Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:42 PM GMT

PDB ID	:	3UDC
Title	:	Crystal structure of a membrane protein
Authors	:	Li, W.; Ge, J.; Yang, M.
Deposited on	:	2011-10-28
Resolution	:	3.35 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:

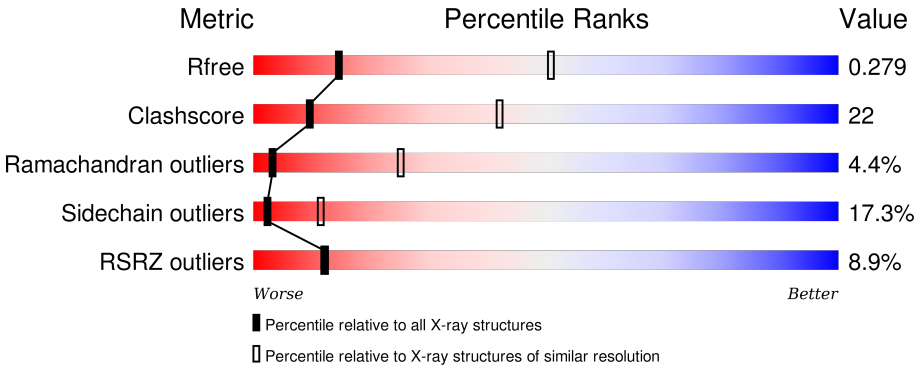
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.35 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	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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	285	11% 47% 37% 9% • 6%
1	B	285	9% 50% 34% 9% • 6%
1	C	285	7% 47% 36% 10% • 6%
1	D	285	11% 50% 33% 9% • 6%
1	E	285	10% 48% 35% 10% • 6%

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Mol	Chain	Length	Quality of chain
1	F	285	8% 48% 34% 11% • 6%
1	G	285	2% 48% 35% 10% • 6%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14903 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 Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel.

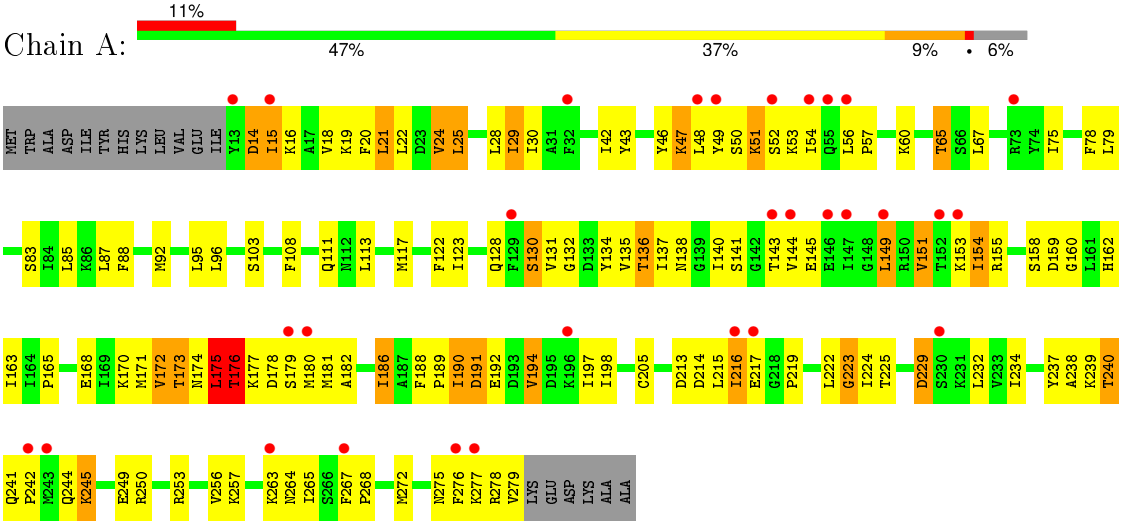
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	B	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	C	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	D	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	E	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	F	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	G	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			

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.

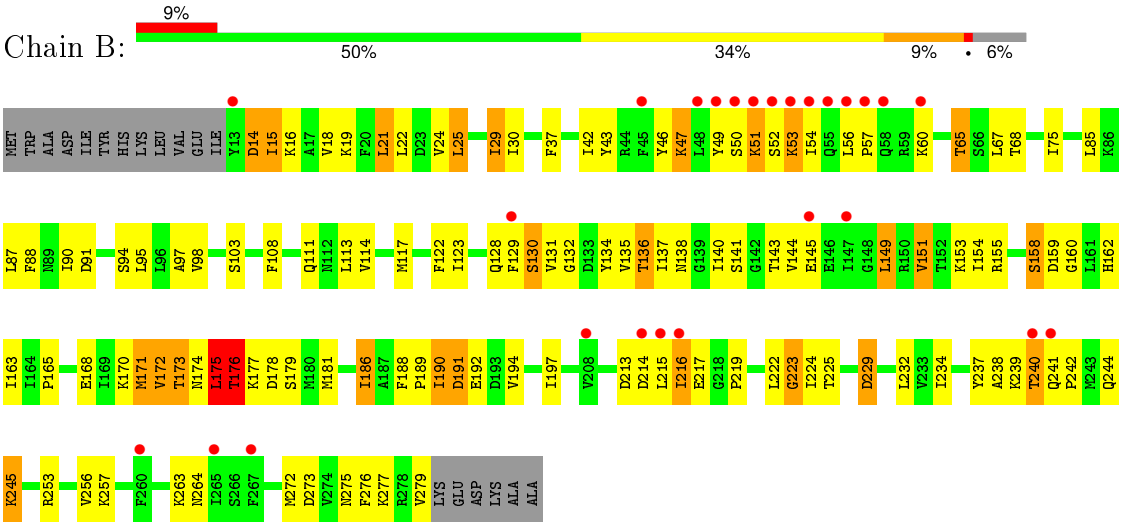
• Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel

Chain A:



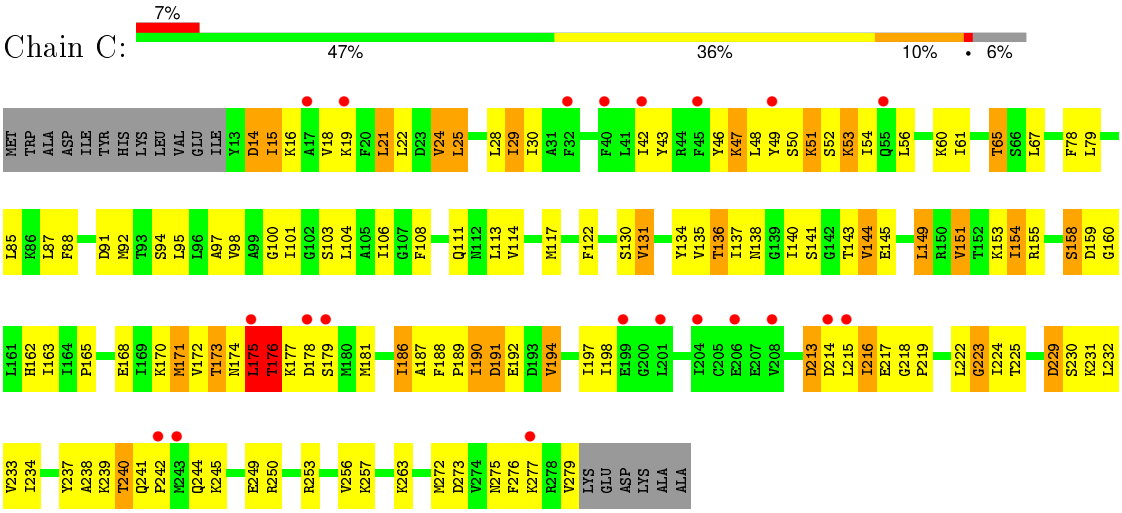
• Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel

Chain B:



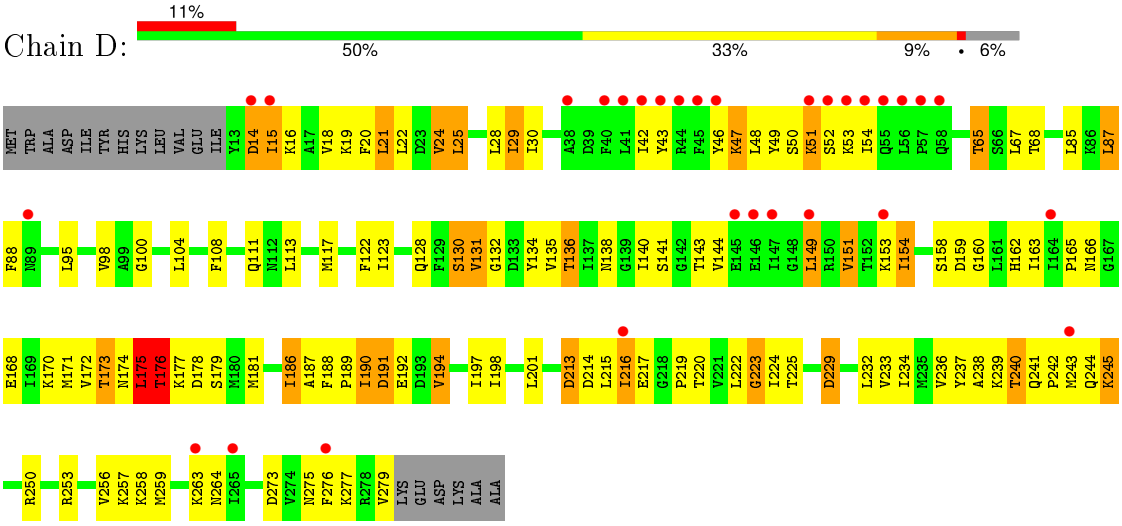
• Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel

Chain C:



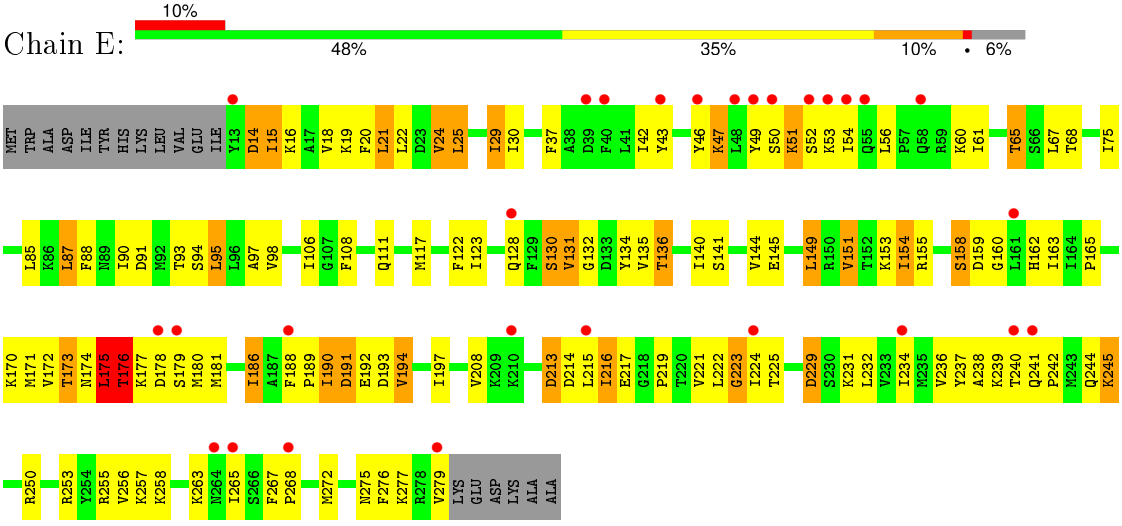
• Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel

Chain D:



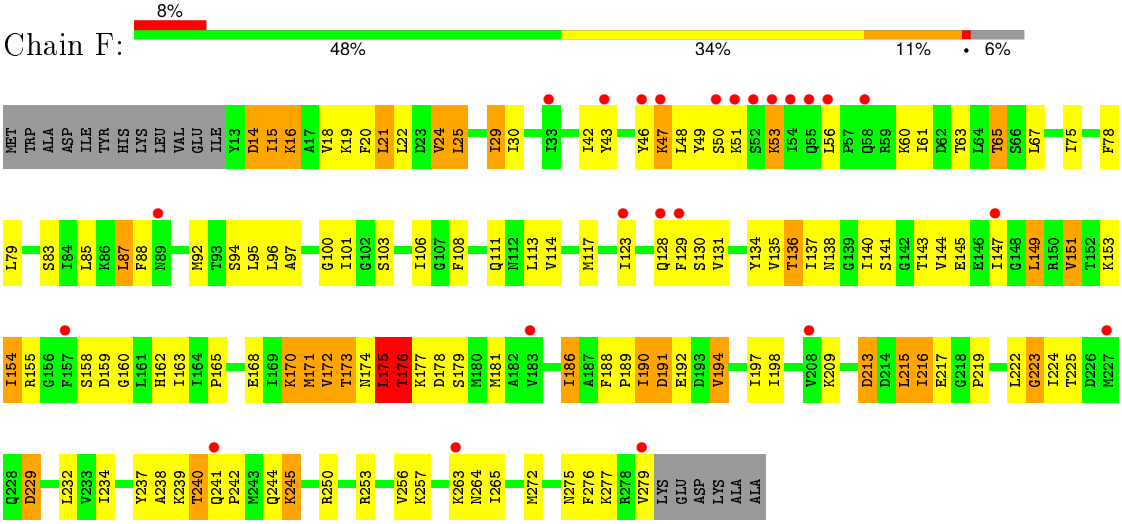
• Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel

Chain E:



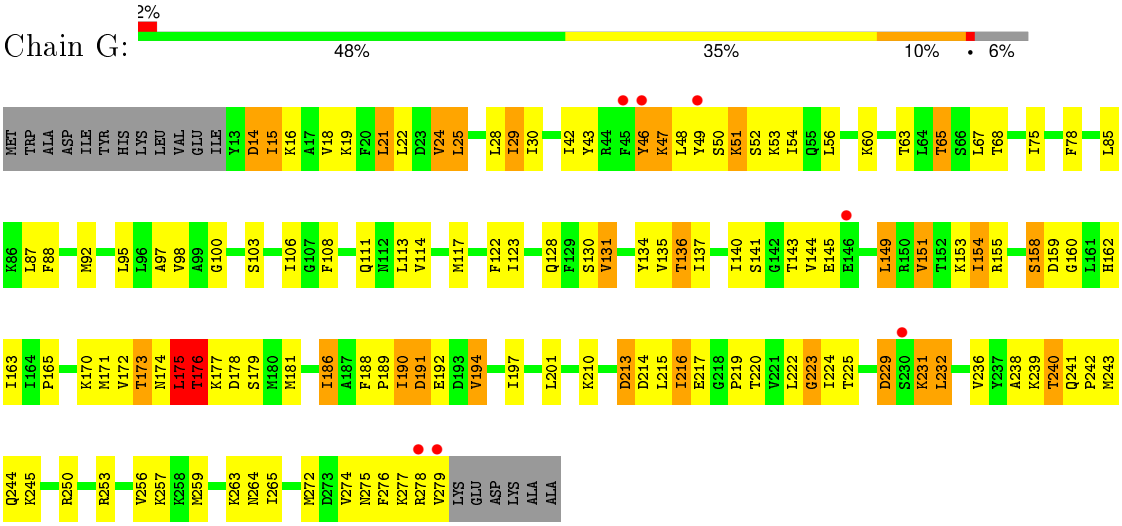
• Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel

Chain F:



• Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.05Å 139.47Å 224.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.08 – 3.35 42.08 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.08-3.35) 98.9 (42.08-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.248 , 0.274 0.261 , 0.279	Depositor DCC
R_{free} test set	1878 reflections (4.52%)	DCC
Wilson B-factor (Å^2)	111.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 67.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 43422 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14903	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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	0.50	0/2165	0.63	0/2915
1	B	0.48	0/2165	0.63	0/2915
1	C	0.47	0/2165	0.64	0/2915
1	D	0.49	0/2165	0.64	0/2915
1	E	0.49	0/2165	0.65	0/2915
1	F	0.47	0/2165	0.65	0/2915
1	G	0.49	0/2165	0.63	0/2915
All	All	0.49	0/15155	0.64	0/20405

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	2129	0	2223	123	1
1	B	2129	0	2223	111	0
1	C	2129	0	2223	122	0
1	D	2129	0	2223	114	0
1	E	2129	0	2223	121	0
1	F	2129	0	2223	121	0
1	G	2129	0	2223	117	1
All	All	14903	0	15561	681	1

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 22.

All (681) 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:D:162:HIS:HD2	1:E:173:THR:HB	1.19	1.04
1:A:173:THR:HB	1:B:162:HIS:HD2	1.24	1.02
1:A:162:HIS:HD2	1:D:173:THR:HB	1.24	1.02
1:G:217:GLU:HB3	1:G:239:LYS:HB2	1.43	1.00
1:C:173:THR:HB	1:F:162:HIS:HD2	1.24	0.99
1:E:162:HIS:HD2	1:F:173:THR:HB	1.23	0.99
1:A:217:GLU:HB3	1:A:239:LYS:HB2	1.44	0.97
1:B:217:GLU:HB3	1:B:239:LYS:HB2	1.47	0.97
1:D:217:GLU:HB3	1:D:239:LYS:HB2	1.45	0.97
1:C:217:GLU:HB3	1:C:239:LYS:HB2	1.44	0.96
1:B:173:THR:HB	1:G:162:HIS:HD2	1.30	0.95
1:F:217:GLU:HB3	1:F:239:LYS:HB2	1.50	0.94
1:D:158:SER:HA	1:E:181:MET:HB3	1.49	0.94
1:E:217:GLU:HB3	1:E:239:LYS:HB2	1.50	0.92
1:D:162:HIS:CD2	1:E:173:THR:HB	2.06	0.91
1:C:162:HIS:HD2	1:G:173:THR:HB	1.35	0.89
1:E:162:HIS:CD2	1:F:173:THR:HB	2.10	0.86
1:C:173:THR:HB	1:F:162:HIS:CD2	2.09	0.86
1:B:277:LYS:HE2	1:G:275:ASN:OD1	1.75	0.85
1:A:173:THR:HB	1:B:162:HIS:CD2	2.11	0.85
1:A:162:HIS:CD2	1:D:173:THR:HB	2.10	0.84
1:C:158:SER:HA	1:G:181:MET:HB3	1.59	0.84
1:D:134:TYR:CD2	1:D:175:LEU:HD23	2.13	0.83
1:C:134:TYR:CD2	1:C:175:LEU:HD23	2.14	0.83
1:G:134:TYR:CD2	1:G:175:LEU:HD23	2.13	0.83
1:B:134:TYR:CD2	1:B:175:LEU:HD23	2.14	0.82
1:A:134:TYR:CD2	1:A:175:LEU:HD23	2.14	0.82
1:C:134:TYR:HD2	1:C:175:LEU:HD23	1.45	0.81
1:B:173:THR:HB	1:G:162:HIS:CD2	2.16	0.81
1:D:15:ILE:H	1:D:16:LYS:HZ3	1.28	0.81
1:E:134:TYR:CD2	1:E:175:LEU:HD23	2.16	0.81
1:E:275:ASN:OD1	1:F:277:LYS:HE2	1.81	0.80
1:E:88:PHE:CD1	1:F:30:ILE:HB	2.17	0.80
1:D:275:ASN:OD1	1:E:277:LYS:HE2	1.80	0.80
1:F:134:TYR:CD2	1:F:175:LEU:HD23	2.17	0.79
1:G:134:TYR:HD2	1:G:175:LEU:HD23	1.45	0.78
1:A:134:TYR:HD2	1:A:175:LEU:HD23	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:134:TYR:HD2	1:E:175:LEU:HD23	1.48	0.78
1:D:215:LEU:HD22	1:D:219:PRO:HD3	1.66	0.78
1:D:134:TYR:HD2	1:D:175:LEU:HD23	1.48	0.76
1:A:277:LYS:HE2	1:B:275:ASN:OD1	1.86	0.76
1:C:15:ILE:H	1:C:16:LYS:HZ3	1.32	0.76
1:A:158:SER:HA	1:D:181:MET:HB3	1.66	0.76
1:B:15:ILE:H	1:B:16:LYS:HZ3	1.31	0.74
1:A:217:GLU:CB	1:A:239:LYS:HB2	2.17	0.74
1:E:88:PHE:HD1	1:F:30:ILE:HB	1.51	0.74
1:B:190:ILE:O	1:G:257:LYS:NZ	2.21	0.74
1:B:181:MET:HB3	1:G:158:SER:HA	1.69	0.74
1:D:217:GLU:CB	1:D:239:LYS:HB2	2.18	0.74
1:B:176:THR:OG1	1:B:177:LYS:N	2.20	0.74
1:A:30:ILE:HB	1:B:88:PHE:CD1	2.23	0.74
1:G:217:GLU:CB	1:G:239:LYS:HB2	2.17	0.73
1:B:217:GLU:CB	1:B:239:LYS:HB2	2.19	0.73
1:B:134:TYR:HD2	1:B:175:LEU:HD23	1.51	0.73
1:F:14:ASP:HA	1:F:16:LYS:HZ3	1.54	0.73
1:C:162:HIS:CD2	1:G:173:THR:HB	2.21	0.72
1:F:134:TYR:HD2	1:F:175:LEU:HD23	1.51	0.72
1:E:176:THR:OG1	1:E:177:LYS:N	2.18	0.72
1:G:215:LEU:HD22	1:G:219:PRO:HD3	1.71	0.72
1:E:215:LEU:HD22	1:E:219:PRO:HD3	1.72	0.71
1:F:176:THR:OG1	1:F:177:LYS:N	2.23	0.70
1:C:176:THR:OG1	1:C:177:LYS:N	2.23	0.70
1:C:181:MET:HB3	1:F:158:SER:HA	1.73	0.70
1:C:30:ILE:HB	1:F:88:PHE:CD1	2.27	0.69
1:G:213:ASP:N	1:G:213:ASP:OD2	2.25	0.69
1:C:277:LYS:HE2	1:F:275:ASN:OD1	1.93	0.69
1:C:217:GLU:CB	1:C:239:LYS:HB2	2.18	0.68
1:C:30:ILE:HB	1:F:88:PHE:HD1	1.58	0.68
1:F:215:LEU:HD22	1:F:219:PRO:HD3	1.73	0.68
1:A:173:THR:CB	1:B:162:HIS:HD2	2.04	0.68
1:E:186:ILE:HG21	1:E:256:VAL:HG11	1.75	0.68
1:G:14:ASP:HA	1:G:16:LYS:HZ3	1.58	0.68
1:A:14:ASP:HA	1:A:16:LYS:HZ3	1.59	0.68
1:F:217:GLU:CB	1:F:239:LYS:HB2	2.23	0.67
1:C:215:LEU:HD22	1:C:219:PRO:HD3	1.77	0.67
1:C:190:ILE:O	1:F:257:LYS:NZ	2.26	0.67
1:G:176:THR:OG1	1:G:177:LYS:N	2.21	0.67
1:E:213:ASP:N	1:E:213:ASP:OD2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:HD22	1:B:219:PRO:HD3	1.76	0.67
1:E:14:ASP:HA	1:E:16:LYS:HZ3	1.60	0.67
1:D:46:TYR:HD1	1:D:65:THR:HG21	1.61	0.66
1:A:257:LYS:NZ	1:D:190:ILE:O	2.27	0.66
1:F:135:VAL:HG12	1:F:174:ASN:HA	1.77	0.66
1:A:275:ASN:OD1	1:D:277:LYS:HE2	1.95	0.66
1:D:176:THR:OG1	1:D:177:LYS:N	2.27	0.66
1:A:30:ILE:HB	1:B:88:PHE:HD1	1.60	0.66
1:G:217:GLU:HB3	1:G:239:LYS:CB	2.25	0.66
1:C:257:LYS:HE2	1:G:194:VAL:HG22	1.76	0.66
1:F:213:ASP:OD2	1:F:213:ASP:N	2.27	0.66
1:G:189:PRO:HD2	1:G:192:GLU:HG3	1.77	0.65
1:C:213:ASP:OD2	1:C:213:ASP:N	2.28	0.65
1:C:173:THR:CB	1:F:162:HIS:HD2	2.03	0.65
1:E:162:HIS:HD2	1:F:173:THR:CB	2.04	0.65
1:A:217:GLU:HB3	1:A:239:LYS:CB	2.22	0.65
1:A:215:LEU:HD22	1:A:219:PRO:HD3	1.76	0.65
1:A:176:THR:OG1	1:A:177:LYS:N	2.29	0.65
1:E:189:PRO:HD2	1:E:192:GLU:HG3	1.78	0.65
1:C:88:PHE:HD1	1:G:30:ILE:HB	1.61	0.65
1:B:213:ASP:N	1:B:213:ASP:OD2	2.30	0.65
1:D:162:HIS:HD2	1:E:173:THR:CB	2.03	0.64
1:F:15:ILE:H	1:F:16:LYS:HZ3	1.45	0.64
1:C:117:MET:HG2	1:C:149:LEU:HD13	1.80	0.64
1:C:217:GLU:HB3	1:C:239:LYS:CB	2.24	0.64
1:D:257:LYS:NZ	1:E:190:ILE:O	2.29	0.64
1:D:213:ASP:N	1:D:213:ASP:OD2	2.29	0.64
1:G:15:ILE:H	1:G:16:LYS:HZ3	1.45	0.64
1:E:46:TYR:HD1	1:E:65:THR:HG21	1.62	0.64
1:A:25:LEU:O	1:A:29:ILE:HG23	1.98	0.64
1:C:275:ASN:OD1	1:G:277:LYS:HE2	1.98	0.64
1:D:217:GLU:HB3	1:D:239:LYS:CB	2.25	0.63
1:C:88:PHE:CD1	1:G:30:ILE:HB	2.33	0.63
1:B:137:ILE:HD12	1:B:154:ILE:CD1	2.27	0.63
1:E:15:ILE:H	1:E:16:LYS:HZ3	1.47	0.63
1:A:117:MET:HG2	1:A:149:LEU:HD13	1.81	0.63
1:B:25:LEU:O	1:B:29:ILE:HG23	1.98	0.63
1:B:173:THR:CB	1:G:162:HIS:HD2	2.08	0.63
1:B:46:TYR:HD1	1:B:65:THR:HG21	1.64	0.63
1:A:46:TYR:HD1	1:A:65:THR:HG21	1.64	0.63
1:G:186:ILE:HG21	1:G:256:VAL:HG11	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:HG21	1:B:256:VAL:HG11	1.80	0.63
1:F:137:ILE:HD12	1:F:154:ILE:CD1	2.29	0.63
1:E:257:LYS:NZ	1:F:190:ILE:O	2.31	0.62
1:A:15:ILE:H	1:A:16:LYS:HZ3	1.47	0.62
1:E:46:TYR:CD1	1:E:65:THR:HG21	2.35	0.62
1:A:103:SER:OG	1:B:97:ALA:O	2.16	0.62
1:E:217:GLU:CB	1:E:239:LYS:HB2	2.25	0.62
1:G:46:TYR:HD1	1:G:65:THR:HG21	1.64	0.62
1:A:181:MET:HB3	1:B:158:SER:HA	1.82	0.62
1:B:135:VAL:HG12	1:B:174:ASN:HA	1.81	0.62
1:F:25:LEU:O	1:F:29:ILE:HG23	2.00	0.62
1:E:158:SER:HA	1:F:181:MET:HB3	1.80	0.62
1:D:113:LEU:HD11	1:E:122:PHE:CZ	2.35	0.62
1:B:75:ILE:HD13	1:G:98:VAL:HG11	1.79	0.62
1:D:46:TYR:CD1	1:D:65:THR:HG21	2.35	0.61
1:F:46:TYR:HD1	1:F:65:THR:HG21	1.64	0.61
1:A:189:PRO:HD2	1:A:192:GLU:HG3	1.82	0.61
1:C:43:TYR:O	1:C:46:TYR:HB3	2.00	0.61
1:A:162:HIS:HD2	1:D:173:THR:CB	2.07	0.61
1:E:160:GLY:HA3	1:F:175:LEU:HD12	1.83	0.61
1:B:219:PRO:HA	1:B:238:ALA:HB2	1.83	0.61
1:F:46:TYR:CD1	1:F:65:THR:HG21	2.35	0.61
1:A:92:MET:HG3	1:B:91:ASP:OD2	2.01	0.61
1:G:117:MET:HG2	1:G:149:LEU:HD13	1.82	0.61
1:C:186:ILE:HG21	1:C:256:VAL:HG11	1.83	0.60
1:E:91:ASP:OD2	1:F:92:MET:HG3	2.01	0.60
1:E:25:LEU:O	1:E:29:ILE:HG23	2.01	0.60
1:D:186:ILE:HG21	1:D:256:VAL:HG11	1.83	0.60
1:E:117:MET:HG2	1:E:149:LEU:HD13	1.83	0.60
1:C:46:TYR:HD1	1:C:65:THR:HG21	1.66	0.60
1:A:213:ASP:N	1:A:213:ASP:OD2	2.34	0.60
1:A:219:PRO:HA	1:A:238:ALA:HB2	1.84	0.60
1:D:88:PHE:HD1	1:E:30:ILE:HB	1.66	0.60
1:E:135:VAL:HG12	1:E:174:ASN:HA	1.84	0.60
1:G:219:PRO:HA	1:G:238:ALA:HB2	1.84	0.59
1:A:46:TYR:CD1	1:A:65:THR:HG21	2.37	0.59
1:C:257:LYS:NZ	1:G:190:ILE:O	2.36	0.59
1:D:25:LEU:O	1:D:29:ILE:HG23	2.02	0.59
1:B:189:PRO:HD2	1:B:192:GLU:HG3	1.84	0.59
1:E:189:PRO:HB2	1:E:191:ASP:HB3	1.85	0.59
1:A:43:TYR:O	1:A:46:TYR:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:ARG:HD2	1:E:224:ILE:O	2.02	0.59
1:C:219:PRO:HA	1:C:238:ALA:HB2	1.84	0.59
1:F:186:ILE:HG21	1:F:256:VAL:HG11	1.83	0.59
1:A:186:ILE:HG21	1:A:256:VAL:HG11	1.84	0.59
1:D:216:ILE:HG12	1:D:239:LYS:HB3	1.84	0.59
1:B:46:TYR:CD1	1:B:65:THR:HG21	2.37	0.59
1:G:43:TYR:O	1:G:46:TYR:HB3	2.03	0.59
1:B:117:MET:HG2	1:B:149:LEU:HD13	1.84	0.59
1:D:135:VAL:HG12	1:D:174:ASN:HA	1.84	0.59
1:D:276:PHE:CZ	1:E:276:PHE:CE1	2.91	0.59
1:D:219:PRO:HA	1:D:238:ALA:HB2	1.83	0.58
1:C:46:TYR:CD1	1:C:65:THR:HG21	2.38	0.58
1:E:136:THR:HB	1:E:141:SER:OG	2.04	0.58
1:D:189:PRO:HD2	1:D:192:GLU:HG3	1.85	0.58
1:C:273:ASP:HB2	1:G:275:ASN:HB2	1.85	0.58
1:G:25:LEU:O	1:G:29:ILE:HG23	2.03	0.58
1:G:46:TYR:CD1	1:G:65:THR:HG21	2.37	0.58
1:D:216:ILE:HD11	1:D:239:LYS:HD2	1.85	0.58
1:A:276:PHE:CE1	1:B:276:PHE:CZ	2.92	0.58
1:E:43:TYR:O	1:E:46:TYR:HB3	2.04	0.58
1:D:160:GLY:HA3	1:E:175:LEU:HD12	1.84	0.58
1:C:272:MET:O	1:G:274:VAL:HA	2.03	0.57
1:E:47:LYS:NZ	1:E:47:LYS:HB2	2.18	0.57
1:C:137:ILE:HD12	1:C:154:ILE:CD1	2.34	0.57
1:F:117:MET:HG2	1:F:149:LEU:HD13	1.86	0.57
1:D:43:TYR:O	1:D:46:TYR:HB3	2.05	0.57
1:F:189:PRO:HD2	1:F:192:GLU:HG3	1.86	0.57
1:D:108:PHE:O	1:D:111:GLN:HG2	2.04	0.57
1:C:135:VAL:HG12	1:C:174:ASN:HA	1.87	0.57
1:B:217:GLU:HB3	1:B:239:LYS:CB	2.29	0.57
1:C:175:LEU:HD12	1:F:160:GLY:HA3	1.85	0.57
1:B:175:LEU:HD12	1:G:160:GLY:HA3	1.86	0.57
1:C:117:MET:HG2	1:C:149:LEU:CD1	2.35	0.57
1:C:25:LEU:O	1:C:29:ILE:HG23	2.05	0.57
1:B:47:LYS:HB2	1:B:47:LYS:NZ	2.19	0.57
1:A:190:ILE:O	1:B:257:LYS:NZ	2.38	0.57
1:C:189:PRO:HD2	1:C:192:GLU:HG3	1.87	0.57
1:A:189:PRO:HB2	1:A:191:ASP:HB3	1.86	0.57
1:E:42:ILE:HD11	1:E:68:THR:HG22	1.87	0.56
1:G:175:LEU:O	1:G:176:THR:C	2.43	0.56
1:E:175:LEU:O	1:E:176:THR:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:189:PRO:HB2	1:G:191:ASP:HB3	1.87	0.56
1:D:88:PHE:CD1	1:E:30:ILE:HB	2.41	0.56
1:E:97:ALA:O	1:F:103:SER:OG	2.22	0.56
1:B:103:SER:OG	1:G:97:ALA:O	2.21	0.56
1:G:136:THR:HB	1:G:141:SER:OG	2.05	0.56
1:C:108:PHE:O	1:C:111:GLN:HG2	2.05	0.56
1:E:217:GLU:HB3	1:E:239:LYS:CB	2.29	0.56
1:B:43:TYR:O	1:B:46:TYR:HB3	2.05	0.56
1:F:217:GLU:HB3	1:F:239:LYS:CB	2.31	0.56
1:F:43:TYR:O	1:F:46:TYR:HB3	2.06	0.56
1:C:188:PHE:CE2	1:C:197:ILE:HG21	2.40	0.56
1:E:188:PHE:HE2	1:E:234:ILE:HG13	1.71	0.56
1:C:97:ALA:O	1:G:103:SER:OG	2.23	0.56
1:C:103:SER:OG	1:F:97:ALA:O	2.20	0.56
1:G:201:LEU:HD23	1:G:259:MET:HE1	1.88	0.56
1:B:175:LEU:O	1:B:176:THR:C	2.43	0.55
1:E:188:PHE:CG	1:E:197:ILE:HD13	2.42	0.55
1:D:117:MET:HG2	1:D:149:LEU:HD13	1.88	0.55
1:A:136:THR:HB	1:A:141:SER:OG	2.06	0.55
1:F:219:PRO:HA	1:F:238:ALA:HB2	1.88	0.55
1:F:188:PHE:CG	1:F:197:ILE:HD13	2.42	0.55
1:G:135:VAL:HG12	1:G:174:ASN:HA	1.88	0.55
1:A:135:VAL:HG12	1:A:174:ASN:HA	1.87	0.55
1:A:137:ILE:HD12	1:A:154:ILE:CD1	2.37	0.55
1:F:47:LYS:NZ	1:F:47:LYS:HB2	2.21	0.55
1:A:188:PHE:CG	1:A:197:ILE:HD13	2.42	0.55
1:G:47:LYS:NZ	1:G:47:LYS:HB2	2.22	0.55
1:A:47:LYS:NZ	1:A:47:LYS:HB2	2.22	0.55
1:C:189:PRO:HB2	1:C:191:ASP:HB3	1.89	0.54
1:D:188:PHE:CG	1:D:197:ILE:HD13	2.42	0.54
1:D:188:PHE:HE2	1:D:234:ILE:HG13	1.72	0.54
1:B:30:ILE:HB	1:G:88:PHE:HD1	1.71	0.54
1:C:175:LEU:O	1:C:176:THR:C	2.46	0.54
1:F:175:LEU:O	1:F:176:THR:C	2.46	0.54
1:F:188:PHE:CE2	1:F:197:ILE:HG21	2.41	0.54
1:D:47:LYS:HB2	1:D:47:LYS:NZ	2.23	0.54
1:C:257:LYS:CE	1:G:194:VAL:HG22	2.38	0.54
1:F:216:ILE:HD11	1:F:239:LYS:HD2	1.89	0.54
1:B:189:PRO:HB2	1:B:191:ASP:HB3	1.89	0.54
1:A:216:ILE:HG12	1:A:239:LYS:HB3	1.88	0.54
1:C:21:LEU:O	1:C:25:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LYS:HG2	1:B:163:ILE:HG12	1.90	0.54
1:A:253:ARG:HD2	1:D:224:ILE:O	2.07	0.54
1:G:188:PHE:CG	1:G:197:ILE:HD13	2.43	0.54
1:A:108:PHE:O	1:A:111:GLN:HG2	2.08	0.54
1:D:153:LYS:HG2	1:D:163:ILE:HG12	1.88	0.54
1:D:175:LEU:O	1:D:176:THR:C	2.46	0.54
1:C:136:THR:HB	1:C:141:SER:OG	2.09	0.53
1:D:136:THR:HB	1:D:141:SER:OG	2.09	0.53
1:D:98:VAL:HG11	1:E:75:ILE:HD13	1.90	0.53
1:F:189:PRO:HB2	1:F:191:ASP:HB3	1.90	0.53
1:B:188:PHE:CG	1:B:197:ILE:HD13	2.44	0.53
1:F:216:ILE:HG12	1:F:239:LYS:HB3	1.90	0.53
1:A:188:PHE:CE2	1:A:197:ILE:HG21	2.44	0.53
1:G:154:ILE:O	1:G:154:ILE:HG22	2.08	0.53
1:F:151:VAL:HG23	1:F:165:PRO:HA	1.91	0.53
1:C:273:ASP:CB	1:G:275:ASN:HB2	2.39	0.53
1:D:257:LYS:CE	1:E:194:VAL:HG22	2.39	0.53
1:C:253:ARG:HD2	1:G:224:ILE:O	2.08	0.53
1:G:108:PHE:O	1:G:111:GLN:HG2	2.09	0.53
1:A:21:LEU:O	1:A:25:LEU:HB2	2.08	0.52
1:B:136:THR:HB	1:B:141:SER:OG	2.09	0.52
1:C:91:ASP:OD2	1:G:92:MET:HG3	2.09	0.52
1:E:98:VAL:CG1	1:F:75:ILE:HD13	2.40	0.52
1:E:134:TYR:H	1:E:176:THR:HG21	1.74	0.52
1:F:188:PHE:HE2	1:F:234:ILE:HG13	1.75	0.52
1:D:189:PRO:HB2	1:D:191:ASP:HB3	1.91	0.52
1:B:21:LEU:O	1:B:25:LEU:HB2	2.10	0.52
1:E:117:MET:HG2	1:E:149:LEU:CD1	2.40	0.52
1:D:98:VAL:CG1	1:E:75:ILE:HD13	2.40	0.52
1:D:250:ARG:CZ	1:E:222:LEU:HD12	2.40	0.52
1:B:30:ILE:HB	1:G:88:PHE:CD1	2.45	0.52
1:E:221:VAL:HG22	1:E:236:VAL:HG12	1.92	0.52
1:B:216:ILE:HG12	1:B:239:LYS:HB3	1.92	0.51
1:G:186:ILE:HD12	1:G:256:VAL:HG21	1.91	0.51
1:A:113:LEU:HD11	1:D:122:PHE:CZ	2.44	0.51
1:C:47:LYS:NZ	1:C:47:LYS:HB2	2.25	0.51
1:F:153:LYS:HG2	1:F:163:ILE:HG12	1.91	0.51
1:E:219:PRO:HA	1:E:238:ALA:HB2	1.92	0.51
1:A:190:ILE:O	1:A:192:GLU:N	2.42	0.51
1:C:188:PHE:CG	1:C:197:ILE:HD13	2.45	0.51
1:A:151:VAL:HG23	1:A:165:PRO:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LEU:O	1:D:25:LEU:HB2	2.10	0.51
1:C:276:PHE:CZ	1:G:276:PHE:CE1	2.98	0.51
1:E:56:LEU:HD12	1:E:60:LYS:CB	2.41	0.51
1:A:134:TYR:H	1:A:176:THR:HG21	1.75	0.51
1:C:153:LYS:HG2	1:C:163:ILE:HG12	1.93	0.51
1:A:241:GLN:HG3	1:A:242:PRO:HD2	1.93	0.51
1:B:134:TYR:H	1:B:176:THR:HG21	1.76	0.50
1:G:216:ILE:HG12	1:G:239:LYS:HB3	1.93	0.50
1:B:75:ILE:HD13	1:G:98:VAL:CG1	2.41	0.50
1:F:136:THR:HB	1:F:141:SER:OG	2.11	0.50
1:C:224:ILE:O	1:F:253:ARG:HD2	2.11	0.50
1:D:134:TYR:H	1:D:176:THR:HG21	1.77	0.50
1:G:188:PHE:CE2	1:G:197:ILE:HG21	2.47	0.50
1:C:162:HIS:HD2	1:G:173:THR:CB	2.15	0.50
1:G:21:LEU:O	1:G:25:LEU:HB2	2.11	0.50
1:F:134:TYR:H	1:F:176:THR:HG21	1.76	0.50
1:E:108:PHE:O	1:E:111:GLN:HG2	2.12	0.50
1:A:257:LYS:HE2	1:D:194:VAL:HG22	1.94	0.50
1:D:113:LEU:CD1	1:E:122:PHE:CE2	2.95	0.50
1:D:113:LEU:HD13	1:E:122:PHE:CE2	2.46	0.50
1:C:276:PHE:CZ	1:G:276:PHE:CZ	3.00	0.50
1:B:108:PHE:O	1:B:111:GLN:HG2	2.11	0.50
1:C:188:PHE:HE2	1:C:234:ILE:HG13	1.76	0.50
1:B:188:PHE:HE2	1:B:234:ILE:HG13	1.77	0.50
1:A:153:LYS:HG2	1:A:163:ILE:HG12	1.94	0.50
1:E:197:ILE:HG12	1:E:265:ILE:HD13	1.94	0.50
1:E:188:PHE:CE2	1:E:197:ILE:HG21	2.47	0.50
1:A:175:LEU:O	1:A:176:THR:C	2.48	0.49
1:B:137:ILE:HD12	1:B:154:ILE:HD12	1.94	0.49
1:G:181:MET:O	1:G:245:LYS:HE2	2.12	0.49
1:E:98:VAL:HG11	1:F:75:ILE:HD13	1.93	0.49
1:B:214:ASP:HB2	1:B:244:GLN:HG3	1.94	0.49
1:F:14:ASP:HA	1:F:16:LYS:NZ	2.26	0.49
1:G:117:MET:HG2	1:G:149:LEU:CD1	2.42	0.49
1:C:106:ILE:HA	1:G:114:VAL:HG11	1.93	0.49
1:F:21:LEU:O	1:F:25:LEU:HB2	2.11	0.49
1:E:21:LEU:O	1:E:25:LEU:HB2	2.11	0.49
1:G:151:VAL:HG23	1:G:165:PRO:HA	1.94	0.49
1:F:190:ILE:O	1:F:192:GLU:N	2.46	0.49
1:D:188:PHE:CE2	1:D:197:ILE:HG21	2.48	0.49
1:B:122:PHE:CZ	1:G:113:LEU:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:LYS:HG2	1:E:163:ILE:HG12	1.95	0.49
1:A:216:ILE:HD11	1:A:239:LYS:HD2	1.95	0.49
1:D:14:ASP:HA	1:D:16:LYS:HZ1	1.78	0.49
1:A:154:ILE:HG22	1:A:154:ILE:O	2.13	0.49
1:E:222:LEU:HD22	1:E:237:TYR:CD1	2.47	0.49
1:D:222:LEU:HD22	1:D:237:TYR:CD1	2.48	0.49
1:F:15:ILE:H	1:F:16:LYS:NZ	2.11	0.48
1:D:257:LYS:HE2	1:E:194:VAL:HG22	1.95	0.48
1:A:214:ASP:HB2	1:A:244:GLN:HG3	1.95	0.48
1:G:134:TYR:H	1:G:176:THR:HG21	1.79	0.48
1:E:222:LEU:O	1:E:223:GLY:O	2.30	0.48
1:C:241:GLN:HG3	1:C:242:PRO:HD2	1.94	0.48
1:A:278:ARG:HB2	1:A:278:ARG:CZ	2.43	0.48
1:F:154:ILE:HG22	1:F:154:ILE:O	2.13	0.48
1:D:154:ILE:HG22	1:D:154:ILE:O	2.14	0.48
1:B:117:MET:HG2	1:B:149:LEU:CD1	2.44	0.48
1:A:51:LYS:HA	1:A:51:LYS:HD2	1.63	0.48
1:B:177:LYS:O	1:B:179:SER:N	2.45	0.48
1:A:177:LYS:O	1:A:179:SER:N	2.44	0.48
1:C:154:ILE:O	1:C:154:ILE:HG22	2.13	0.48
1:E:130:SER:O	1:E:132:GLY:N	2.47	0.48
1:D:18:VAL:HG13	1:D:19:LYS:N	2.29	0.48
1:G:222:LEU:O	1:G:223:GLY:O	2.32	0.48
1:B:14:ASP:HA	1:B:16:LYS:HZ1	1.78	0.48
1:B:151:VAL:HG23	1:B:165:PRO:HA	1.96	0.48
1:D:241:GLN:HG3	1:D:242:PRO:HD2	1.95	0.48
1:B:222:LEU:HD12	1:G:250:ARG:CZ	2.44	0.48
1:C:179:SER:HB2	1:C:240:THR:O	2.14	0.47
1:C:273:ASP:HB3	1:G:275:ASN:ND2	2.29	0.47
1:A:29:ILE:HG13	1:A:30:ILE:N	2.29	0.47
1:F:117:MET:HG2	1:F:149:LEU:CD1	2.43	0.47
1:C:134:TYR:H	1:C:176:THR:HG21	1.78	0.47
1:F:241:GLN:HG3	1:F:242:PRO:HD2	1.95	0.47
1:E:188:PHE:CE2	1:E:234:ILE:HG13	2.49	0.47
1:G:18:VAL:HG13	1:G:19:LYS:N	2.29	0.47
1:F:179:SER:HB2	1:F:240:THR:O	2.14	0.47
1:C:14:ASP:HA	1:C:16:LYS:HZ1	1.80	0.47
1:C:214:ASP:HB2	1:C:244:GLN:HG3	1.95	0.47
1:G:51:LYS:HA	1:G:51:LYS:HD2	1.64	0.47
1:B:29:ILE:HG13	1:B:30:ILE:N	2.30	0.47
1:F:181:MET:O	1:F:245:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:LEU:HD23	1:F:79:LEU:HD11	1.96	0.47
1:C:14:ASP:HA	1:C:16:LYS:NZ	2.30	0.47
1:G:197:ILE:HG12	1:G:265:ILE:HD13	1.95	0.47
1:F:108:PHE:O	1:F:111:GLN:HG2	2.14	0.47
1:C:151:VAL:HG23	1:C:165:PRO:HA	1.96	0.47
1:A:52:SER:O	1:A:54:ILE:HG13	2.15	0.47
1:D:214:ASP:HB2	1:D:244:GLN:HG3	1.95	0.47
1:B:272:MET:HB3	1:B:272:MET:HE2	1.79	0.47
1:C:100:GLY:O	1:C:104:LEU:HG	2.14	0.47
1:C:18:VAL:HG13	1:C:19:LYS:N	2.30	0.47
1:A:222:LEU:O	1:A:223:GLY:O	2.33	0.47
1:G:242:PRO:O	1:G:243:MET:HB2	2.14	0.47
1:A:257:LYS:CE	1:D:194:VAL:HG22	2.44	0.47
1:E:51:LYS:HA	1:E:51:LYS:HD2	1.59	0.47
1:B:181:MET:O	1:B:245:LYS:HE2	2.15	0.47
1:B:154:ILE:O	1:B:154:ILE:HG22	2.14	0.47
1:B:224:ILE:O	1:G:253:ARG:HD2	2.15	0.47
1:D:14:ASP:HA	1:D:16:LYS:NZ	2.30	0.46
1:A:92:MET:HE2	1:A:92:MET:HA	1.97	0.46
1:B:222:LEU:HD22	1:B:237:TYR:CD1	2.49	0.46
1:E:154:ILE:HG22	1:E:154:ILE:O	2.14	0.46
1:A:194:VAL:O	1:A:198:ILE:HG13	2.16	0.46
1:G:14:ASP:HA	1:G:16:LYS:NZ	2.27	0.46
1:G:60:LYS:O	1:G:63:THR:HG22	2.15	0.46
1:G:153:LYS:HG2	1:G:163:ILE:HG12	1.97	0.46
1:G:60:LYS:HD3	1:G:60:LYS:HA	1.81	0.46
1:G:177:LYS:O	1:G:179:SER:N	2.43	0.46
1:C:177:LYS:HA	1:C:177:LYS:HD2	1.80	0.46
1:A:194:VAL:HG22	1:B:257:LYS:HE2	1.97	0.46
1:C:98:VAL:HG11	1:G:75:ILE:HD13	1.98	0.46
1:F:190:ILE:H	1:F:190:ILE:HG12	1.44	0.46
1:G:42:ILE:HD11	1:G:68:THR:HG22	1.97	0.46
1:A:186:ILE:HD12	1:A:256:VAL:HG21	1.98	0.46
1:E:56:LEU:HD12	1:E:60:LYS:HB2	1.98	0.46
1:E:151:VAL:HG23	1:E:165:PRO:HA	1.97	0.46
1:A:172:VAL:O	1:A:172:VAL:HG22	2.16	0.46
1:E:14:ASP:HA	1:E:16:LYS:NZ	2.29	0.46
1:C:186:ILE:HD12	1:C:256:VAL:HG21	1.97	0.46
1:G:231:LYS:HB2	1:G:231:LYS:NZ	2.31	0.46
1:F:272:MET:HE2	1:F:272:MET:HB3	1.80	0.46
1:A:14:ASP:HA	1:A:16:LYS:NZ	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:SER:HB2	1:B:240:THR:O	2.16	0.46
1:C:51:LYS:HA	1:C:51:LYS:HD2	1.64	0.46
1:A:175:LEU:HD12	1:B:160:GLY:HA3	1.98	0.45
1:F:194:VAL:O	1:F:198:ILE:HG13	2.15	0.45
1:E:276:PHE:CZ	1:F:276:PHE:CE1	3.03	0.45
1:B:188:PHE:CE2	1:B:197:ILE:HG21	2.52	0.45
1:A:224:ILE:O	1:B:253:ARG:HD2	2.16	0.45
1:C:194:VAL:HG22	1:F:257:LYS:HE2	1.98	0.45
1:C:171:MET:HB3	1:C:171:MET:HE3	1.86	0.45
1:C:216:ILE:HG12	1:C:239:LYS:HB3	1.97	0.45
1:B:18:VAL:HG13	1:B:19:LYS:N	2.31	0.45
1:F:15:ILE:N	1:F:16:LYS:HZ3	2.11	0.45
1:F:197:ILE:HG12	1:F:265:ILE:HD13	1.98	0.45
1:A:18:VAL:HG13	1:A:19:LYS:N	2.31	0.45
1:A:145:GLU:OE2	1:A:155:ARG:HD2	2.16	0.45
1:C:190:ILE:O	1:C:192:GLU:N	2.49	0.45
1:B:42:ILE:HD11	1:B:68:THR:HG22	1.99	0.45
1:F:137:ILE:HD12	1:F:154:ILE:HD12	1.98	0.45
1:F:222:LEU:O	1:F:223:GLY:O	2.35	0.45
1:A:113:LEU:HD13	1:D:122:PHE:CE2	2.52	0.45
1:D:130:SER:O	1:D:132:GLY:N	2.49	0.45
1:B:114:VAL:HG11	1:G:106:ILE:HA	1.98	0.45
1:E:180:MET:HE2	1:E:245:LYS:HD2	1.98	0.45
1:A:15:ILE:N	1:A:16:LYS:HZ3	2.13	0.45
1:A:117:MET:HG2	1:A:149:LEU:CD1	2.46	0.45
1:B:186:ILE:HG12	1:B:186:ILE:H	1.63	0.45
1:A:75:ILE:HD13	1:B:98:VAL:HG11	1.99	0.45
1:A:92:MET:CE	1:A:92:MET:HA	2.47	0.45
1:B:145:GLU:OE2	1:B:155:ARG:HD2	2.16	0.45
1:D:258:LYS:HA	1:D:258:LYS:HD3	1.86	0.45
1:F:177:LYS:HD2	1:F:177:LYS:HA	1.75	0.45
1:A:275:ASN:HB2	1:B:273:ASP:HB2	1.99	0.45
1:G:47:LYS:HA	1:G:50:SER:HB3	1.98	0.45
1:A:250:ARG:CZ	1:D:222:LEU:HD12	2.46	0.45
1:B:222:LEU:O	1:B:223:GLY:O	2.35	0.45
1:E:250:ARG:CZ	1:F:222:LEU:HD12	2.46	0.45
1:E:177:LYS:HD2	1:E:177:LYS:HA	1.75	0.45
1:D:42:ILE:O	1:D:46:TYR:HB2	2.17	0.45
1:F:186:ILE:HD12	1:F:256:VAL:HG21	1.99	0.45
1:C:137:ILE:HD12	1:C:154:ILE:HD12	1.98	0.45
1:B:222:LEU:HD22	1:B:237:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ALA:HB2	1:C:233:VAL:HG22	1.98	0.45
1:C:145:GLU:OE2	1:C:155:ARG:HD2	2.17	0.45
1:A:122:PHE:CZ	1:B:113:LEU:HD11	2.51	0.45
1:A:130:SER:O	1:A:132:GLY:N	2.51	0.44
1:C:114:VAL:HG11	1:F:106:ILE:HA	1.98	0.44
1:B:190:ILE:O	1:B:192:GLU:N	2.50	0.44
1:G:190:ILE:O	1:G:192:GLU:N	2.51	0.44
1:A:75:ILE:HD13	1:B:98:VAL:CG1	2.47	0.44
1:F:56:LEU:HD12	1:F:60:LYS:CB	2.47	0.44
1:A:179:SER:HB2	1:A:240:THR:O	2.18	0.44
1:E:190:ILE:O	1:E:192:GLU:N	2.51	0.44
1:E:47:LYS:HA	1:E:50:SER:HB3	1.99	0.44
1:D:188:PHE:CE2	1:D:234:ILE:HG13	2.52	0.44
1:E:90:ILE:HA	1:F:83:SER:OG	2.18	0.44
1:D:51:LYS:HD2	1:D:51:LYS:HA	1.65	0.44
1:G:214:ASP:HB2	1:G:244:GLN:HG3	1.99	0.44
1:B:14:ASP:HA	1:B:16:LYS:NZ	2.32	0.44
1:G:15:ILE:N	1:G:16:LYS:HZ3	2.13	0.44
1:B:46:TYR:CD2	1:B:46:TYR:C	2.91	0.44
1:B:186:ILE:HD12	1:B:256:VAL:HG21	1.99	0.44
1:A:60:LYS:HD3	1:A:60:LYS:HA	1.80	0.44
1:F:188:PHE:CE2	1:F:234:ILE:HG13	2.52	0.44
1:A:20:PHE:O	1:A:24:VAL:HG12	2.18	0.44
1:B:53:LYS:HB3	1:B:53:LYS:HE2	1.78	0.44
1:A:197:ILE:HG12	1:A:265:ILE:HD13	2.00	0.44
1:F:79:LEU:HD23	1:F:79:LEU:HA	1.61	0.44
1:F:20:PHE:O	1:F:24:VAL:HG12	2.18	0.44
1:C:79:LEU:HA	1:C:79:LEU:HD23	1.72	0.44
1:A:138:ASN:ND2	1:A:168:GLU:O	2.50	0.44
1:F:137:ILE:HD12	1:F:154:ILE:HD11	2.00	0.43
1:D:186:ILE:H	1:D:186:ILE:HG12	1.69	0.43
1:G:100:GLY:HA2	1:G:103:SER:HB2	1.99	0.43
1:D:47:LYS:HA	1:D:50:SER:HB3	1.99	0.43
1:G:241:GLN:HG3	1:G:242:PRO:HD2	1.99	0.43
1:C:138:ASN:ND2	1:C:168:GLU:O	2.51	0.43
1:C:53:LYS:HB3	1:C:53:LYS:HE2	1.76	0.43
1:G:56:LEU:HD12	1:G:60:LYS:HB2	2.00	0.43
1:F:60:LYS:HA	1:F:60:LYS:HD3	1.86	0.43
1:D:87:LEU:HA	1:D:87:LEU:HD12	1.69	0.43
1:F:18:VAL:HG13	1:F:19:LYS:N	2.33	0.43
1:E:42:ILE:O	1:E:46:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:TYR:CD2	1:G:46:TYR:C	2.92	0.43
1:C:122:PHE:CZ	1:F:113:LEU:HD11	2.54	0.43
1:E:123:ILE:HA	1:E:128:GLN:HG3	2.00	0.43
1:D:179:SER:HB2	1:D:240:THR:O	2.19	0.43
1:B:56:LEU:HD12	1:B:60:LYS:CB	2.48	0.43
1:C:56:LEU:HD12	1:C:60:LYS:CB	2.49	0.43
1:B:42:ILE:O	1:B:46:TYR:HB2	2.18	0.43
1:E:272:MET:HB3	1:E:272:MET:HE2	1.80	0.43
1:G:272:MET:HB3	1:G:272:MET:HE2	1.78	0.43
1:C:177:LYS:O	1:C:179:SER:N	2.46	0.43
1:C:160:GLY:HA3	1:G:175:LEU:HD12	2.01	0.43
1:F:29:ILE:HG13	1:F:30:ILE:N	2.33	0.43
1:D:181:MET:HB2	1:D:181:MET:HE2	1.90	0.43
1:F:16:LYS:HE2	1:F:16:LYS:HB2	1.89	0.43
1:F:186:ILE:HG12	1:F:186:ILE:H	1.63	0.43
1:D:222:LEU:O	1:D:223:GLY:O	2.37	0.43
1:E:18:VAL:HG13	1:E:19:LYS:N	2.33	0.43
1:F:87:LEU:HA	1:F:87:LEU:HD12	1.79	0.43
1:C:216:ILE:HD11	1:C:239:LYS:HD2	2.01	0.43
1:D:42:ILE:HD11	1:D:68:THR:HG22	2.00	0.43
1:C:276:PHE:CE1	1:F:276:PHE:CZ	3.07	0.43
1:E:216:ILE:HG12	1:E:239:LYS:HB3	1.99	0.43
1:C:16:LYS:HB2	1:C:16:LYS:HE2	1.84	0.43
1:A:275:ASN:HB2	1:B:273:ASP:CB	2.49	0.43
1:E:61:ILE:O	1:E:65:THR:HB	2.19	0.43
1:A:47:LYS:HA	1:A:50:SER:HB3	2.00	0.43
1:D:100:GLY:O	1:D:104:LEU:HG	2.19	0.43
1:F:129:PHE:CD2	1:F:147:ILE:HD11	2.53	0.43
1:D:138:ASN:ND2	1:D:168:GLU:O	2.52	0.43
1:A:272:MET:HE2	1:A:272:MET:HB3	1.84	0.43
1:G:216:ILE:HD11	1:G:239:LYS:HD2	1.99	0.43
1:C:61:ILE:O	1:C:65:THR:HB	2.19	0.43
1:G:137:ILE:HD12	1:G:154:ILE:CD1	2.49	0.43
1:C:222:LEU:O	1:C:223:GLY:O	2.37	0.43
1:B:52:SER:O	1:B:54:ILE:N	2.50	0.43
1:D:177:LYS:HA	1:D:177:LYS:HD2	1.74	0.42
1:A:181:MET:O	1:A:245:LYS:HE2	2.19	0.42
1:E:108:PHE:HB3	1:F:111:GLN:OE1	2.18	0.42
1:A:56:LEU:HA	1:A:57:PRO:HD3	1.92	0.42
1:C:78:PHE:CE2	1:F:94:SER:HB3	2.54	0.42
1:F:123:ILE:HA	1:F:128:GLN:HG3	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASN:HD22	1:B:273:ASP:HB3	1.84	0.42
1:C:47:LYS:HA	1:C:50:SER:HB3	2.01	0.42
1:C:18:VAL:HG13	1:C:19:LYS:H	1.83	0.42
1:C:222:LEU:HD22	1:C:237:TYR:CD1	2.54	0.42
1:E:145:GLU:OE2	1:E:155:ARG:HD2	2.18	0.42
1:E:87:LEU:HA	1:E:87:LEU:HD12	1.77	0.42
1:E:46:TYR:CD2	1:E:46:TYR:C	2.93	0.42
1:G:197:ILE:CG1	1:G:265:ILE:HD13	2.49	0.42
1:B:60:LYS:HA	1:B:60:LYS:HD3	1.84	0.42
1:D:123:ILE:HA	1:D:128:GLN:HG3	2.02	0.42
1:B:123:ILE:HA	1:B:128:GLN:HG3	2.02	0.42
1:C:273:ASP:HB3	1:G:275:ASN:HD22	1.84	0.42
1:D:174:ASN:ND2	1:D:177:LYS:HD3	2.35	0.42
1:A:177:LYS:HA	1:A:177:LYS:HD2	1.77	0.42
1:E:186:ILE:HD12	1:E:256:VAL:HG21	2.01	0.42
1:G:16:LYS:HB2	1:G:16:LYS:HE2	1.87	0.42
1:B:216:ILE:HD11	1:B:239:LYS:HD2	2.00	0.42
1:A:42:ILE:O	1:A:46:TYR:HB2	2.19	0.42
1:G:42:ILE:O	1:G:46:TYR:HB2	2.20	0.42
1:B:47:LYS:HA	1:B:50:SER:HB3	2.01	0.42
1:A:52:SER:O	1:A:54:ILE:N	2.52	0.42
1:F:222:LEU:HD22	1:F:237:TYR:CD1	2.53	0.42
1:D:187:ALA:HB2	1:D:233:VAL:HG22	2.02	0.42
1:G:179:SER:HB2	1:G:240:THR:O	2.19	0.42
1:A:134:TYR:H	1:A:176:THR:CG2	2.31	0.42
1:A:113:LEU:CD1	1:D:122:PHE:CE2	3.03	0.42
1:E:253:ARG:HD2	1:F:224:ILE:O	2.19	0.42
1:E:94:SER:HB3	1:F:78:PHE:CE2	2.54	0.42
1:A:88:PHE:HD1	1:D:30:ILE:HB	1.84	0.42
1:A:180:MET:HE2	1:A:245:LYS:HD2	2.01	0.42
1:C:42:ILE:O	1:C:46:TYR:HB2	2.20	0.42
1:C:24:VAL:O	1:C:28:LEU:HG	2.19	0.42
1:G:131:VAL:HG12	1:G:131:VAL:O	2.20	0.42
1:C:113:LEU:HD11	1:G:122:PHE:CZ	2.55	0.42
1:B:177:LYS:HA	1:B:177:LYS:HD2	1.76	0.42
1:C:194:VAL:O	1:C:198:ILE:HG13	2.20	0.42
1:D:190:ILE:HG12	1:D:190:ILE:H	1.51	0.42
1:F:100:GLY:HA2	1:F:103:SER:HB2	2.02	0.42
1:C:188:PHE:CE2	1:C:234:ILE:HG13	2.54	0.42
1:C:231:LYS:HB2	1:C:231:LYS:NZ	2.35	0.42
1:B:171:MET:HB3	1:B:171:MET:HE3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:VAL:O	1:E:131:VAL:HG12	2.20	0.42
1:F:145:GLU:OE2	1:F:155:ARG:HD2	2.18	0.42
1:G:123:ILE:HA	1:G:128:GLN:HG3	2.02	0.42
1:A:188:PHE:HE2	1:A:234:ILE:HG13	1.85	0.42
1:A:182:ALA:HB1	1:A:249:GLU:HG3	2.02	0.42
1:F:172:VAL:HG22	1:F:172:VAL:O	2.20	0.42
1:D:131:VAL:O	1:D:131:VAL:HG12	2.20	0.42
1:E:93:THR:CG2	1:F:96:LEU:HB2	2.50	0.42
1:A:276:PHE:CZ	1:D:276:PHE:CE1	3.07	0.42
1:F:47:LYS:HA	1:F:50:SER:HB3	2.01	0.42
1:D:250:ARG:NE	1:E:222:LEU:HD12	2.34	0.42
1:E:51:LYS:HD3	1:E:51:LYS:N	2.34	0.42
1:G:145:GLU:OE2	1:G:155:ARG:HD2	2.20	0.42
1:C:134:TYR:H	1:C:176:THR:CG2	2.33	0.41
1:D:117:MET:HG2	1:D:149:LEU:CD1	2.48	0.41
1:G:56:LEU:HD12	1:G:60:LYS:CB	2.49	0.41
1:A:24:VAL:O	1:A:28:LEU:HG	2.19	0.41
1:A:83:SER:OG	1:B:90:ILE:HA	2.19	0.41
1:G:29:ILE:HG13	1:G:30:ILE:N	2.34	0.41
1:A:96:LEU:HD12	1:B:97:ALA:HB2	2.02	0.41
1:E:29:ILE:HG13	1:E:30:ILE:N	2.35	0.41
1:D:18:VAL:HG13	1:D:19:LYS:H	1.83	0.41
1:E:241:GLN:HG3	1:E:242:PRO:HD2	2.02	0.41
1:G:278:ARG:CZ	1:G:278:ARG:HB2	2.50	0.41
1:C:250:ARG:CZ	1:G:222:LEU:HD12	2.50	0.41
1:F:56:LEU:HD12	1:F:60:LYS:HB2	2.01	0.41
1:B:56:LEU:HD12	1:B:60:LYS:HB2	2.02	0.41
1:B:129:PHE:CE1	1:B:172:VAL:HG21	2.56	0.41
1:D:151:VAL:HG23	1:D:165:PRO:HA	2.01	0.41
1:F:53:LYS:HE2	1:F:53:LYS:HB3	1.75	0.41
1:E:20:PHE:O	1:E:24:VAL:HG12	2.20	0.41
1:B:130:SER:O	1:B:132:GLY:N	2.53	0.41
1:C:249:GLU:O	1:C:253:ARG:HG3	2.20	0.41
1:E:106:ILE:HA	1:F:114:VAL:HG11	2.02	0.41
1:E:193:ASP:C	1:E:193:ASP:OD1	2.58	0.41
1:F:177:LYS:O	1:F:179:SER:N	2.48	0.41
1:F:209:LYS:HE3	1:F:209:LYS:HB2	1.81	0.41
1:C:218:GLY:HA3	1:C:219:PRO:HA	1.91	0.41
1:C:46:TYR:CD2	1:C:46:TYR:C	2.94	0.41
1:C:272:MET:HE2	1:C:272:MET:HB3	1.82	0.41
1:E:222:LEU:HD22	1:E:237:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LYS:HE3	1:A:19:LYS:HB3	1.78	0.41
1:B:56:LEU:HA	1:B:57:PRO:HD3	1.93	0.41
1:B:138:ASN:ND2	1:B:168:GLU:O	2.54	0.41
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.70	0.41
1:E:258:LYS:HA	1:E:258:LYS:HD3	1.89	0.41
1:C:52:SER:O	1:C:54:ILE:N	2.53	0.41
1:E:216:ILE:HD11	1:E:239:LYS:HD2	2.02	0.41
1:A:275:ASN:ND2	1:B:273:ASP:HB3	2.35	0.41
1:D:19:LYS:HE3	1:D:19:LYS:HB3	1.80	0.41
1:A:222:LEU:HD22	1:A:237:TYR:CD1	2.56	0.41
1:A:78:PHE:CE2	1:B:94:SER:HB3	2.56	0.41
1:F:138:ASN:ND2	1:F:168:GLU:O	2.54	0.41
1:D:215:LEU:O	1:D:215:LEU:HD12	2.20	0.41
1:A:276:PHE:CZ	1:B:276:PHE:CZ	3.09	0.41
1:A:137:ILE:HD12	1:A:154:ILE:HD12	2.03	0.41
1:C:222:LEU:HD12	1:F:250:ARG:CZ	2.51	0.41
1:D:201:LEU:HD23	1:D:259:MET:HE3	2.03	0.41
1:D:194:VAL:O	1:D:198:ILE:HG13	2.20	0.41
1:E:257:LYS:HE2	1:F:194:VAL:HG22	2.03	0.41
1:F:42:ILE:O	1:F:46:TYR:HB2	2.21	0.41
1:D:186:ILE:HD12	1:D:256:VAL:HG21	2.02	0.41
1:E:47:LYS:HZ2	1:E:47:LYS:HB2	1.83	0.41
1:C:56:LEU:HD12	1:C:60:LYS:HB2	2.02	0.41
1:C:92:MET:HA	1:C:92:MET:CE	2.51	0.41
1:G:24:VAL:O	1:G:28:LEU:HG	2.21	0.41
1:C:94:SER:HB3	1:G:78:PHE:CE2	2.56	0.41
1:E:214:ASP:HB2	1:E:244:GLN:HG3	2.02	0.41
1:B:51:LYS:HD2	1:B:51:LYS:HA	1.67	0.41
1:E:177:LYS:O	1:E:179:SER:N	2.49	0.41
1:C:190:ILE:HG12	1:C:230:SER:C	2.41	0.41
1:F:61:ILE:O	1:F:65:THR:HB	2.21	0.41
1:B:241:GLN:HG3	1:B:242:PRO:HD2	2.02	0.41
1:A:267:PHE:HB3	1:A:268:PRO:HD2	2.03	0.41
1:D:20:PHE:O	1:D:24:VAL:HG12	2.21	0.41
1:D:24:VAL:O	1:D:28:LEU:HG	2.21	0.41
1:C:257:LYS:HD3	1:C:257:LYS:O	2.21	0.40
1:A:46:TYR:C	1:A:46:TYR:CD2	2.95	0.40
1:D:222:LEU:HD22	1:D:237:TYR:CE1	2.56	0.40
1:F:19:LYS:HE3	1:F:19:LYS:HB3	1.78	0.40
1:A:88:PHE:CD1	1:D:30:ILE:HB	2.56	0.40
1:A:123:ILE:HA	1:A:128:GLN:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:SER:O	1:G:54:ILE:N	2.51	0.40
1:G:232:LEU:HD23	1:G:232:LEU:O	2.21	0.40
1:G:220:THR:O	1:G:236:VAL:HA	2.21	0.40
1:A:160:GLY:HA3	1:D:175:LEU:HD12	2.03	0.40
1:D:134:TYR:H	1:D:176:THR:CG2	2.34	0.40
1:D:181:MET:O	1:D:245:LYS:HE2	2.22	0.40
1:E:15:ILE:N	1:E:16:LYS:HZ3	2.15	0.40
1:C:106:ILE:HG22	1:F:101:ILE:HG23	2.02	0.40
1:F:60:LYS:O	1:F:63:THR:HG22	2.21	0.40
1:C:131:VAL:HA	1:C:144:VAL:CG2	2.51	0.40
1:E:208:VAL:CG2	1:E:255:ARG:HD2	2.50	0.40
1:D:162:HIS:HA	1:E:173:THR:HA	2.04	0.40
1:G:177:LYS:HA	1:G:177:LYS:HD2	1.74	0.40
1:G:257:LYS:C	1:G:257:LYS:HD3	2.41	0.40
1:A:205:CYS:SG	1:A:219:PRO:HB2	2.62	0.40
1:A:56:LEU:HD12	1:A:60:LYS:CB	2.51	0.40
1:F:171:MET:HE3	1:F:171:MET:HB3	1.78	0.40
1:E:267:PHE:HB3	1:E:268:PRO:HD2	2.03	0.40
1:E:134:TYR:H	1:E:176:THR:CG2	2.34	0.40
1:F:244:GLN:O	1:F:245:LYS:C	2.60	0.40
1:D:149:LEU:O	1:D:166:ASN:ND2	2.53	0.40
1:D:273:ASP:HB3	1:E:275:ASN:ND2	2.37	0.40
1:E:186:ILE:HG12	1:E:186:ILE:H	1.66	0.40
1:D:242:PRO:O	1:D:243:MET:HB2	2.21	0.40
1:A:18:VAL:HG13	1:A:19:LYS:H	1.86	0.40
1:C:101:ILE:HD13	1:G:106:ILE:HG21	2.04	0.40
1:E:52:SER:O	1:E:54:ILE:N	2.55	0.40
1:D:220:THR:O	1:D:236:VAL:HA	2.21	0.40
1:D:52:SER:O	1:D:54:ILE:N	2.52	0.40

All (1) 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:278:ARG:NH2	1:G:210:LYS:C[4_455]	2.06	0.14

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	265/285 (93%)	233 (88%)	20 (8%)	12 (4%)	3	24
1	B	265/285 (93%)	236 (89%)	17 (6%)	12 (4%)	3	24
1	C	265/285 (93%)	233 (88%)	21 (8%)	11 (4%)	3	27
1	D	265/285 (93%)	233 (88%)	20 (8%)	12 (4%)	3	24
1	E	265/285 (93%)	234 (88%)	20 (8%)	11 (4%)	3	27
1	F	265/285 (93%)	234 (88%)	19 (7%)	12 (4%)	3	24
1	G	265/285 (93%)	235 (89%)	19 (7%)	11 (4%)	3	27
All	All	1855/1995 (93%)	1638 (88%)	136 (7%)	81 (4%)	3	25

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	191	ASP
1	A	223	GLY
1	B	14	ASP
1	B	191	ASP
1	B	223	GLY
1	C	14	ASP
1	C	191	ASP
1	C	223	GLY
1	D	14	ASP
1	D	191	ASP
1	D	223	GLY
1	E	14	ASP
1	E	191	ASP
1	E	223	GLY
1	F	14	ASP
1	F	191	ASP
1	F	223	GLY

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Mol	Chain	Res	Type
1	G	14	ASP
1	G	191	ASP
1	G	223	GLY
1	A	131	VAL
1	A	170	LYS
1	A	175	LEU
1	A	229	ASP
1	B	131	VAL
1	B	170	LYS
1	B	175	LEU
1	B	229	ASP
1	C	170	LYS
1	C	175	LEU
1	C	229	ASP
1	D	131	VAL
1	D	170	LYS
1	D	175	LEU
1	D	229	ASP
1	E	131	VAL
1	E	170	LYS
1	E	175	LEU
1	E	229	ASP
1	F	131	VAL
1	F	170	LYS
1	F	175	LEU
1	F	229	ASP
1	G	170	LYS
1	G	175	LEU
1	G	229	ASP
1	A	178	ASP
1	B	53	LYS
1	C	53	LYS
1	C	131	VAL
1	C	178	ASP
1	D	53	LYS
1	E	53	LYS
1	E	178	ASP
1	F	53	LYS
1	F	245	LYS
1	G	53	LYS
1	G	178	ASP
1	A	53	LYS

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Mol	Chain	Res	Type
1	B	176	THR
1	B	178	ASP
1	C	176	THR
1	D	176	THR
1	D	178	ASP
1	E	176	THR
1	F	176	THR
1	F	178	ASP
1	G	131	VAL
1	G	176	THR
1	A	176	THR
1	A	245	LYS
1	A	264	ASN
1	B	245	LYS
1	C	245	LYS
1	D	245	LYS
1	D	264	ASN
1	E	245	LYS
1	F	264	ASN
1	G	264	ASN
1	B	264	ASN

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	236/251 (94%)	197 (84%)	39 (16%)	3 13
1	B	236/251 (94%)	197 (84%)	39 (16%)	3 13
1	C	236/251 (94%)	195 (83%)	41 (17%)	2 11
1	D	236/251 (94%)	196 (83%)	40 (17%)	2 12
1	E	236/251 (94%)	195 (83%)	41 (17%)	2 11
1	F	236/251 (94%)	193 (82%)	43 (18%)	2 9
1	G	236/251 (94%)	193 (82%)	43 (18%)	2 9
All	All	1652/1757 (94%)	1366 (83%)	286 (17%)	2 11

All (286) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	21	LEU
1	A	22	LEU
1	A	24	VAL
1	A	25	LEU
1	A	29	ILE
1	A	47	LYS
1	A	48	LEU
1	A	49	TYR
1	A	51	LYS
1	A	65	THR
1	A	67	LEU
1	A	85	LEU
1	A	87	LEU
1	A	95	LEU
1	A	130	SER
1	A	136	THR
1	A	140	ILE
1	A	143	THR
1	A	144	VAL
1	A	149	LEU
1	A	151	VAL
1	A	154	ILE
1	A	159	ASP
1	A	171	MET
1	A	172	VAL
1	A	173	THR
1	A	175	LEU
1	A	176	THR
1	A	186	ILE
1	A	190	ILE
1	A	194	VAL
1	A	216	ILE
1	A	225	THR
1	A	229	ASP
1	A	232	LEU
1	A	240	THR
1	A	263	LYS
1	A	279	VAL
1	B	15	ILE
1	B	21	LEU
1	B	22	LEU

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Mol	Chain	Res	Type
1	B	24	VAL
1	B	25	LEU
1	B	29	ILE
1	B	37	PHE
1	B	47	LYS
1	B	49	TYR
1	B	51	LYS
1	B	65	THR
1	B	67	LEU
1	B	85	LEU
1	B	87	LEU
1	B	95	LEU
1	B	130	SER
1	B	136	THR
1	B	140	ILE
1	B	143	THR
1	B	144	VAL
1	B	149	LEU
1	B	151	VAL
1	B	158	SER
1	B	159	ASP
1	B	171	MET
1	B	172	VAL
1	B	173	THR
1	B	175	LEU
1	B	176	THR
1	B	186	ILE
1	B	190	ILE
1	B	194	VAL
1	B	216	ILE
1	B	225	THR
1	B	229	ASP
1	B	232	LEU
1	B	240	THR
1	B	263	LYS
1	B	279	VAL
1	C	15	ILE
1	C	21	LEU
1	C	22	LEU
1	C	24	VAL
1	C	25	LEU
1	C	29	ILE

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Mol	Chain	Res	Type
1	C	47	LYS
1	C	48	LEU
1	C	49	TYR
1	C	51	LYS
1	C	65	THR
1	C	67	LEU
1	C	85	LEU
1	C	87	LEU
1	C	95	LEU
1	C	130	SER
1	C	136	THR
1	C	140	ILE
1	C	143	THR
1	C	144	VAL
1	C	149	LEU
1	C	151	VAL
1	C	154	ILE
1	C	158	SER
1	C	159	ASP
1	C	171	MET
1	C	172	VAL
1	C	173	THR
1	C	175	LEU
1	C	176	THR
1	C	186	ILE
1	C	190	ILE
1	C	194	VAL
1	C	213	ASP
1	C	216	ILE
1	C	225	THR
1	C	229	ASP
1	C	232	LEU
1	C	240	THR
1	C	263	LYS
1	C	279	VAL
1	D	15	ILE
1	D	21	LEU
1	D	22	LEU
1	D	24	VAL
1	D	25	LEU
1	D	29	ILE
1	D	47	LYS

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Mol	Chain	Res	Type
1	D	48	LEU
1	D	49	TYR
1	D	51	LYS
1	D	65	THR
1	D	67	LEU
1	D	85	LEU
1	D	87	LEU
1	D	95	LEU
1	D	130	SER
1	D	136	THR
1	D	140	ILE
1	D	143	THR
1	D	144	VAL
1	D	149	LEU
1	D	151	VAL
1	D	154	ILE
1	D	159	ASP
1	D	171	MET
1	D	172	VAL
1	D	173	THR
1	D	175	LEU
1	D	176	THR
1	D	186	ILE
1	D	190	ILE
1	D	194	VAL
1	D	213	ASP
1	D	216	ILE
1	D	225	THR
1	D	229	ASP
1	D	232	LEU
1	D	240	THR
1	D	263	LYS
1	D	279	VAL
1	E	15	ILE
1	E	21	LEU
1	E	22	LEU
1	E	24	VAL
1	E	25	LEU
1	E	29	ILE
1	E	37	PHE
1	E	47	LYS
1	E	49	TYR

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Mol	Chain	Res	Type
1	E	51	LYS
1	E	65	THR
1	E	67	LEU
1	E	85	LEU
1	E	87	LEU
1	E	95	LEU
1	E	130	SER
1	E	136	THR
1	E	140	ILE
1	E	144	VAL
1	E	149	LEU
1	E	151	VAL
1	E	154	ILE
1	E	158	SER
1	E	159	ASP
1	E	171	MET
1	E	172	VAL
1	E	173	THR
1	E	175	LEU
1	E	176	THR
1	E	186	ILE
1	E	190	ILE
1	E	194	VAL
1	E	213	ASP
1	E	216	ILE
1	E	225	THR
1	E	229	ASP
1	E	231	LYS
1	E	232	LEU
1	E	240	THR
1	E	263	LYS
1	E	279	VAL
1	F	15	ILE
1	F	16	LYS
1	F	21	LEU
1	F	22	LEU
1	F	24	VAL
1	F	25	LEU
1	F	29	ILE
1	F	47	LYS
1	F	48	LEU
1	F	49	TYR

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Mol	Chain	Res	Type
1	F	51	LYS
1	F	65	THR
1	F	67	LEU
1	F	85	LEU
1	F	87	LEU
1	F	95	LEU
1	F	130	SER
1	F	136	THR
1	F	140	ILE
1	F	143	THR
1	F	144	VAL
1	F	149	LEU
1	F	151	VAL
1	F	154	ILE
1	F	159	ASP
1	F	170	LYS
1	F	171	MET
1	F	172	VAL
1	F	173	THR
1	F	175	LEU
1	F	176	THR
1	F	186	ILE
1	F	190	ILE
1	F	194	VAL
1	F	213	ASP
1	F	215	LEU
1	F	216	ILE
1	F	225	THR
1	F	229	ASP
1	F	232	LEU
1	F	240	THR
1	F	263	LYS
1	F	279	VAL
1	G	15	ILE
1	G	21	LEU
1	G	22	LEU
1	G	24	VAL
1	G	25	LEU
1	G	29	ILE
1	G	46	TYR
1	G	47	LYS
1	G	48	LEU

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Mol	Chain	Res	Type
1	G	49	TYR
1	G	51	LYS
1	G	65	THR
1	G	67	LEU
1	G	85	LEU
1	G	87	LEU
1	G	95	LEU
1	G	130	SER
1	G	136	THR
1	G	140	ILE
1	G	143	THR
1	G	144	VAL
1	G	149	LEU
1	G	151	VAL
1	G	154	ILE
1	G	158	SER
1	G	159	ASP
1	G	171	MET
1	G	172	VAL
1	G	173	THR
1	G	175	LEU
1	G	176	THR
1	G	186	ILE
1	G	190	ILE
1	G	194	VAL
1	G	213	ASP
1	G	216	ILE
1	G	225	THR
1	G	229	ASP
1	G	231	LYS
1	G	232	LEU
1	G	240	THR
1	G	263	LYS
1	G	279	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	HIS
1	B	162	HIS
1	C	162	HIS
1	D	162	HIS

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Mol	Chain	Res	Type
1	E	162	HIS
1	F	162	HIS
1	G	162	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	267/285 (93%)	0.67	30 (11%) 7 6	98, 136, 200, 250	0
1	B	267/285 (93%)	0.69	26 (9%) 10 11	99, 133, 200, 249	0
1	C	267/285 (93%)	0.56	21 (7%) 15 16	94, 131, 198, 249	0
1	D	267/285 (93%)	0.69	30 (11%) 7 6	100, 135, 200, 252	0
1	E	267/285 (93%)	0.64	28 (10%) 8 8	98, 134, 199, 266	0
1	F	267/285 (93%)	0.62	24 (8%) 12 12	94, 134, 200, 248	0
1	G	267/285 (93%)	0.42	7 (2%) 59 59	90, 131, 199, 249	0
All	All	1869/1995 (93%)	0.61	166 (8%) 12 12	90, 134, 200, 266	0

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	LYS	10.0
1	B	49	TYR	9.6
1	G	279	VAL	7.5
1	D	54	ILE	7.5
1	D	56	LEU	7.2
1	B	48	LEU	7.1
1	D	55	GLN	6.8
1	B	51	LYS	6.0
1	D	146	GLU	5.7
1	A	146	GLU	5.3
1	B	56	LEU	5.3
1	A	49	TYR	5.3
1	D	42	ILE	5.2
1	E	53	LYS	5.1
1	B	214	ASP	4.9
1	A	276	PHE	4.9
1	D	45	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	E	46	TYR	4.8
1	F	51	LYS	4.8
1	E	178	ASP	4.7
1	E	279	VAL	4.7
1	B	50	SER	4.7
1	F	54	ILE	4.6
1	F	279	VAL	4.6
1	F	53	LYS	4.4
1	B	58	GLN	4.4
1	E	50	SER	4.3
1	D	41	LEU	4.2
1	E	43	TYR	4.1
1	A	55	GLN	4.0
1	C	179	SER	3.9
1	F	50	SER	3.8
1	F	52	SER	3.8
1	F	128	GLN	3.8
1	E	268	PRO	3.8
1	C	243	MET	3.6
1	B	52	SER	3.6
1	A	56	LEU	3.6
1	A	152	THR	3.5
1	C	55	GLN	3.5
1	A	243	MET	3.4
1	F	47	LYS	3.4
1	F	208	VAL	3.4
1	D	145	GLU	3.4
1	A	15	ILE	3.3
1	B	45	PHE	3.3
1	E	215	LEU	3.3
1	A	52	SER	3.3
1	C	178	ASP	3.3
1	D	51	LYS	3.2
1	A	143	THR	3.2
1	C	49	TYR	3.2
1	D	52	SER	3.1
1	F	129	PHE	3.1
1	D	147	ILE	3.1
1	B	13	TYR	3.1
1	D	265	ILE	3.1
1	B	54	ILE	3.1
1	C	242	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	179	SER	3.1
1	E	188	PHE	3.0
1	D	46	TYR	3.0
1	A	147	ILE	3.0
1	C	40	PHE	2.9
1	E	241	GLN	2.9
1	F	43	TYR	2.9
1	B	55	GLN	2.9
1	F	147	ILE	2.9
1	E	52	SER	2.9
1	D	243	MET	2.9
1	A	216	ILE	2.8
1	E	54	ILE	2.8
1	B	129	PHE	2.8
1	F	89	ASN	2.8
1	E	55	GLN	2.8
1	E	40	PHE	2.8
1	E	264	ASN	2.8
1	E	13	TYR	2.8
1	D	38	ALA	2.7
1	A	32	PHE	2.7
1	D	15	ILE	2.7
1	D	153	LYS	2.7
1	C	208	VAL	2.6
1	B	57	PRO	2.6
1	D	58	GLN	2.6
1	A	48	LEU	2.6
1	B	215	LEU	2.6
1	D	43	TYR	2.5
1	A	230	SER	2.5
1	A	242	PRO	2.5
1	E	58	GLN	2.5
1	D	44	ARG	2.5
1	E	128	GLN	2.5
1	E	48	LEU	2.5
1	F	56	LEU	2.5
1	A	144	VAL	2.5
1	A	13	TYR	2.5
1	C	201	LEU	2.5
1	D	57	PRO	2.5
1	C	32	PHE	2.5
1	A	73	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	55	GLN	2.4
1	G	46	TYR	2.4
1	F	241	GLN	2.4
1	B	267	PHE	2.4
1	G	146	GLU	2.4
1	B	60	LYS	2.4
1	C	17	ALA	2.4
1	E	39	ASP	2.4
1	G	230	SER	2.4
1	E	161	LEU	2.4
1	A	277	LYS	2.4
1	G	278	ARG	2.4
1	F	263	LYS	2.4
1	D	164	ILE	2.4
1	C	45	PHE	2.4
1	A	196	LYS	2.3
1	E	49	TYR	2.3
1	D	216	ILE	2.3
1	C	215	LEU	2.3
1	E	240	THR	2.3
1	B	216	ILE	2.3
1	C	204	ILE	2.3
1	F	46	TYR	2.3
1	F	183	VAL	2.3
1	F	227	MET	2.3
1	D	40	PHE	2.3
1	A	180	MET	2.3
1	E	265	ILE	2.3
1	G	45	PHE	2.3
1	A	153	LYS	2.2
1	C	199	GLU	2.2
1	C	206	GLU	2.2
1	A	129	PHE	2.2
1	A	179	SER	2.2
1	C	42	ILE	2.2
1	D	14	ASP	2.2
1	B	208	VAL	2.2
1	C	277	LYS	2.2
1	D	149	LEU	2.2
1	F	123	ILE	2.2
1	B	147	ILE	2.1
1	C	214	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	33	ILE	2.1
1	G	49	TYR	2.1
1	B	260	PHE	2.1
1	D	53	LYS	2.1
1	F	58	GLN	2.1
1	A	217	GLU	2.1
1	E	224	ILE	2.1
1	E	234	ILE	2.1
1	C	175	LEU	2.1
1	D	276	PHE	2.1
1	A	149	LEU	2.1
1	A	54	ILE	2.1
1	B	241	GLN	2.1
1	B	145	GLU	2.1
1	B	265	ILE	2.0
1	B	240	THR	2.0
1	D	89	ASN	2.0
1	C	19	LYS	2.0
1	D	263	LYS	2.0
1	E	210	LYS	2.0
1	F	157	PHE	2.0
1	A	263	LYS	2.0
1	A	267	PHE	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.