Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 01:39 AM GMT

PDB ID	:	2DU7
Title	:	Crystal structure of Methanococcus jannacshii O-phosphoseryl-tRNA synthetase
Authors	:	Fukunaga, R.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-07-20
Resolution	:	3.60 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:

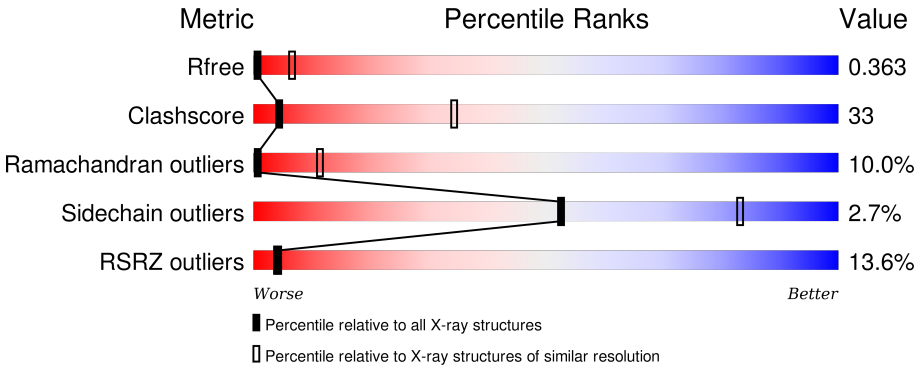
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	549	14% 45% 45% 7% .
1	B	549	11% 46% 46% 7% .
1	C	549	12% 45% 46% 7% .
1	D	549	15% 46% 46% 7% .

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 17516 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 O-phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4379	2826	727	807	19			
1	B	539	Total	C	N	O	S	0	0	0
			4379	2826	727	807	19			
1	C	539	Total	C	N	O	S	0	0	0
			4379	2826	727	807	19			
1	D	539	Total	C	N	O	S	0	0	0
			4379	2826	727	807	19			

3 Residue-property plots (i)

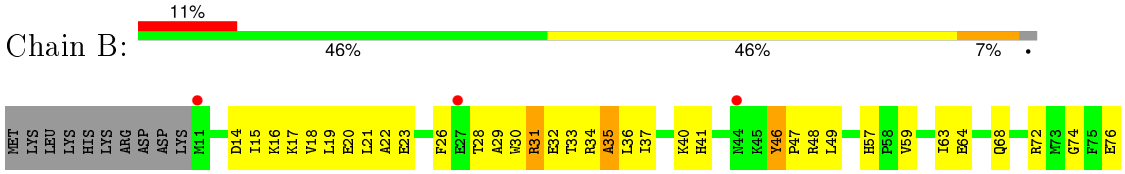
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

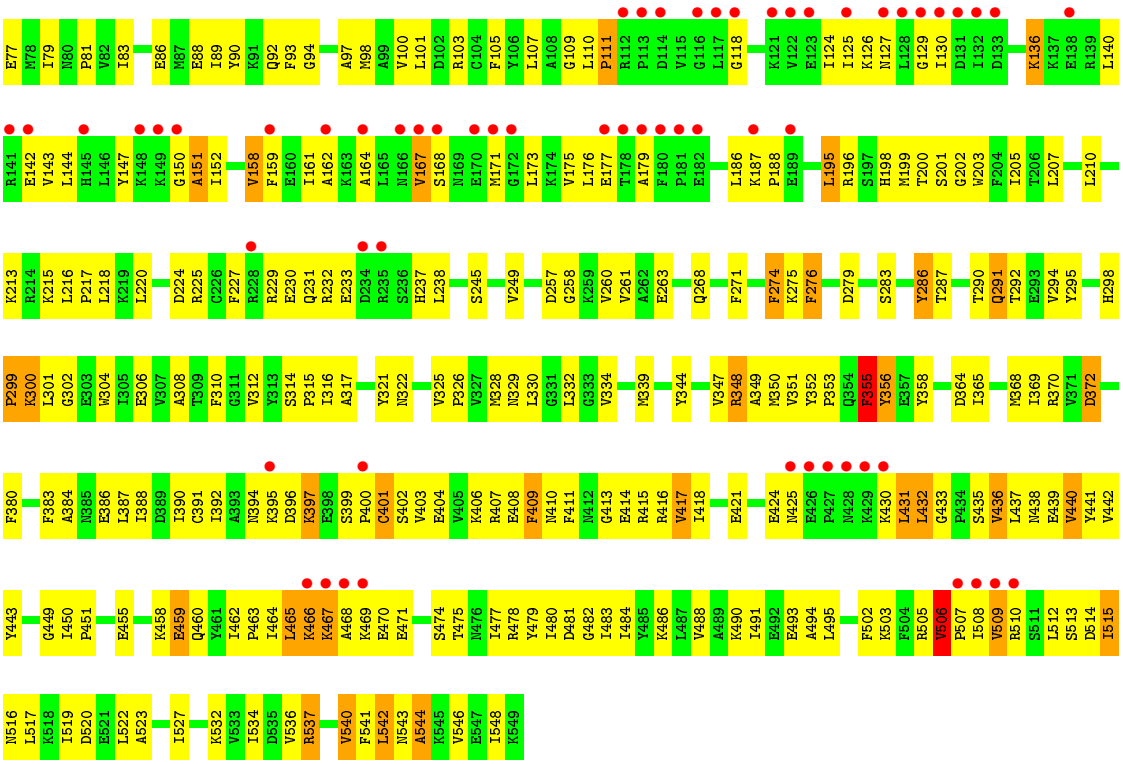
- Molecule 1: O-phosphoseryl-tRNA synthetase

Chain A:

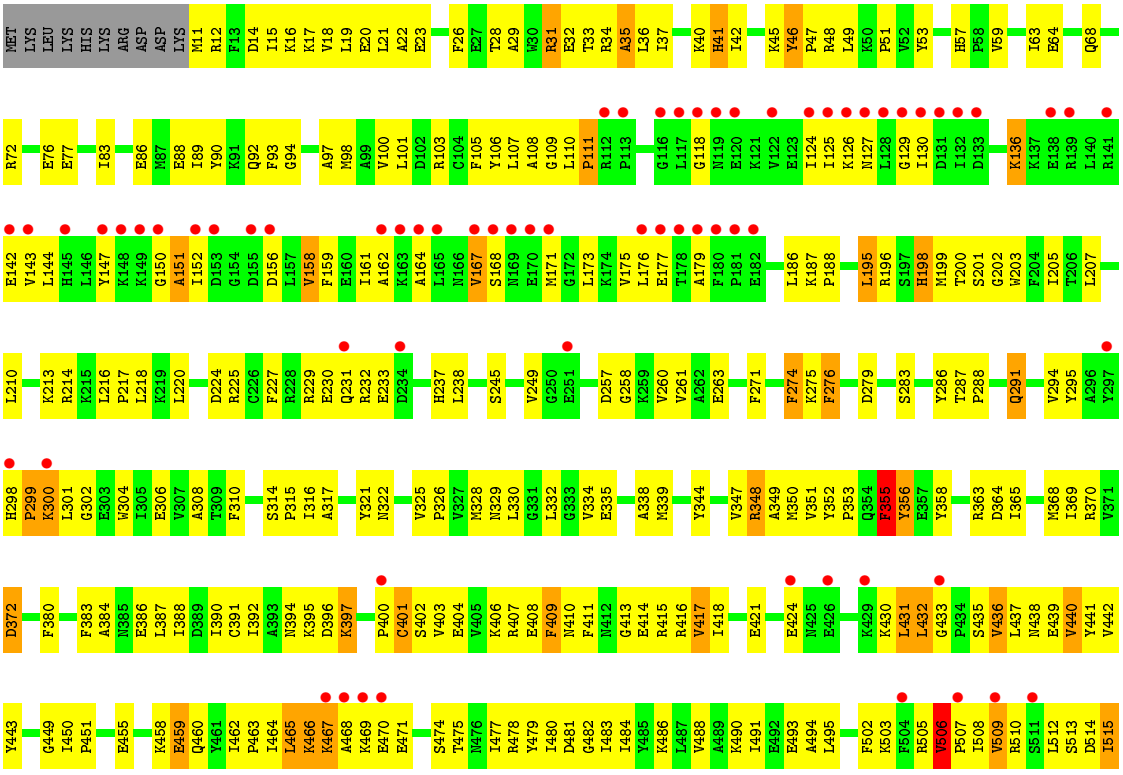
- Molecule 1: O-phosphoseryl-tRNA synthetase

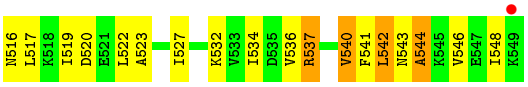
Chain B:



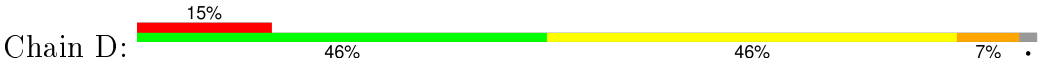


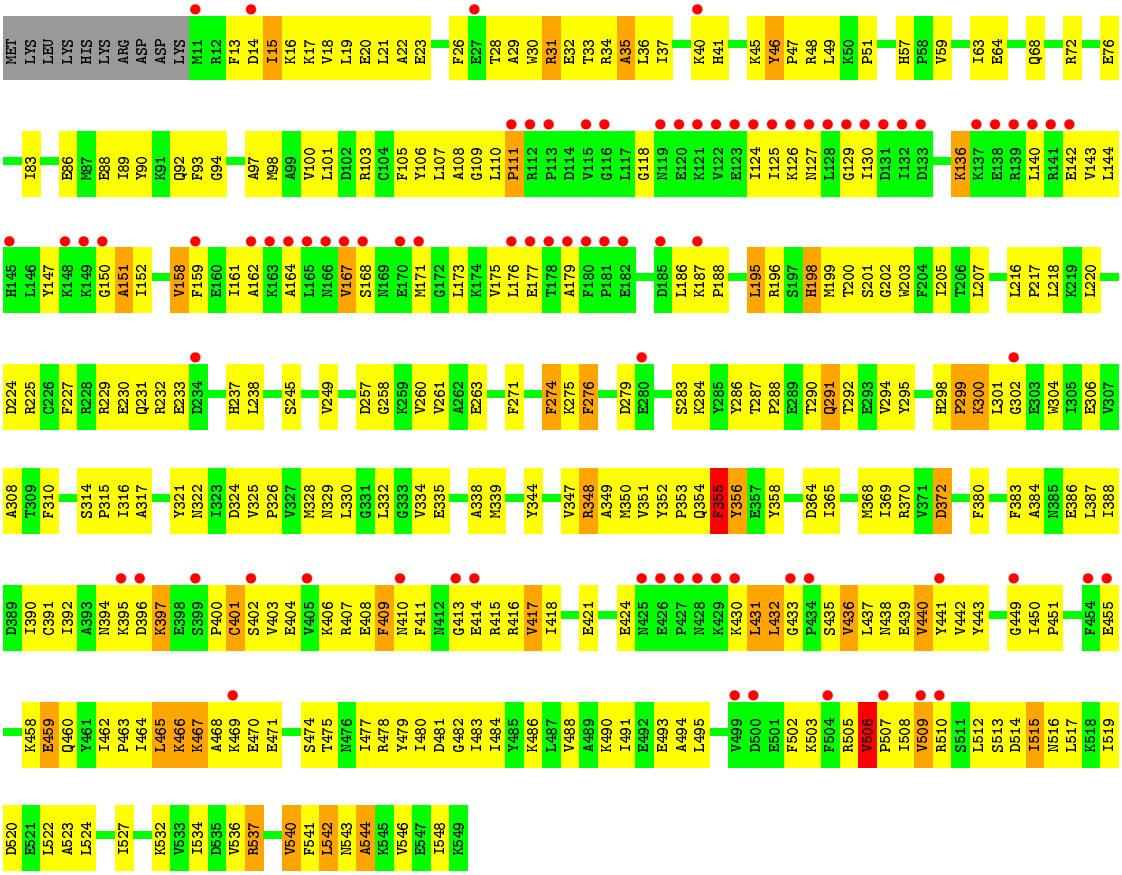
• Molecule 1: O-phosphoseryl-tRNA synthetase





• Molecule 1: O-phosphoseryl-tRNA synthetase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	196.35Å 299.45Å 125.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.79 – 3.60 19.79 – 3.60	Depositor EDS
% Data completeness (in resolution range)	97.5 (19.79-3.60) 97.6 (19.79-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 3.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.330 , 0.387 0.314 , 0.363	Depositor DCC
R_{free} test set	4236 reflections (10.08%)	DCC
Wilson B-factor (Å^2)	118.1	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 101.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 42030 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	17516	wwPDB-VP
Average B, all atoms (Å^2)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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	0.26	0/4468	0.48	0/6023
1	B	0.27	0/4468	0.48	0/6023
1	C	0.27	0/4468	0.48	0/6023
1	D	0.26	0/4468	0.48	0/6023
All	All	0.27	0/17872	0.48	0/24092

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	4379	0	4462	326	2
1	B	4379	0	4462	318	0
1	C	4379	0	4462	299	0
1	D	4379	0	4462	311	0
All	All	17516	0	17848	1161	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 33.

All (1161) 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:28:THR:HA	1:A:31:ARG:HE	1.06	1.17
1:B:28:THR:HA	1:B:31:ARG:HE	1.06	1.11
1:C:28:THR:HA	1:C:31:ARG:HE	1.06	1.10
1:D:28:THR:HA	1:D:31:ARG:HE	1.06	1.07
1:D:31:ARG:H	1:D:31:ARG:HD3	1.18	1.07
1:D:506:VAL:HG23	1:D:507:PRO:HD3	1.38	1.06
1:C:31:ARG:H	1:C:31:ARG:HD3	1.18	1.05
1:A:506:VAL:HG23	1:A:507:PRO:HD3	1.39	1.04
1:B:31:ARG:H	1:B:31:ARG:HD3	1.19	1.03
1:A:31:ARG:HD3	1:A:31:ARG:H	1.18	1.02
1:C:506:VAL:HG23	1:C:507:PRO:HD3	1.40	1.01
1:B:506:VAL:HG23	1:B:507:PRO:HD3	1.39	0.98
1:A:283:SER:H	1:A:291:GLN:HE22	1.11	0.95
1:A:158:VAL:HG13	1:A:159:PHE:H	1.33	0.94
1:C:283:SER:H	1:C:291:GLN:HE22	1.12	0.93
1:D:28:THR:HA	1:D:31:ARG:NE	1.85	0.92
1:B:68:GLN:HE22	1:D:72:ARG:HH11	1.16	0.92
1:A:28:THR:HA	1:A:31:ARG:NE	1.85	0.92
1:C:28:THR:HA	1:C:31:ARG:NE	1.85	0.92
1:D:158:VAL:HG13	1:D:159:PHE:H	1.33	0.92
1:A:354:GLN:HB3	1:B:210:LEU:HD13	1.50	0.91
1:B:28:THR:HA	1:B:31:ARG:NE	1.85	0.91
1:C:158:VAL:HG13	1:C:159:PHE:H	1.33	0.91
1:B:283:SER:H	1:B:291:GLN:HE22	1.12	0.90
1:B:158:VAL:HG13	1:B:159:PHE:H	1.33	0.90
1:A:161:ILE:HG12	1:A:167:VAL:HG11	1.55	0.89
1:B:161:ILE:HG12	1:B:167:VAL:HG11	1.55	0.89
1:D:283:SER:H	1:D:291:GLN:HE22	1.12	0.89
1:C:161:ILE:HG12	1:C:167:VAL:HG11	1.56	0.88
1:B:274:PHE:HD1	1:B:275:LYS:H	1.22	0.88
1:D:161:ILE:HG12	1:D:167:VAL:HG11	1.56	0.87
1:C:210:LEU:HD13	1:D:354:GLN:HB3	1.56	0.87
1:C:395:LYS:HG2	1:C:396:ASP:H	1.41	0.86
1:C:274:PHE:HD1	1:C:275:LYS:H	1.22	0.86
1:A:395:LYS:HG2	1:A:396:ASP:H	1.40	0.86
1:B:395:LYS:HG2	1:B:396:ASP:H	1.40	0.85
1:A:30:TRP:CZ2	1:D:288:PRO:HG3	2.11	0.85
1:A:274:PHE:HD1	1:A:275:LYS:H	1.23	0.84
1:D:436:VAL:HB	1:D:480:ILE:HG23	1.59	0.84
1:C:436:VAL:HB	1:C:480:ILE:HG23	1.60	0.84
1:D:395:LYS:HG2	1:D:396:ASP:H	1.40	0.84
1:B:436:VAL:HB	1:B:480:ILE:HG23	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:PHE:HD1	1:D:275:LYS:H	1.23	0.83
1:A:97:ALA:HA	1:A:100:VAL:HG12	1.60	0.83
1:D:89:ILE:HG21	1:D:101:LEU:HD21	1.61	0.83
1:B:97:ALA:HA	1:B:100:VAL:HG12	1.61	0.83
1:A:436:VAL:HB	1:A:480:ILE:HG23	1.59	0.82
1:D:97:ALA:HA	1:D:100:VAL:HG12	1.60	0.82
1:C:89:ILE:HG21	1:C:101:LEU:HD21	1.61	0.82
1:C:97:ALA:HA	1:C:100:VAL:HG12	1.61	0.81
1:B:300:LYS:HG2	1:B:301:LEU:H	1.45	0.81
1:A:89:ILE:HG21	1:A:101:LEU:HD21	1.62	0.81
1:C:503:LYS:HB3	1:C:543:ASN:HB3	1.63	0.81
1:B:89:ILE:HG21	1:B:101:LEU:HD21	1.62	0.81
1:A:300:LYS:HG2	1:A:301:LEU:H	1.45	0.81
1:D:111:PRO:HD3	1:D:188:PRO:HA	1.63	0.80
1:C:111:PRO:HD3	1:C:188:PRO:HA	1.63	0.80
1:A:503:LYS:HB3	1:A:543:ASN:HB3	1.64	0.80
1:C:283:SER:H	1:C:291:GLN:NE2	1.80	0.80
1:C:300:LYS:HG2	1:C:301:LEU:H	1.45	0.80
1:D:283:SER:H	1:D:291:GLN:NE2	1.80	0.80
1:D:300:LYS:HG2	1:D:301:LEU:H	1.45	0.79
1:B:72:ARG:HH11	1:D:68:GLN:HE22	1.27	0.79
1:B:111:PRO:HD3	1:B:188:PRO:HA	1.63	0.79
1:A:111:PRO:HD3	1:A:188:PRO:HA	1.63	0.79
1:A:68:GLN:HE22	1:C:72:ARG:HH11	1.27	0.79
1:B:418:ILE:HG12	1:B:548:ILE:HG23	1.65	0.79
1:A:22:ALA:HA	1:A:26:PHE:HD1	1.48	0.79
1:B:503:LYS:HB3	1:B:543:ASN:HB3	1.64	0.78
1:D:503:LYS:HB3	1:D:543:ASN:HB3	1.64	0.78
1:A:418:ILE:HG12	1:A:548:ILE:HG23	1.64	0.78
1:A:326:PRO:HB3	1:D:37:ILE:HG21	1.64	0.78
1:B:22:ALA:HA	1:B:26:PHE:HD1	1.48	0.78
1:B:283:SER:H	1:B:291:GLN:NE2	1.81	0.78
1:A:283:SER:H	1:A:291:GLN:NE2	1.80	0.78
1:A:72:ARG:HH11	1:C:68:GLN:HE22	1.28	0.78
1:B:30:TRP:CE2	1:C:288:PRO:HG3	2.19	0.78
1:C:22:ALA:HA	1:C:26:PHE:HD1	1.48	0.77
1:C:418:ILE:HG12	1:C:548:ILE:HG23	1.65	0.77
1:D:22:ALA:HA	1:D:26:PHE:HD1	1.48	0.77
1:D:418:ILE:HG12	1:D:548:ILE:HG23	1.65	0.77
1:A:404:GLU:O	1:A:406:LYS:HG2	1.85	0.76
1:B:404:GLU:O	1:B:406:LYS:HG2	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LEU:HB3	1:B:249:VAL:HB	1.68	0.76
1:C:404:GLU:O	1:C:406:LYS:HG2	1.85	0.76
1:D:404:GLU:O	1:D:406:LYS:HG2	1.85	0.76
1:A:98:MET:SD	1:B:176:LEU:HD12	2.25	0.75
1:C:370:ARG:O	1:C:517:LEU:HA	1.86	0.75
1:D:86:GLU:O	1:D:89:ILE:HG22	1.87	0.75
1:D:218:LEU:HB3	1:D:249:VAL:HB	1.68	0.75
1:A:86:GLU:O	1:A:89:ILE:HG22	1.86	0.75
1:C:86:GLU:O	1:C:89:ILE:HG22	1.86	0.74
1:A:218:LEU:HB3	1:A:249:VAL:HB	1.68	0.74
1:D:370:ARG:O	1:D:517:LEU:HA	1.87	0.74
1:A:523:ALA:O	1:A:527:ILE:HG12	1.88	0.74
1:B:86:GLU:O	1:B:89:ILE:HG22	1.87	0.74
1:C:218:LEU:HB3	1:C:249:VAL:HB	1.68	0.74
1:C:439:GLU:HB2	1:C:441:TYR:CE1	2.23	0.74
1:C:76:GLU:HB3	1:C:220:LEU:HD23	1.70	0.73
1:C:31:ARG:H	1:C:31:ARG:CD	1.96	0.73
1:B:370:ARG:O	1:B:517:LEU:HA	1.87	0.73
1:B:523:ALA:O	1:B:527:ILE:HG12	1.88	0.73
1:D:523:ALA:O	1:D:527:ILE:HG12	1.88	0.73
1:A:370:ARG:O	1:A:517:LEU:HA	1.87	0.73
1:A:76:GLU:HB3	1:A:220:LEU:HD23	1.71	0.73
1:D:439:GLU:HB2	1:D:441:TYR:CE1	2.24	0.73
1:A:439:GLU:HB2	1:A:441:TYR:CE1	2.24	0.72
1:B:439:GLU:HB2	1:B:441:TYR:CE1	2.25	0.72
1:C:462:ILE:HB	1:C:463:PRO:HD3	1.72	0.72
1:C:523:ALA:O	1:C:527:ILE:HG12	1.89	0.71
1:C:348:ARG:HH11	1:C:349:ALA:HA	1.55	0.71
1:D:462:ILE:HB	1:D:463:PRO:HD3	1.72	0.71
1:A:46:TYR:HA	1:A:49:LEU:H	1.55	0.71
1:B:46:TYR:HA	1:B:49:LEU:H	1.55	0.71
1:D:46:TYR:HA	1:D:49:LEU:H	1.55	0.71
1:D:76:GLU:HB3	1:D:220:LEU:HD23	1.71	0.70
1:B:76:GLU:HB3	1:B:220:LEU:HD23	1.71	0.70
1:B:462:ILE:HB	1:B:463:PRO:HD3	1.72	0.70
1:C:205:ILE:HD13	1:C:321:TYR:HE2	1.56	0.70
1:A:462:ILE:HB	1:A:463:PRO:HD3	1.72	0.70
1:A:205:ILE:HD13	1:A:321:TYR:HE2	1.57	0.70
1:C:46:TYR:HA	1:C:49:LEU:H	1.56	0.70
1:A:326:PRO:HB3	1:D:37:ILE:CG2	2.22	0.70
1:A:348:ARG:HH11	1:A:349:ALA:HA	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:HD13	1:B:107:LEU:HD21	1.74	0.69
1:D:348:ARG:HH11	1:D:349:ALA:HA	1.56	0.69
1:B:31:ARG:H	1:B:31:ARG:CD	1.97	0.69
1:A:354:GLN:CB	1:B:210:LEU:HD13	2.22	0.69
1:D:205:ILE:HD13	1:D:321:TYR:HE2	1.56	0.69
1:B:348:ARG:HH11	1:B:349:ALA:HA	1.56	0.69
1:C:348:ARG:HH22	1:C:356:TYR:HB2	1.58	0.69
1:A:229:ARG:NE	1:B:109:GLY:HA3	2.07	0.69
1:B:536:VAL:HG23	1:B:537:ARG:H	1.58	0.68
1:B:205:ILE:HD13	1:B:321:TYR:HE2	1.56	0.68
1:A:348:ARG:HH22	1:A:356:TYR:HB2	1.58	0.68
1:C:83:ILE:HD13	1:C:107:LEU:HD21	1.74	0.68
1:A:64:GLU:HG3	1:B:64:GLU:OE1	1.94	0.68
1:D:83:ILE:HD13	1:D:107:LEU:HD21	1.74	0.68
1:B:372:ASP:HB3	1:B:516:ASN:OD1	1.94	0.68
1:B:348:ARG:HH22	1:B:356:TYR:HB2	1.59	0.68
1:A:507:PRO:HG2	1:A:514:ASP:HB2	1.74	0.68
1:A:438:ASN:ND2	1:A:451:PRO:HD3	2.09	0.68
1:A:372:ASP:HB3	1:A:516:ASN:OD1	1.94	0.68
1:B:507:PRO:HG2	1:B:514:ASP:HB2	1.75	0.68
1:A:83:ILE:HD13	1:A:107:LEU:HD21	1.74	0.68
1:A:536:VAL:HG23	1:A:537:ARG:H	1.59	0.67
1:C:507:PRO:HG2	1:C:514:ASP:HB2	1.75	0.67
1:D:507:PRO:HG2	1:D:514:ASP:HB2	1.74	0.67
1:B:68:GLN:HE22	1:D:72:ARG:NH1	1.90	0.67
1:D:348:ARG:HH22	1:D:356:TYR:HB2	1.58	0.67
1:B:369:ILE:HD12	1:B:475:THR:HG21	1.77	0.67
1:A:64:GLU:OE1	1:B:64:GLU:HG3	1.95	0.67
1:C:438:ASN:ND2	1:C:451:PRO:HD3	2.10	0.67
1:C:369:ILE:HD12	1:C:475:THR:HG21	1.77	0.67
1:A:57:HIS:CE1	1:B:79:ILE:HD12	2.30	0.66
1:D:536:VAL:HG23	1:D:537:ARG:H	1.59	0.66
1:D:512:LEU:HA	1:D:536:VAL:HG21	1.77	0.66
1:C:536:VAL:HG23	1:C:537:ARG:H	1.58	0.66
1:D:438:ASN:ND2	1:D:451:PRO:HD3	2.10	0.66
1:C:512:LEU:HA	1:C:536:VAL:HG21	1.78	0.66
1:C:372:ASP:HB3	1:C:516:ASN:OD1	1.96	0.66
1:A:339:MET:SD	1:A:347:VAL:HG22	2.35	0.66
1:B:158:VAL:HG13	1:B:159:PHE:N	2.10	0.66
1:C:158:VAL:HG13	1:C:159:PHE:N	2.10	0.66
1:D:372:ASP:HB3	1:D:516:ASN:OD1	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:HA	1:A:536:VAL:HG21	1.77	0.65
1:D:287:THR:HG22	1:D:314:SER:HA	1.77	0.65
1:B:438:ASN:ND2	1:B:451:PRO:HD3	2.10	0.65
1:A:260:VAL:HG22	1:D:51:PRO:HB3	1.76	0.65
1:D:369:ILE:HD12	1:D:475:THR:HG21	1.78	0.65
1:A:435:SER:HB2	1:A:438:ASN:OD1	1.97	0.65
1:A:287:THR:HG22	1:A:314:SER:HA	1.78	0.65
1:C:108:ALA:HB3	1:D:106:TYR:HB2	1.79	0.65
1:C:287:THR:HG22	1:C:314:SER:HA	1.77	0.65
1:D:158:VAL:HG13	1:D:159:PHE:N	2.10	0.65
1:B:287:THR:HG22	1:B:314:SER:HA	1.79	0.65
1:A:506:VAL:CG2	1:A:507:PRO:HD3	2.23	0.64
1:D:339:MET:SD	1:D:347:VAL:HG22	2.36	0.64
1:B:512:LEU:HA	1:B:536:VAL:HG21	1.78	0.64
1:B:506:VAL:CG2	1:B:507:PRO:HD3	2.23	0.64
1:A:158:VAL:HG13	1:A:159:PHE:N	2.09	0.64
1:A:369:ILE:HD12	1:A:475:THR:HG21	1.78	0.64
1:C:339:MET:SD	1:C:347:VAL:HG22	2.38	0.64
1:A:344:TYR:CD2	1:A:350:MET:HB2	2.33	0.64
1:B:344:TYR:CD2	1:B:350:MET:HB2	2.33	0.64
1:A:31:ARG:CD	1:A:31:ARG:H	1.96	0.63
1:D:435:SER:HB2	1:D:438:ASN:OD1	1.98	0.63
1:B:435:SER:HB2	1:B:438:ASN:OD1	1.98	0.63
1:A:477:ILE:HG21	1:A:517:LEU:HD21	1.81	0.63
1:C:435:SER:HB2	1:C:438:ASN:OD1	1.98	0.63
1:B:536:VAL:HG23	1:B:537:ARG:N	2.14	0.63
1:B:339:MET:SD	1:B:347:VAL:HG22	2.38	0.63
1:C:395:LYS:HG3	1:C:430:LYS:HG2	1.81	0.63
1:C:344:TYR:CD2	1:C:350:MET:HB2	2.34	0.63
1:C:430:LYS:HD2	1:C:433:GLY:O	1.99	0.63
1:D:31:ARG:CD	1:D:31:ARG:H	1.96	0.62
1:C:477:ILE:HG21	1:C:517:LEU:HD21	1.80	0.62
1:D:536:VAL:HG23	1:D:537:ARG:N	2.15	0.62
1:C:98:MET:SD	1:D:176:LEU:HD12	2.38	0.62
1:B:477:ILE:HG21	1:B:517:LEU:HD21	1.81	0.62
1:A:395:LYS:HG3	1:A:430:LYS:HG2	1.81	0.62
1:B:430:LYS:HD2	1:B:433:GLY:O	1.99	0.62
1:D:430:LYS:HD2	1:D:433:GLY:O	2.00	0.62
1:A:352:TYR:HE2	1:B:81:PRO:N	1.97	0.62
1:D:477:ILE:HG21	1:D:517:LEU:HD21	1.81	0.62
1:C:536:VAL:HG23	1:C:537:ARG:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:ILE:O	1:D:510:ARG:HG3	1.99	0.62
1:C:508:ILE:O	1:C:510:ARG:HG3	2.00	0.62
1:C:506:VAL:CG2	1:C:507:PRO:HD3	2.24	0.61
1:D:344:TYR:CD2	1:D:350:MET:HB2	2.34	0.61
1:B:195:LEU:HD13	1:B:227:PHE:CG	2.35	0.61
1:A:230:GLU:HB3	1:A:233:GLU:HG3	1.82	0.61
1:A:287:THR:CG2	1:A:314:SER:HA	2.30	0.61
1:C:432:LEU:HD12	1:C:432:LEU:N	2.16	0.61
1:B:395:LYS:HG3	1:B:430:LYS:HG2	1.81	0.61
1:C:287:THR:CG2	1:C:314:SER:HA	2.31	0.61
1:B:230:GLU:HB3	1:B:233:GLU:HG3	1.82	0.61
1:D:195:LEU:HD13	1:D:227:PHE:CG	2.35	0.61
1:A:322:ASN:ND2	1:D:15:ILE:HD11	2.16	0.61
1:A:322:ASN:HD21	1:D:15:ILE:HD11	1.66	0.61
1:C:230:GLU:HB3	1:C:233:GLU:HG3	1.82	0.61
1:A:430:LYS:HD2	1:A:433:GLY:O	2.00	0.61
1:C:186:LEU:HD23	1:C:187:LYS:N	2.16	0.61
1:A:195:LEU:HD13	1:A:227:PHE:CG	2.36	0.61
1:C:283:SER:N	1:C:291:GLN:HE22	1.93	0.60
1:D:287:THR:CG2	1:D:314:SER:HA	2.31	0.60
1:B:287:THR:CG2	1:B:314:SER:HA	2.31	0.60
1:A:508:ILE:O	1:A:510:ARG:HG3	2.00	0.60
1:C:109:GLY:O	1:C:111:PRO:HD3	2.01	0.60
1:D:230:GLU:HB3	1:D:233:GLU:HG3	1.82	0.60
1:A:229:ARG:HE	1:B:109:GLY:HA3	1.65	0.60
1:A:57:HIS:CD2	1:B:79:ILE:HG13	2.36	0.60
1:B:508:ILE:O	1:B:510:ARG:HG3	2.01	0.60
1:A:284:LYS:HA	1:D:30:TRP:CZ2	2.36	0.60
1:B:72:ARG:NH1	1:D:68:GLN:HE22	1.98	0.60
1:D:46:TYR:CD1	1:D:47:PRO:HA	2.37	0.60
1:D:186:LEU:HD23	1:D:187:LYS:N	2.16	0.60
1:C:195:LEU:HD13	1:C:227:PHE:CG	2.36	0.60
1:D:395:LYS:HG3	1:D:430:LYS:HG2	1.82	0.60
1:A:536:VAL:HG23	1:A:537:ARG:N	2.15	0.60
1:A:196:ARG:NH1	1:A:199:MET:HE1	2.17	0.60
1:A:109:GLY:O	1:A:111:PRO:HD3	2.01	0.59
1:A:440:VAL:HA	1:A:449:GLY:HA3	1.84	0.59
1:B:440:VAL:HA	1:B:449:GLY:HA3	1.84	0.59
1:A:46:TYR:CD1	1:A:47:PRO:HA	2.37	0.59
1:B:432:LEU:N	1:B:432:LEU:HD12	2.17	0.59
1:D:506:VAL:CG2	1:D:507:PRO:HD3	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HD23	1:B:187:LYS:N	2.17	0.59
1:C:401:CYS:SG	1:C:402:SER:N	2.74	0.59
1:B:387:LEU:O	1:B:387:LEU:HD13	2.03	0.59
1:B:68:GLN:NE2	1:D:72:ARG:HH11	1.95	0.59
1:D:109:GLY:O	1:D:111:PRO:HD3	2.01	0.59
1:B:46:TYR:CD1	1:B:47:PRO:HA	2.37	0.59
1:C:46:TYR:CD1	1:C:47:PRO:HA	2.38	0.59
1:B:196:ARG:NH1	1:B:199:MET:HE1	2.18	0.59
1:A:186:LEU:HD23	1:A:187:LYS:N	2.16	0.59
1:A:432:LEU:HD12	1:A:432:LEU:N	2.18	0.59
1:D:325:VAL:HG23	1:D:326:PRO:HD2	1.85	0.59
1:C:522:LEU:O	1:C:523:ALA:HB3	2.03	0.59
1:C:440:VAL:HA	1:C:449:GLY:HA3	1.85	0.59
1:C:210:LEU:HD13	1:D:354:GLN:CB	2.31	0.59
1:B:109:GLY:O	1:B:111:PRO:HD3	2.01	0.59
1:C:325:VAL:HG23	1:C:326:PRO:HD2	1.85	0.59
1:D:432:LEU:N	1:D:432:LEU:HD12	2.17	0.59
1:D:440:VAL:HA	1:D:449:GLY:HA3	1.84	0.59
1:A:30:TRP:CH2	1:D:288:PRO:HG3	2.38	0.59
1:C:271:PHE:CZ	1:C:298:HIS:HB2	2.38	0.59
1:A:294:VAL:HB	1:A:308:ALA:HB3	1.85	0.59
1:B:502:PHE:HD2	1:B:546:VAL:HG13	1.68	0.58
1:D:271:PHE:CZ	1:D:298:HIS:HB2	2.38	0.58
1:B:294:VAL:HB	1:B:308:ALA:HB3	1.85	0.58
1:A:271:PHE:CZ	1:A:298:HIS:HB2	2.38	0.58
1:C:502:PHE:HD2	1:C:546:VAL:HG13	1.68	0.58
1:B:401:CYS:SG	1:B:402:SER:N	2.76	0.58
1:D:508:ILE:HD12	1:D:508:ILE:O	2.04	0.58
1:A:322:ASN:ND2	1:D:15:ILE:CD1	2.67	0.58
1:B:271:PHE:CZ	1:B:298:HIS:HB2	2.39	0.58
1:D:384:ALA:HA	1:D:488:VAL:HG21	1.86	0.58
1:C:294:VAL:HB	1:C:308:ALA:HB3	1.85	0.58
1:A:401:CYS:SG	1:A:402:SER:N	2.77	0.57
1:B:93:PHE:HB2	1:B:97:ALA:HB2	1.86	0.57
1:D:502:PHE:HD2	1:D:546:VAL:HG13	1.69	0.57
1:D:387:LEU:O	1:D:387:LEU:HD13	2.03	0.57
1:C:93:PHE:HB2	1:C:97:ALA:HB2	1.87	0.57
1:D:37:ILE:HG13	1:D:37:ILE:O	2.04	0.57
1:A:161:ILE:HG12	1:A:167:VAL:CG1	2.33	0.57
1:B:275:LYS:HG3	1:C:363:ARG:HH12	1.70	0.57
1:D:93:PHE:HB2	1:D:97:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:387:LEU:HD12	1:D:484:ILE:HG23	1.86	0.57
1:C:37:ILE:HG13	1:C:37:ILE:O	2.04	0.57
1:B:527:ILE:O	1:B:532:LYS:HB2	2.04	0.57
1:A:37:ILE:O	1:A:37:ILE:HG13	2.05	0.57
1:A:384:ALA:HA	1:A:488:VAL:HG21	1.86	0.57
1:A:64:GLU:CD	1:B:64:GLU:HG3	2.24	0.57
1:C:387:LEU:HD12	1:C:484:ILE:HG23	1.87	0.57
1:D:514:ASP:C	1:D:516:ASN:N	2.58	0.57
1:A:325:VAL:HG23	1:A:326:PRO:HD2	1.86	0.57
1:A:527:ILE:O	1:A:532:LYS:HB2	2.04	0.57
1:D:103:ARG:HA	1:D:229:ARG:HB3	1.87	0.57
1:B:414:GLU:O	1:B:416:ARG:HG2	2.05	0.57
1:A:387:LEU:O	1:A:387:LEU:HD13	2.04	0.57
1:A:527:ILE:HG21	1:A:534:ILE:HD11	1.86	0.57
1:B:527:ILE:HG21	1:B:534:ILE:HD11	1.86	0.57
1:A:395:LYS:HG2	1:A:396:ASP:N	2.17	0.56
1:C:527:ILE:O	1:C:532:LYS:HB2	2.05	0.56
1:B:37:ILE:O	1:B:37:ILE:HG13	2.05	0.56
1:C:384:ALA:HA	1:C:488:VAL:HG21	1.86	0.56
1:C:161:ILE:HG12	1:C:167:VAL:CG1	2.34	0.56
1:B:387:LEU:HD12	1:B:484:ILE:HG23	1.87	0.56
1:A:37:ILE:HG21	1:D:326:PRO:HB3	1.88	0.56
1:A:387:LEU:HD12	1:A:484:ILE:HG23	1.86	0.56
1:C:31:ARG:N	1:C:31:ARG:HD3	2.04	0.56
1:C:64:GLU:OE1	1:D:64:GLU:HG3	2.04	0.56
1:C:64:GLU:HG3	1:D:64:GLU:OE1	2.04	0.56
1:B:325:VAL:HG23	1:B:326:PRO:HD2	1.86	0.56
1:D:294:VAL:HB	1:D:308:ALA:HB3	1.86	0.56
1:D:527:ILE:O	1:D:532:LYS:HB2	2.05	0.56
1:A:502:PHE:HD2	1:A:546:VAL:HG13	1.69	0.56
1:A:512:LEU:HB3	1:A:536:VAL:HG11	1.87	0.56
1:D:512:LEU:HB3	1:D:536:VAL:HG11	1.87	0.56
1:C:387:LEU:HD13	1:C:387:LEU:O	2.05	0.56
1:D:196:ARG:NH1	1:D:199:MET:HE1	2.21	0.56
1:D:31:ARG:N	1:D:31:ARG:HD3	2.04	0.56
1:A:540:VAL:O	1:A:541:PHE:HB2	2.05	0.56
1:A:522:LEU:O	1:A:523:ALA:HB3	2.06	0.56
1:D:522:LEU:O	1:D:523:ALA:HB3	2.06	0.56
1:A:414:GLU:O	1:A:416:ARG:HG2	2.06	0.56
1:B:514:ASP:C	1:B:516:ASN:N	2.59	0.56
1:D:395:LYS:HG2	1:D:396:ASP:N	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:HB2	1:A:97:ALA:HB2	1.86	0.56
1:A:103:ARG:HA	1:A:229:ARG:HB3	1.87	0.56
1:D:527:ILE:HG21	1:D:534:ILE:HD11	1.87	0.56
1:C:103:ARG:HA	1:C:229:ARG:HB3	1.88	0.56
1:A:30:TRP:CE2	1:D:288:PRO:HG3	2.41	0.56
1:B:508:ILE:O	1:B:508:ILE:HD12	2.06	0.56
1:D:401:CYS:SG	1:D:402:SER:N	2.78	0.56
1:D:414:GLU:O	1:D:416:ARG:HG2	2.06	0.56
1:B:384:ALA:HA	1:B:488:VAL:HG21	1.87	0.56
1:B:283:SER:N	1:B:291:GLN:HE22	1.94	0.56
1:B:103:ARG:HA	1:B:229:ARG:HB3	1.87	0.55
1:B:540:VAL:O	1:B:541:PHE:HB2	2.05	0.55
1:C:527:ILE:HG21	1:C:534:ILE:HD11	1.87	0.55
1:A:260:VAL:CG2	1:D:51:PRO:HB3	2.35	0.55
1:D:508:ILE:HD12	1:D:510:ARG:HG3	1.88	0.55
1:C:508:ILE:HD12	1:C:510:ARG:HG3	1.88	0.55
1:C:540:VAL:O	1:C:541:PHE:HB2	2.05	0.55
1:D:540:VAL:O	1:D:541:PHE:HB2	2.05	0.55
1:D:161:ILE:HG12	1:D:167:VAL:CG1	2.33	0.55
1:D:396:ASP:O	1:D:397:LYS:HB2	2.07	0.55
1:C:508:ILE:O	1:C:508:ILE:HD12	2.06	0.55
1:A:227:PHE:HZ	1:B:227:PHE:HZ	1.55	0.55
1:A:372:ASP:H	1:A:517:LEU:H	1.55	0.55
1:C:409:PHE:HD1	1:C:409:PHE:H	1.54	0.55
1:C:396:ASP:O	1:C:397:LYS:HB2	2.06	0.55
1:B:258:GLY:HA3	1:B:310:PHE:CD2	2.42	0.55
1:A:409:PHE:HD1	1:A:409:PHE:H	1.53	0.55
1:C:258:GLY:HA3	1:C:310:PHE:CD2	2.41	0.55
1:A:109:GLY:HA3	1:B:229:ARG:NH1	2.21	0.55
1:C:512:LEU:HB3	1:C:536:VAL:HG11	1.88	0.55
1:B:508:ILE:HD12	1:B:510:ARG:HG3	1.88	0.55
1:A:298:HIS:O	1:A:300:LYS:N	2.40	0.55
1:D:35:ALA:C	1:D:37:ILE:H	2.10	0.55
1:B:466:LYS:HD3	1:B:470:GLU:OE2	2.07	0.55
1:A:316:ILE:HG23	1:A:317:ALA:H	1.72	0.55
1:B:372:ASP:H	1:B:517:LEU:H	1.56	0.54
1:C:298:HIS:O	1:C:300:LYS:N	2.40	0.54
1:A:508:ILE:HD12	1:A:508:ILE:O	2.07	0.54
1:C:35:ALA:C	1:C:37:ILE:H	2.09	0.54
1:C:414:GLU:O	1:C:416:ARG:HG2	2.06	0.54
1:D:283:SER:N	1:D:291:GLN:HE22	1.93	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASP:O	1:A:397:LYS:HB2	2.07	0.54
1:B:512:LEU:HB3	1:B:536:VAL:HG11	1.87	0.54
1:C:156:ASP:OD2	1:D:284:LYS:HE3	2.07	0.54
1:B:505:ARG:O	1:B:506:VAL:HG13	2.07	0.54
1:C:395:LYS:HG2	1:C:396:ASP:N	2.17	0.54
1:B:522:LEU:O	1:B:523:ALA:HB3	2.07	0.54
1:A:35:ALA:C	1:A:37:ILE:H	2.09	0.54
1:C:466:LYS:HD3	1:C:470:GLU:OE2	2.07	0.54
1:C:505:ARG:O	1:C:506:VAL:HG13	2.08	0.54
1:D:258:GLY:HA3	1:D:310:PHE:CD2	2.42	0.54
1:B:386:GLU:O	1:B:390:ILE:HG13	2.08	0.54
1:D:466:LYS:HD3	1:D:470:GLU:OE2	2.07	0.54
1:A:283:SER:N	1:A:291:GLN:HE22	1.93	0.54
1:A:258:GLY:HA3	1:A:310:PHE:CD2	2.41	0.54
1:B:35:ALA:C	1:B:37:ILE:H	2.10	0.54
1:B:257:ASP:O	1:B:261:VAL:HG23	2.07	0.54
1:C:513:SER:O	1:C:514:ASP:HB3	2.08	0.54
1:B:396:ASP:O	1:B:397:LYS:HB2	2.06	0.54
1:D:505:ARG:O	1:D:506:VAL:HG13	2.08	0.54
1:B:395:LYS:HG2	1:B:396:ASP:N	2.16	0.54
1:A:508:ILE:HD12	1:A:510:ARG:HG3	1.88	0.54
1:A:466:LYS:HD3	1:A:470:GLU:OE2	2.08	0.54
1:C:372:ASP:H	1:C:517:LEU:H	1.56	0.54
1:B:161:ILE:HG12	1:B:167:VAL:CG1	2.33	0.54
1:D:386:GLU:O	1:D:390:ILE:HG13	2.08	0.54
1:D:494:ALA:HB2	1:D:502:PHE:HZ	1.73	0.54
1:A:386:GLU:O	1:A:390:ILE:HG13	2.08	0.54
1:D:372:ASP:H	1:D:517:LEU:H	1.55	0.53
1:A:257:ASP:O	1:A:261:VAL:HG23	2.08	0.53
1:D:92:GLN:HE22	1:D:201:SER:HA	1.73	0.53
1:C:16:LYS:HA	1:C:19:LEU:HB3	1.90	0.53
1:A:505:ARG:O	1:A:506:VAL:HG13	2.08	0.53
1:B:16:LYS:HA	1:B:19:LEU:HB3	1.90	0.53
1:D:513:SER:O	1:D:514:ASP:HB3	2.09	0.53
1:A:494:ALA:HB2	1:A:502:PHE:HZ	1.73	0.53
1:B:92:GLN:HE22	1:B:201:SER:HA	1.73	0.53
1:A:514:ASP:C	1:A:516:ASN:N	2.58	0.53
1:D:316:ILE:HG23	1:D:317:ALA:H	1.74	0.53
1:D:105:PHE:CE1	1:D:229:ARG:HG3	2.44	0.53
1:A:158:VAL:CG1	1:A:159:PHE:H	2.16	0.53
1:B:298:HIS:O	1:B:300:LYS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:ALA:HB2	1:C:502:PHE:HZ	1.74	0.53
1:B:494:ALA:HB2	1:B:502:PHE:HZ	1.74	0.53
1:A:72:ARG:NH1	1:C:68:GLN:HE22	2.02	0.53
1:A:92:GLN:HE22	1:A:201:SER:HA	1.73	0.53
1:C:386:GLU:O	1:C:390:ILE:HG13	2.09	0.53
1:D:298:HIS:O	1:D:300:LYS:N	2.41	0.53
1:B:105:PHE:CE1	1:B:229:ARG:HG3	2.44	0.53
1:C:106:TYR:HB2	1:D:108:ALA:HB3	1.88	0.53
1:D:502:PHE:CD2	1:D:546:VAL:HG13	2.44	0.53
1:C:105:PHE:CE1	1:C:229:ARG:HG3	2.44	0.53
1:D:310:PHE:HB3	1:D:330:LEU:HD13	1.91	0.53
1:C:92:GLN:HE22	1:C:201:SER:HA	1.73	0.53
1:D:150:GLY:O	1:D:152:ILE:HG13	2.09	0.53
1:D:16:LYS:HA	1:D:19:LEU:HB3	1.91	0.53
1:C:514:ASP:O	1:C:515:ILE:HB	2.09	0.52
1:C:316:ILE:HG23	1:C:317:ALA:H	1.73	0.52
1:B:513:SER:O	1:B:514:ASP:HB3	2.09	0.52
1:C:502:PHE:CD2	1:C:546:VAL:HG13	2.44	0.52
1:A:105:PHE:CE1	1:A:229:ARG:HG3	2.44	0.52
1:A:16:LYS:HA	1:A:19:LEU:HB3	1.90	0.52
1:A:503:LYS:CB	1:A:543:ASN:HB3	2.38	0.52
1:B:502:PHE:CD2	1:B:546:VAL:HG13	2.44	0.52
1:B:150:GLY:O	1:B:152:ILE:HG13	2.09	0.52
1:C:229:ARG:HG2	1:C:229:ARG:HH21	1.74	0.52
1:C:48:ARG:HG3	1:C:48:ARG:HH21	1.73	0.52
1:D:257:ASP:O	1:D:261:VAL:HG23	2.09	0.52
1:A:515:ILE:HG22	1:A:515:ILE:O	2.10	0.52
1:A:109:GLY:HA3	1:B:229:ARG:NE	2.24	0.52
1:D:229:ARG:HH21	1:D:229:ARG:HG2	1.75	0.52
1:A:37:ILE:HG22	1:D:326:PRO:HG3	1.92	0.52
1:C:150:GLY:O	1:C:152:ILE:HG13	2.09	0.52
1:D:301:LEU:HG	1:D:302:GLY:N	2.25	0.52
1:D:48:ARG:HG3	1:D:48:ARG:HH21	1.75	0.52
1:A:310:PHE:HB3	1:A:330:LEU:HD13	1.91	0.52
1:C:199:MET:HE1	1:C:224:ASP:HB3	1.92	0.52
1:C:257:ASP:O	1:C:261:VAL:HG23	2.09	0.52
1:D:32:GLU:O	1:D:34:ARG:N	2.43	0.52
1:C:515:ILE:HG22	1:C:515:ILE:O	2.10	0.52
1:A:111:PRO:CD	1:A:188:PRO:HA	2.39	0.52
1:B:450:ILE:HD11	1:B:465:LEU:HD11	1.92	0.52
1:B:48:ARG:HG3	1:B:48:ARG:HH21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LEU:C	1:B:332:LEU:HD23	2.31	0.52
1:B:316:ILE:HG23	1:B:317:ALA:H	1.73	0.52
1:A:513:SER:O	1:A:514:ASP:HB3	2.09	0.51
1:B:514:ASP:O	1:B:515:ILE:HB	2.11	0.51
1:D:310:PHE:HB3	1:D:330:LEU:CD1	2.40	0.51
1:A:324:ASP:HA	1:D:13:PHE:CE1	2.44	0.51
1:A:301:LEU:HG	1:A:302:GLY:N	2.26	0.51
1:A:150:GLY:O	1:A:152:ILE:HG13	2.09	0.51
1:A:458:LYS:C	1:A:460:GLN:H	2.14	0.51
1:C:519:ILE:HG22	1:C:520:ASP:O	2.10	0.51
1:C:32:GLU:O	1:C:34:ARG:N	2.44	0.51
1:C:396:ASP:N	1:C:430:LYS:HA	2.26	0.51
1:A:502:PHE:CD2	1:A:546:VAL:HG13	2.45	0.51
1:C:450:ILE:HD11	1:C:465:LEU:HD11	1.92	0.51
1:D:515:ILE:HG22	1:D:515:ILE:O	2.10	0.51
1:A:229:ARG:HH21	1:A:229:ARG:HG2	1.75	0.51
1:B:391:CYS:HB3	1:B:432:LEU:HD21	1.93	0.51
1:D:126:LYS:HG3	1:D:127:ASN:ND2	2.25	0.51
1:C:310:PHE:HB3	1:C:330:LEU:HD13	1.91	0.51
1:A:32:GLU:O	1:A:34:ARG:N	2.44	0.51
1:C:176:LEU:HD12	1:D:98:MET:SD	2.50	0.51
1:A:126:LYS:HG3	1:A:127:ASN:ND2	2.25	0.51
1:A:332:LEU:HD23	1:A:332:LEU:C	2.31	0.51
1:B:421:GLU:O	1:B:544:ALA:HB1	2.11	0.51
1:A:198:HIS:CE1	1:A:329:ASN:HD21	2.29	0.51
1:C:276:PHE:HD2	1:C:294:VAL:HG22	1.76	0.51
1:B:310:PHE:HB3	1:B:330:LEU:CD1	2.40	0.51
1:A:514:ASP:O	1:A:515:ILE:HB	2.10	0.51
1:A:396:ASP:N	1:A:430:LYS:HA	2.26	0.51
1:D:494:ALA:HB2	1:D:502:PHE:CZ	2.46	0.51
1:D:450:ILE:HD11	1:D:465:LEU:HD11	1.92	0.51
1:A:450:ILE:HD11	1:A:465:LEU:HD11	1.93	0.51
1:B:310:PHE:HB3	1:B:330:LEU:HD13	1.92	0.51
1:C:310:PHE:HB3	1:C:330:LEU:CD1	2.41	0.51
1:B:519:ILE:HG22	1:B:520:ASP:O	2.11	0.51
1:B:515:ILE:O	1:B:515:ILE:HG22	2.10	0.51
1:A:68:GLN:HE22	1:C:72:ARG:NH1	2.00	0.51
1:D:421:GLU:O	1:D:544:ALA:HB1	2.11	0.51
1:C:126:LYS:HG3	1:C:127:ASN:ND2	2.25	0.51
1:B:458:LYS:C	1:B:460:GLN:H	2.13	0.51
1:B:126:LYS:HG3	1:B:127:ASN:ND2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:PHE:HD1	1:D:409:PHE:H	1.53	0.51
1:C:214:ARG:HD3	1:D:354:GLN:OE1	2.10	0.51
1:C:421:GLU:O	1:C:544:ALA:HB1	2.10	0.51
1:B:540:VAL:HG12	1:B:541:PHE:N	2.25	0.51
1:A:391:CYS:HB3	1:A:432:LEU:HD21	1.93	0.51
1:D:519:ILE:HG22	1:D:520:ASP:O	2.11	0.51
1:C:299:PRO:O	1:C:300:LYS:HB2	2.11	0.51
1:C:107:LEU:HD23	1:D:105:PHE:CG	2.46	0.51
1:A:310:PHE:HB3	1:A:330:LEU:CD1	2.41	0.51
1:D:276:PHE:HD2	1:D:294:VAL:HG22	1.76	0.51
1:A:14:ASP:HB2	1:A:17:LYS:CB	2.41	0.51
1:D:57:HIS:HE1	1:D:59:VAL:HG23	1.76	0.51
1:B:396:ASP:N	1:B:430:LYS:HA	2.26	0.50
1:C:503:LYS:CB	1:C:543:ASN:HB3	2.38	0.50
1:A:494:ALA:HB2	1:A:502:PHE:CZ	2.46	0.50
1:B:14:ASP:HB2	1:B:17:LYS:CB	2.42	0.50
1:B:301:LEU:HG	1:B:302:GLY:N	2.25	0.50
1:C:540:VAL:HG12	1:C:541:PHE:N	2.25	0.50
1:D:503:LYS:CB	1:D:543:ASN:HB3	2.38	0.50
1:B:224:ASP:CG	1:B:225:ARG:H	2.15	0.50
1:C:380:PHE:HZ	1:C:495:LEU:HD12	1.76	0.50
1:D:380:PHE:HZ	1:D:495:LEU:HD12	1.76	0.50
1:A:48:ARG:HG3	1:A:48:ARG:HH21	1.75	0.50
1:B:369:ILE:HD12	1:B:475:THR:CG2	2.41	0.50
1:D:514:ASP:O	1:D:515:ILE:HB	2.12	0.50
1:A:486:LYS:HB2	1:A:516:ASN:ND2	2.27	0.50
1:C:514:ASP:C	1:C:516:ASN:N	2.60	0.50
1:A:299:PRO:O	1:A:300:LYS:HB2	2.11	0.50
1:B:229:ARG:HG2	1:B:229:ARG:HH21	1.75	0.50
1:C:391:CYS:HB3	1:C:432:LEU:HD21	1.94	0.50
1:B:260:VAL:HG22	1:C:51:PRO:HB3	1.93	0.50
1:C:14:ASP:HB2	1:C:17:LYS:CB	2.42	0.50
1:D:458:LYS:C	1:D:460:GLN:H	2.14	0.50
1:C:301:LEU:HG	1:C:302:GLY:N	2.25	0.50
1:D:522:LEU:H	1:D:522:LEU:HD12	1.77	0.50
1:C:522:LEU:HD12	1:C:522:LEU:H	1.76	0.50
1:A:380:PHE:HZ	1:A:495:LEU:HD12	1.76	0.50
1:A:316:ILE:HG23	1:A:317:ALA:N	2.27	0.50
1:D:14:ASP:HB2	1:D:17:LYS:CB	2.41	0.50
1:B:380:PHE:HZ	1:B:495:LEU:HD12	1.77	0.50
1:C:57:HIS:HE1	1:C:59:VAL:HG23	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:PRO:O	1:B:300:LYS:HB2	2.11	0.50
1:C:494:ALA:HB2	1:C:502:PHE:CZ	2.47	0.50
1:A:540:VAL:HG12	1:A:541:PHE:N	2.26	0.50
1:D:540:VAL:HG12	1:D:541:PHE:N	2.26	0.50
1:A:369:ILE:HD12	1:A:475:THR:CG2	2.42	0.50
1:B:409:PHE:H	1:B:409:PHE:HD1	1.54	0.50
1:C:216:LEU:HB3	1:C:217:PRO:HA	1.93	0.50
1:C:198:HIS:CE1	1:C:329:ASN:HD21	2.30	0.50
1:B:32:GLU:O	1:B:34:ARG:N	2.44	0.50
1:A:514:ASP:C	1:A:516:ASN:H	2.15	0.50
1:B:503:LYS:CB	1:B:543:ASN:HB3	2.38	0.50
1:A:56:PRO:HA	1:B:77:GLU:HB3	1.94	0.50
1:D:310:PHE:HB3	1:D:330:LEU:HA	1.94	0.50
1:D:486:LYS:HB2	1:D:516:ASN:ND2	2.27	0.50
1:C:111:PRO:CD	1:C:188:PRO:HA	2.39	0.50
1:A:109:GLY:HA3	1:B:229:ARG:CZ	2.42	0.50
1:A:519:ILE:HG22	1:A:520:ASP:O	2.11	0.50
1:D:216:LEU:HB3	1:D:217:PRO:HA	1.94	0.50
1:A:216:LEU:HB3	1:A:217:PRO:HA	1.92	0.50
1:B:486:LYS:HB2	1:B:516:ASN:ND2	2.26	0.50
1:A:421:GLU:O	1:A:544:ALA:HB1	2.12	0.50
1:D:332:LEU:C	1:D:332:LEU:HD23	2.31	0.50
1:A:64:GLU:HG3	1:B:64:GLU:CD	2.33	0.49
1:D:416:ARG:HG3	1:D:417:VAL:HG23	1.94	0.49
1:C:196:ARG:NH1	1:C:199:MET:HE1	2.26	0.49
1:A:310:PHE:HB3	1:A:330:LEU:HA	1.94	0.49
1:D:391:CYS:HB3	1:D:432:LEU:HD21	1.93	0.49
1:D:316:ILE:HG23	1:D:317:ALA:N	2.27	0.49
1:B:47:PRO:HG2	1:B:474:SER:O	2.12	0.49
1:A:57:HIS:HE1	1:A:59:VAL:HG23	1.77	0.49
1:D:410:ASN:HA	1:D:415:ARG:O	2.13	0.49
1:D:396:ASP:N	1:D:430:LYS:HA	2.26	0.49
1:B:522:LEU:H	1:B:522:LEU:HD12	1.76	0.49
1:C:369:ILE:HD12	1:C:475:THR:CG2	2.42	0.49
1:D:14:ASP:HB2	1:D:17:LYS:HB3	1.95	0.49
1:D:111:PRO:CD	1:D:188:PRO:HA	2.39	0.49
1:C:310:PHE:HB3	1:C:330:LEU:HA	1.94	0.49
1:C:224:ASP:CG	1:C:225:ARG:H	2.16	0.49
1:B:198:HIS:CE1	1:B:329:ASN:HD21	2.31	0.49
1:D:299:PRO:O	1:D:300:LYS:HB2	2.11	0.49
1:A:522:LEU:HD12	1:A:522:LEU:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:PRO:HG2	1:D:474:SER:O	2.13	0.49
1:C:410:ASN:HA	1:C:415:ARG:O	2.13	0.49
1:C:458:LYS:C	1:C:460:GLN:H	2.14	0.49
1:C:332:LEU:C	1:C:332:LEU:HD23	2.32	0.49
1:C:28:THR:O	1:C:31:ARG:HG2	2.12	0.49
1:D:28:THR:O	1:D:31:ARG:HG2	2.13	0.49
1:A:144:LEU:HG	1:A:159:PHE:CE1	2.48	0.49
1:C:83:ILE:HD13	1:C:107:LEU:CD2	2.43	0.49
1:A:224:ASP:CG	1:A:225:ARG:H	2.15	0.49
1:B:14:ASP:HB2	1:B:17:LYS:HB3	1.94	0.49
1:A:28:THR:O	1:A:31:ARG:HG2	2.13	0.49
1:A:276:PHE:HD2	1:A:294:VAL:HG22	1.77	0.49
1:D:175:VAL:O	1:D:176:LEU:HD23	2.13	0.49
1:B:238:LEU:HD22	1:B:238:LEU:N	2.28	0.49
1:B:216:LEU:HB3	1:B:217:PRO:HA	1.93	0.49
1:C:350:MET:O	1:C:353:PRO:HD3	2.13	0.49
1:B:310:PHE:HB3	1:B:330:LEU:HA	1.94	0.49
1:D:198:HIS:CE1	1:D:329:ASN:HD21	2.30	0.49
1:D:514:ASP:C	1:D:516:ASN:H	2.15	0.49
1:C:486:LYS:HB2	1:C:516:ASN:ND2	2.28	0.49
1:B:83:ILE:HD13	1:B:107:LEU:CD2	2.43	0.49
1:B:199:MET:HB2	1:B:245:SER:HB2	1.95	0.49
1:B:416:ARG:HG3	1:B:417:VAL:HG23	1.95	0.49
1:A:387:LEU:CD1	1:A:484:ILE:HD12	2.43	0.49
1:D:224:ASP:CG	1:D:225:ARG:H	2.16	0.49
1:A:416:ARG:HG3	1:A:417:VAL:HG23	1.94	0.49
1:A:14:ASP:HB2	1:A:17:LYS:HB3	1.94	0.49
1:B:21:LEU:N	1:B:21:LEU:HD12	2.28	0.49
1:B:57:HIS:HE1	1:B:59:VAL:HG23	1.78	0.49
1:C:295:TYR:HA	1:C:306:GLU:HA	1.95	0.49
1:A:410:ASN:HA	1:A:415:ARG:O	2.13	0.49
1:D:541:PHE:O	1:D:542:LEU:C	2.52	0.48
1:A:356:TYR:N	1:B:213:LYS:HZ3	2.11	0.48
1:A:198:HIS:CE1	1:A:245:SER:HG	2.31	0.48
1:A:238:LEU:N	1:A:238:LEU:HD22	2.28	0.48
1:B:494:ALA:HB2	1:B:502:PHE:CZ	2.47	0.48
1:C:401:CYS:SG	1:C:403:VAL:HG23	2.53	0.48
1:B:276:PHE:HD2	1:B:294:VAL:HG22	1.78	0.48
1:C:316:ILE:HG23	1:C:317:ALA:N	2.27	0.48
1:C:59:VAL:O	1:C:63:ILE:HG13	2.13	0.48
1:B:410:ASN:HA	1:B:415:ARG:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:O	1:A:176:LEU:HD23	2.13	0.48
1:A:364:ASP:O	1:A:368:MET:HG3	2.13	0.48
1:B:364:ASP:O	1:B:368:MET:HG3	2.13	0.48
1:B:31:ARG:N	1:B:31:ARG:HD3	2.04	0.48
1:B:370:ARG:HH21	1:B:370:ARG:HG2	1.78	0.48
1:D:350:MET:O	1:D:353:PRO:HD3	2.13	0.48
1:B:316:ILE:HG23	1:B:317:ALA:N	2.27	0.48
1:A:111:PRO:HD2	1:A:186:LEU:HD21	1.95	0.48
1:A:68:GLN:NE2	1:C:72:ARG:HH11	2.06	0.48
1:B:175:VAL:O	1:B:176:LEU:HD23	2.14	0.48
1:D:369:ILE:HD12	1:D:475:THR:CG2	2.42	0.48
1:B:350:MET:O	1:B:353:PRO:HD3	2.13	0.48
1:A:199:MET:HB2	1:A:245:SER:HB2	1.95	0.48
1:B:387:LEU:CD1	1:B:484:ILE:HD12	2.43	0.48
1:D:295:TYR:HA	1:D:306:GLU:HA	1.95	0.48
1:C:238:LEU:N	1:C:238:LEU:HD22	2.28	0.48
1:D:238:LEU:HD22	1:D:238:LEU:N	2.28	0.48
1:D:431:LEU:O	1:D:431:LEU:HD13	2.14	0.48
1:D:482:GLY:O	1:D:516:ASN:ND2	2.44	0.48
1:A:431:LEU:HB3	1:A:432:LEU:HD12	1.95	0.48
1:D:21:LEU:N	1:D:21:LEU:HD12	2.29	0.48
1:C:541:PHE:O	1:C:542:LEU:C	2.52	0.48
1:D:387:LEU:CD1	1:D:484:ILE:HD12	2.43	0.48
1:B:111:PRO:HD2	1:B:186:LEU:HD21	1.95	0.48
1:C:47:PRO:HG2	1:C:474:SER:O	2.13	0.48
1:D:508:ILE:O	1:D:509:VAL:C	2.52	0.48
1:B:195:LEU:HD13	1:B:227:PHE:CD1	2.49	0.48
1:C:175:VAL:O	1:C:176:LEU:HD23	2.13	0.48
1:D:59:VAL:O	1:D:63:ILE:HG13	2.13	0.48
1:C:14:ASP:HB2	1:C:17:LYS:HB3	1.95	0.48
1:A:295:TYR:HA	1:A:306:GLU:HA	1.95	0.48
1:B:28:THR:O	1:B:31:ARG:HG2	2.13	0.48
1:D:195:LEU:HD13	1:D:227:PHE:CD1	2.49	0.48
1:A:431:LEU:HD13	1:A:431:LEU:O	2.14	0.48
1:C:48:ARG:HG3	1:C:48:ARG:NH2	2.29	0.48
1:D:380:PHE:CZ	1:D:495:LEU:HD12	2.49	0.48
1:A:176:LEU:HD12	1:B:98:MET:SD	2.53	0.48
1:D:507:PRO:CG	1:D:514:ASP:HB2	2.43	0.48
1:C:144:LEU:HG	1:C:159:PHE:CE1	2.49	0.48
1:B:431:LEU:HB3	1:B:432:LEU:HD12	1.96	0.48
1:D:364:ASP:O	1:D:368:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:ASN:O	1:C:517:LEU:HB2	2.14	0.47
1:D:136:LYS:HE3	1:D:167:VAL:HG23	1.96	0.47
1:B:30:TRP:CZ2	1:C:288:PRO:HG3	2.49	0.47
1:D:20:GLU:C	1:D:22:ALA:H	2.17	0.47
1:A:350:MET:O	1:A:353:PRO:HD3	2.13	0.47
1:C:508:ILE:O	1:C:509:VAL:C	2.52	0.47
1:C:416:ARG:HG3	1:C:417:VAL:HG23	1.95	0.47
1:B:260:VAL:CG2	1:C:51:PRO:HB3	2.43	0.47
1:C:199:MET:HB2	1:C:245:SER:HB2	1.96	0.47
1:B:216:LEU:HD12	1:B:216:LEU:N	2.29	0.47
1:C:21:LEU:N	1:C:21:LEU:HD12	2.29	0.47
1:C:364:ASP:O	1:C:368:MET:HG3	2.13	0.47
1:A:479:TYR:O	1:A:483:ILE:HG13	2.14	0.47
1:A:352:TYR:HE2	1:B:81:PRO:CA	2.27	0.47
1:B:59:VAL:O	1:B:63:ILE:HG13	2.14	0.47
1:B:144:LEU:HG	1:B:159:PHE:CE1	2.49	0.47
1:D:508:ILE:C	1:D:508:ILE:HD12	2.34	0.47
1:A:512:LEU:CA	1:A:536:VAL:HG21	2.44	0.47
1:D:199:MET:HE1	1:D:224:ASP:HB3	1.95	0.47
1:A:380:PHE:CZ	1:A:495:LEU:HD12	2.48	0.47
1:A:21:LEU:N	1:A:21:LEU:HD12	2.29	0.47
1:C:352:TYR:HB3	1:C:355:PHE:HD2	1.79	0.47
1:A:541:PHE:O	1:A:542:LEU:C	2.52	0.47
1:B:136:LYS:HE3	1:B:167:VAL:HG23	1.97	0.47
1:A:548:ILE:HG22	1:A:548:ILE:O	2.15	0.47
1:A:83:ILE:HD13	1:A:107:LEU:CD2	2.43	0.47
1:C:380:PHE:CZ	1:C:495:LEU:HD12	2.49	0.47
1:A:436:VAL:HA	1:A:479:TYR:HB2	1.97	0.47
1:C:136:LYS:HE3	1:C:167:VAL:HG23	1.97	0.47
1:D:111:PRO:HD2	1:D:186:LEU:HD21	1.95	0.47
1:C:548:ILE:HG22	1:C:548:ILE:O	2.15	0.47
1:D:548:ILE:HG22	1:D:548:ILE:O	2.15	0.47
1:A:47:PRO:HG2	1:A:474:SER:O	2.13	0.47
1:A:195:LEU:HD13	1:A:227:PHE:CD1	2.49	0.47
1:A:508:ILE:O	1:A:509:VAL:C	2.53	0.47
1:B:508:ILE:C	1:B:508:ILE:HD12	2.35	0.47
1:D:216:LEU:HD12	1:D:216:LEU:N	2.30	0.47
1:C:514:ASP:C	1:C:516:ASN:H	2.17	0.47
1:D:144:LEU:HG	1:D:159:PHE:CE1	2.50	0.47
1:A:260:VAL:HG23	1:D:51:PRO:HD3	1.95	0.47
1:C:436:VAL:HA	1:C:479:TYR:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:MET:H	1:B:173:LEU:CD1	2.28	0.47
1:A:161:ILE:HG13	1:A:162:ALA:N	2.30	0.47
1:C:195:LEU:HD13	1:C:227:PHE:CD1	2.50	0.47
1:D:199:MET:HB2	1:D:245:SER:HB2	1.95	0.47
1:C:176:LEU:HD12	1:D:98:MET:HE1	1.97	0.47
1:C:161:ILE:HG13	1:C:162:ALA:N	2.30	0.47
1:A:352:TYR:HB3	1:A:355:PHE:HD2	1.80	0.47
1:A:508:ILE:C	1:A:508:ILE:HD12	2.36	0.47
1:C:387:LEU:CD1	1:C:484:ILE:HD12	2.44	0.47
1:C:301:LEU:HG	1:C:302:GLY:H	1.80	0.46
1:A:229:ARG:CZ	1:B:109:GLY:HA3	2.45	0.46
1:A:20:GLU:C	1:A:22:ALA:H	2.18	0.46
1:C:508:ILE:HD12	1:C:508:ILE:C	2.36	0.46
1:A:216:LEU:HD12	1:A:216:LEU:N	2.30	0.46
1:D:352:TYR:HB3	1:D:355:PHE:HD2	1.80	0.46
1:D:436:VAL:HA	1:D:479:TYR:HB2	1.97	0.46
1:C:370:ARG:HH21	1:C:370:ARG:HG2	1.80	0.46
1:B:436:VAL:HA	1:B:479:TYR:HB2	1.97	0.46
1:B:508:ILE:O	1:B:509:VAL:C	2.53	0.46
1:B:431:LEU:HD13	1:B:431:LEU:O	2.15	0.46
1:D:455:GLU:H	1:D:459:GLU:HG3	1.81	0.46
1:B:301:LEU:HG	1:B:302:GLY:H	1.80	0.46
1:B:72:ARG:HH11	1:D:68:GLN:NE2	2.04	0.46
1:B:548:ILE:O	1:B:548:ILE:HG22	2.15	0.46
1:B:502:PHE:HB2	1:B:546:VAL:CG1	2.45	0.46
1:B:541:PHE:O	1:B:542:LEU:C	2.53	0.46
1:D:48:ARG:HG3	1:D:48:ARG:NH2	2.30	0.46
1:C:438:ASN:O	1:C:478:ARG:HA	2.15	0.46
1:C:216:LEU:N	1:C:216:LEU:HD12	2.31	0.46
1:C:171:MET:H	1:C:173:LEU:CD1	2.28	0.46
1:B:300:LYS:CG	1:B:301:LEU:H	2.20	0.46
1:D:502:PHE:HB2	1:D:546:VAL:CG1	2.45	0.46
1:A:443:TYR:CG	1:A:464:ILE:HG23	2.50	0.46
1:B:295:TYR:HA	1:B:306:GLU:HA	1.95	0.46
1:D:370:ARG:HH21	1:D:370:ARG:HG2	1.79	0.46
1:A:370:ARG:HH21	1:A:370:ARG:HG2	1.80	0.46
1:A:516:ASN:O	1:A:517:LEU:HB2	2.16	0.46
1:A:358:TYR:HD2	1:B:213:LYS:HD3	1.80	0.46
1:A:59:VAL:O	1:A:63:ILE:HG13	2.14	0.46
1:D:431:LEU:HB3	1:D:432:LEU:HD12	1.96	0.46
1:C:455:GLU:H	1:C:459:GLU:HG3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:LEU:HG	1:D:302:GLY:H	1.79	0.46
1:A:57:HIS:H	1:B:77:GLU:HB3	1.80	0.46
1:A:411:PHE:HB3	1:A:415:ARG:HB2	1.98	0.46
1:B:443:TYR:CG	1:B:464:ILE:HG23	2.51	0.46
1:B:514:ASP:C	1:B:516:ASN:H	2.16	0.46
1:B:283:SER:N	1:B:291:GLN:NE2	2.59	0.46
1:B:161:ILE:HG13	1:B:162:ALA:N	2.30	0.46
1:D:161:ILE:HG13	1:D:162:ALA:N	2.30	0.46
1:C:111:PRO:HD2	1:C:186:LEU:HD21	1.96	0.46
1:B:111:PRO:CD	1:B:188:PRO:HA	2.39	0.46
1:B:20:GLU:C	1:B:22:ALA:H	2.18	0.46
1:C:431:LEU:HB3	1:C:432:LEU:HD12	1.98	0.46
1:A:387:LEU:HD12	1:A:484:ILE:HD12	1.98	0.46
1:B:380:PHE:CZ	1:B:495:LEU:HD12	2.50	0.46
1:A:455:GLU:H	1:A:459:GLU:HG3	1.80	0.46
1:A:171:MET:H	1:A:173:LEU:CD1	2.28	0.46
1:B:167:VAL:HG13	1:B:168:SER:N	2.31	0.46
1:C:502:PHE:HB2	1:C:546:VAL:CG1	2.45	0.46
1:C:213:LYS:NZ	1:D:355:PHE:C	2.69	0.46
1:A:136:LYS:HE3	1:A:167:VAL:HG23	1.97	0.46
1:B:48:ARG:HG3	1:B:48:ARG:NH2	2.30	0.46
1:B:411:PHE:HB3	1:B:415:ARG:HB2	1.98	0.46
1:A:18:VAL:HA	1:A:21:LEU:HD13	1.98	0.46
1:B:352:TYR:HB3	1:B:355:PHE:HD2	1.80	0.46
1:A:167:VAL:HG13	1:A:168:SER:N	2.31	0.45
1:A:301:LEU:CG	1:A:302:GLY:H	2.30	0.45
1:D:103:ARG:CA	1:D:229:ARG:HB3	2.46	0.45
1:D:438:ASN:O	1:D:478:ARG:HA	2.16	0.45
1:B:401:CYS:SG	1:B:403:VAL:HG23	2.56	0.45
1:A:13:PHE:CE1	1:D:324:ASP:HA	2.51	0.45
1:C:479:TYR:O	1:C:483:ILE:HG13	2.16	0.45
1:D:171:MET:H	1:D:173:LEU:CD1	2.29	0.45
1:B:167:VAL:HG13	1:B:168:SER:H	1.81	0.45
1:D:301:LEU:CG	1:D:302:GLY:H	2.29	0.45
1:A:348:ARG:HH12	1:A:356:TYR:HB3	1.81	0.45
1:A:351:VAL:O	1:B:79:ILE:HB	2.16	0.45
1:A:368:MET:CE	1:B:215:LYS:HD2	2.46	0.45
1:C:20:GLU:C	1:C:22:ALA:H	2.17	0.45
1:D:411:PHE:HB3	1:D:415:ARG:HB2	1.98	0.45
1:C:443:TYR:CG	1:C:464:ILE:HG23	2.52	0.45
1:D:147:TYR:O	1:D:151:ALA:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:TYR:CG	1:D:464:ILE:HG23	2.51	0.45
1:A:167:VAL:HG13	1:A:168:SER:H	1.81	0.45
1:A:90:TYR:O	1:A:94:GLY:HA2	2.17	0.45
1:A:424:GLU:OE1	1:A:542:LEU:HD23	2.17	0.45
1:A:502:PHE:HB2	1:A:546:VAL:CG1	2.46	0.45
1:D:300:LYS:CG	1:D:301:LEU:H	2.20	0.45
1:A:103:ARG:CA	1:A:229:ARG:HB3	2.46	0.45
1:B:103:ARG:CA	1:B:229:ARG:HB3	2.46	0.45
1:C:167:VAL:HG13	1:C:168:SER:N	2.32	0.45
1:B:274:PHE:HD1	1:B:275:LYS:N	2.03	0.45
1:C:431:LEU:O	1:C:431:LEU:HD13	2.16	0.45
1:B:387:LEU:HD12	1:B:484:ILE:HD12	1.97	0.45
1:C:64:GLU:HG3	1:D:64:GLU:CD	2.35	0.45
1:B:507:PRO:CG	1:B:514:ASP:HB2	2.44	0.45
1:C:301:LEU:CG	1:C:302:GLY:H	2.29	0.45
1:B:348:ARG:HH12	1:B:356:TYR:HB3	1.82	0.45
1:C:411:PHE:HB3	1:C:415:ARG:HB2	1.98	0.45
1:C:167:VAL:HG13	1:C:168:SER:H	1.82	0.45
1:A:90:TYR:HD2	1:A:97:ALA:HB3	1.82	0.45
1:B:424:GLU:OE1	1:B:542:LEU:HD23	2.17	0.45
1:C:103:ARG:CA	1:C:229:ARG:HB3	2.47	0.45
1:C:325:VAL:CG2	1:C:326:PRO:HD2	2.47	0.45
1:D:18:VAL:HA	1:D:21:LEU:HD13	1.98	0.45
1:C:18:VAL:HA	1:C:21:LEU:HD13	1.99	0.45
1:C:41:HIS:ND1	1:C:42:ILE:N	2.52	0.45
1:C:424:GLU:OE1	1:C:542:LEU:HD23	2.16	0.45
1:B:512:LEU:CA	1:B:536:VAL:HG21	2.46	0.45
1:D:387:LEU:HD12	1:D:484:ILE:HD12	1.98	0.45
1:A:31:ARG:N	1:A:31:ARG:HD3	2.03	0.45
1:D:516:ASN:O	1:D:517:LEU:HB2	2.16	0.45
1:D:167:VAL:HG13	1:D:168:SER:H	1.82	0.45
1:D:424:GLU:OE1	1:D:542:LEU:HD23	2.17	0.45
1:A:48:ARG:HG3	1:A:48:ARG:NH2	2.31	0.45
1:D:110:LEU:HD13	1:D:110:LEU:C	2.37	0.45
1:D:167:VAL:HG13	1:D:168:SER:N	2.31	0.45
1:B:90:TYR:O	1:B:94:GLY:HA2	2.17	0.45
1:B:90:TYR:HD2	1:B:97:ALA:HB3	1.82	0.45
1:A:300:LYS:CG	1:A:301:LEU:H	2.20	0.45
1:D:401:CYS:SG	1:D:403:VAL:HG23	2.57	0.45
1:B:455:GLU:H	1:B:459:GLU:HG3	1.81	0.45
1:D:479:TYR:O	1:D:483:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ASN:O	1:B:517:LEU:HB2	2.16	0.44
1:D:395:LYS:CG	1:D:430:LYS:HG2	2.47	0.44
1:C:90:TYR:HD2	1:C:97:ALA:HB3	1.81	0.44
1:A:301:LEU:HG	1:A:302:GLY:H	1.80	0.44
1:C:387:LEU:HD12	1:C:484:ILE:HD12	1.99	0.44
1:C:90:TYR:O	1:C:94:GLY:HA2	2.17	0.44
1:A:57:HIS:N	1:B:77:GLU:HB3	2.31	0.44
1:D:512:LEU:CA	1:D:536:VAL:HG21	2.45	0.44
1:C:512:LEU:CA	1:C:536:VAL:HG21	2.45	0.44
1:D:395:LYS:CG	1:D:396:ASP:H	2.14	0.44
1:D:263:GLU:HG3	1:D:274:PHE:HZ	1.83	0.44
1:A:97:ALA:HA	1:A:100:VAL:CG1	2.41	0.44
1:D:348:ARG:HH12	1:D:356:TYR:HB3	1.81	0.44
1:C:435:SER:O	1:C:437:LEU:N	2.51	0.44
1:A:199:MET:HE1	1:A:224:ASP:HB3	1.99	0.44
1:B:97:ALA:HA	1:B:100:VAL:CG1	2.41	0.44
1:B:301:LEU:CG	1:B:302:GLY:H	2.30	0.44
1:A:502:PHE:HB3	1:A:503:LYS:H	1.48	0.44
1:C:348:ARG:HH12	1:C:356:TYR:HB3	1.82	0.44
1:C:36:LEU:N	1:C:36:LEU:HD22	2.33	0.44
1:A:507:PRO:CG	1:A:514:ASP:HB2	2.43	0.44
1:A:158:VAL:HG22	1:A:159:PHE:CD2	2.52	0.44
1:A:395:LYS:CG	1:A:430:LYS:HG2	2.47	0.44
1:C:301:LEU:CG	1:C:302:GLY:N	2.81	0.44
1:B:438:ASN:O	1:B:478:ARG:HA	2.17	0.44
1:B:260:VAL:HG13	1:B:261:VAL:N	2.32	0.44
1:A:110:LEU:C	1:A:110:LEU:HD13	2.38	0.44
1:C:31:ARG:N	1:C:31:ARG:CD	2.74	0.44
1:A:438:ASN:O	1:A:478:ARG:HA	2.18	0.44
1:B:479:TYR:O	1:B:483:ILE:HG13	2.18	0.44
1:C:396:ASP:CA	1:C:430:LYS:HA	2.48	0.44
1:D:90:TYR:O	1:D:94:GLY:HA2	2.17	0.44
1:A:227:PHE:HZ	1:B:227:PHE:CZ	2.34	0.44
1:C:63:ILE:HG12	1:C:334:VAL:HG11	1.99	0.44
1:C:147:TYR:O	1:C:151:ALA:HB2	2.18	0.44
1:C:110:LEU:HD13	1:C:110:LEU:C	2.38	0.44
1:B:482:GLY:HA3	1:B:515:ILE:O	2.18	0.44
1:C:522:LEU:N	1:C:522:LEU:HD12	2.33	0.44
1:A:401:CYS:SG	1:A:403:VAL:HG23	2.58	0.44
1:D:63:ILE:HG12	1:D:334:VAL:HG11	2.00	0.44
1:B:147:TYR:O	1:B:151:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ILE:CD1	1:D:179:ALA:HB1	2.48	0.44
1:B:263:GLU:HG3	1:B:274:PHE:HZ	1.83	0.44
1:D:35:ALA:O	1:D:36:LEU:HB2	2.18	0.44
1:C:230:GLU:HB3	1:C:233:GLU:CG	2.48	0.44
1:D:230:GLU:HB3	1:D:233:GLU:CG	2.48	0.44
1:C:227:PHE:N	1:C:227:PHE:CD1	2.86	0.44
1:C:490:LYS:O	1:C:491:ILE:C	2.57	0.44
1:D:483:ILE:O	1:D:486:LYS:HB3	2.18	0.44
1:C:507:PRO:CG	1:C:514:ASP:HB2	2.44	0.44
1:D:90:TYR:HD2	1:D:97:ALA:HB3	1.82	0.44
1:D:301:LEU:CG	1:D:302:GLY:N	2.81	0.44
1:D:36:LEU:N	1:D:36:LEU:HD22	2.33	0.44
1:B:522:LEU:N	1:B:522:LEU:HD12	2.33	0.44
1:B:230:GLU:HB3	1:B:233:GLU:CG	2.48	0.44
1:B:199:MET:HE1	1:B:224:ASP:HB3	1.99	0.44
1:A:147:TYR:O	1:A:151:ALA:HB2	2.17	0.44
1:A:301:LEU:CG	1:A:302:GLY:N	2.81	0.43
1:B:72:ARG:HE	1:D:68:GLN:NE2	2.15	0.43
1:B:435:SER:O	1:B:437:LEU:N	2.51	0.43
1:B:36:LEU:N	1:B:36:LEU:HD22	2.32	0.43
1:B:325:VAL:CG2	1:B:326:PRO:HD2	2.48	0.43
1:C:130:ILE:CD1	1:C:179:ALA:HB1	2.48	0.43
1:C:469:LYS:HG2	1:C:469:LYS:O	2.18	0.43
1:C:200:THR:C	1:C:202:GLY:N	2.72	0.43
1:C:158:VAL:HG22	1:C:159:PHE:CD2	2.53	0.43
1:C:107:LEU:HD23	1:D:105:PHE:CD1	2.53	0.43
1:B:388:ILE:HG12	1:B:484:ILE:HG13	2.00	0.43
1:D:158:VAL:HG22	1:D:159:PHE:CD2	2.53	0.43
1:A:395:LYS:CG	1:A:396:ASP:N	2.80	0.43
1:B:301:LEU:CG	1:B:302:GLY:N	2.81	0.43
1:A:541:PHE:O	1:A:543:ASN:N	2.52	0.43
1:C:365:ILE:O	1:C:369:ILE:HG13	2.18	0.43
1:C:287:THR:HG22	1:C:315:PRO:HD3	2.01	0.43
1:C:35:ALA:O	1:C:36:LEU:HB2	2.18	0.43
1:C:380:PHE:O	1:C:383:PHE:HB3	2.18	0.43
1:B:18:VAL:HA	1:B:21:LEU:HD13	1.99	0.43
1:A:41:HIS:ND1	1:A:42:ILE:N	2.53	0.43
1:B:110:LEU:HD13	1:B:110:LEU:C	2.38	0.43
1:D:469:LYS:O	1:D:469:LYS:HG2	2.18	0.43
1:A:130:ILE:CD1	1:A:179:ALA:HB1	2.49	0.43
1:D:159:PHE:HB3	1:D:171:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:HG22	1:B:159:PHE:CD2	2.54	0.43
1:B:396:ASP:OD2	1:B:397:LYS:N	2.51	0.43
1:D:396:ASP:CA	1:D:430:LYS:HA	2.49	0.43
1:A:109:GLY:HA3	1:B:229:ARG:HH11	1.83	0.43
1:A:35:ALA:O	1:A:36:LEU:HB2	2.19	0.43
1:D:203:TRP:CE3	1:D:203:TRP:HA	2.54	0.43
1:A:54:GLY:N	1:B:74:GLY:HA2	2.33	0.43
1:A:435:SER:O	1:A:437:LEU:N	2.51	0.43
1:D:35:ALA:C	1:D:37:ILE:N	2.72	0.43
1:A:441:TYR:CG	1:A:465:LEU:HB2	2.54	0.43
1:D:83:ILE:HD13	1:D:107:LEU:CD2	2.43	0.43
1:A:230:GLU:HB3	1:A:233:GLU:CG	2.48	0.43
1:D:387:LEU:HD12	1:D:484:ILE:CG2	2.49	0.43
1:A:380:PHE:O	1:A:383:PHE:HB3	2.18	0.43
1:A:335:GLU:O	1:A:338:ALA:HB3	2.19	0.43
1:A:483:ILE:O	1:A:486:LYS:HB3	2.18	0.43
1:D:89:ILE:HD13	1:D:101:LEU:CD2	2.49	0.43
1:C:541:PHE:O	1:C:543:ASN:N	2.51	0.43
1:C:441:TYR:CG	1:C:465:LEU:HB2	2.54	0.43
1:B:224:ASP:CG	1:B:225:ARG:N	2.72	0.43
1:A:36:LEU:N	1:A:36:LEU:HD22	2.33	0.43
1:B:35:ALA:O	1:B:36:LEU:HB2	2.18	0.43
1:B:130:ILE:CD1	1:B:179:ALA:HB1	2.48	0.43
1:B:158:VAL:CG1	1:B:159:PHE:H	2.16	0.43
1:A:396:ASP:OD2	1:A:397:LYS:N	2.50	0.43
1:B:72:ARG:HE	1:D:68:GLN:HE22	1.67	0.43
1:A:325:VAL:CG2	1:A:326:PRO:HD2	2.48	0.43
1:A:287:THR:HG22	1:A:315:PRO:HD3	2.00	0.43
1:B:35:ALA:C	1:B:37:ILE:N	2.72	0.43
1:A:203:TRP:O	1:A:207:LEU:N	2.51	0.43
1:B:396:ASP:CA	1:B:430:LYS:HA	2.49	0.43
1:D:274:PHE:HD1	1:D:275:LYS:N	2.04	0.43
1:A:205:ILE:HD13	1:A:321:TYR:CE2	2.46	0.43
1:D:435:SER:O	1:D:437:LEU:N	2.52	0.43
1:D:365:ILE:O	1:D:369:ILE:HG13	2.19	0.43
1:A:365:ILE:HB	1:A:442:VAL:HG11	2.01	0.43
1:B:380:PHE:O	1:B:383:PHE:HB3	2.18	0.43
1:D:328:MET:SD	1:D:328:MET:C	2.97	0.43
1:C:516:ASN:HB3	1:C:517:LEU:H	1.68	0.43
1:B:513:SER:C	1:B:514:ASP:O	2.57	0.43
1:D:173:LEU:HD12	1:D:173:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASP:CA	1:A:430:LYS:HA	2.49	0.43
1:B:543:ASN:O	1:B:544:ALA:O	2.37	0.43
1:D:502:PHE:HB2	1:D:546:VAL:HG13	2.01	0.43
1:D:522:LEU:N	1:D:522:LEU:HD12	2.33	0.43
1:B:441:TYR:CG	1:B:465:LEU:HB2	2.54	0.43
1:D:325:VAL:CG2	1:D:326:PRO:HD2	2.47	0.43
1:D:260:VAL:HG13	1:D:261:VAL:N	2.33	0.43
1:C:260:VAL:HG13	1:C:261:VAL:N	2.34	0.43
1:A:79:ILE:HD12	1:B:57:HIS:CE1	2.54	0.43
1:A:88:GLU:OE1	1:A:88:GLU:HA	2.19	0.43
1:C:203:TRP:HA	1:C:203:TRP:CE3	2.54	0.43
1:C:203:TRP:O	1:C:207:LEU:N	2.52	0.43
1:D:97:ALA:HA	1:D:100:VAL:CG1	2.40	0.43
1:B:205:ILE:HD13	1:B:321:TYR:CE2	2.46	0.43
1:A:260:VAL:HG13	1:A:261:VAL:N	2.34	0.43
1:D:380:PHE:O	1:D:383:PHE:HB3	2.19	0.43
1:B:380:PHE:CE1	1:B:409:PHE:HE2	2.37	0.43
1:C:213:LYS:HZ2	1:D:355:PHE:C	2.23	0.43
1:B:365:ILE:HB	1:B:442:VAL:HG11	2.01	0.42
1:A:224:ASP:CG	1:A:225:ARG:N	2.73	0.42
1:B:63:ILE:HG12	1:B:334:VAL:HG11	2.00	0.42
1:A:203:TRP:CE3	1:A:203:TRP:HA	2.54	0.42
1:A:469:LYS:HG2	1:A:469:LYS:O	2.18	0.42
1:D:482:GLY:HA3	1:D:515:ILE:O	2.19	0.42
1:A:435:SER:OG	1:A:436:VAL:N	2.52	0.42
1:B:483:ILE:O	1:B:486:LYS:HB3	2.19	0.42
1:A:105:PHE:CD1	1:B:107:LEU:HB3	2.54	0.42
1:B:541:PHE:O	1:B:543:ASN:N	2.52	0.42
1:D:541:PHE:O	1:D:543:ASN:N	2.52	0.42
1:D:287:THR:HG22	1:D:315:PRO:HD3	2.01	0.42
1:D:365:ILE:HB	1:D:442:VAL:HG11	2.01	0.42
1:B:387:LEU:HD12	1:B:484:ILE:CG2	2.49	0.42
1:B:203:TRP:HA	1:B:203:TRP:CE3	2.54	0.42
1:B:203:TRP:O	1:B:207:LEU:N	2.51	0.42
1:B:490:LYS:O	1:B:491:ILE:C	2.57	0.42
1:C:482:GLY:HA3	1:C:515:ILE:O	2.18	0.42
1:C:482:GLY:O	1:C:516:ASN:ND2	2.46	0.42
1:A:26:PHE:CE1	1:A:29:ALA:HB3	2.55	0.42
1:C:205:ILE:HD13	1:C:321:TYR:CE2	2.45	0.42
1:C:108:ALA:H	1:D:106:TYR:H	1.66	0.42
1:B:365:ILE:O	1:B:369:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:C	1:A:37:ILE:N	2.71	0.42
1:D:388:ILE:HG12	1:D:484:ILE:HG13	2.01	0.42
1:A:387:LEU:HD12	1:A:484:ILE:CG2	2.49	0.42
1:A:388:ILE:HG12	1:A:484:ILE:HG13	2.02	0.42
1:C:224:ASP:CG	1:C:225:ARG:N	2.73	0.42
1:D:203:TRP:O	1:D:207:LEU:N	2.51	0.42
1:B:469:LYS:HG2	1:B:469:LYS:O	2.18	0.42
1:A:279:ASP:HB3	1:A:291:GLN:HG2	2.01	0.42
1:B:173:LEU:HD12	1:B:173:LEU:N	2.34	0.42
1:D:490:LYS:O	1:D:491:ILE:C	2.58	0.42
1:C:395:LYS:CG	1:C:430:LYS:HG2	2.47	0.42
1:D:395:LYS:CG	1:D:396:ASP:N	2.80	0.42
1:C:502:PHE:HB2	1:C:546:VAL:HG13	2.02	0.42
1:D:502:PHE:HB3	1:D:503:LYS:H	1.48	0.42
1:D:26:PHE:CE1	1:D:29:ALA:HB3	2.54	0.42
1:D:441:TYR:CG	1:D:465:LEU:HB2	2.54	0.42
1:A:227:PHE:N	1:A:227:PHE:CD1	2.88	0.42
1:A:200:THR:C	1:A:202:GLY:N	2.72	0.42
1:A:173:LEU:HD12	1:A:173:LEU:N	2.34	0.42
1:C:263:GLU:HG3	1:C:274:PHE:HZ	1.83	0.42
1:C:543:ASN:O	1:C:544:ALA:O	2.38	0.42
1:A:46:TYR:HA	1:A:48:ARG:N	2.35	0.42
1:C:35:ALA:C	1:C:37:ILE:N	2.71	0.42
1:D:224:ASP:CG	1:D:225:ARG:N	2.73	0.42
1:C:77:GLU:HB3	1:D:57:HIS:H	1.84	0.42
1:D:200:THR:C	1:D:202:GLY:H	2.23	0.42
1:C:396:ASP:OD2	1:C:397:LYS:N	2.51	0.42
1:A:263:GLU:HG3	1:A:274:PHE:HZ	1.84	0.42
1:B:502:PHE:HB2	1:B:546:VAL:HG13	2.02	0.42
1:D:543:ASN:O	1:D:544:ALA:O	2.38	0.42
1:C:26:PHE:CE1	1:C:29:ALA:HB3	2.55	0.42
1:B:287:THR:HG22	1:B:315:PRO:HD3	2.01	0.42
1:C:413:GLY:C	1:C:415:ARG:H	2.23	0.42
1:D:200:THR:C	1:D:202:GLY:N	2.73	0.42
1:D:290:THR:O	1:D:292:THR:HG23	2.20	0.42
1:C:395:LYS:CG	1:C:396:ASP:N	2.80	0.42
1:D:263:GLU:HG3	1:D:274:PHE:CZ	2.55	0.42
1:A:522:LEU:HD12	1:A:522:LEU:N	2.34	0.42
1:A:380:PHE:CE1	1:A:409:PHE:HE2	2.38	0.42
1:A:490:LYS:O	1:A:491:ILE:C	2.58	0.42
1:D:279:ASP:HB3	1:D:291:GLN:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:GLU:HG3	1:A:274:PHE:CZ	2.55	0.42
1:B:26:PHE:CE1	1:B:29:ALA:HB3	2.55	0.42
1:A:63:ILE:HG12	1:A:334:VAL:HG11	2.01	0.42
1:B:227:PHE:CD1	1:B:227:PHE:N	2.88	0.42
1:D:227:PHE:N	1:D:227:PHE:CD1	2.88	0.42
1:D:392:ILE:HD11	1:D:480:ILE:CD1	2.50	0.42
1:A:506:VAL:H	1:A:507:PRO:CD	2.33	0.42
1:B:159:PHE:HB3	1:B:171:MET:SD	2.60	0.42
1:C:107:LEU:HD12	1:C:107:LEU:N	2.35	0.42
1:A:512:LEU:C	1:A:512:LEU:HD12	2.40	0.42
1:A:413:GLY:C	1:A:415:ARG:H	2.24	0.42
1:B:88:GLU:OE1	1:B:88:GLU:HA	2.20	0.42
1:B:328:MET:C	1:B:328:MET:SD	2.99	0.42
1:C:506:VAL:H	1:C:507:PRO:CD	2.33	0.41
1:B:370:ARG:NH2	1:B:370:ARG:HG2	2.35	0.41
1:B:392:ILE:HD11	1:B:480:ILE:CD1	2.50	0.41
1:C:173:LEU:HD12	1:C:173:LEU:N	2.34	0.41
1:B:263:GLU:HG3	1:B:274:PHE:CZ	2.55	0.41
1:C:89:ILE:HD13	1:C:101:LEU:CD2	2.50	0.41
1:D:512:LEU:C	1:D:512:LEU:HD12	2.41	0.41
1:C:388:ILE:HG12	1:C:484:ILE:HG13	2.01	0.41
1:C:380:PHE:CE1	1:C:409:PHE:HE2	2.38	0.41
1:D:380:PHE:CE1	1:D:409:PHE:HE2	2.38	0.41
1:D:413:GLY:C	1:D:415:ARG:H	2.23	0.41
1:C:467:LYS:O	1:C:468:ALA:HB3	2.20	0.41
1:A:290:THR:O	1:A:292:THR:HG23	2.20	0.41
1:D:88:GLU:OE1	1:D:88:GLU:HA	2.20	0.41
1:D:467:LYS:O	1:D:468:ALA:HB3	2.20	0.41
1:C:483:ILE:O	1:C:486:LYS:HB3	2.19	0.41
1:B:482:GLY:O	1:B:516:ASN:ND2	2.46	0.41
1:D:46:TYR:HA	1:D:48:ARG:N	2.35	0.41
1:C:156:ASP:CG	1:D:284:LYS:HE3	2.40	0.41
1:A:467:LYS:O	1:A:468:ALA:HB3	2.20	0.41
1:A:328:MET:SD	1:A:328:MET:C	2.98	0.41
1:D:516:ASN:HB3	1:D:517:LEU:H	1.67	0.41
1:A:513:SER:C	1:A:514:ASP:O	2.57	0.41
1:A:543:ASN:O	1:A:544:ALA:O	2.38	0.41
1:D:522:LEU:O	1:D:524:LEU:N	2.50	0.41
1:B:46:TYR:HA	1:B:48:ARG:N	2.35	0.41
1:A:57:HIS:H	1:B:77:GLU:CG	2.33	0.41
1:C:200:THR:C	1:C:202:GLY:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:GLY:O	1:A:516:ASN:ND2	2.44	0.41
1:C:159:PHE:HB3	1:C:171:MET:SD	2.61	0.41
1:B:89:ILE:HD13	1:B:101:LEU:CD2	2.50	0.41
1:C:88:GLU:HA	1:C:88:GLU:OE1	2.20	0.41
1:B:467:LYS:O	1:B:468:ALA:HB3	2.20	0.41
1:B:200:THR:C	1:B:202:GLY:H	2.24	0.41
1:D:513:SER:C	1:D:514:ASP:O	2.57	0.41
1:A:482:GLY:HA3	1:A:515:ILE:O	2.20	0.41
1:C:395:LYS:CG	1:C:396:ASP:H	2.14	0.41
1:C:263:GLU:HG3	1:C:274:PHE:CZ	2.55	0.41
1:B:395:LYS:CG	1:B:396:ASP:N	2.80	0.41
1:A:502:PHE:HB2	1:A:546:VAL:HG13	2.02	0.41
1:A:109:GLY:HA3	1:B:229:ARG:HE	1.85	0.41
1:B:502:PHE:O	1:B:503:LYS:HB2	2.20	0.41
1:B:20:GLU:C	1:B:22:ALA:N	2.74	0.41
1:A:441:TYR:CE2	1:A:474:SER:HB2	2.55	0.41
1:C:365:ILE:HB	1:C:442:VAL:HG11	2.02	0.41
1:A:308:ALA:HB1	1:A:330:LEU:HD11	2.02	0.41
1:A:352:TYR:CE2	1:B:81:PRO:HA	2.55	0.41
1:B:290:THR:O	1:B:292:THR:HG23	2.21	0.41
1:D:506:VAL:H	1:D:507:PRO:CD	2.34	0.41
1:C:513:SER:C	1:C:514:ASP:O	2.58	0.41
1:B:89:ILE:HD11	1:B:100:VAL:CG1	2.51	0.41
1:C:441:TYR:CE2	1:C:474:SER:HB2	2.55	0.41
1:C:522:LEU:O	1:C:523:ALA:CB	2.68	0.41
1:B:512:LEU:C	1:B:512:LEU:HD12	2.41	0.41
1:D:32:GLU:C	1:D:34:ARG:N	2.74	0.41
1:B:458:LYS:O	1:B:460:GLN:N	2.49	0.41
1:C:335:GLU:O	1:C:338:ALA:HB3	2.20	0.41
1:C:502:PHE:O	1:C:503:LYS:HB2	2.20	0.41
1:C:387:LEU:HD12	1:C:484:ILE:CG2	2.50	0.41
1:B:279:ASP:HB3	1:B:291:GLN:HG2	2.02	0.41
1:A:502:PHE:O	1:A:503:LYS:HB2	2.21	0.41
1:D:20:GLU:C	1:D:22:ALA:N	2.74	0.41
1:C:45:LYS:O	1:C:46:TYR:HB3	2.21	0.41
1:D:441:TYR:CE2	1:D:474:SER:HB2	2.56	0.41
1:B:441:TYR:CE2	1:B:474:SER:HB2	2.56	0.41
1:D:107:LEU:HD12	1:D:107:LEU:N	2.36	0.41
1:A:57:HIS:HB2	1:B:77:GLU:HG2	2.01	0.41
1:A:365:ILE:O	1:A:369:ILE:HG13	2.20	0.41
1:D:351:VAL:HB	1:D:352:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:C	1:A:202:GLY:H	2.23	0.41
1:C:392:ILE:HD11	1:C:480:ILE:CD1	2.51	0.41
1:B:506:VAL:H	1:B:507:PRO:CD	2.33	0.41
1:B:395:LYS:CG	1:B:430:LYS:HG2	2.48	0.41
1:D:396:ASP:OD2	1:D:397:LYS:N	2.51	0.41
1:C:89:ILE:HD11	1:C:100:VAL:CG1	2.51	0.41
1:A:20:GLU:C	1:A:22:ALA:N	2.74	0.41
1:D:502:PHE:O	1:D:503:LYS:HB2	2.20	0.41
1:C:88:GLU:OE2	1:C:205:ILE:HD12	2.21	0.41
1:C:108:ALA:O	1:D:105:PHE:HA	2.21	0.41
1:B:387:LEU:C	1:B:387:LEU:HD13	2.41	0.41
1:D:308:ALA:HB1	1:D:330:LEU:HD11	2.03	0.41
1:C:351:VAL:HB	1:C:352:TYR:CD1	2.56	0.41
1:B:399:SER:HB3	1:B:425:ASN:HA	2.03	0.41
1:A:370:ARG:NH2	1:A:370:ARG:HG2	2.36	0.41
1:C:279:ASP:HB3	1:C:291:GLN:HG2	2.03	0.41
1:A:89:ILE:HD13	1:A:101:LEU:CD2	2.51	0.41
1:C:20:GLU:C	1:C:22:ALA:N	2.74	0.41
1:A:45:LYS:O	1:A:46:TYR:HB3	2.21	0.41
1:C:512:LEU:C	1:C:512:LEU:HD12	2.42	0.41
1:C:200:THR:O	1:C:202:GLY:N	2.54	0.41
1:D:140:LEU:N	1:D:140:LEU:HD12	2.36	0.41
1:A:89:ILE:HD11	1:A:100:VAL:CG1	2.50	0.40
1:A:316:ILE:O	1:A:319:ALA:HB3	2.20	0.40
1:C:11:MET:HE3	1:C:12:ARG:H	1.86	0.40
1:A:392:ILE:HD11	1:A:480:ILE:CD1	2.50	0.40
1:A:159:PHE:HB3	1:A:171:MET:SD	2.61	0.40
1:C:90:TYR:CD2	1:C:97:ALA:HB3	2.56	0.40
1:C:301:LEU:HD12	1:C:302:GLY:H	1.86	0.40
1:D:45:LYS:O	1:D:46:TYR:HB3	2.22	0.40
1:A:57:HIS:NE2	1:B:79:ILE:HD12	2.36	0.40
1:A:261:VAL:HG12	1:A:330:LEU:HD23	2.03	0.40
1:B:32:GLU:C	1:B:34:ARG:N	2.75	0.40
1:B:413:GLY:C	1:B:415:ARG:H	2.24	0.40
1:D:335:GLU:O	1:D:338:ALA:HB3	2.21	0.40
1:A:140:LEU:N	1:A:140:LEU:HD12	2.36	0.40
1:C:328:MET:SD	1:C:328:MET:C	2.99	0.40
1:B:301:LEU:HD12	1:B:302:GLY:H	1.86	0.40
1:D:298:HIS:ND1	1:D:299:PRO:HD2	2.37	0.40
1:A:352:TYR:CE2	1:B:81:PRO:CA	3.05	0.40
1:D:387:LEU:HD13	1:D:387:LEU:C	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLN:HG2	1:C:53:TYR:CE2	2.57	0.40
1:B:286:TYR:HA	1:B:312:VAL:O	2.22	0.40
1:B:396:ASP:HA	1:B:430:LYS:HA	2.04	0.40
1:C:298:HIS:ND1	1:C:299:PRO:HD2	2.37	0.40
1:B:107:LEU:N	1:B:107:LEU:HD12	2.36	0.40
1:C:32:GLU:C	1:C:34:ARG:N	2.74	0.40
1:A:32:GLU:C	1:A:34:ARG:N	2.74	0.40
1:C:513:SER:O	1:C:514:ASP:CB	2.69	0.40
1:A:396:ASP:HA	1:A:430:LYS:HA	2.03	0.40
1:C:105:PHE:CD1	1:D:107:LEU:HD23	2.57	0.40
1:B:351:VAL:HB	1:B:352:TYR:CD1	2.57	0.40
1:B:140:LEU:N	1:B:140:LEU:HD12	2.36	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:LYS:CB	1:A:174:LYS:CB[3_655]	2.14	0.06
1:A:143:VAL:CG1	1:A:143:VAL:CG1[3_655]	2.16	0.04

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	537/549 (98%)	345 (64%)	138 (26%)	54 (10%)	1 11
1	B	537/549 (98%)	346 (64%)	138 (26%)	53 (10%)	1 12
1	C	537/549 (98%)	344 (64%)	139 (26%)	54 (10%)	1 11
1	D	537/549 (98%)	345 (64%)	138 (26%)	54 (10%)	1 11
All	All	2148/2196 (98%)	1380 (64%)	553 (26%)	215 (10%)	1 11

All (215) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	124	ILE
1	A	151	ALA
1	A	167	VAL
1	A	195	LEU
1	A	358	TYR
1	A	397	LYS
1	A	407	ARG
1	A	471	GLU
1	A	506	VAL
1	A	509	VAL
1	A	540	VAL
1	A	544	ALA
1	B	33	THR
1	B	124	ILE
1	B	151	ALA
1	B	167	VAL
1	B	195	LEU
1	B	358	TYR
1	B	397	LYS
1	B	407	ARG
1	B	471	GLU
1	B	506	VAL
1	B	509	VAL
1	B	540	VAL
1	B	544	ALA
1	C	33	THR
1	C	124	ILE
1	C	151	ALA
1	C	167	VAL
1	C	195	LEU
1	C	358	TYR
1	C	397	LYS
1	C	407	ARG
1	C	471	GLU
1	C	506	VAL
1	C	509	VAL
1	C	540	VAL
1	C	544	ALA
1	D	33	THR
1	D	124	ILE
1	D	151	ALA
1	D	167	VAL

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Mol	Chain	Res	Type
1	D	195	LEU
1	D	358	TYR
1	D	397	LYS
1	D	407	ARG
1	D	471	GLU
1	D	506	VAL
1	D	509	VAL
1	D	540	VAL
1	D	544	ALA
1	A	15	ILE
1	A	35	ALA
1	A	40	LYS
1	A	232	ARG
1	A	300	LYS
1	A	394	ASN
1	A	400	PRO
1	A	466	LYS
1	A	542	LEU
1	B	15	ILE
1	B	35	ALA
1	B	158	VAL
1	B	232	ARG
1	B	300	LYS
1	B	394	ASN
1	B	400	PRO
1	B	466	LYS
1	B	542	LEU
1	C	15	ILE
1	C	35	ALA
1	C	40	LYS
1	C	158	VAL
1	C	232	ARG
1	C	300	LYS
1	C	394	ASN
1	C	400	PRO
1	C	466	LYS
1	C	542	LEU
1	D	15	ILE
1	D	35	ALA
1	D	158	VAL
1	D	232	ARG
1	D	300	LYS

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Mol	Chain	Res	Type
1	D	394	ASN
1	D	400	PRO
1	D	466	LYS
1	D	542	LEU
1	A	41	HIS
1	A	136	LYS
1	A	158	VAL
1	A	231	GLN
1	A	299	PRO
1	A	304	TRP
1	A	356	TYR
1	A	372	ASP
1	A	465	LEU
1	A	467	LYS
1	A	537	ARG
1	B	40	LYS
1	B	41	HIS
1	B	136	LYS
1	B	231	GLN
1	B	299	PRO
1	B	304	TRP
1	B	356	TYR
1	B	372	ASP
1	B	465	LEU
1	B	467	LYS
1	B	537	ARG
1	C	41	HIS
1	C	136	LYS
1	C	231	GLN
1	C	299	PRO
1	C	304	TRP
1	C	356	TYR
1	C	372	ASP
1	C	465	LEU
1	C	467	LYS
1	C	537	ARG
1	D	40	LYS
1	D	41	HIS
1	D	136	LYS
1	D	231	GLN
1	D	299	PRO
1	D	304	TRP

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Mol	Chain	Res	Type
1	D	356	TYR
1	D	372	ASP
1	D	465	LEU
1	D	467	LYS
1	D	537	ARG
1	A	142	GLU
1	A	177	GLU
1	A	237	HIS
1	A	291	GLN
1	A	355	PHE
1	A	401	CYS
1	A	459	GLU
1	A	481	ASP
1	B	142	GLU
1	B	177	GLU
1	B	237	HIS
1	B	291	GLN
1	B	355	PHE
1	B	401	CYS
1	B	459	GLU
1	C	142	GLU
1	C	177	GLU
1	C	237	HIS
1	C	291	GLN
1	C	355	PHE
1	C	401	CYS
1	C	459	GLU
1	D	142	GLU
1	D	177	GLU
1	D	237	HIS
1	D	291	GLN
1	D	355	PHE
1	D	401	CYS
1	D	459	GLU
1	A	23	GLU
1	A	46	TYR
1	A	111	PRO
1	A	164	ALA
1	B	23	GLU
1	B	46	TYR
1	B	111	PRO
1	B	164	ALA

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Mol	Chain	Res	Type
1	B	481	ASP
1	C	23	GLU
1	C	46	TYR
1	C	111	PRO
1	C	164	ALA
1	C	481	ASP
1	D	46	TYR
1	D	111	PRO
1	D	164	ALA
1	D	481	ASP
1	A	118	GLY
1	A	198	HIS
1	A	436	VAL
1	A	515	ILE
1	B	118	GLY
1	B	436	VAL
1	B	515	ILE
1	C	118	GLY
1	C	198	HIS
1	C	436	VAL
1	C	515	ILE
1	D	23	GLU
1	D	118	GLY
1	D	198	HIS
1	D	436	VAL
1	D	515	ILE
1	A	417	VAL
1	B	417	VAL
1	C	417	VAL
1	D	417	VAL
1	A	125	ILE
1	A	129	GLY
1	A	440	VAL
1	B	125	ILE
1	B	129	GLY
1	B	440	VAL
1	C	125	ILE
1	C	129	GLY
1	C	440	VAL
1	D	125	ILE
1	D	129	GLY
1	D	440	VAL

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Mol	Chain	Res	Type
1	A	143	VAL
1	B	143	VAL
1	C	143	VAL
1	D	143	VAL

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	481/491 (98%)	468 (97%)	13 (3%)	52 83
1	B	481/491 (98%)	468 (97%)	13 (3%)	52 83
1	C	481/491 (98%)	468 (97%)	13 (3%)	52 83
1	D	481/491 (98%)	468 (97%)	13 (3%)	52 83
All	All	1924/1964 (98%)	1872 (97%)	52 (3%)	52 83

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ARG
1	A	274	PHE
1	A	276	PHE
1	A	286	TYR
1	A	322	ASN
1	A	348	ARG
1	A	355	PHE
1	A	408	GLU
1	A	409	PHE
1	A	431	LEU
1	A	432	LEU
1	A	493	GLU
1	A	506	VAL
1	B	31	ARG
1	B	274	PHE
1	B	276	PHE
1	B	286	TYR

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Mol	Chain	Res	Type
1	B	322	ASN
1	B	348	ARG
1	B	355	PHE
1	B	408	GLU
1	B	409	PHE
1	B	431	LEU
1	B	432	LEU
1	B	493	GLU
1	B	506	VAL
1	C	31	ARG
1	C	274	PHE
1	C	276	PHE
1	C	286	TYR
1	C	322	ASN
1	C	348	ARG
1	C	355	PHE
1	C	408	GLU
1	C	409	PHE
1	C	431	LEU
1	C	432	LEU
1	C	493	GLU
1	C	506	VAL
1	D	31	ARG
1	D	274	PHE
1	D	276	PHE
1	D	286	TYR
1	D	322	ASN
1	D	348	ARG
1	D	355	PHE
1	D	408	GLU
1	D	409	PHE
1	D	431	LEU
1	D	432	LEU
1	D	493	GLU
1	D	506	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	127	ASN
1	A	231	GLN

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Mol	Chain	Res	Type
1	A	242	HIS
1	A	291	GLN
1	A	322	ASN
1	A	329	ASN
1	A	382	ASN
1	A	412	ASN
1	A	476	ASN
1	B	68	GLN
1	B	127	ASN
1	B	231	GLN
1	B	242	HIS
1	B	291	GLN
1	B	322	ASN
1	B	329	ASN
1	B	382	ASN
1	B	412	ASN
1	B	476	ASN
1	C	68	GLN
1	C	127	ASN
1	C	231	GLN
1	C	242	HIS
1	C	291	GLN
1	C	322	ASN
1	C	329	ASN
1	C	382	ASN
1	C	412	ASN
1	C	476	ASN
1	D	68	GLN
1	D	127	ASN
1	D	231	GLN
1	D	242	HIS
1	D	291	GLN
1	D	322	ASN
1	D	329	ASN
1	D	382	ASN
1	D	412	ASN
1	D	476	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	539/549 (98%)	0.53	79 (14%)	3 3	37, 149, 203, 203	0
1	B	539/549 (98%)	0.26	63 (11%)	6 5	15, 116, 203, 203	0
1	C	539/549 (98%)	0.26	68 (12%)	5 5	13, 104, 203, 203	0
1	D	539/549 (98%)	0.55	83 (15%)	3 2	26, 151, 203, 203	0
All	All	2156/2196 (98%)	0.40	293 (13%)	4 4	13, 131, 203, 203	0

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	133	ASP	10.4
1	D	171	MET	9.9
1	D	425	ASN	9.8
1	C	138	GLU	9.7
1	D	179	ALA	9.7
1	B	130	ILE	9.5
1	A	508	ILE	9.4
1	D	128	LEU	9.0
1	D	162	ALA	8.7
1	D	131	ASP	8.3
1	A	148	LYS	8.2
1	D	500	ASP	8.2
1	A	179	ALA	8.1
1	A	181	PRO	8.0
1	B	508	ILE	7.9
1	A	164	ALA	7.9
1	D	426	GLU	7.5
1	A	180	PHE	7.5
1	C	118	GLY	7.5
1	B	132	ILE	7.4
1	C	133	ASP	7.3

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Mol	Chain	Res	Type	RSRZ
1	D	127	ASN	7.2
1	B	178	THR	7.1
1	C	125	ILE	7.1
1	D	177	GLU	7.0
1	C	128	LEU	6.9
1	C	171	MET	6.9
1	D	402	SER	6.9
1	D	138	GLU	6.9
1	B	509	VAL	6.9
1	A	429	LYS	6.7
1	C	177	GLU	6.7
1	D	181	PRO	6.6
1	A	426	GLU	6.5
1	D	434	PRO	6.4
1	B	131	ASP	6.4
1	A	163	LYS	6.4
1	B	507	PRO	6.2
1	B	127	ASN	6.2
1	D	129	GLY	6.2
1	A	177	GLU	6.1
1	A	427	PRO	6.0
1	C	127	ASN	5.9
1	A	149	LYS	5.9
1	A	27	GLU	5.9
1	D	413	GLY	5.7
1	A	162	ALA	5.7
1	B	428	ASN	5.5
1	B	145	HIS	5.5
1	D	166	ASN	5.5
1	D	132	ILE	5.5
1	C	168	SER	5.4
1	D	125	ILE	5.4
1	D	427	PRO	5.3
1	B	133	ASP	5.3
1	D	165	LEU	5.3
1	A	127	ASN	5.2
1	A	165	LEU	5.1
1	D	142	GLU	5.1
1	B	429	LYS	5.1
1	A	469	LYS	5.1
1	D	428	ASN	5.0
1	A	150	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	467	LYS	5.0
1	C	132	ILE	5.0
1	C	131	ASP	5.0
1	C	116	GLY	5.0
1	A	133	ASP	4.9
1	C	504	PHE	4.9
1	A	126	LYS	4.9
1	D	119	ASN	4.9
1	B	150	GLY	4.9
1	D	145	HIS	4.9
1	D	170	GLU	4.8
1	D	113	PRO	4.8
1	D	509	VAL	4.8
1	B	112	ARG	4.8
1	D	302	GLY	4.7
1	A	178	THR	4.7
1	C	164	ALA	4.7
1	D	163	LYS	4.7
1	D	430	LYS	4.7
1	C	129	GLY	4.7
1	C	163	LYS	4.7
1	A	510	ARG	4.7
1	B	427	PRO	4.7
1	B	234	ASP	4.7
1	A	169	ASN	4.6
1	B	113	PRO	4.6
1	C	507	PRO	4.6
1	A	187	LYS	4.5
1	A	135	GLU	4.4
1	A	189	GLU	4.4
1	C	234	ASP	4.4
1	D	410	ASN	4.4
1	D	126	LYS	4.4
1	B	129	GLY	4.4
1	C	509	VAL	4.4
1	A	24	LYS	4.3
1	A	549	LYS	4.3
1	B	179	ALA	4.3
1	C	469	LYS	4.3
1	B	172	GLY	4.3
1	A	166	ASN	4.2
1	C	126	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	145	HIS	4.2
1	B	123	GLU	4.2
1	A	111	PRO	4.2
1	B	170	GLU	4.2
1	A	231	GLN	4.2
1	C	112	ARG	4.2
1	D	507	PRO	4.2
1	D	182	GLU	4.2
1	D	168	SER	4.1
1	B	187	LYS	4.1
1	C	178	THR	4.1
1	D	178	THR	4.1
1	C	170	GLU	4.1
1	C	176	LEU	4.1
1	A	509	VAL	4.0
1	C	156	ASP	4.0
1	C	179	ALA	4.0
1	C	152	ILE	4.0
1	B	166	ASN	4.0
1	C	117	LEU	4.0
1	B	167	VAL	3.9
1	D	455	GLU	3.9
1	D	137	LYS	3.9
1	C	181	PRO	3.9
1	C	468	ALA	3.9
1	B	469	LYS	3.9
1	C	180	PHE	3.9
1	C	155	ASP	3.9
1	A	14	ASP	3.8
1	C	122	VAL	3.8
1	D	449	GLY	3.8
1	A	23	GLU	3.8
1	A	468	ALA	3.8
1	B	171	MET	3.7
1	C	424	GLU	3.7
1	A	182	GLU	3.7
1	D	121	LYS	3.7
1	B	148	LYS	3.7
1	B	122	VAL	3.7
1	A	151	ALA	3.7
1	D	116	GLY	3.7
1	A	507	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	414	GLU	3.7
1	D	111	PRO	3.7
1	D	499	VAL	3.6
1	C	120	GLU	3.6
1	D	185	ASP	3.6
1	B	118	GLY	3.6
1	C	298	HIS	3.6
1	A	113	PRO	3.5
1	D	510	ARG	3.5
1	B	142	GLU	3.5
1	A	289	GLU	3.5
1	A	511	SER	3.5
1	D	124	ILE	3.5
1	A	129	GLY	3.5
1	A	136	LYS	3.5
1	C	297	TYR	3.5
1	B	466	LYS	3.5
1	D	187	LYS	3.5
1	A	235	ARG	3.4
1	A	137	LYS	3.4
1	C	124	ILE	3.4
1	D	130	ILE	3.4
1	B	177	GLU	3.4
1	D	140	LEU	3.4
1	D	469	LYS	3.4
1	D	405	VAL	3.4
1	D	159	PHE	3.3
1	B	189	GLU	3.3
1	C	167	VAL	3.3
1	A	404	GLU	3.3
1	B	168	SER	3.2
1	C	142	GLU	3.2
1	C	130	ILE	3.2
1	D	27	GLU	3.1
1	C	150	GLY	3.1
1	B	149	LYS	3.1
1	C	429	LYS	3.1
1	D	123	GLU	3.1
1	D	164	ALA	3.1
1	A	174	LYS	3.1
1	D	148	LYS	3.1
1	B	426	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	119	ASN	3.0
1	C	169	ASN	3.0
1	D	149	LYS	3.0
1	A	413	GLY	3.0
1	B	11	MET	2.9
1	C	511	SER	2.9
1	D	429	LYS	2.9
1	D	11	MET	2.9
1	A	124	ILE	2.9
1	A	123	GLU	2.9
1	C	549	LYS	2.9
1	A	119	ASN	2.8
1	A	416	ARG	2.8
1	A	505	ARG	2.8
1	A	188	PRO	2.8
1	B	400	PRO	2.8
1	B	181	PRO	2.8
1	B	27	GLU	2.7
1	D	112	ARG	2.7
1	C	148	LYS	2.7
1	D	120	GLU	2.7
1	C	231	GLN	2.7
1	A	297	TYR	2.6
1	A	132	ILE	2.6
1	C	182	GLU	2.6
1	A	25	ASP	2.6
1	C	113	PRO	2.6
1	C	143	VAL	2.6
1	B	164	ALA	2.6
1	B	468	ALA	2.6
1	C	433	GLY	2.6
1	A	463	PRO	2.6
1	B	228	ARG	2.6
1	C	141	ARG	2.6
1	B	121	LYS	2.5
1	D	141	ARG	2.5
1	A	120	GLU	2.5
1	D	234	ASP	2.5
1	C	165	LEU	2.5
1	D	414	GLU	2.5
1	A	125	ILE	2.5
1	A	114	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	114	ASP	2.5
1	D	167	VAL	2.4
1	B	510	ARG	2.4
1	A	428	ASN	2.4
1	C	470	GLU	2.4
1	D	14	ASP	2.4
1	A	122	VAL	2.4
1	B	138	GLU	2.4
1	B	395	LYS	2.4
1	C	426	GLU	2.4
1	C	400	PRO	2.4
1	D	395	LYS	2.4
1	B	180	PHE	2.4
1	C	153	ASP	2.4
1	D	454	PHE	2.3
1	C	162	ALA	2.3
1	A	170	GLU	2.3
1	A	467	LYS	2.3
1	C	139	ARG	2.3
1	D	399	SER	2.3
1	B	162	ALA	2.3
1	B	182	GLU	2.3
1	A	138	GLU	2.3
1	C	251	GLU	2.3
1	A	139	ARG	2.3
1	A	159	PHE	2.2
1	A	424	GLU	2.2
1	D	139	ARG	2.2
1	B	117	LEU	2.2
1	A	185	ASP	2.2
1	A	506	VAL	2.2
1	B	116	GLY	2.2
1	A	128	LEU	2.2
1	B	128	LEU	2.2
1	B	141	ARG	2.2
1	B	125	ILE	2.2
1	C	467	LYS	2.2
1	A	98	MET	2.2
1	A	419	LYS	2.2
1	C	300	LYS	2.2
1	B	425	ASN	2.2
1	A	131	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	504	PHE	2.2
1	A	142	GLU	2.1
1	C	149	LYS	2.1
1	D	150	GLY	2.1
1	D	396	ASP	2.1
1	B	430	LYS	2.1
1	D	176	LEU	2.1
1	B	44	ASN	2.1
1	C	147	TYR	2.1
1	A	130	ILE	2.1
1	D	122	VAL	2.1
1	D	280	GLU	2.1
1	B	159	PHE	2.0
1	D	40	LYS	2.0
1	D	433	GLY	2.0
1	D	115	VAL	2.0
1	A	504	PHE	2.0
1	D	180	PHE	2.0
1	D	441	TYR	2.0
1	B	235	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.