:C:330:HIS:HE1	1.37	0.72
1:A:100:GLU:HG3	1:A:100:GLU:O	1.90	0.72
1:C:233:GLU:O	1:C:233:GLU:HG3	1.87	0.71
1:C:131:VAL:HG12	1:C:132:GLU:H	1.53	0.71
1:C:56:VAL:HG21	1:C:304:MET:HG3	1.71	0.71
1:B:196:LYS:N	1:B:196:LYS:HD3	2.04	0.71
1:C:254:LEU:HD23	1:C:255:GLN:N	2.06	0.71
1:C:135:ASP:OD1	1:C:138:ASN:HB2	1.89	0.71
1:C:244:ILE:HG21	1:C:270:THR:CG2	2.20	0.71
1:A:279:ARG:HB3	1:A:279:ARG:HH11	1.56	0.71
1:C:127:TYR:O	1:C:129:THR:HG22	1.90	0.71
1:C:34:ILE:HG13	1:C:330:HIS:CD2	2.25	0.71
1:C:148:ASN:O	1:C:151:VAL:HG12	1.91	0.71
1:B:30:SER:HB3	1:B:33:SER:HB3	1.73	0.71
1:C:307:ILE:CD1	1:C:307:ILE:H	1.93	0.71
1:A:231:VAL:HG22	1:A:246:LEU:CD1	2.21	0.71
1:B:186:TRP:HH2	1:B:243:MET:HG2	1.54	0.70
1:B:247:LEU:HD21	1:B:364:HIS:O	1.91	0.70
1:C:111:LYS:HD3	1:C:135:ASP:HB2	1.73	0.70
1:A:295:LEU:O	1:A:299:LEU:HB2	1.91	0.70
1:C:241:LEU:HD22	1:C:374:ARG:O	1.91	0.70
1:A:38:LEU:HD12	1:A:57:LEU:HD11	1.74	0.70
1:B:337:THR:CG2	1:B:339:GLU:HB2	2.20	0.70
1:A:262:THR:H	1:A:265:LYS:HG2	1.56	0.70
1:C:241:LEU:CD2	1:C:375:GLN:HA	2.22	0.69
1:B:44:GLY:HA3	1:B:317:MET:HG3	1.74	0.69
1:A:221:PHE:CZ	1:A:230:LYS:HD2	2.28	0.69
1:B:81:VAL:HG11	1:B:83:HIS:NE2	2.06	0.69
1:B:34:ILE:HG13	1:B:330:HIS:CD2	2.27	0.69
1:C:33:SER:C	1:C:178:ASN:HD21	1.95	0.69
1:A:15:LEU:HD13	1:A:302:MET:HE1	1.73	0.69
1:C:236:TYR:HB2	1:C:241:LEU:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:TYR:HE1	1:C:243:MET:HB2	1.58	0.69
1:B:44:GLY:HA3	1:B:317:MET:CG	2.23	0.69
1:A:221:PHE:HZ	1:A:230:LYS:HD2	1.57	0.68
1:C:168:ILE:HD11	1:C:175:VAL:HG21	1.75	0.68
1:C:307:ILE:HD13	1:C:307:ILE:N	2.05	0.68
1:C:30:SER:H	1:C:330:HIS:CE1	2.11	0.68
1:B:16:PHE:HE1	1:B:27:ILE:HD11	1.57	0.68
1:B:312:ALA:HB3	1:B:324:VAL:HG13	1.76	0.68
1:B:244:ILE:HG21	1:B:270:THR:CG2	2.23	0.68
1:A:244:ILE:HG21	1:A:270:THR:CG2	2.22	0.68
1:C:246:LEU:O	1:C:369:PHE:HB2	1.92	0.68
1:B:38:LEU:HD12	1:B:57:LEU:HD11	1.75	0.68
1:A:144:ARG:HA	1:A:147:ILE:HD12	1.76	0.68
1:B:37:ALA:O	1:B:176:LEU:HD21	1.92	0.68
1:A:35:THR:HB	1:A:85:PHE:HZ	1.59	0.68
1:C:159:ILE:HG23	1:C:331:LYS:HD3	1.74	0.68
1:B:236:TYR:HB2	1:B:241:LEU:O	1.93	0.68
1:A:48:ASN:O	1:A:52:GLN:HG2	1.93	0.68
1:C:110:GLU:OE1	1:C:112:THR:HG23	1.93	0.68
1:A:231:VAL:HG22	1:A:246:LEU:HD11	1.75	0.68
1:B:54:LYS:HB3	1:B:60:ASP:HB2	1.76	0.68
1:A:150:TRP:CE2	1:A:154:GLN:HG3	2.28	0.68
1:B:262:THR:O	1:B:265:LYS:HB2	1.93	0.67
1:C:246:LEU:HB2	1:C:370:LEU:HD12	1.76	0.67
1:A:141:GLU:HG2	1:A:142:GLU:N	2.09	0.67
1:B:56:VAL:HG21	1:B:304:MET:HG3	1.77	0.67
1:A:201:TRP:O	1:A:368:PRO:HD3	1.95	0.67
1:C:198:GLU:HG3	1:C:199:LYS:H	1.58	0.67
1:B:81:VAL:N	1:B:84:GLN:HE22	1.92	0.67
1:A:15:LEU:HD13	1:A:302:MET:CE	2.25	0.67
1:A:16:PHE:HE1	1:A:27:ILE:HD11	1.59	0.67
1:C:251:ILE:HD13	1:C:367:HIS:HB3	1.77	0.67
1:B:131:VAL:HG12	1:B:132:GLU:H	1.60	0.66
1:A:106:LYS:HD2	1:A:108:PHE:CE1	2.30	0.66
1:A:123:ILE:CD1	1:A:130:SER:HA	2.25	0.66
1:A:262:THR:O	1:A:265:LYS:HB2	1.96	0.66
1:A:106:LYS:HG2	1:A:130:SER:O	1.96	0.66
1:A:55:LYS:NZ	1:A:303:GLY:HA3	2.10	0.66
1:A:374:ARG:HG3	1:A:375:GLN:N	2.11	0.66
1:C:198:GLU:O	1:C:209:SER:HA	1.96	0.66
1:C:9:THR:HG22	1:C:381:ILE:HD13	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:MET:HG3	1:B:13:PHE:N	2.12	0.65
1:A:36:SER:HB3	1:A:85:PHE:CE2	2.31	0.65
1:B:373:ILE:HB	1:B:383:PHE:HB2	1.77	0.65
1:C:387:PHE:CZ	1:C:390:PRO:HB3	2.29	0.65
1:A:55:LYS:HZ1	1:A:303:GLY:HA3	1.62	0.65
1:C:143:SER:O	1:C:146:LYS:HB2	1.96	0.65
1:B:248:PRO:HG3	1:B:254:LEU:HB3	1.78	0.65
1:C:185:GLN:NE2	1:C:339:GLU:HB3	2.11	0.65
1:B:106:LYS:HB3	1:B:108:PHE:HE1	1.62	0.65
1:C:194:ASP:O	1:C:214:ARG:HD2	1.96	0.65
1:C:1:SER:OG	1:C:88:LEU:HD21	1.97	0.65
1:C:245:VAL:HG13	1:C:369:PHE:CD1	2.32	0.65
1:B:143:SER:O	1:B:146:LYS:HB2	1.95	0.65
1:B:200:PHE:HB2	1:B:210:ILE:HD13	1.79	0.65
1:C:227:VAL:HG11	1:C:257:LEU:HD13	1.79	0.65
1:A:164:PRO:O	1:A:167:ASN:HB2	1.97	0.65
1:B:49:THR:HG23	1:B:307:ILE:HG13	1.79	0.65
1:A:26:ASN:HD21	1:A:389:SER:HA	1.61	0.65
1:C:34:ILE:N	1:C:178:ASN:HD21	1.95	0.65
1:A:224:LEU:HD23	1:A:231:VAL:HG23	1.79	0.65
1:A:55:LYS:HA	2:A:445:HOH:O	1.96	0.64
1:C:86:GLN:O	1:C:90:THR:HG23	1.98	0.64
1:B:49:THR:CG2	1:B:307:ILE:HG13	2.27	0.64
1:A:241:LEU:HD22	1:A:375:GLN:HA	1.79	0.64
1:C:201:TRP:O	1:C:368:PRO:HD3	1.97	0.64
1:B:214:ARG:HG3	1:B:215:GLN:N	2.12	0.64
1:C:48:ASN:O	1:C:52:GLN:HG2	1.98	0.64
1:B:99:TYR:HA	1:B:184:GLY:HA2	1.80	0.64
1:B:244:ILE:HG21	1:B:270:THR:HG22	1.78	0.64
1:C:178:ASN:ND2	1:C:330:HIS:HD2	1.95	0.64
1:A:295:LEU:HB2	1:A:299:LEU:HD23	1.80	0.64
1:B:238:GLY:O	1:B:239:LYS:HB2	1.96	0.64
1:B:102:LYS:HB3	1:B:155:THR:HA	1.80	0.63
1:B:200:PHE:O	1:B:202:PRO:HD3	1.98	0.63
1:B:11:PHE:CZ	1:B:15:LEU:HD22	2.32	0.63
1:B:5:SER:O	1:B:9:THR:HG23	1.97	0.63
1:A:55:LYS:HG3	1:A:56:VAL:N	2.13	0.63
1:A:202:PRO:HD2	1:A:206:THR:O	1.99	0.63
1:B:235:PRO:HA	1:B:242:SER:HB3	1.80	0.63
1:A:27:ILE:O	1:A:385:GLY:HA2	1.99	0.63
1:A:243:MET:HG3	1:A:243:MET:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:SER:O	1:B:319:GLY:N	2.30	0.63
1:A:106:LYS:CG	1:A:130:SER:O	2.47	0.63
1:B:366:ASN:HD22	1:B:366:ASN:H	0.77	0.63
1:A:367:HIS:HB2	1:A:368:PRO:HD2	1.81	0.63
1:B:57:LEU:HD23	1:B:59:PHE:CE2	2.33	0.62
1:C:294:ASP:HA	1:C:328:VAL:O	1.99	0.62
1:C:241:LEU:HD23	1:C:375:GLN:HA	1.79	0.62
1:A:162:LEU:O	1:A:162:LEU:HD22	1.99	0.62
1:A:30:SER:H	1:A:330:HIS:CE1	2.17	0.62
1:A:86:GLN:O	1:A:90:THR:HG23	1.98	0.62
1:C:244:ILE:HG21	1:C:270:THR:HG22	1.80	0.62
1:A:101:LEU:HD12	1:A:101:LEU:O	1.98	0.62
1:A:108:PHE:CE2	1:A:147:ILE:HG23	2.35	0.62
1:C:280:VAL:HG22	1:C:361:GLU:HB3	1.82	0.62
1:B:282:LEU:HD11	1:B:284:LEU:HB2	1.81	0.62
1:B:229:ALA:CB	1:B:248:PRO:HA	2.29	0.62
1:B:350:VAL:CG1	1:B:351:GLY:N	2.63	0.62
1:C:366:ASN:HD22	1:C:366:ASN:N	1.96	0.62
1:C:227:VAL:CG2	1:C:257:LEU:HA	2.30	0.62
1:A:18:GLN:HG3	1:A:302:MET:HE2	1.82	0.61
1:C:362:GLU:HB3	1:C:364:HIS:CE1	2.35	0.61
1:A:168:ILE:HD11	1:A:175:VAL:HG21	1.81	0.61
1:B:214:ARG:HH21	1:B:216:TYR:HB2	1.65	0.61
1:A:210:ILE:HD12	1:A:285:PRO:HB3	1.81	0.61
1:A:148:ASN:O	1:A:151:VAL:HG12	2.01	0.61
1:A:157:GLU:HG2	1:A:160:LYS:NZ	2.16	0.61
1:B:84:GLN:HA	1:B:87:LYS:HE3	1.83	0.61
1:B:270:THR:HG21	1:B:372:PHE:CZ	2.35	0.61
1:C:268:GLU:HG2	1:C:269:TRP:HD1	1.64	0.61
1:C:38:LEU:CD1	1:C:57:LEU:HD11	2.24	0.61
1:C:368:PRO:HB3	1:C:388:SER:HA	1.82	0.61
1:A:246:LEU:HB2	1:A:370:LEU:HD12	1.83	0.61
1:A:108:PHE:CZ	1:A:147:ILE:HG23	2.35	0.61
1:B:225:GLU:HA	1:B:225:GLU:OE1	2.00	0.61
1:B:156:ASN:HB2	1:B:158:LYS:HG2	1.82	0.61
1:B:270:THR:HG21	1:B:372:PHE:CE2	2.36	0.61
1:A:300:ARG:HA	1:A:304:MET:O	2.00	0.61
1:C:315:SER:O	1:C:319:GLY:N	2.34	0.61
1:C:28:PHE:HB2	1:C:289:VAL:HG11	1.83	0.60
1:C:12:MET:CE	1:C:31:PRO:HG3	2.31	0.60
1:A:92:PHE:N	1:A:92:PHE:CD2	2.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ASN:H	1:C:2:ASN:HD22	1.45	0.60
1:C:247:LEU:HD21	1:C:364:HIS:O	2.01	0.60
1:A:81:VAL:O	1:A:84:GLN:HG2	2.01	0.60
1:B:12:MET:HE1	1:B:31:PRO:HG3	1.83	0.60
1:B:48:ASN:O	1:B:52:GLN:HG2	2.00	0.60
1:C:106:LYS:HD2	1:C:108:PHE:CE1	2.35	0.60
1:B:213:MET:SD	1:B:286:ARG:HG2	2.41	0.60
1:A:267:MET:HB2	2:A:443:HOH:O	2.01	0.60
1:B:236:TYR:HE1	1:B:243:MET:HB3	1.65	0.60
1:A:84:GLN:O	1:A:88:LEU:HD23	2.00	0.60
1:C:105:ASN:HB2	2:C:425:HOH:O	2.00	0.60
1:B:246:LEU:O	1:B:369:PHE:HB2	2.01	0.60
1:B:203:ASN:OD1	1:B:206:THR:N	2.34	0.60
1:B:368:PRO:HB3	1:B:388:SER:HA	1.83	0.60
1:B:12:MET:HE3	1:B:381:ILE:HG21	1.83	0.60
1:C:231:VAL:HG22	1:C:246:LEU:CD1	2.31	0.60
1:B:134:VAL:HG23	1:B:146:LYS:NZ	2.17	0.59
1:C:276:ARG:O	1:C:278:THR:HG23	2.01	0.59
1:A:315:SER:HA	1:A:320:SER:O	2.01	0.59
1:B:16:PHE:C	1:B:18:GLN:H	2.06	0.59
1:B:85:PHE:O	1:B:89:LEU:HD12	2.02	0.59
1:A:386:ARG:O	1:A:386:ARG:HG3	2.00	0.59
1:A:368:PRO:HA	1:A:387:PHE:O	2.02	0.59
1:A:25:ASN:OD1	1:A:390:PRO:HG2	2.02	0.59
1:C:12:MET:HG3	1:C:13:PHE:N	2.17	0.59
1:B:221:PHE:CZ	1:B:230:LYS:HD2	2.37	0.59
1:B:101:LEU:O	1:B:101:LEU:HD12	2.02	0.59
1:B:186:TRP:HH2	1:B:243:MET:CG	2.15	0.59
1:A:219:PHE:CB	1:A:232:LEU:HD11	2.32	0.59
1:A:16:PHE:CE1	1:A:27:ILE:HD11	2.38	0.59
1:A:198:GLU:HG3	1:A:199:LYS:N	2.16	0.59
1:A:123:ILE:HD11	1:A:130:SER:HA	1.84	0.59
1:A:123:ILE:HG13	1:A:124:LYS:N	2.17	0.59
1:B:246:LEU:HB2	1:B:370:LEU:HD12	1.85	0.59
1:C:92:PHE:O	1:C:101:LEU:HD11	2.02	0.58
1:A:131:VAL:HG12	1:A:132:GLU:H	1.68	0.58
1:C:15:LEU:HG	1:C:19:PHE:CE1	2.38	0.58
1:C:312:ALA:CB	1:C:324:VAL:HG12	2.28	0.58
1:C:196:LYS:N	1:C:214:ARG:HH22	1.96	0.58
1:C:315:SER:HA	1:C:320:SER:O	2.03	0.58
1:A:111:LYS:HD3	1:A:135:ASP:OD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TRP:CH2	1:A:243:MET:HG2	2.37	0.58
1:C:219:PHE:CB	1:C:232:LEU:HD11	2.33	0.58
1:C:81:VAL:C	1:C:83:HIS:H	2.06	0.58
1:C:190:PHE:HD2	1:C:213:MET:HB3	1.68	0.58
1:B:284:LEU:HD23	1:B:285:PRO:O	2.04	0.58
1:B:144:ARG:HA	1:B:147:ILE:HD12	1.86	0.58
1:B:55:LYS:HG3	1:B:56:VAL:N	2.19	0.58
1:A:12:MET:HG3	1:A:13:PHE:N	2.18	0.58
1:C:227:VAL:HG21	1:C:257:LEU:HA	1.86	0.58
1:A:132:GLU:HG3	1:A:132:GLU:O	2.04	0.58
1:B:101:LEU:HA	1:B:181:TYR:O	2.04	0.58
1:C:366:ASN:ND2	1:C:366:ASN:N	2.51	0.58
1:C:229:ALA:CB	1:C:248:PRO:HA	2.34	0.58
1:B:241:LEU:HD22	1:B:374:ARG:O	2.04	0.57
1:B:13:PHE:O	1:B:16:PHE:HB3	2.04	0.57
1:A:57:LEU:HB3	1:A:59:PHE:CE1	2.39	0.57
1:A:184:GLY:HA3	1:A:236:TYR:CE2	2.39	0.57
1:C:227:VAL:HG23	1:C:260:LYS:HG3	1.86	0.57
1:B:159:ILE:HG23	1:B:331:LYS:HD3	1.86	0.57
1:A:115:PHE:CZ	1:A:131:VAL:HG11	2.40	0.57
1:C:35:THR:HB	1:C:85:PHE:HZ	1.69	0.57
1:C:141:GLU:CG	1:C:142:GLU:H	2.18	0.57
1:C:13:PHE:CE2	1:C:263:ALA:HA	2.39	0.57
1:C:262:THR:OG1	1:C:264:GLU:HG2	2.04	0.57
1:C:131:VAL:HG12	1:C:132:GLU:N	2.18	0.57
1:C:27:ILE:O	1:C:385:GLY:HA2	2.05	0.57
1:C:92:PHE:HB3	1:C:101:LEU:CD2	2.27	0.57
1:B:16:PHE:O	1:B:18:GLN:N	2.34	0.57
1:C:55:LYS:HG3	1:C:56:VAL:N	2.19	0.57
1:A:236:TYR:HB2	1:A:241:LEU:O	2.05	0.57
1:B:81:VAL:HG21	1:B:83:HIS:CE1	2.39	0.57
1:B:30:SER:H	1:B:330:HIS:CE1	2.23	0.57
1:B:200:PHE:HA	1:B:366:ASN:O	2.05	0.57
1:B:227:VAL:HG21	1:B:257:LEU:HA	1.87	0.57
1:C:219:PHE:HB3	1:C:232:LEU:HD11	1.87	0.57
1:A:84:GLN:HB3	1:A:87:LYS:NZ	2.20	0.56
1:A:288:LYS:HB3	1:A:335:GLU:HG3	1.87	0.56
1:A:176:LEU:HD12	1:A:177:VAL:N	2.20	0.56
1:A:366:ASN:H	1:A:366:ASN:ND2	2.03	0.56
1:C:34:ILE:HA	1:C:178:ASN:HD21	1.68	0.56
1:B:94:LYS:HG2	1:B:94:LYS:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ILE:HD12	1:B:130:SER:HA	1.86	0.56
1:B:81:VAL:HG12	1:B:82:HIS:H	1.71	0.56
1:A:34:ILE:HG13	1:A:330:HIS:CD2	2.40	0.56
1:B:217:THR:OG1	1:B:218:SER:N	2.37	0.56
1:A:23:LYS:HZ2	1:A:27:ILE:HG22	1.70	0.56
1:A:21:LYS:NZ	1:B:117:GLN:OE1	2.39	0.56
1:C:114:LEU:O	1:C:318:THR:HG22	2.06	0.56
1:C:13:PHE:HE2	1:C:263:ALA:HA	1.70	0.56
1:B:244:ILE:HD11	1:B:374:ARG:NH1	2.20	0.56
1:A:298:THR:O	1:A:302:MET:HG3	2.06	0.56
1:C:119:TYR:CE2	1:C:317:MET:HG2	2.41	0.56
1:A:11:PHE:CZ	1:A:15:LEU:HD22	2.41	0.56
1:C:299:LEU:HB3	1:C:304:MET:HE2	1.88	0.56
1:C:178:ASN:O	1:C:330:HIS:HA	2.06	0.56
1:A:141:GLU:HG2	1:A:142:GLU:H	1.69	0.56
1:B:254:LEU:O	1:B:257:LEU:HB3	2.06	0.56
1:C:159:ILE:CG2	1:C:331:LYS:HD3	2.36	0.56
1:A:254:LEU:O	1:A:257:LEU:HB3	2.05	0.56
1:C:28:PHE:CE1	1:C:334:VAL:HB	2.40	0.55
1:B:98:ALA:HA	1:B:237:LYS:HB3	1.88	0.55
1:B:229:ALA:HB2	1:B:248:PRO:HA	1.88	0.55
1:A:161:ASN:HD22	1:A:161:ASN:N	2.04	0.55
1:B:148:ASN:O	1:B:151:VAL:HG12	2.06	0.55
1:B:100:GLU:O	1:B:182:PHE:HA	2.06	0.55
1:B:107:LEU:HB3	1:B:131:VAL:HG13	1.89	0.55
1:C:164:PRO:HD2	1:C:167:ASN:CG	2.26	0.55
1:A:210:ILE:HD11	1:A:212:MET:HE2	1.89	0.55
1:B:25:ASN:O	1:B:386:ARG:HD2	2.07	0.55
1:B:189:LYS:HD3	1:B:344:ALA:HB2	1.88	0.55
1:B:227:VAL:CG2	1:B:257:LEU:HA	2.36	0.55
1:B:34:ILE:HA	1:B:178:ASN:ND2	2.22	0.55
1:B:189:LYS:HG2	1:B:190:PHE:N	2.19	0.55
1:B:231:VAL:HG23	1:B:246:LEU:CD1	2.37	0.55
1:C:203:ASN:OD1	1:C:206:THR:N	2.40	0.55
1:C:38:LEU:CB	1:C:57:LEU:HD21	2.37	0.55
1:C:27:ILE:HG13	1:C:27:ILE:O	2.06	0.55
1:A:282:LEU:HD12	1:A:283:HIS:H	1.66	0.55
1:C:300:ARG:HA	1:C:304:MET:O	2.07	0.55
1:A:281:ASP:O	1:A:362:GLU:HB2	2.06	0.55
1:B:127:TYR:O	1:B:129:THR:N	2.40	0.55
1:A:46:LYS:CE	1:A:47:ASP:H	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:SER:O	1:A:319:GLY:N	2.36	0.55
1:C:85:PHE:O	1:C:89:LEU:HB2	2.07	0.55
1:A:83:HIS:HB3	1:A:84:GLN:OE1	2.07	0.55
1:C:108:PHE:CZ	1:C:147:ILE:HG23	2.41	0.55
1:C:144:ARG:HA	1:C:147:ILE:HD12	1.88	0.55
1:A:43:LEU:HD12	1:A:123:ILE:HG22	1.87	0.54
1:C:102:LYS:CB	1:C:155:THR:HA	2.32	0.54
1:B:187:GLU:OE1	1:B:239:LYS:HD2	2.08	0.54
1:A:381:ILE:CD1	1:A:381:ILE:H	2.16	0.54
1:C:5:SER:OG	1:C:380:SER:HA	2.07	0.54
1:A:227:VAL:HG21	1:A:257:LEU:HA	1.89	0.54
1:B:164:PRO:HG2	1:B:167:ASN:ND2	2.22	0.54
1:A:12:MET:CE	1:A:31:PRO:HG3	2.38	0.54
1:B:189:LYS:HA	1:B:340:GLY:HA3	1.90	0.54
1:C:48:ASN:HA	1:C:51:GLN:HE21	1.71	0.54
1:B:162:LEU:HD23	1:B:331:LYS:HD2	1.89	0.54
1:C:220:HIS:CD2	1:C:275:MET:HB3	2.40	0.54
1:B:84:GLN:HG3	1:B:87:LYS:HZ1	1.72	0.54
1:A:227:VAL:CG2	1:A:257:LEU:HA	2.37	0.54
1:B:286:ARG:NH1	1:B:337:THR:OG1	2.41	0.54
1:C:280:VAL:HA	1:C:361:GLU:O	2.07	0.54
1:A:241:LEU:CD2	1:A:375:GLN:HA	2.38	0.54
1:C:123:ILE:O	1:C:127:TYR:N	2.39	0.54
1:A:123:ILE:HD12	1:A:130:SER:HA	1.89	0.54
1:C:134:VAL:HG23	1:C:146:LYS:NZ	2.23	0.54
1:C:15:LEU:HG	1:C:19:PHE:HE1	1.73	0.54
1:C:102:LYS:HE3	1:C:156:ASN:ND2	2.23	0.54
1:C:34:ILE:CA	1:C:178:ASN:HD21	2.21	0.54
1:C:374:ARG:HG3	1:C:375:GLN:N	2.22	0.54
1:B:13:PHE:HE2	1:B:263:ALA:HA	1.72	0.54
1:B:81:VAL:HG23	1:B:84:GLN:HE22	1.71	0.54
1:C:282:LEU:HD12	1:C:283:HIS:N	2.22	0.54
1:A:381:ILE:HD12	1:A:381:ILE:N	2.17	0.54
1:C:202:PRO:HB3	1:C:389:SER:HB2	1.90	0.53
1:A:219:PHE:HB3	1:A:232:LEU:HD11	1.91	0.53
1:A:382:LEU:HD12	1:A:383:PHE:CD2	2.43	0.53
1:A:300:ARG:CZ	1:B:114:LEU:HD22	2.38	0.53
1:B:164:PRO:HD2	1:B:167:ASN:OD1	2.08	0.53
1:B:33:SER:OG	1:B:178:ASN:OD1	2.26	0.53
1:B:186:TRP:CE3	1:B:234:ILE:HG22	2.43	0.53
1:B:374:ARG:HH11	1:B:376:ASN:HD21	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HA	1:A:178:ASN:ND2	2.23	0.53
1:C:16:PHE:HE1	1:C:27:ILE:CD1	2.07	0.53
1:C:295:LEU:O	1:C:299:LEU:HB2	2.08	0.53
1:C:162:LEU:HD12	1:C:177:VAL:HG13	1.90	0.53
1:B:243:MET:HB2	1:B:373:ILE:HG12	1.91	0.53
1:C:140:PRO:O	1:C:143:SER:HB2	2.08	0.53
1:B:219:PHE:O	1:B:277:GLU:HA	2.08	0.53
1:B:370:LEU:HD12	1:B:370:LEU:O	2.09	0.53
1:A:219:PHE:O	1:A:277:GLU:HA	2.08	0.53
1:A:23:LYS:NZ	1:A:27:ILE:HG22	2.24	0.53
1:C:2:ASN:ND2	1:C:2:ASN:N	2.54	0.53
1:B:102:LYS:HG3	1:B:156:ASN:OD1	2.09	0.53
1:A:371:PHE:O	1:A:372:PHE:HB3	2.09	0.53
1:A:20:ARG:CZ	1:A:258:GLU:HB3	2.39	0.53
1:C:119:TYR:CZ	1:C:317:MET:HG2	2.44	0.53
1:A:101:LEU:HA	1:A:181:TYR:O	2.09	0.53
1:C:372:PHE:HB2	1:C:383:PHE:O	2.09	0.52
1:A:110:GLU:OE2	1:A:112:THR:HG23	2.09	0.52
1:A:2:ASN:OD1	1:A:2:ASN:N	2.41	0.52
1:A:81:VAL:HG22	1:A:82:HIS:N	2.24	0.52
1:A:267:MET:HE3	2:A:464:HOH:O	2.08	0.52
1:C:23:LYS:HE3	1:C:23:LYS:HA	1.90	0.52
1:A:238:GLY:O	1:A:239:LYS:HB2	2.09	0.52
1:C:217:THR:OG1	1:C:218:SER:N	2.43	0.52
1:A:4:LEU:HD12	1:A:84:GLN:HB2	1.91	0.52
1:B:119:TYR:O	1:B:122:ALA:N	2.42	0.52
1:C:87:LYS:HG2	1:C:88:LEU:CD2	2.38	0.52
1:C:314:LEU:HD13	1:C:317:MET:SD	2.49	0.52
1:C:247:LEU:HD12	1:C:248:PRO:HD2	1.90	0.52
1:C:11:PHE:CZ	1:C:15:LEU:HD22	2.45	0.52
1:B:102:LYS:O	1:B:180:ILE:HA	2.09	0.52
1:C:38:LEU:HD12	1:C:57:LEU:CD1	2.27	0.52
1:C:49:THR:CG2	1:C:307:ILE:HG23	2.40	0.52
1:A:46:LYS:CD	1:A:47:ASP:H	2.23	0.52
1:C:279:ARG:HB2	1:C:360:ASN:HD22	1.75	0.52
1:C:29:TYR:HB3	1:C:293:TYR:HE1	1.74	0.52
1:C:244:ILE:HG21	1:C:270:THR:HG21	1.90	0.52
1:A:220:HIS:HD2	1:A:275:MET:HB3	1.75	0.52
1:A:12:MET:HE1	1:A:31:PRO:HG3	1.91	0.52
1:A:106:LYS:HB3	1:A:108:PHE:HE1	1.75	0.52
1:A:30:SER:H	1:A:330:HIS:HE1	1.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:PHE:CZ	1:C:383:PHE:CD1	2.98	0.51
1:B:243:MET:CG	1:B:243:MET:O	2.58	0.51
1:C:221:PHE:HZ	1:C:230:LYS:HD2	1.74	0.51
1:B:84:GLN:HG3	1:B:87:LYS:NZ	2.25	0.51
1:C:190:PHE:CD2	1:C:213:MET:HB3	2.45	0.51
1:B:355:SER:HB2	1:B:358:SER:HB3	1.92	0.51
1:C:186:TRP:CE3	1:C:234:ILE:HG22	2.46	0.51
1:C:123:ILE:HG13	1:C:124:LYS:N	2.25	0.51
1:B:268:GLU:HG2	1:B:269:TRP:CD1	2.44	0.51
1:B:296:LYS:HE3	1:B:300:ARG:NH2	2.26	0.51
1:C:102:LYS:HE3	1:C:156:ASN:HD21	1.75	0.51
1:A:23:LYS:HE3	1:A:291:GLU:OE1	2.10	0.51
1:A:246:LEU:O	1:A:369:PHE:HB2	2.10	0.51
1:A:131:VAL:HG12	1:A:132:GLU:N	2.24	0.51
1:B:295:LEU:HB2	1:B:299:LEU:HD22	1.92	0.51
1:A:278:THR:O	1:A:280:VAL:HG23	2.11	0.51
1:B:15:LEU:HG	1:B:19:PHE:CE1	2.46	0.51
1:A:236:TYR:HE1	1:A:243:MET:HB3	1.75	0.51
1:B:313:ASP:OD1	1:B:321:ARG:HD2	2.11	0.51
1:A:174:LEU:O	1:A:175:VAL:HG23	2.11	0.51
1:A:272:LEU:HA	1:A:275:MET:HB2	1.91	0.51
1:B:372:PHE:HB2	1:B:383:PHE:O	2.11	0.51
1:A:202:PRO:HD3	1:A:207:TYR:HA	1.92	0.51
1:C:144:ARG:NH1	1:C:163:ILE:O	2.43	0.51
1:C:111:LYS:HD3	1:C:135:ASP:CB	2.40	0.51
1:A:108:PHE:CD2	1:A:147:ILE:HG12	2.46	0.51
1:B:127:TYR:O	1:B:129:THR:HG22	2.10	0.51
1:B:190:PHE:HB2	1:B:338:GLU:CA	2.41	0.51
1:C:313:ASP:CG	1:C:321:ARG:HD2	2.31	0.51
1:A:81:VAL:HG13	1:A:82:HIS:N	2.20	0.51
1:B:104:ALA:HB1	1:B:150:TRP:CZ3	2.47	0.50
1:A:30:SER:OG	1:A:33:SER:HB3	2.10	0.50
1:A:157:GLU:HG2	1:A:160:LYS:HZ3	1.76	0.50
1:C:12:MET:HE1	1:C:31:PRO:HG3	1.92	0.50
1:A:201:TRP:N	1:A:366:ASN:O	2.38	0.50
1:A:40:MET:O	1:A:43:LEU:HB2	2.11	0.50
1:C:154:GLN:NE2	1:C:154:GLN:O	2.45	0.50
1:B:245:VAL:HG13	1:B:369:PHE:CD1	2.46	0.50
1:B:231:VAL:HB	1:B:246:LEU:HD11	1.94	0.50
1:B:210:ILE:HG21	1:B:390:PRO:CG	2.41	0.50
1:B:295:LEU:CB	1:B:299:LEU:HD22	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:THR:HG22	1:A:85:PHE:CE1	2.47	0.50
1:B:190:PHE:HB2	1:B:338:GLU:HA	1.93	0.50
1:B:12:MET:CE	1:B:31:PRO:HG3	2.42	0.50
1:A:296:LYS:NZ	1:A:308:PHE:HB3	2.27	0.50
1:B:221:PHE:HZ	1:B:230:LYS:HD2	1.74	0.50
1:B:350:VAL:HG13	1:B:351:GLY:H	1.77	0.50
1:C:229:ALA:HB2	1:C:248:PRO:HA	1.93	0.50
1:A:111:LYS:O	1:A:113:TYR:N	2.45	0.50
1:C:226:ASP:N	1:C:226:ASP:OD2	2.45	0.50
1:B:40:MET:CE	1:B:107:LEU:HB2	2.41	0.50
1:C:48:ASN:OD1	1:C:51:GLN:NE2	2.44	0.50
1:C:56:VAL:HG11	1:C:299:LEU:HD12	1.92	0.49
1:C:32:ILE:CG2	1:C:33:SER:N	2.74	0.49
1:B:156:ASN:O	1:B:157:GLU:HB2	2.12	0.49
1:C:123:ILE:CD1	1:C:130:SER:HA	2.42	0.49
1:A:115:PHE:HA	1:A:317:MET:O	2.12	0.49
1:B:374:ARG:HH11	1:B:376:ASN:ND2	2.10	0.49
1:C:254:LEU:O	1:C:257:LEU:HB3	2.12	0.49
1:A:224:LEU:HB2	1:A:229:ALA:O	2.12	0.49
1:B:268:GLU:HG2	1:B:269:TRP:HD1	1.78	0.49
1:A:174:LEU:HB3	1:A:325:LEU:HA	1.93	0.49
1:A:221:PHE:CD2	1:A:222:ALA:N	2.80	0.49
1:B:105:ASN:HD21	1:B:178:ASN:CG	2.15	0.49
1:B:105:ASN:ND2	1:B:178:ASN:OD1	2.46	0.49
1:B:374:ARG:NH1	1:B:376:ASN:ND2	2.61	0.49
1:A:23:LYS:HD3	1:A:27:ILE:HG22	1.93	0.49
1:B:295:LEU:HB2	1:B:299:LEU:CD2	2.42	0.49
1:A:387:PHE:CZ	1:A:389:SER:HB2	2.47	0.49
1:A:124:LYS:O	1:A:128:GLN:HA	2.13	0.49
1:B:157:GLU:HB3	1:B:160:LYS:NZ	2.28	0.49
1:B:227:VAL:HA	1:B:256:LYS:HE3	1.94	0.49
1:A:174:LEU:HD22	1:A:323:LEU:HG	1.94	0.49
1:C:268:GLU:HG2	1:C:269:TRP:CD1	2.46	0.49
1:B:31:PRO:O	1:B:35:THR:OG1	2.31	0.49
1:A:189:LYS:HG3	1:A:340:GLY:H	1.77	0.49
1:C:278:THR:O	1:C:280:VAL:HG23	2.13	0.49
1:C:210:ILE:HG21	1:C:390:PRO:CG	2.43	0.49
1:A:151:VAL:CG1	1:A:152:GLU:N	2.76	0.49
1:B:237:LYS:HE3	1:B:341:ALA:HB2	1.95	0.49
1:A:23:LYS:HZ2	1:A:26:ASN:C	2.16	0.49
1:A:307:ILE:H	1:A:307:ILE:CD1	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ARG:NH1	1:C:258:GLU:OE1	2.45	0.49
1:C:148:ASN:ND2	1:C:161:ASN:HA	2.27	0.49
1:C:185:GLN:HE22	1:C:339:GLU:HB3	1.78	0.48
1:A:161:ASN:ND2	1:A:161:ASN:N	2.61	0.48
1:A:261:LEU:HD22	1:A:266:LEU:HD23	1.94	0.48
1:C:102:LYS:O	1:C:155:THR:HG22	2.13	0.48
1:B:131:VAL:HG12	1:B:132:GLU:N	2.27	0.48
1:A:280:VAL:HG13	1:A:362:GLU:HA	1.95	0.48
1:C:108:PHE:CE2	1:C:147:ILE:HG23	2.48	0.48
1:B:337:THR:HG23	1:B:339:GLU:H	1.78	0.48
1:B:174:LEU:HD21	1:B:317:MET:CE	2.42	0.48
1:B:42:LEU:HB2	1:B:53:ILE:HG21	1.94	0.48
1:A:200:PHE:O	1:A:202:PRO:HD3	2.12	0.48
1:C:264:GLU:N	1:C:264:GLU:CD	2.58	0.48
1:B:85:PHE:O	1:B:89:LEU:HB2	2.13	0.48
1:A:216:TYR:HA	1:A:281:ASP:HA	1.95	0.48
1:B:210:ILE:HG21	1:B:390:PRO:HG2	1.94	0.48
1:A:6:GLU:O	1:A:9:THR:OG1	2.25	0.48
1:C:151:VAL:CG1	1:C:152:GLU:N	2.76	0.48
1:B:337:THR:HG21	1:B:339:GLU:HB2	1.96	0.48
1:B:44:GLY:HA3	1:B:317:MET:HG2	1.93	0.48
1:A:181:TYR:C	1:A:181:TYR:CD2	2.87	0.48
1:A:135:ASP:OD1	1:A:138:ASN:HB2	2.14	0.48
1:B:219:PHE:CB	1:B:232:LEU:HD11	2.44	0.48
1:B:32:ILE:CG2	1:B:33:SER:N	2.76	0.48
1:A:57:LEU:O	1:A:58:HIS:HB2	2.13	0.48
1:B:349:VAL:O	1:B:349:VAL:HG23	2.13	0.48
1:B:186:TRP:HE3	1:B:235:PRO:O	1.96	0.48
1:C:82:HIS:CD2	1:C:82:HIS:H	2.31	0.48
1:B:1:SER:O	1:B:4:LEU:HB3	2.13	0.48
1:A:115:PHE:CE1	1:A:131:VAL:HG11	2.48	0.48
1:A:235:PRO:HA	1:A:242:SER:CB	2.43	0.48
1:B:155:THR:C	1:B:157:GLU:H	2.15	0.48
1:A:388:SER:OG	1:A:390:PRO:HD3	2.13	0.48
1:A:143:SER:O	1:A:146:LYS:HB2	2.14	0.48
1:B:232:LEU:CD2	1:B:282:LEU:HD22	2.44	0.47
1:B:200:PHE:HB2	1:B:210:ILE:CD1	2.42	0.47
1:C:162:LEU:O	1:C:329:LEU:HD12	2.14	0.47
1:A:338:GLU:H	1:A:338:GLU:HG2	1.37	0.47
1:C:368:PRO:HA	1:C:387:PHE:O	2.14	0.47
1:A:309:ASN:O	1:A:311:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:GLN:O	1:B:237:LYS:N	2.40	0.47
1:B:186:TRP:HZ3	1:B:234:ILE:O	1.98	0.47
1:B:81:VAL:N	1:B:84:GLN:NE2	2.62	0.47
1:C:32:ILE:HG23	1:C:33:SER:N	2.29	0.47
1:B:35:THR:HB	1:B:85:PHE:CZ	2.36	0.47
1:A:38:LEU:HD12	1:A:57:LEU:CD1	2.43	0.47
1:A:232:LEU:HD23	1:A:282:LEU:HD22	1.96	0.47
1:C:190:PHE:HB2	1:C:338:GLU:HA	1.95	0.47
1:C:43:LEU:HB3	1:C:119:TYR:HE1	1.78	0.47
1:B:206:THR:HG22	1:B:207:TYR:N	2.30	0.47
1:A:188:LYS:HD2	1:A:217:THR:HG21	1.95	0.47
1:C:194:ASP:N	1:C:194:ASP:OD1	2.46	0.47
1:B:14:ASP:O	1:B:18:GLN:HG2	2.15	0.47
1:C:45:ALA:HB2	1:C:314:LEU:CD2	2.45	0.47
1:A:117:GLN:HA	1:A:120:LEU:HD12	1.96	0.47
1:C:127:TYR:O	1:C:129:THR:N	2.47	0.47
1:A:35:THR:HG22	1:A:85:PHE:HE1	1.79	0.47
1:B:134:VAL:HG23	1:B:146:LYS:CE	2.45	0.47
1:B:231:VAL:CG2	1:B:246:LEU:HD11	2.45	0.47
1:B:374:ARG:HD3	1:B:376:ASN:ND2	2.30	0.47
1:C:254:LEU:HA	1:C:257:LEU:HB3	1.95	0.47
1:C:111:LYS:HE2	1:C:135:ASP:OD2	2.15	0.47
1:B:114:LEU:O	1:B:318:THR:HG22	2.15	0.47
1:A:321:ARG:HB3	1:A:321:ARG:HE	1.32	0.47
1:A:264:GLU:HG2	2:A:408:HOH:O	2.14	0.47
1:A:233:GLU:HB3	1:A:275:MET:HE2	1.96	0.47
1:B:162:LEU:HD13	1:B:329:LEU:HB3	1.96	0.47
1:C:181:TYR:C	1:C:181:TYR:CD2	2.88	0.46
1:A:245:VAL:O	1:A:246:LEU:HD12	2.15	0.46
1:B:198:GLU:HG3	1:B:199:LYS:N	2.28	0.46
1:C:96:THR:HG21	1:C:99:TYR:CE2	2.50	0.46
1:A:23:LYS:HZ1	1:A:26:ASN:N	2.12	0.46
1:B:190:PHE:HB2	1:B:338:GLU:O	2.16	0.46
1:B:156:ASN:O	1:B:157:GLU:CB	2.63	0.46
1:A:201:TRP:CE3	1:A:207:TYR:HB3	2.50	0.46
1:C:20:ARG:NH2	1:C:258:GLU:HB3	2.30	0.46
1:A:297:ASP:O	1:A:301:THR:HG23	2.14	0.46
1:B:84:GLN:N	1:B:84:GLN:OE1	2.40	0.46
1:B:350:VAL:HG13	1:B:351:GLY:N	2.29	0.46
1:B:111:LYS:HA	1:B:133:SER:HB3	1.97	0.46
1:B:5:SER:OG	1:B:380:SER:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:MET:O	1:B:243:MET:HG3	2.15	0.46
1:A:247:LEU:HB2	1:A:363:PHE:CE1	2.51	0.46
1:C:84:GLN:HG3	1:C:87:LYS:HZ1	1.74	0.46
1:A:23:LYS:HB3	1:A:27:ILE:HG22	1.97	0.46
1:C:210:ILE:CD1	1:C:285:PRO:HB3	2.38	0.46
1:C:20:ARG:HH22	1:C:259:GLU:N	2.14	0.46
1:A:47:ASP:HB3	1:A:48:ASN:H	1.62	0.46
1:B:262:THR:H	1:B:265:LYS:HB2	1.81	0.46
1:A:157:GLU:OE1	1:A:160:LYS:NZ	2.49	0.46
1:C:85:PHE:O	1:C:89:LEU:HD12	2.15	0.46
1:B:198:GLU:O	1:B:209:SER:HA	2.16	0.46
1:C:103:ILE:HG23	1:C:180:ILE:HD12	1.97	0.46
1:B:215:GLN:HE21	1:B:215:GLN:HB2	1.58	0.46
1:A:222:ALA:CB	1:A:275:MET:HG3	2.28	0.46
1:C:28:PHE:HD2	1:C:385:GLY:HA3	1.81	0.46
1:C:227:VAL:HG22	1:C:257:LEU:HA	1.98	0.46
1:A:227:VAL:HG21	1:A:257:LEU:HD12	1.98	0.46
1:A:296:LYS:HB3	2:A:402:HOH:O	2.14	0.46
1:A:42:LEU:HD11	1:A:54:LYS:HE3	1.98	0.46
1:C:13:PHE:O	1:C:16:PHE:HB3	2.16	0.46
1:B:227:VAL:HG21	1:B:257:LEU:HD12	1.97	0.46
1:C:213:MET:HB2	1:C:213:MET:HE2	1.70	0.46
1:A:42:LEU:HD21	1:A:54:LYS:HE2	1.97	0.46
1:B:183:LYS:HD2	1:B:335:GLU:HB3	1.98	0.46
1:A:184:GLY:HA3	1:A:236:TYR:CD2	2.51	0.46
1:C:29:TYR:HB3	1:C:293:TYR:CE1	2.50	0.46
1:B:141:GLU:CD	1:B:142:GLU:H	2.19	0.45
1:A:232:LEU:HB2	1:A:363:PHE:CD2	2.51	0.45
1:A:102:LYS:CB	1:A:155:THR:HA	2.40	0.45
1:B:28:PHE:H	1:B:291:GLU:HG3	1.80	0.45
1:C:203:ASN:ND2	1:C:206:THR:HB	2.31	0.45
1:B:283:HIS:HD2	1:B:362:GLU:OE2	1.99	0.45
1:C:265:LYS:HA	1:C:265:LYS:HD2	1.72	0.45
1:A:295:LEU:HB2	1:A:299:LEU:CD2	2.46	0.45
1:A:299:LEU:HB3	1:A:304:MET:HE2	1.99	0.45
1:C:218:SER:OG	1:C:279:ARG:HD2	2.17	0.45
1:B:221:PHE:CD2	1:B:222:ALA:N	2.85	0.45
1:B:32:ILE:HB	1:B:382:LEU:HA	1.98	0.45
1:C:159:ILE:HD12	1:C:181:TYR:HB2	1.98	0.45
1:C:102:LYS:HD3	1:C:102:LYS:HA	1.76	0.45
1:C:148:ASN:CG	1:C:161:ASN:HA	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:TRP:CH2	1:B:243:MET:HG2	2.42	0.45
1:B:282:LEU:HD12	1:B:283:HIS:N	2.32	0.45
1:A:84:GLN:HB3	1:A:87:LYS:HZ1	1.82	0.45
1:B:12:MET:HE1	1:B:384:TYR:HB2	1.99	0.45
1:B:88:LEU:O	1:B:91:GLU:HB3	2.17	0.45
1:B:254:LEU:HA	1:B:257:LEU:HB3	1.98	0.45
1:B:193:GLU:C	1:B:195:THR:H	2.20	0.45
1:C:38:LEU:HB3	1:C:57:LEU:HD21	1.99	0.45
1:B:162:LEU:HD22	1:B:162:LEU:O	2.17	0.45
1:B:389:SER:HA	1:B:390:PRO:HD3	1.69	0.45
1:C:233:GLU:OE1	1:C:242:SER:HB2	2.16	0.45
1:A:380:SER:O	1:A:382:LEU:HD23	2.16	0.45
1:C:262:THR:O	1:C:265:LYS:HB2	2.17	0.45
1:B:40:MET:HE2	1:B:107:LEU:HB2	1.99	0.45
1:B:266:LEU:O	1:B:268:GLU:N	2.49	0.45
1:C:247:LEU:HD22	1:C:365:CYS:SG	2.57	0.45
1:B:90:THR:HA	1:B:93:ASN:HD22	1.81	0.45
1:C:196:LYS:H	1:C:214:ARG:CZ	2.30	0.45
1:A:224:LEU:HD23	1:A:231:VAL:CG2	2.46	0.45
1:B:110:GLU:OE2	1:B:136:PHE:N	2.50	0.45
1:C:81:VAL:C	1:C:83:HIS:N	2.68	0.45
1:B:167:ASN:N	1:B:167:ASN:HD22	2.15	0.44
1:C:23:LYS:HG3	1:C:25:ASN:H	1.82	0.44
1:B:378:THR:O	1:B:379:ASN:C	2.55	0.44
1:B:105:ASN:HD22	1:B:105:ASN:HA	1.59	0.44
1:A:188:LYS:NZ	1:A:218:SER:O	2.50	0.44
1:A:28:PHE:CE1	1:A:334:VAL:HB	2.53	0.44
1:B:12:MET:SD	1:B:384:TYR:CD1	3.11	0.44
1:A:59:PHE:N	1:A:59:PHE:CD1	2.82	0.44
1:A:92:PHE:N	1:A:92:PHE:HD2	2.11	0.44
1:C:244:ILE:N	1:C:244:ILE:HD12	2.32	0.44
1:A:262:THR:N	1:A:265:LYS:HG2	2.29	0.44
1:B:110:GLU:HA	1:B:134:VAL:O	2.18	0.44
1:B:247:LEU:HB2	1:B:363:PHE:CE1	2.53	0.44
1:A:389:SER:N	1:A:390:PRO:HD3	2.32	0.44
1:C:33:SER:OG	1:C:178:ASN:OD1	2.31	0.44
1:C:1:SER:O	1:C:4:LEU:N	2.51	0.44
1:B:15:LEU:O	1:B:18:GLN:HB2	2.18	0.44
1:A:190:PHE:CD2	1:A:213:MET:HB3	2.52	0.44
1:B:233:GLU:OE2	1:B:272:LEU:HD11	2.17	0.44
1:A:297:ASP:OD2	1:A:300:ARG:NH1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:TRP:CD1	1:A:269:TRP:N	2.83	0.44
1:B:298:THR:O	1:B:302:MET:CG	2.54	0.44
1:C:221:PHE:CG	1:C:222:ALA:N	2.86	0.44
1:A:200:PHE:HA	1:A:366:ASN:O	2.17	0.44
1:B:16:PHE:C	1:B:18:GLN:N	2.71	0.44
1:B:265:LYS:HE2	1:B:269:TRP:CZ2	2.53	0.44
1:C:338:GLU:HG2	1:C:338:GLU:H	1.35	0.44
1:C:318:THR:C	1:C:320:SER:H	2.20	0.44
1:B:168:ILE:HA	1:B:168:ILE:HD13	1.88	0.44
1:C:332:ALA:HB1	1:C:383:PHE:HE1	1.82	0.44
1:B:34:ILE:HG12	1:B:295:LEU:HD11	2.00	0.44
1:C:34:ILE:CA	1:C:178:ASN:ND2	2.73	0.44
1:B:164:PRO:HG2	1:B:167:ASN:HD21	1.83	0.44
1:A:232:LEU:CD2	1:A:282:LEU:HD22	2.48	0.44
1:B:190:PHE:CD1	1:B:215:GLN:NE2	2.86	0.44
1:C:289:VAL:HG23	1:C:334:VAL:HG12	1.99	0.44
1:C:99:TYR:CD1	1:C:100:GLU:N	2.86	0.44
1:C:196:LYS:O	1:C:214:ARG:NH2	2.51	0.44
1:C:81:VAL:HB	1:C:82:HIS:H	1.49	0.44
1:C:217:THR:HA	1:C:279:ARG:NH2	2.33	0.44
1:B:355:SER:O	1:B:356:PRO:C	2.56	0.44
1:B:125:LYS:HE3	1:B:126:PHE:CE1	2.53	0.44
1:C:334:VAL:HG22	1:C:335:GLU:H	1.83	0.44
1:A:375:GLN:O	1:A:379:ASN:N	2.51	0.44
1:C:123:ILE:HD12	1:C:130:SER:HA	2.00	0.44
1:A:143:SER:O	1:A:147:ILE:HG13	2.18	0.44
1:B:99:TYR:CA	1:B:184:GLY:HA2	2.46	0.44
1:C:21:LYS:H	1:C:21:LYS:HG2	1.45	0.44
1:A:220:HIS:HB2	1:A:233:GLU:HG2	2.00	0.44
1:B:246:LEU:HA	1:B:246:LEU:HD12	1.64	0.44
1:B:220:HIS:O	1:B:275:MET:HG2	2.18	0.44
1:C:160:LYS:HB2	1:C:161:ASN:ND2	2.33	0.44
1:A:221:PHE:CG	1:A:222:ALA:N	2.85	0.43
1:A:9:THR:O	1:A:12:MET:CG	2.66	0.43
1:A:270:THR:HG21	1:A:372:PHE:CE2	2.53	0.43
1:B:190:PHE:O	1:B:338:GLU:HB2	2.18	0.43
1:B:244:ILE:HD13	1:B:372:PHE:CZ	2.53	0.43
1:C:374:ARG:HD2	1:C:379:ASN:HA	2.00	0.43
1:C:44:GLY:O	1:C:314:LEU:HA	2.18	0.43
1:A:190:PHE:HB2	1:A:338:GLU:CA	2.48	0.43
1:C:40:MET:HE1	1:C:107:LEU:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASN:N	1:B:329:LEU:O	2.50	0.43
1:B:55:LYS:HG3	1:B:56:VAL:H	1.82	0.43
1:C:99:TYR:HD1	1:C:100:GLU:N	2.15	0.43
1:C:381:ILE:CD1	1:C:381:ILE:H	2.20	0.43
1:C:185:GLN:CD	1:C:339:GLU:HB3	2.37	0.43
1:C:48:ASN:O	1:C:51:GLN:HB3	2.18	0.43
1:B:345:ALA:O	1:B:346:ALA:HB2	2.18	0.43
1:A:134:VAL:HG22	1:A:143:SER:OG	2.17	0.43
1:C:306:ASP:O	1:C:309:ASN:OD1	2.36	0.43
1:C:174:LEU:HB3	1:C:325:LEU:HA	2.00	0.43
1:B:244:ILE:HD11	1:B:374:ARG:NE	2.29	0.43
1:B:220:HIS:CE1	1:B:277:GLU:HG3	2.54	0.43
1:C:144:ARG:NH2	1:C:165:GLU:HG2	2.34	0.43
1:C:216:TYR:HA	1:C:281:ASP:HA	2.00	0.43
1:B:40:MET:O	1:B:43:LEU:HB2	2.18	0.43
1:A:374:ARG:HD2	1:A:379:ASN:HA	2.01	0.43
1:B:254:LEU:O	1:B:257:LEU:N	2.51	0.43
1:A:111:LYS:HE2	1:A:111:LYS:HB2	1.77	0.43
1:B:102:LYS:HB2	1:B:181:TYR:HB3	2.01	0.43
1:B:28:PHE:CZ	1:B:383:PHE:CD1	3.07	0.43
1:B:283:HIS:HB2	1:B:364:HIS:HA	2.01	0.43
1:C:92:PHE:C	1:C:94:LYS:H	2.21	0.43
1:A:206:THR:HG22	1:A:207:TYR:N	2.34	0.43
1:A:244:ILE:N	1:A:244:ILE:HD12	2.33	0.43
1:A:186:TRP:O	1:A:340:GLY:HA3	2.19	0.43
1:C:203:ASN:OD1	1:C:206:THR:HB	2.18	0.43
1:C:224:LEU:HD12	1:C:226:ASP:OD2	2.18	0.43
1:A:261:LEU:HD22	1:A:266:LEU:CD2	2.48	0.43
1:B:154:GLN:O	1:B:154:GLN:HG3	2.19	0.43
1:B:186:TRP:CZ3	1:B:234:ILE:HG22	2.54	0.43
1:B:37:ALA:HB2	1:B:105:ASN:ND2	2.34	0.43
1:A:219:PHE:HB2	1:A:232:LEU:HD11	2.01	0.43
1:A:27:ILE:O	1:A:385:GLY:CA	2.65	0.43
1:B:38:LEU:HD12	1:B:57:LEU:HD21	2.00	0.43
1:A:40:MET:HE2	1:A:107:LEU:HB2	2.01	0.43
1:C:190:PHE:HB2	1:C:338:GLU:CA	2.49	0.43
1:B:86:GLN:NE2	1:B:125:LYS:HG3	2.34	0.43
1:B:161:ASN:N	1:B:161:ASN:ND2	2.67	0.43
1:A:15:LEU:CD1	1:A:302:MET:HE1	2.44	0.43
1:C:106:LYS:HB2	1:C:150:TRP:CH2	2.54	0.43
1:B:50:ALA:O	1:B:54:LYS:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:GLU:HG3	1:C:198:GLU:H	1.83	0.43
1:A:157:GLU:HG2	1:A:160:LYS:HZ2	1.83	0.43
1:B:235:PRO:CA	1:B:242:SER:HB3	2.49	0.42
1:A:190:PHE:HB2	1:A:338:GLU:HA	2.01	0.42
1:C:52:GLN:H	1:C:52:GLN:HG2	1.47	0.42
1:B:378:THR:C	1:B:379:ASN:OD1	2.57	0.42
1:B:86:GLN:NE2	1:B:126:PHE:HA	2.34	0.42
1:A:220:HIS:CD2	1:A:275:MET:HB3	2.53	0.42
1:C:94:LYS:HG2	1:C:96:THR:HB	2.01	0.42
1:A:364:HIS:CD2	1:A:366:ASN:ND2	2.87	0.42
1:A:28:PHE:CZ	1:A:383:PHE:CD1	3.07	0.42
1:B:321:ARG:HB3	1:B:321:ARG:HE	1.61	0.42
1:B:262:THR:OG1	1:B:265:LYS:HD3	2.19	0.42
1:C:185:GLN:O	1:C:237:LYS:N	2.49	0.42
1:A:168:ILE:HD13	1:A:168:ILE:HA	1.85	0.42
1:C:38:LEU:HB2	1:C:57:LEU:HD21	2.01	0.42
1:B:34:ILE:HA	1:B:178:ASN:HD21	1.84	0.42
1:C:30:SER:CB	1:C:180:ILE:HG21	2.50	0.42
1:B:27:ILE:O	1:B:385:GLY:HA2	2.19	0.42
1:B:174:LEU:HD21	1:B:317:MET:HE3	2.01	0.42
1:B:309:ASN:O	1:B:324:VAL:CG1	2.66	0.42
1:B:38:LEU:CB	1:B:57:LEU:HD21	2.49	0.42
1:B:224:LEU:HB2	1:B:229:ALA:O	2.19	0.42
1:C:189:LYS:HG2	1:C:190:PHE:H	1.82	0.42
1:A:225:GLU:H	1:A:225:GLU:HG3	1.58	0.42
1:B:212:MET:HE1	1:B:365:CYS:O	2.20	0.42
1:A:218:SER:HB2	1:A:277:GLU:OE2	2.19	0.42
1:A:307:ILE:O	1:A:324:VAL:HG13	2.18	0.42
1:B:46:LYS:HG3	1:B:315:SER:HB2	2.01	0.42
1:B:97:ASP:O	1:B:99:TYR:N	2.52	0.42
1:A:266:LEU:O	1:A:268:GLU:N	2.52	0.42
1:B:290:GLU:HG3	1:B:290:GLU:O	2.19	0.42
1:C:295:LEU:HB2	1:C:299:LEU:HD23	2.01	0.42
1:B:368:PRO:HA	1:B:387:PHE:O	2.19	0.42
1:A:185:GLN:HB3	1:A:340:GLY:HA2	2.00	0.42
1:A:24:GLU:HA	1:A:386:ARG:HH12	1.84	0.42
1:B:86:GLN:HE22	1:B:125:LYS:HG3	1.85	0.42
1:B:175:VAL:HG12	1:B:175:VAL:O	2.19	0.42
1:B:46:LYS:O	1:B:313:ASP:HB3	2.19	0.42
1:C:198:GLU:HG3	1:C:199:LYS:N	2.31	0.42
1:C:189:LYS:HA	1:C:340:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ASN:HA	1:C:51:GLN:HB3	2.01	0.42
1:A:254:LEU:HA	1:A:257:LEU:HB3	2.00	0.42
1:B:162:LEU:CD1	1:B:329:LEU:HB3	2.49	0.42
1:B:159:ILE:HD11	1:B:180:ILE:O	2.19	0.42
1:C:32:ILE:HD12	1:C:32:ILE:HA	1.89	0.42
1:C:44:GLY:HA3	1:C:317:MET:CG	2.38	0.42
1:B:84:GLN:CD	1:B:84:GLN:H	2.17	0.42
1:C:98:ALA:HA	1:C:237:LYS:HD2	2.02	0.42
1:A:148:ASN:O	1:A:151:VAL:N	2.52	0.42
1:C:232:LEU:HB2	1:C:363:PHE:CE2	2.54	0.42
1:A:367:HIS:HB2	1:A:368:PRO:CD	2.49	0.42
1:A:84:GLN:H	1:A:84:GLN:CD	2.21	0.42
1:B:120:LEU:HD23	1:B:131:VAL:HG23	2.02	0.42
1:B:196:LYS:CD	1:B:196:LYS:N	2.77	0.42
1:B:44:GLY:CA	1:B:317:MET:HG3	2.48	0.42
1:B:111:LYS:HG3	1:B:111:LYS:H	1.56	0.42
1:C:14:ASP:O	1:C:18:GLN:HG2	2.20	0.42
1:B:299:LEU:HG	1:B:304:MET:HE2	2.02	0.42
1:B:382:LEU:HD12	1:B:383:PHE:CD2	2.54	0.42
1:B:92:PHE:CD2	1:B:92:PHE:N	2.86	0.42
1:A:298:THR:HG22	1:A:302:MET:CE	2.50	0.42
1:B:27:ILE:HG13	1:B:27:ILE:O	2.20	0.42
1:B:32:ILE:HA	1:B:32:ILE:HD12	1.93	0.42
1:B:32:ILE:O	1:B:33:SER:C	2.58	0.42
1:C:34:ILE:CD1	1:C:295:LEU:HD11	2.50	0.42
1:A:255:GLN:HG2	1:A:259:GLU:OE2	2.19	0.42
1:C:37:ALA:O	1:C:176:LEU:HD21	2.20	0.42
1:B:281:ASP:O	1:B:362:GLU:HA	2.19	0.41
1:A:381:ILE:CG2	1:A:383:PHE:O	2.68	0.41
1:A:2:ASN:C	1:A:4:LEU:N	2.72	0.41
1:A:101:LEU:HB3	1:A:182:PHE:HD2	1.84	0.41
1:C:186:TRP:CZ3	1:C:234:ILE:HG22	2.55	0.41
1:C:289:VAL:HG23	1:C:334:VAL:CG1	2.50	0.41
1:A:28:PHE:HE1	1:A:334:VAL:HB	1.85	0.41
1:B:8:ASN:ND2	1:B:381:ILE:O	2.53	0.41
1:A:243:MET:HA	1:A:373:ILE:HA	2.02	0.41
1:B:317:MET:HE2	1:B:317:MET:HB3	1.95	0.41
1:B:44:GLY:O	1:B:317:MET:HG3	2.20	0.41
1:A:164:PRO:HD2	1:A:167:ASN:OD1	2.19	0.41
1:C:261:LEU:HA	1:C:261:LEU:HD23	1.66	0.41
1:B:244:ILE:CG2	1:B:245:VAL:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:HB3	1:A:27:ILE:CG2	2.50	0.41
1:A:198:GLU:O	1:A:209:SER:HA	2.21	0.41
1:A:299:LEU:HD13	1:A:299:LEU:HA	1.85	0.41
1:A:183:LYS:HD2	1:A:335:GLU:HB3	2.02	0.41
1:C:54:LYS:O	1:C:59:PHE:N	2.47	0.41
1:C:157:GLU:O	1:C:160:LYS:HD3	2.20	0.41
1:C:286:ARG:HH11	1:C:338:GLU:HG2	1.85	0.41
1:C:27:ILE:CG1	1:C:27:ILE:O	2.68	0.41
1:B:55:LYS:CG	1:B:56:VAL:N	2.83	0.41
1:C:56:VAL:CG2	1:C:304:MET:HG3	2.45	0.41
1:C:43:LEU:HD23	1:C:43:LEU:HA	1.90	0.41
1:B:227:VAL:HG23	1:B:256:LYS:HD3	2.02	0.41
1:C:369:PHE:HE1	1:C:371:PHE:HB3	1.86	0.41
1:C:101:LEU:HD12	1:C:101:LEU:O	2.20	0.41
1:A:203:ASN:OD1	1:A:206:THR:N	2.51	0.41
1:A:28:PHE:H	1:A:291:GLU:HG3	1.85	0.41
1:C:200:PHE:O	1:C:207:TYR:HA	2.21	0.41
1:A:147:ILE:HG13	1:A:147:ILE:H	1.42	0.41
1:B:162:LEU:HD21	1:B:331:LYS:HB2	2.03	0.41
1:A:80:ASN:HD22	1:A:81:VAL:HG12	1.79	0.41
1:A:189:LYS:HG2	1:A:190:PHE:H	1.86	0.41
1:A:298:THR:HG22	1:A:302:MET:HE3	2.02	0.41
1:A:188:LYS:HE3	1:A:219:PHE:CE1	2.55	0.41
1:A:81:VAL:CG1	1:A:82:HIS:H	2.20	0.41
1:A:84:GLN:HB3	1:A:87:LYS:HZ2	1.86	0.41
1:C:30:SER:HB2	1:C:180:ILE:HG21	2.03	0.41
1:C:374:ARG:HA	1:C:381:ILE:HA	2.03	0.41
1:C:240:ASP:O	1:C:241:LEU:HD23	2.21	0.41
1:B:12:MET:HE1	1:B:384:TYR:CB	2.51	0.41
1:B:123:ILE:HG13	1:B:124:LYS:N	2.35	0.41
1:B:91:GLU:O	1:B:94:LYS:HB3	2.21	0.41
1:B:119:TYR:CZ	1:B:317:MET:HG2	2.56	0.41
1:C:338:GLU:O	1:C:339:GLU:C	2.59	0.41
1:A:32:ILE:CG2	1:A:33:SER:N	2.84	0.41
1:A:32:ILE:HG23	1:A:33:SER:N	2.36	0.41
1:B:350:VAL:HG12	1:B:351:GLY:N	2.36	0.41
1:A:254:LEU:HD23	1:A:255:GLN:N	2.36	0.41
1:B:371:PHE:N	1:B:371:PHE:CD1	2.89	0.41
1:B:159:ILE:HD12	1:B:181:TYR:HB2	2.04	0.41
1:B:231:VAL:HG23	1:B:246:LEU:HD11	2.03	0.41
1:A:120:LEU:O	1:A:124:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG11	1:A:257:LEU:HD13	2.02	0.41
1:B:198:GLU:HB2	1:B:212:MET:HB3	2.03	0.40
1:B:219:PHE:HB3	1:B:232:LEU:HD11	2.02	0.40
1:C:162:LEU:C	1:C:163:ILE:HG13	2.42	0.40
1:C:163:ILE:HG23	1:C:167:ASN:HB2	2.03	0.40
1:B:4:LEU:HD22	1:B:4:LEU:C	2.41	0.40
1:B:147:ILE:CG2	1:B:177:VAL:HG21	2.51	0.40
1:A:227:VAL:O	1:A:228:GLN:HB2	2.21	0.40
1:C:107:LEU:HA	1:C:107:LEU:HD13	1.85	0.40
1:B:345:ALA:HB3	2:B:414:HOH:O	2.21	0.40
1:B:197:GLU:HG3	1:B:198:GLU:H	1.86	0.40
1:A:13:PHE:O	1:A:16:PHE:HB3	2.21	0.40
1:A:12:MET:HE3	1:A:381:ILE:HG21	2.04	0.40
1:B:4:LEU:HD22	1:B:4:LEU:O	2.21	0.40
1:A:150:TRP:CZ2	1:A:154:GLN:HG3	2.55	0.40
1:B:224:LEU:HB3	1:B:227:VAL:HG12	2.02	0.40
1:C:215:GLN:HG3	1:C:217:THR:HG22	2.02	0.40
1:A:263:ALA:N	2:A:408:HOH:O	2.54	0.40
1:B:285:PRO:HD3	1:B:365:CYS:HB2	2.02	0.40
1:C:101:LEU:HA	1:C:181:TYR:O	2.21	0.40
1:C:200:PHE:CD1	1:C:390:PRO:HD2	2.56	0.40
1:B:110:GLU:HG3	1:B:112:THR:HG23	2.04	0.40
1:B:181:TYR:C	1:B:181:TYR:CD2	2.95	0.40
1:B:185:GLN:N	1:B:236:TYR:HD2	2.19	0.40
1:B:28:PHE:CE1	1:B:334:VAL:HB	2.57	0.40
1:B:92:PHE:HB3	1:B:101:LEU:CD2	2.40	0.40
1:A:201:TRP:O	1:A:368:PRO:CD	2.67	0.40
1:A:361:GLU:HG3	1:A:362:GLU:N	2.34	0.40
1:B:188:LYS:O	1:B:189:LYS:O	2.39	0.40
1:A:242:SER:OG	1:A:376:ASN:ND2	2.52	0.40
1:C:46:LYS:NZ	1:C:46:LYS:HB3	2.37	0.40
1:A:23:LYS:HZ1	1:A:25:ASN:HB2	1.86	0.40
1:A:288:LYS:HB3	1:A:335:GLU:CG	2.49	0.40
1:A:118:GLU:O	1:A:121:ASP:HB2	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	344/401 (86%)	271 (79%)	63 (18%)	10 (3%)	6 14
1	B	367/401 (92%)	277 (76%)	64 (17%)	26 (7%)	1 2
1	C	344/401 (86%)	276 (80%)	60 (17%)	8 (2%)	8 20
All	All	1055/1203 (88%)	824 (78%)	187 (18%)	44 (4%)	3 7

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	VAL
1	A	112	THR
1	A	137	ALA
1	B	128	GLN
1	B	189	LYS
1	B	342	GLU
1	B	344	ALA
1	B	345	ALA
1	B	346	ALA
1	C	128	GLN
1	C	189	LYS
1	A	189	LYS
1	A	310	GLY
1	B	17	GLN
1	B	307	ILE
1	C	376	ASN
1	A	267	MET
1	B	95	SER
1	B	98	ALA
1	B	100	GLU
1	B	192	LYS
1	B	267	MET
1	B	295	LEU
1	B	300	ARG

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Mol	Chain	Res	Type
1	C	192	LYS
1	C	267	MET
1	A	175	VAL
1	A	307	ILE
1	B	25	ASN
1	B	112	THR
1	B	137	ALA
1	B	157	GLU
1	B	296	LYS
1	C	100	GLU
1	C	295	LEU
1	C	296	LYS
1	A	295	LEU
1	A	372	PHE
1	B	148	ASN
1	B	175	VAL
1	B	197	GLU
1	B	347	THR
1	B	379	ASN
1	B	53	ILE

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	319/356 (90%)	221 (69%)	98 (31%)	0 1
1	B	332/356 (93%)	224 (68%)	108 (32%)	0 0
1	C	319/356 (90%)	229 (72%)	90 (28%)	0 1
All	All	970/1068 (91%)	674 (70%)	296 (30%)	0 1

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	3	SER

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Mol	Chain	Res	Type
1	A	4	LEU
1	A	12	MET
1	A	15	LEU
1	A	20	ARG
1	A	22	SER
1	A	27	ILE
1	A	33	SER
1	A	40	MET
1	A	46	LYS
1	A	51	GLN
1	A	52	GLN
1	A	55	LYS
1	A	57	LEU
1	A	84	GLN
1	A	85	PHE
1	A	87	LYS
1	A	89	LEU
1	A	92	PHE
1	A	94	LYS
1	A	95	SER
1	A	100	GLU
1	A	101	LEU
1	A	106	LYS
1	A	107	LEU
1	A	111	LYS
1	A	114	LEU
1	A	118	GLU
1	A	124	LYS
1	A	130	SER
1	A	132	GLU
1	A	133	SER
1	A	147	ILE
1	A	151	VAL
1	A	160	LYS
1	A	162	LEU
1	A	167	ASN
1	A	168	ILE
1	A	170	SER
1	A	173	THR
1	A	174	LEU
1	A	176	LEU
1	A	187	GLU

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Mol	Chain	Res	Type
1	A	191	ASN
1	A	192	LYS
1	A	196	LYS
1	A	197	GLU
1	A	205	ASN
1	A	208	LYS
1	A	214	ARG
1	A	216	TYR
1	A	218	SER
1	A	220	HIS
1	A	224	LEU
1	A	225	GLU
1	A	227	VAL
1	A	233	GLU
1	A	237	LYS
1	A	239	LYS
1	A	240	ASP
1	A	241	LEU
1	A	243	MET
1	A	250	GLU
1	A	252	ASP
1	A	254	LEU
1	A	256	LYS
1	A	259	GLU
1	A	265	LYS
1	A	266	LEU
1	A	267	MET
1	A	275	MET
1	A	276	ARG
1	A	277	GLU
1	A	279	ARG
1	A	286	ARG
1	A	289	VAL
1	A	290	GLU
1	A	295	LEU
1	A	299	LEU
1	A	300	ARG
1	A	301	THR
1	A	307	ILE
1	A	325	LEU
1	A	326	SER
1	A	335	GLU

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Mol	Chain	Res	Type
1	A	338	GLU
1	A	339	GLU
1	A	360	ASN
1	A	362	GLU
1	A	366	ASN
1	A	370	LEU
1	A	374	ARG
1	A	377	LYS
1	A	378	THR
1	A	379	ASN
1	A	382	LEU
1	A	384	TYR
1	B	2	ASN
1	B	4	LEU
1	B	12	MET
1	B	20	ARG
1	B	22	SER
1	B	24	GLU
1	B	26	ASN
1	B	30	SER
1	B	35	THR
1	B	36	SER
1	B	41	VAL
1	B	46	LYS
1	B	54	LYS
1	B	55	LYS
1	B	57	LEU
1	B	60	ASP
1	B	81	VAL
1	B	85	PHE
1	B	87	LYS
1	B	89	LEU
1	B	94	LYS
1	B	100	GLU
1	B	105	ASN
1	B	107	LEU
1	B	111	LYS
1	B	118	GLU
1	B	124	LYS
1	B	125	LYS
1	B	130	SER
1	B	132	GLU

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Mol	Chain	Res	Type
1	B	141	GLU
1	B	143	SER
1	B	144	ARG
1	B	147	ILE
1	B	151	VAL
1	B	160	LYS
1	B	161	ASN
1	B	162	LEU
1	B	165	GLU
1	B	170	SER
1	B	173	THR
1	B	187	GLU
1	B	191	ASN
1	B	192	LYS
1	B	193	GLU
1	B	196	LYS
1	B	197	GLU
1	B	198	GLU
1	B	214	ARG
1	B	215	GLN
1	B	216	TYR
1	B	217	THR
1	B	218	SER
1	B	220	HIS
1	B	225	GLU
1	B	230	LYS
1	B	233	GLU
1	B	240	ASP
1	B	241	LEU
1	B	242	SER
1	B	243	MET
1	B	246	LEU
1	B	250	GLU
1	B	251	ILE
1	B	252	ASP
1	B	255	GLN
1	B	260	LYS
1	B	264	GLU
1	B	265	LYS
1	B	266	LEU
1	B	267	MET
1	B	268	GLU

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Mol	Chain	Res	Type
1	B	270	THR
1	B	271	SER
1	B	275	MET
1	B	276	ARG
1	B	277	GLU
1	B	282	LEU
1	B	286	ARG
1	B	289	VAL
1	B	290	GLU
1	B	295	LEU
1	B	299	LEU
1	B	300	ARG
1	B	301	THR
1	B	305	VAL
1	B	307	ILE
1	B	315	SER
1	B	321	ARG
1	B	324	VAL
1	B	325	LEU
1	B	326	SER
1	B	333	PHE
1	B	334	VAL
1	B	335	GLU
1	B	339	GLU
1	B	347	THR
1	B	354	SER
1	B	361	GLU
1	B	362	GLU
1	B	366	ASN
1	B	374	ARG
1	B	378	THR
1	B	379	ASN
1	B	380	SER
1	B	382	LEU
1	B	386	ARG
1	B	388	SER
1	C	1	SER
1	C	2	ASN
1	C	3	SER
1	C	4	LEU
1	C	6	GLU
1	C	12	MET

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Mol	Chain	Res	Type
1	C	20	ARG
1	C	21	LYS
1	C	23	LYS
1	C	24	GLU
1	C	35	THR
1	C	46	LYS
1	C	47	ASP
1	C	51	GLN
1	C	52	GLN
1	C	57	LEU
1	C	81	VAL
1	C	85	PHE
1	C	87	LYS
1	C	89	LEU
1	C	95	SER
1	C	100	GLU
1	C	106	LYS
1	C	107	LEU
1	C	118	GLU
1	C	124	LYS
1	C	125	LYS
1	C	130	SER
1	C	141	GLU
1	C	144	ARG
1	C	147	ILE
1	C	151	VAL
1	C	154	GLN
1	C	160	LYS
1	C	162	LEU
1	C	167	ASN
1	C	170	SER
1	C	173	THR
1	C	187	GLU
1	C	191	ASN
1	C	193	GLU
1	C	194	ASP
1	C	197	GLU
1	C	198	GLU
1	C	214	ARG
1	C	215	GLN
1	C	217	THR
1	C	218	SER

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Mol	Chain	Res	Type
1	C	220	HIS
1	C	224	LEU
1	C	226	ASP
1	C	227	VAL
1	C	233	GLU
1	C	240	ASP
1	C	241	LEU
1	C	243	MET
1	C	252	ASP
1	C	254	LEU
1	C	255	GLN
1	C	256	LYS
1	C	259	GLU
1	C	260	LYS
1	C	261	LEU
1	C	265	LYS
1	C	266	LEU
1	C	267	MET
1	C	268	GLU
1	C	270	THR
1	C	275	MET
1	C	282	LEU
1	C	289	VAL
1	C	299	LEU
1	C	305	VAL
1	C	307	ILE
1	C	311	ASP
1	C	315	SER
1	C	325	LEU
1	C	326	SER
1	C	333	PHE
1	C	335	GLU
1	C	338	GLU
1	C	366	ASN
1	C	370	LEU
1	C	374	ARG
1	C	377	LYS
1	C	378	THR
1	C	379	ASN
1	C	382	LEU
1	C	386	ARG
1	C	389	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	51	GLN
1	A	80	ASN
1	A	105	ASN
1	A	161	ASN
1	A	178	ASN
1	A	215	GLN
1	A	220	HIS
1	A	228	GLN
1	A	330	HIS
1	A	366	ASN
1	B	25	ASN
1	B	86	GLN
1	B	93	ASN
1	B	105	ASN
1	B	161	ASN
1	B	167	ASN
1	B	220	HIS
1	B	283	HIS
1	B	330	HIS
1	B	366	ASN
1	B	376	ASN
1	C	2	ASN
1	C	25	ASN
1	C	51	GLN
1	C	93	ASN
1	C	105	ASN
1	C	154	GLN
1	C	156	ASN
1	C	161	ASN
1	C	167	ASN
1	C	178	ASN
1	C	215	GLN
1	C	220	HIS
1	C	283	HIS
1	C	330	HIS
1	C	366	ASN

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	350/401 (87%)	0.15	5 (1%)	78 77	23, 68, 97, 100	0
1	B	371/401 (92%)	0.07	2 (0%)	91 93	17, 61, 95, 100	0
1	C	350/401 (87%)	0.19	5 (1%)	78 77	26, 68, 97, 100	0
All	All	1071/1203 (89%)	0.14	12 (1%)	82 83	17, 66, 97, 100	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169	GLY	3.8
1	C	168	ILE	3.4
1	A	267	MET	3.1
1	A	92	PHE	2.8
1	B	168	ILE	2.8
1	A	85	PHE	2.2
1	C	140	PRO	2.2
1	B	169	GLY	2.1
1	C	269	TRP	2.1
1	A	89	LEU	2.1
1	C	390	PRO	2.1
1	A	23	LYS	2.1

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.