Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 08:30 pm BST

PDB ID	:	2ZW3
Title	:	Structure of the connexin-26 gap junction channel at 3.5 angstrom resolution
Authors	:	Maeda, S.; Nakagawa, S.; Suga, M.; Yamashita, E.; Oshima, A.; Fujiyoshi, Y.; Tsukihara, T.
Deposited on	:	2008-12-01
Resolution	:	3.50 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

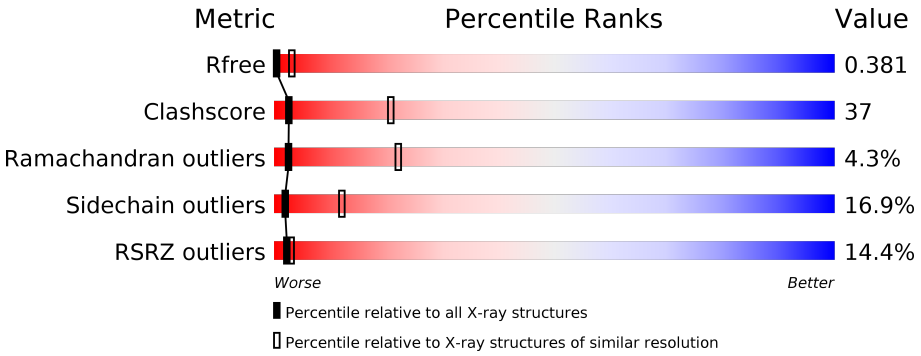
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 respectively. 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	226	8% 36% 43% 9% • 11%
1	B	226	16% 36% 43% 8% • 11%
1	C	226	16% 35% 43% 9% • 11%
1	D	226	13% 36% 43% 8% • 11%
1	E	226	14% 34% 46% 8% • 11%
1	F	226	11% 37% 42% 8% • 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9834 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 Gap junction beta-2 protein.

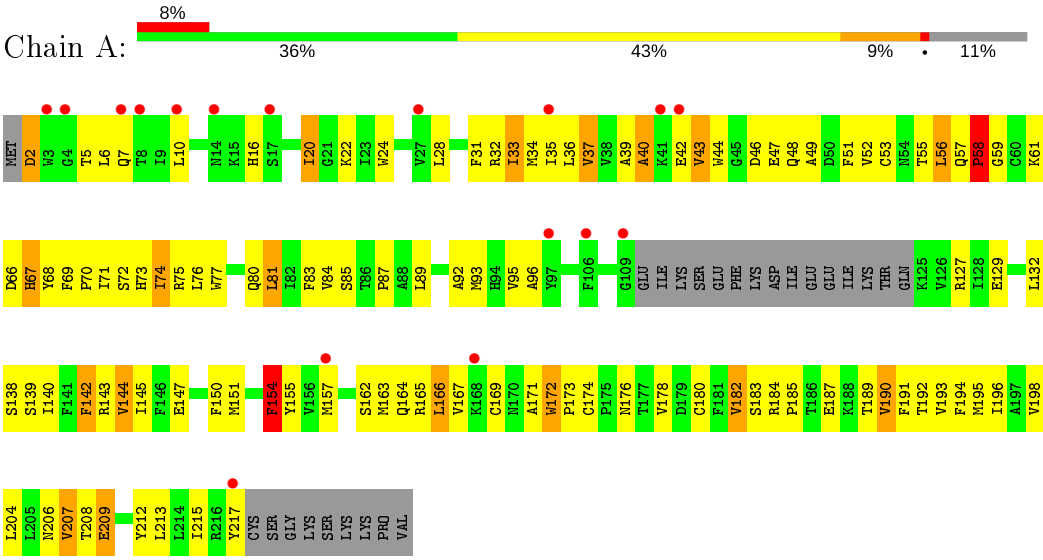
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1639	1088	269	268	14			
1	B	201	Total	C	N	O	S	0	0	0
			1639	1088	269	268	14			
1	C	201	Total	C	N	O	S	0	0	0
			1639	1088	269	268	14			
1	D	201	Total	C	N	O	S	0	0	0
			1639	1088	269	268	14			
1	E	201	Total	C	N	O	S	0	0	0
			1639	1088	269	268	14			
1	F	201	Total	C	N	O	S	0	0	0
			1639	1088	269	268	14			

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

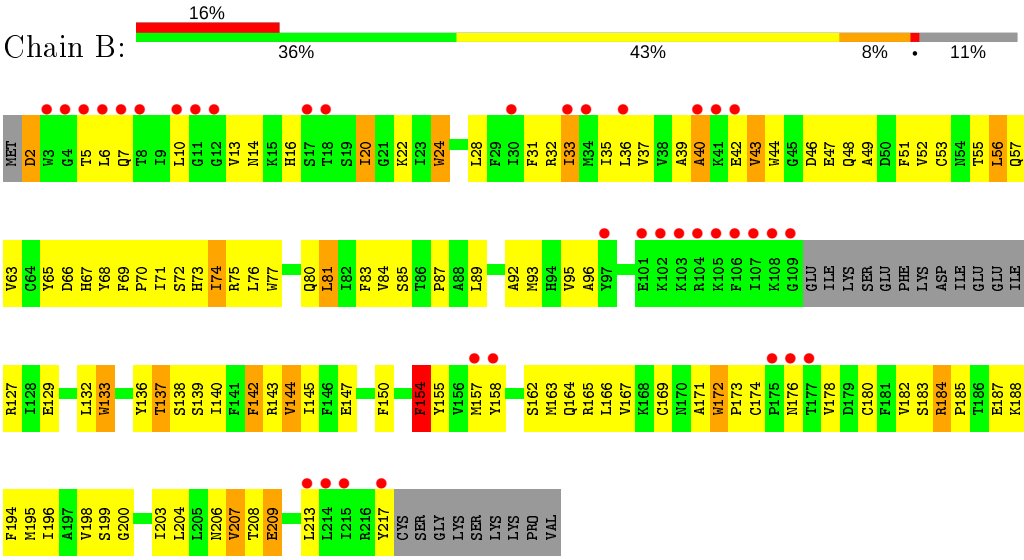
- Molecule 1: Gap junction beta-2 protein

Chain A:

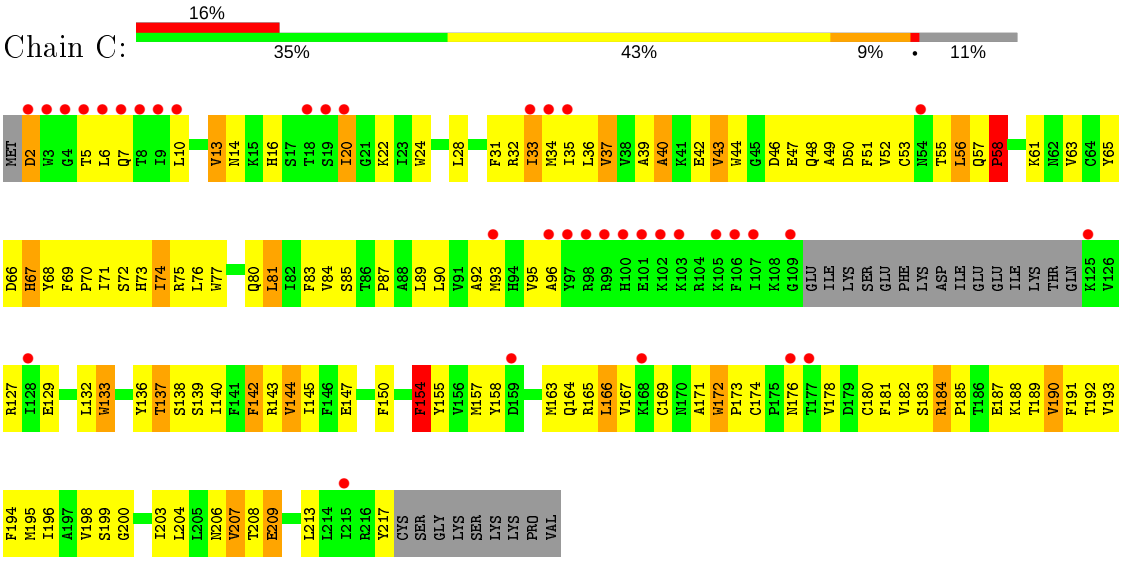


- Molecule 1: Gap junction beta-2 protein

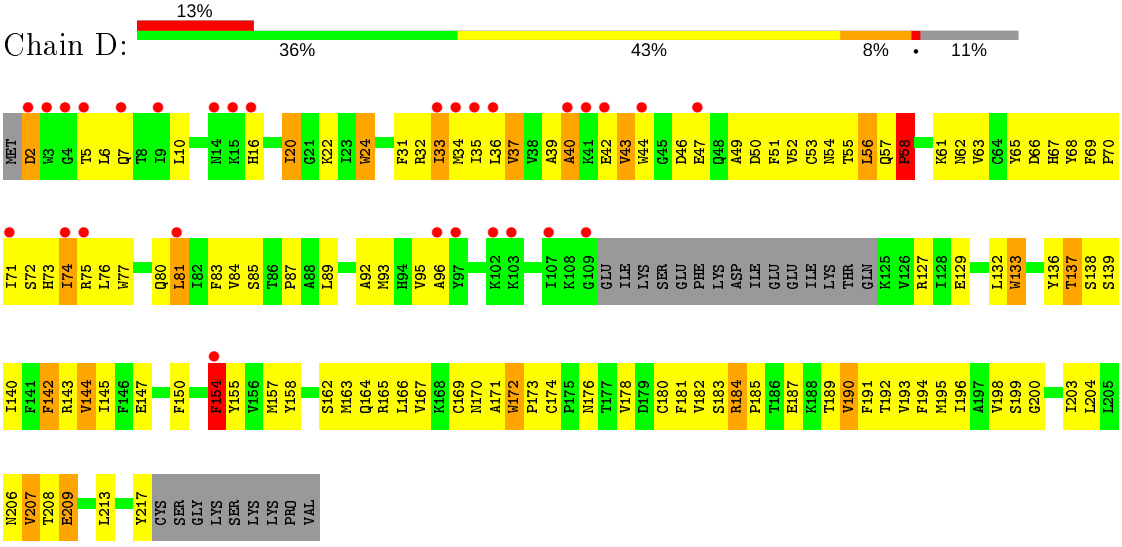
Chain B:



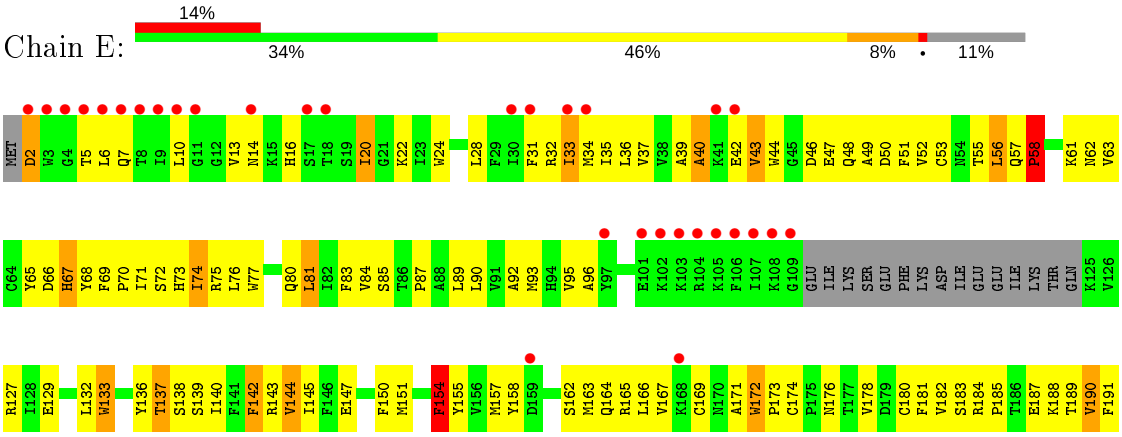
- Molecule 1: Gap junction beta-2 protein



- Molecule 1: Gap junction beta-2 protein

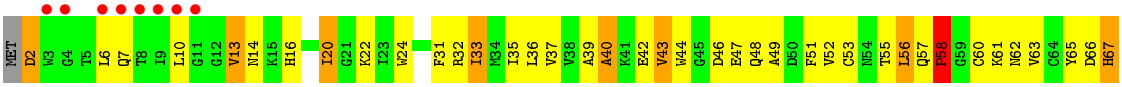


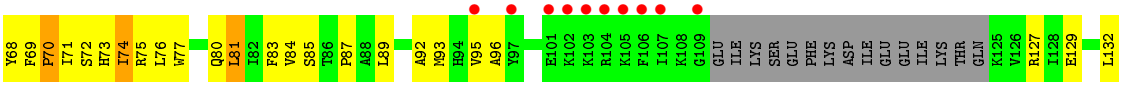
- Molecule 1: Gap junction beta-2 protein

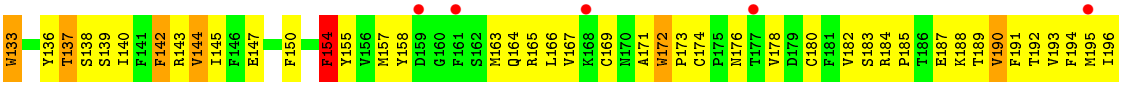


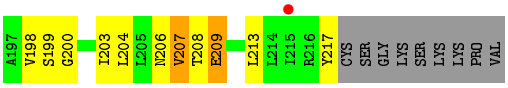
- Molecule 1: Gap junction beta-2 protein

Chain F:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	167.62Å 111.25Å 155.39Å 90.00° 114.04° 90.00°	Depositor
Resolution (Å)	22.00 – 3.50 141.91 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (22.00-3.50) 94.6 (141.91-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.337 , 0.351 0.344 , 0.381	Depositor DCC
R_{free} test set	1583 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	104.7	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.72	EDS
Total number of atoms	9834	wwPDB-VP
Average B, all atoms (Å^2)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.57	0/1686	0.63	0/2291
1	B	0.56	0/1686	0.63	0/2291
1	C	0.57	0/1686	0.63	0/2291
1	D	0.56	0/1686	0.63	0/2291
1	E	0.56	0/1686	0.63	0/2291
1	F	0.58	1/1686 (0.1%)	0.63	0/2291
All	All	0.57	1/10116 (0.0%)	0.63	0/13746

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	60	CYS	CB-SG	-5.46	1.73	1.81

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	1639	0	1647	130	0
1	B	1639	0	1647	139	0
1	C	1639	0	1647	138	0
1	D	1639	0	1647	138	0
1	E	1639	0	1647	146	0
1	F	1639	0	1647	138	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9834	0	9882	720	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (720) 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:F:68:TYR:CE1	1:F:167:VAL:HG21	1.71	1.25
1:A:68:TYR:CE1	1:A:167:VAL:HG21	1.71	1.24
1:E:68:TYR:CE1	1:E:167:VAL:HG21	1.73	1.23
1:C:68:TYR:CE1	1:C:167:VAL:HG21	1.73	1.23
1:B:68:TYR:CE1	1:B:167:VAL:HG21	1.75	1.22
1:D:68:TYR:CE1	1:D:167:VAL:HG21	1.76	1.18
1:E:80:GLN:HE21	1:E:150:PHE:HB2	1.07	1.13
1:F:80:GLN:HE21	1:F:150:PHE:HB2	1.09	1.12
1:D:80:GLN:HE21	1:D:150:PHE:HB2	1.09	1.10
1:B:80:GLN:HE21	1:B:150:PHE:HB2	1.09	1.10
1:C:80:GLN:HE21	1:C:150:PHE:HB2	1.08	1.10
1:D:144:VAL:HG22	1:D:206:ASN:HB3	1.35	1.08
1:A:80:GLN:HE21	1:A:150:PHE:HB2	1.11	1.08
1:B:144:VAL:HG22	1:B:206:ASN:HB3	1.35	1.08
1:C:144:VAL:HG22	1:C:206:ASN:HB3	1.35	1.08
1:E:144:VAL:HG22	1:E:206:ASN:HB3	1.37	1.05
1:F:80:GLN:NE2	1:F:150:PHE:HB2	1.71	1.05
1:A:144:VAL:HG22	1:A:206:ASN:HB3	1.35	1.05
1:E:80:GLN:NE2	1:E:150:PHE:HB2	1.72	1.05
1:D:80:GLN:NE2	1:D:150:PHE:HB2	1.72	1.04
1:F:144:VAL:HG22	1:F:206:ASN:HB3	1.36	1.03
1:F:7:GLN:HG3	1:F:89:LEU:HD11	1.39	1.02
1:C:80:GLN:NE2	1:C:150:PHE:HB2	1.73	1.02
1:B:7:GLN:HG3	1:B:89:LEU:HD11	1.40	1.01
1:B:80:GLN:NE2	1:B:150:PHE:HB2	1.74	1.00
1:B:68:TYR:HE1	1:B:167:VAL:HG21	1.22	0.98
1:A:7:GLN:HG3	1:A:89:LEU:HD11	1.45	0.98
1:E:80:GLN:HE21	1:E:150:PHE:CB	1.77	0.98
1:F:68:TYR:HE1	1:F:167:VAL:HG21	1.20	0.98
1:A:80:GLN:NE2	1:A:150:PHE:HB2	1.78	0.97
1:D:80:GLN:HE21	1:D:150:PHE:CB	1.76	0.97
1:F:80:GLN:HE21	1:F:150:PHE:CB	1.79	0.95
1:A:68:TYR:HE1	1:A:167:VAL:HG21	1.23	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:TYR:HE1	1:D:167:VAL:HG21	1.28	0.95
1:D:7:GLN:HG3	1:D:89:LEU:HD11	1.45	0.95
1:B:43:VAL:HG12	1:C:75:ARG:HH11	1.32	0.94
1:D:165:ARG:HD3	1:E:63:VAL:HG13	1.50	0.94
1:C:187:GLU:HB2	1:D:70:PRO:O	1.68	0.94
1:E:187:GLU:HB2	1:F:70:PRO:O	1.67	0.94
1:A:80:GLN:HE21	1:A:150:PHE:CB	1.79	0.94
1:B:80:GLN:HE21	1:B:150:PHE:CB	1.78	0.94
1:D:43:VAL:HG12	1:E:75:ARG:HH11	1.33	0.94
1:C:80:GLN:HE21	1:C:150:PHE:CB	1.80	0.93
1:E:43:VAL:HG12	1:F:75:ARG:HH11	1.33	0.93
1:B:33:ILE:HD12	1:B:81:LEU:HD12	1.52	0.92
1:B:187:GLU:HB2	1:C:70:PRO:O	1.69	0.92
1:A:187:GLU:HB2	1:B:70:PRO:O	1.69	0.92
1:C:68:TYR:HE1	1:C:167:VAL:HG21	1.23	0.92
1:C:33:ILE:HD12	1:C:81:LEU:HD12	1.51	0.92
1:A:165:ARG:HD3	1:B:63:VAL:HG13	1.51	0.92
1:C:7:GLN:HG3	1:C:89:LEU:HD11	1.51	0.91
1:E:68:TYR:HE1	1:E:167:VAL:HG21	1.24	0.90
1:E:7:GLN:HG3	1:E:89:LEU:HD11	1.51	0.90
1:B:84:VAL:HG21	1:B:147:GLU:HG2	1.54	0.90
1:A:33:ILE:HD12	1:A:81:LEU:HD12	1.53	0.90
1:E:165:ARG:HD3	1:F:63:VAL:HG13	1.52	0.89
1:E:33:ILE:HD12	1:E:81:LEU:HD12	1.53	0.88
1:A:75:ARG:HH11	1:F:43:VAL:HG12	1.38	0.88
1:D:187:GLU:HB2	1:E:70:PRO:O	1.71	0.88
1:A:43:VAL:HG12	1:B:75:ARG:HH11	1.38	0.88
1:F:68:TYR:CE1	1:F:167:VAL:CG2	2.55	0.88
1:A:68:TYR:CE1	1:A:167:VAL:CG2	2.56	0.88
1:E:84:VAL:HG21	1:E:147:GLU:HG2	1.54	0.88
1:E:80:GLN:NE2	1:E:150:PHE:CB	2.36	0.87
1:F:84:VAL:HG21	1:F:147:GLU:HG2	1.56	0.87
1:D:80:GLN:NE2	1:D:150:PHE:CB	2.34	0.87
1:D:33:ILE:HD12	1:D:81:LEU:HD12	1.56	0.87
1:E:68:TYR:CE1	1:E:167:VAL:CG2	2.57	0.87
1:B:68:TYR:CE1	1:B:167:VAL:CG2	2.58	0.86
1:C:84:VAL:HG21	1:C:147:GLU:HG2	1.57	0.86
1:C:68:TYR:CE1	1:C:167:VAL:CG2	2.57	0.86
1:A:84:VAL:HG21	1:A:147:GLU:HG2	1.56	0.86
1:D:68:TYR:CE1	1:D:167:VAL:CG2	2.59	0.86
1:E:140:ILE:HD13	1:E:209:GLU:HB3	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:GLN:NE2	1:B:150:PHE:CB	2.36	0.85
1:C:165:ARG:HD3	1:D:63:VAL:HG13	1.57	0.85
1:C:80:GLN:NE2	1:C:150:PHE:CB	2.39	0.85
1:A:70:PRO:O	1:F:187:GLU:HB2	1.76	0.85
1:F:80:GLN:NE2	1:F:150:PHE:CB	2.35	0.85
1:A:63:VAL:HG13	1:F:165:ARG:HD3	1.55	0.85
1:D:84:VAL:HG21	1:D:147:GLU:HG2	1.59	0.85
1:C:43:VAL:HG12	1:D:75:ARG:HH11	1.40	0.84
1:F:33:ILE:HD12	1:F:81:LEU:HD12	1.58	0.83
1:B:165:ARG:HD3	1:C:63:VAL:HG13	1.57	0.83
1:E:32:ARG:HH11	1:E:198:VAL:HG12	1.43	0.83
1:C:140:ILE:HD13	1:C:209:GLU:HB3	1.60	0.82
1:F:140:ILE:HD13	1:F:209:GLU:HB3	1.60	0.82
1:E:76:LEU:HB3	1:E:154:PHE:CE1	2.16	0.81
1:C:32:ARG:HH11	1:C:198:VAL:HG12	1.46	0.81
1:B:185:PRO:HD2	1:C:66:ASP:OD1	1.81	0.81
1:F:76:LEU:HB3	1:F:154:PHE:CE1	2.16	0.81
1:D:185:PRO:HD2	1:E:66:ASP:OD1	1.80	0.80
1:A:140:ILE:HD13	1:A:209:GLU:HB3	1.61	0.80
1:A:32:ARG:HH11	1:A:198:VAL:HG12	1.47	0.80
1:A:80:GLN:NE2	1:A:150:PHE:CB	2.38	0.80
1:D:140:ILE:HD13	1:D:209:GLU:HB3	1.61	0.80
1:B:140:ILE:HD13	1:B:209:GLU:HB3	1.63	0.80
1:B:76:LEU:HB3	1:B:154:PHE:CE1	2.17	0.80
1:D:76:LEU:HB3	1:D:154:PHE:CE1	2.17	0.80
1:C:76:LEU:HB3	1:C:154:PHE:CE1	2.17	0.80
1:E:185:PRO:HD2	1:F:66:ASP:OD1	1.82	0.79
1:F:32:ARG:HH11	1:F:198:VAL:HG12	1.46	0.79
1:B:32:ARG:HH11	1:B:198:VAL:HG12	1.46	0.79
1:C:185:PRO:HD2	1:D:66:ASP:OD1	1.82	0.79
1:A:39:ALA:HB2	1:A:191:PHE:HD1	1.46	0.79
1:A:76:LEU:HB3	1:A:154:PHE:CE1	2.17	0.78
1:A:66:ASP:OD1	1:F:185:PRO:HD2	1.84	0.78
1:A:185:PRO:HD2	1:B:66:ASP:OD1	1.84	0.77
1:D:32:ARG:HH11	1:D:198:VAL:HG12	1.49	0.77
1:F:140:ILE:HA	1:F:143:ARG:HD2	1.66	0.77
1:E:39:ALA:HB2	1:E:191:PHE:HD1	1.49	0.77
1:E:140:ILE:HA	1:E:143:ARG:HD2	1.66	0.76
1:F:39:ALA:HB2	1:F:191:PHE:HD1	1.49	0.76
1:D:39:ALA:HB2	1:D:191:PHE:HD1	1.50	0.76
1:D:140:ILE:HA	1:D:143:ARG:HD2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ALA:HB2	1:C:191:PHE:HD1	1.50	0.75
1:E:140:ILE:HA	1:E:143:ARG:CD	2.17	0.75
1:A:140:ILE:HA	1:A:143:ARG:CD	2.17	0.75
1:B:140:ILE:HA	1:B:143:ARG:HD2	1.67	0.74
1:A:140:ILE:HA	1:A:143:ARG:HD2	1.67	0.74
1:C:140:ILE:HA	1:C:143:ARG:HD2	1.69	0.74
1:B:39:ALA:HB2	1:B:191:PHE:HD1	1.51	0.74
1:F:68:TYR:HE1	1:F:167:VAL:CG2	1.97	0.74
1:F:140:ILE:HA	1:F:143:ARG:CD	2.18	0.74
1:B:140:ILE:HA	1:B:143:ARG:CD	2.19	0.73
1:E:187:GLU:OE1	1:F:72:SER:N	2.22	0.73
1:D:140:ILE:HA	1:D:143:ARG:CD	2.19	0.72
1:C:140:ILE:HA	1:C:143:ARG:CD	2.20	0.71
1:B:182:VAL:HB	1:B:185:PRO:HG3	1.73	0.71
1:B:36:LEU:HD12	1:B:77:TRP:HB3	1.73	0.70
1:D:182:VAL:HB	1:D:185:PRO:HG3	1.74	0.70
1:C:36:LEU:HD12	1:C:77:TRP:HB3	1.73	0.70
1:C:2:ASP:HB2	1:C:6:LEU:CD1	2.23	0.69
1:A:182:VAL:HB	1:A:185:PRO:HG3	1.73	0.69
1:C:5:THR:HB	1:D:2:ASP:OD1	1.92	0.69
1:E:182:VAL:HB	1:E:185:PRO:HG3	1.75	0.68
1:B:56:LEU:HD12	1:B:56:LEU:N	2.08	0.68
1:C:68:TYR:HE1	1:C:167:VAL:CG2	2.01	0.68
1:A:56:LEU:HD12	1:A:56:LEU:N	2.09	0.68
1:D:187:GLU:OE1	1:E:72:SER:N	2.22	0.68
1:C:182:VAL:HB	1:C:185:PRO:HG3	1.75	0.68
1:B:68:TYR:HE1	1:B:167:VAL:CG2	2.00	0.68
1:F:2:ASP:HB2	1:F:6:LEU:CD1	2.24	0.67
1:F:182:VAL:HB	1:F:185:PRO:HG3	1.76	0.67
1:A:68:TYR:HE1	1:A:167:VAL:CG2	2.01	0.67
1:E:42:GLU:HG2	1:F:75:ARG:CZ	2.23	0.66
1:C:56:LEU:HD12	1:C:56:LEU:N	2.11	0.66
1:C:187:GLU:OE1	1:D:72:SER:N	2.26	0.66
1:F:56:LEU:HD12	1:F:56:LEU:N	2.10	0.66
1:A:36:LEU:HD12	1:A:77:TRP:HB3	1.77	0.65
1:C:57:GLN:HG2	1:C:173:PRO:O	1.97	0.65
1:F:36:LEU:HD12	1:F:77:TRP:HB3	1.78	0.65
1:A:57:GLN:HG2	1:A:173:PRO:O	1.97	0.64
1:D:42:GLU:HG2	1:E:75:ARG:CZ	2.28	0.64
1:A:187:GLU:OE1	1:B:72:SER:N	2.31	0.64
1:A:75:ARG:CZ	1:F:42:GLU:HG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:GLN:HG2	1:D:173:PRO:O	1.98	0.64
1:D:36:LEU:HD12	1:D:77:TRP:HB3	1.80	0.64
1:F:57:GLN:HG2	1:F:173:PRO:O	1.97	0.64
1:C:140:ILE:O	1:C:144:VAL:HG23	1.98	0.64
1:E:36:LEU:HD12	1:E:77:TRP:HB3	1.78	0.64
1:D:185:PRO:CD	1:E:66:ASP:OD1	2.46	0.63
1:A:81:LEU:O	1:A:85:SER:HB2	1.99	0.63
1:E:140:ILE:O	1:E:144:VAL:HG23	1.98	0.63
1:A:140:ILE:O	1:A:144:VAL:HG23	1.99	0.63
1:E:187:GLU:CB	1:F:70:PRO:O	2.46	0.63
1:E:68:TYR:HE1	1:E:167:VAL:CG2	2.02	0.63
1:C:42:GLU:HG2	1:D:75:ARG:CZ	2.29	0.62
1:B:2:ASP:HB2	1:B:6:LEU:CD1	2.28	0.62
1:A:57:GLN:CG	1:A:173:PRO:O	2.47	0.62
1:E:81:LEU:O	1:E:85:SER:HB2	1.99	0.62
1:A:42:GLU:HG2	1:B:75:ARG:CZ	2.29	0.62
1:C:189:THR:O	1:C:192:THR:N	2.31	0.62
1:D:56:LEU:HD12	1:D:56:LEU:N	2.13	0.62
1:D:68:TYR:HE1	1:D:167:VAL:CG2	2.04	0.62
1:C:81:LEU:O	1:C:85:SER:HB2	2.00	0.62
1:D:5:THR:HB	1:E:2:ASP:OD1	2.00	0.62
1:F:140:ILE:O	1:F:144:VAL:HG23	1.99	0.62
1:E:56:LEU:N	1:E:56:LEU:HD12	2.14	0.61
1:B:81:LEU:O	1:B:85:SER:HB2	2.01	0.61
1:D:140:ILE:O	1:D:144:VAL:HG23	2.00	0.61
1:B:187:GLU:OE1	1:C:72:SER:N	2.31	0.61
1:A:5:THR:HB	1:B:2:ASP:OD1	2.00	0.61
1:F:57:GLN:CG	1:F:173:PRO:O	2.49	0.61
1:E:185:PRO:CD	1:F:66:ASP:OD1	2.48	0.61
1:F:2:ASP:HB2	1:F:6:LEU:HD11	1.82	0.61
1:D:81:LEU:O	1:D:85:SER:HB2	2.01	0.61
1:B:174:CYS:HB3	1:B:178:VAL:HG11	1.83	0.60
1:C:142:PHE:O	1:C:145:ILE:HG22	2.02	0.60
1:C:57:GLN:CG	1:C:173:PRO:O	2.48	0.60
1:B:140:ILE:O	1:B:144:VAL:HG23	2.01	0.60
1:B:189:THR:O	1:B:192:THR:N	2.34	0.60
1:A:139:SER:O	1:A:143:ARG:HG3	2.01	0.60
1:B:57:GLN:HG2	1:B:173:PRO:O	2.01	0.60
1:B:185:PRO:CD	1:C:66:ASP:OD1	2.50	0.60
1:C:2:ASP:HB2	1:C:6:LEU:HD11	1.84	0.60
1:E:189:THR:O	1:E:192:THR:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLN:HA	1:A:150:PHE:CD2	2.37	0.60
1:E:2:ASP:HB2	1:E:6:LEU:CD1	2.31	0.60
1:F:81:LEU:O	1:F:85:SER:HB2	2.02	0.60
1:B:57:GLN:CG	1:B:173:PRO:O	2.49	0.59
1:A:72:SER:N	1:F:187:GLU:OE1	2.29	0.59
1:B:42:GLU:HG2	1:C:75:ARG:CZ	2.32	0.59
1:D:80:GLN:NE2	1:D:150:PHE:HB3	2.15	0.59
1:A:185:PRO:CD	1:B:66:ASP:OD1	2.50	0.59
1:D:187:GLU:CB	1:E:70:PRO:O	2.48	0.59
1:D:189:THR:O	1:D:192:THR:N	2.35	0.59
1:C:80:GLN:HA	1:C:150:PHE:CD2	2.38	0.59
1:D:2:ASP:HB2	1:D:6:LEU:HD11	1.85	0.59
1:F:39:ALA:HB2	1:F:191:PHE:CD1	2.37	0.58
1:D:80:GLN:HA	1:D:150:PHE:CD2	2.38	0.58
1:E:5:THR:HB	1:F:2:ASP:OD1	2.03	0.58
1:B:2:ASP:HB2	1:B:6:LEU:HD11	1.85	0.58
1:E:57:GLN:HG2	1:E:173:PRO:O	2.03	0.58
1:A:2:ASP:HB2	1:A:6:LEU:HD11	1.84	0.58
1:C:185:PRO:CD	1:D:66:ASP:OD1	2.49	0.58
1:B:5:THR:HB	1:C:2:ASP:OD1	2.03	0.58
1:F:80:GLN:HA	1:F:150:PHE:CD2	2.39	0.58
1:A:66:ASP:OD1	1:F:185:PRO:CD	2.52	0.58
1:B:40:ALA:HA	1:B:74:ILE:HG12	1.86	0.58
1:D:193:VAL:HG12	1:D:194:PHE:N	2.18	0.58
1:C:187:GLU:CB	1:D:70:PRO:O	2.48	0.58
1:D:2:ASP:HB2	1:D:6:LEU:CD1	2.34	0.58
1:A:80:GLN:NE2	1:A:150:PHE:HB3	2.17	0.58
1:C:68:TYR:C	1:C:69:PHE:HD1	2.07	0.58
1:D:57:GLN:CG	1:D:173:PRO:O	2.52	0.58
1:F:80:GLN:NE2	1:F:150:PHE:HB3	2.19	0.58
1:F:68:TYR:C	1:F:69:PHE:HD1	2.07	0.58
1:A:68:TYR:C	1:A:69:PHE:HD1	2.07	0.57
1:A:35:ILE:HG23	1:A:195:MET:SD	2.45	0.57
1:A:2:ASP:HB2	1:A:6:LEU:CD1	2.34	0.57
1:C:139:SER:O	1:C:143:ARG:HG3	2.05	0.57
1:E:68:TYR:C	1:E:69:PHE:HD1	2.07	0.57
1:A:39:ALA:HB2	1:A:191:PHE:CD1	2.34	0.57
1:B:139:SER:O	1:B:143:ARG:HG3	2.05	0.57
1:E:42:GLU:HG2	1:F:75:ARG:NE	2.19	0.57
1:E:39:ALA:HB2	1:E:191:PHE:CD1	2.36	0.57
1:D:35:ILE:HG23	1:D:195:MET:SD	2.45	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TYR:C	1:B:69:PHE:HD1	2.08	0.56
1:D:139:SER:O	1:D:143:ARG:HG3	2.05	0.56
1:E:80:GLN:HA	1:E:150:PHE:CD2	2.40	0.56
1:C:182:VAL:HG12	1:C:183:SER:H	1.70	0.56
1:C:174:CYS:HB3	1:C:178:VAL:HG11	1.86	0.56
1:E:57:GLN:CG	1:E:173:PRO:O	2.53	0.56
1:A:32:ARG:HH12	1:A:199:SER:CA	2.19	0.56
1:B:80:GLN:HA	1:B:150:PHE:CD2	2.39	0.56
1:D:68:TYR:C	1:D:69:PHE:HD1	2.08	0.56
1:F:139:SER:O	1:F:143:ARG:HG3	2.04	0.56
1:D:68:TYR:CD1	1:D:167:VAL:HG21	2.37	0.56
1:C:35:ILE:HG23	1:C:195:MET:SD	2.45	0.56
1:B:195:MET:O	1:B:199:SER:HB2	2.06	0.56
1:F:189:THR:O	1:F:192:THR:N	2.39	0.56
1:A:172:TRP:CE3	1:A:173:PRO:HG3	2.41	0.56
1:D:52:VAL:O	1:D:180:CYS:HA	2.06	0.56
1:E:35:ILE:HG23	1:E:195:MET:SD	2.45	0.56
1:B:144:VAL:CG2	1:B:206:ASN:HB3	2.24	0.55
1:C:39:ALA:HB2	1:C:191:PHE:CD1	2.38	0.55
1:E:68:TYR:CD1	1:E:167:VAL:HG21	2.37	0.55
1:A:42:GLU:HG2	1:B:75:ARG:NE	2.21	0.55
1:E:174:CYS:HB3	1:E:178:VAL:HG11	1.89	0.55
1:F:144:VAL:CG2	1:F:206:ASN:HB3	2.24	0.55
1:B:193:VAL:HG12	1:B:194:PHE:N	2.22	0.55
1:F:174:CYS:HB3	1:F:178:VAL:HG11	1.89	0.55
1:E:32:ARG:HH12	1:E:199:SER:CA	2.20	0.55
1:B:80:GLN:NE2	1:B:150:PHE:HB3	2.18	0.55
1:B:39:ALA:HB2	1:B:191:PHE:CD1	2.38	0.55
1:E:195:MET:O	1:E:199:SER:HB2	2.06	0.55
1:C:172:TRP:CE3	1:C:173:PRO:HG3	2.42	0.55
1:D:2:ASP:N	1:D:2:ASP:OD2	2.40	0.55
1:A:174:CYS:HB3	1:A:178:VAL:HG11	1.88	0.54
1:D:39:ALA:HB2	1:D:191:PHE:CD1	2.38	0.54
1:A:144:VAL:CG2	1:A:206:ASN:HB3	2.25	0.54
1:B:71:ILE:O	1:B:158:TYR:OH	2.25	0.54
1:C:52:VAL:O	1:C:180:CYS:HA	2.07	0.54
1:E:139:SER:O	1:E:143:ARG:HG3	2.07	0.54
1:C:2:ASP:HB2	1:C:6:LEU:HD12	1.90	0.54
1:D:172:TRP:CE3	1:D:173:PRO:HG3	2.43	0.54
1:B:187:GLU:CB	1:C:70:PRO:O	2.49	0.54
1:D:144:VAL:CG2	1:D:206:ASN:HB3	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:MET:O	1:C:199:SER:HB2	2.07	0.54
1:D:142:PHE:O	1:D:145:ILE:HG22	2.08	0.54
1:E:46:ASP:OD1	1:F:48:GLN:HG2	2.08	0.54
1:F:95:VAL:HG13	1:F:96:ALA:N	2.23	0.54
1:B:190:VAL:HG12	1:B:191:PHE:HD2	1.73	0.54
1:D:53:CYS:HA	1:D:180:CYS:HA	1.90	0.54
1:A:189:THR:O	1:A:192:THR:N	2.40	0.54
1:B:142:PHE:O	1:B:145:ILE:HG22	2.08	0.54
1:B:52:VAL:O	1:B:180:CYS:HA	2.08	0.54
1:D:174:CYS:HB3	1:D:178:VAL:HG11	1.90	0.53
1:F:32:ARG:HH12	1:F:199:SER:CA	2.21	0.53
1:D:190:VAL:HG11	1:E:71:ILE:HG12	1.91	0.53
1:C:32:ARG:HH12	1:C:199:SER:CA	2.22	0.53
1:F:68:TYR:CD1	1:F:167:VAL:HG21	2.35	0.53
1:F:83:PHE:O	1:F:87:PRO:HD3	2.09	0.53
1:B:95:VAL:HG13	1:B:96:ALA:N	2.24	0.53
1:C:53:CYS:HA	1:C:180:CYS:HA	1.90	0.53
1:D:190:VAL:HG12	1:D:191:PHE:HD2	1.74	0.53
1:F:52:VAL:O	1:F:180:CYS:HA	2.07	0.53
1:B:35:ILE:HG23	1:B:195:MET:SD	2.49	0.53
1:D:136:TYR:CE2	1:D:140:ILE:HD11	2.44	0.53
1:D:50:ASP:O	1:E:62:ASN:ND2	2.32	0.53
1:D:42:GLU:HG2	1:E:75:ARG:NE	2.24	0.53
1:F:10:LEU:HB3	1:F:92:ALA:HB1	1.91	0.53
1:A:53:CYS:HA	1:A:180:CYS:HA	1.91	0.53
1:C:80:GLN:NE2	1:C:150:PHE:HB3	2.24	0.53
1:E:80:GLN:NE2	1:E:150:PHE:HB3	2.20	0.53
1:A:142:PHE:O	1:A:145:ILE:HG22	2.09	0.53
1:A:95:VAL:HG13	1:A:96:ALA:N	2.23	0.53
1:B:32:ARG:HH12	1:B:199:SER:CA	2.22	0.53
1:C:40:ALA:HA	1:C:74:ILE:HG12	1.90	0.53
1:C:83:PHE:O	1:C:87:PRO:HD3	2.09	0.53
1:D:182:VAL:HG12	1:D:183:SER:H	1.74	0.53
1:F:53:CYS:HA	1:F:180:CYS:HA	1.91	0.52
1:C:42:GLU:HG2	1:D:75:ARG:NE	2.23	0.52
1:D:46:ASP:OD1	1:E:48:GLN:HG2	2.10	0.52
1:F:190:VAL:HG12	1:F:191:PHE:HD2	1.75	0.52
1:A:195:MET:O	1:A:199:SER:HB2	2.09	0.52
1:C:193:VAL:HG12	1:C:194:PHE:N	2.24	0.52
1:E:142:PHE:O	1:E:145:ILE:HG22	2.09	0.52
1:D:95:VAL:HG13	1:D:96:ALA:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:THR:O	1:E:190:VAL:C	2.47	0.52
1:A:83:PHE:O	1:A:87:PRO:HD3	2.09	0.52
1:B:83:PHE:O	1:B:87:PRO:HD3	2.10	0.52
1:E:95:VAL:HG13	1:E:96:ALA:N	2.25	0.52
1:B:172:TRP:CE3	1:B:173:PRO:HG3	2.45	0.52
1:B:53:CYS:HA	1:B:180:CYS:HA	1.91	0.52
1:C:68:TYR:O	1:C:69:PHE:CD1	2.62	0.52
1:D:40:ALA:HA	1:D:74:ILE:HG12	1.92	0.52
1:F:182:VAL:HG12	1:F:183:SER:H	1.72	0.52
1:A:68:TYR:CD1	1:A:167:VAL:HG21	2.37	0.52
1:D:83:PHE:O	1:D:87:PRO:HD3	2.10	0.52
1:E:13:VAL:HG12	1:E:14:ASN:H	1.74	0.52
1:F:10:LEU:O	1:F:13:VAL:HG22	2.10	0.52
1:A:136:TYR:CE2	1:A:140:ILE:HD11	2.45	0.51
1:A:193:VAL:HG12	1:A:194:PHE:N	2.24	0.51
1:A:40:ALA:HA	1:A:74:ILE:HG12	1.92	0.51
1:E:52:VAL:O	1:E:180:CYS:HA	2.10	0.51
1:F:142:PHE:O	1:F:145:ILE:HG22	2.10	0.51
1:C:172:TRP:HB3	1:C:173:PRO:HD3	1.92	0.51
1:E:190:VAL:HG12	1:E:191:PHE:HD2	1.75	0.51
1:A:75:ARG:NE	1:F:42:GLU:HG2	2.25	0.51
1:B:189:THR:O	1:B:190:VAL:C	2.49	0.51
1:A:187:GLU:CB	1:B:70:PRO:O	2.50	0.51
1:D:195:MET:O	1:D:199:SER:HB2	2.11	0.51
1:E:32:ARG:NH1	1:E:198:VAL:HG12	2.21	0.51
1:D:71:ILE:O	1:D:158:TYR:OH	2.25	0.51
1:E:50:ASP:O	1:F:62:ASN:ND2	2.35	0.51
1:A:52:VAL:O	1:A:180:CYS:HA	2.11	0.51
1:F:71:ILE:O	1:F:158:TYR:OH	2.27	0.51
1:B:56:LEU:CD1	1:B:56:LEU:N	2.74	0.51
1:C:190:VAL:HG12	1:C:191:PHE:HD2	1.76	0.51
1:D:65:TYR:O	1:D:69:PHE:N	2.44	0.51
1:E:193:VAL:HG12	1:E:194:PHE:N	2.25	0.51
1:D:10:LEU:HB3	1:D:92:ALA:HB1	1.92	0.51
1:B:42:GLU:HG2	1:C:75:ARG:NE	2.25	0.51
1:D:32:ARG:HH12	1:D:199:SER:CA	2.23	0.51
1:A:70:PRO:O	1:F:187:GLU:CB	2.55	0.50
1:C:174:CYS:HB3	1:C:178:VAL:CG1	2.41	0.50
1:F:136:TYR:CE2	1:F:140:ILE:HD11	2.46	0.50
1:F:195:MET:O	1:F:199:SER:HB2	2.11	0.50
1:F:35:ILE:HG23	1:F:195:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:TRP:C	1:D:172:TRP:CD1	2.80	0.50
1:E:53:CYS:HA	1:E:180:CYS:HA	1.92	0.50
1:F:40:ALA:HA	1:F:74:ILE:HG12	1.94	0.50
1:A:190:VAL:HG12	1:A:191:PHE:HD2	1.75	0.50
1:E:137:THR:OG1	1:E:213:LEU:HD13	2.10	0.50
1:C:169:CYS:SG	1:C:171:ALA:HB2	2.52	0.50
1:E:2:ASP:HB2	1:E:6:LEU:HD11	1.92	0.50
1:C:13:VAL:HG12	1:C:14:ASN:H	1.77	0.50
1:C:95:VAL:HG13	1:C:96:ALA:N	2.26	0.50
1:F:137:THR:OG1	1:F:213:LEU:HD13	2.12	0.50
1:A:182:VAL:HG12	1:A:183:SER:H	1.76	0.50
1:A:68:TYR:O	1:A:69:PHE:CD1	2.65	0.50
1:B:190:VAL:HG21	1:C:71:ILE:HG12	1.94	0.50
1:E:144:VAL:CG2	1:E:206:ASN:HB3	2.25	0.50
1:F:189:THR:O	1:F:190:VAL:C	2.50	0.50
1:A:44:TRP:CH2	1:A:73:HIS:HB2	2.47	0.50
1:C:172:TRP:C	1:C:172:TRP:CD1	2.84	0.50
1:F:165:ARG:HA	1:F:185:PRO:HG2	1.94	0.50
1:B:68:TYR:O	1:B:69:PHE:CD1	2.65	0.50
1:E:32:ARG:HH12	1:E:199:SER:HA	1.77	0.50
1:A:169:CYS:SG	1:A:171:ALA:HB2	2.52	0.49
1:A:56:LEU:CD1	1:A:56:LEU:N	2.75	0.49
1:C:189:THR:O	1:C:190:VAL:C	2.49	0.49
1:C:137:THR:OG1	1:C:213:LEU:HD13	2.12	0.49
1:C:68:TYR:O	1:C:69:PHE:HD1	1.95	0.49
1:E:129:GLU:O	1:E:133:TRP:HB2	2.12	0.49
1:E:68:TYR:O	1:E:69:PHE:CD1	2.65	0.49
1:E:190:VAL:HG11	1:F:71:ILE:HG12	1.93	0.49
1:A:172:TRP:C	1:A:172:TRP:CD1	2.84	0.49
1:D:189:THR:O	1:D:190:VAL:C	2.51	0.49
1:E:182:VAL:HG12	1:E:183:SER:H	1.76	0.49
1:B:24:TRP:CD1	1:C:90:LEU:HD21	2.47	0.49
1:F:44:TRP:CH2	1:F:73:HIS:HB2	2.47	0.49
1:F:68:TYR:O	1:F:69:PHE:CD1	2.64	0.49
1:E:40:ALA:HA	1:E:74:ILE:HG12	1.93	0.49
1:F:2:ASP:HB2	1:F:6:LEU:HD12	1.93	0.49
1:B:174:CYS:HB3	1:B:178:VAL:CG1	2.43	0.49
1:D:16:HIS:HA	1:D:133:TRP:HZ2	1.78	0.49
1:B:43:VAL:HG22	1:B:44:TRP:CD1	2.47	0.49
1:D:137:THR:OG1	1:D:213:LEU:HD13	2.11	0.49
1:A:190:VAL:HG11	1:B:71:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:CYS:SG	1:B:171:ALA:HB2	2.53	0.49
1:C:129:GLU:O	1:C:133:TRP:HB2	2.12	0.49
1:B:190:VAL:HG11	1:C:71:ILE:HG12	1.94	0.49
1:D:129:GLU:O	1:D:133:TRP:HB2	2.13	0.49
1:F:169:CYS:SG	1:F:171:ALA:HB2	2.53	0.49
1:F:63:VAL:CG1	1:F:171:ALA:HB1	2.41	0.49
1:B:182:VAL:HG12	1:B:183:SER:H	1.77	0.48
1:B:137:THR:OG1	1:B:213:LEU:HD13	2.12	0.48
1:E:2:ASP:N	1:E:2:ASP:OD2	2.45	0.48
1:E:83:PHE:O	1:E:87:PRO:HD3	2.13	0.48
1:A:32:ARG:HH12	1:A:199:SER:HA	1.77	0.48
1:D:63:VAL:CG1	1:D:171:ALA:HB1	2.43	0.48
1:E:57:GLN:NE2	1:E:58:PRO:HD2	2.28	0.48
1:A:129:GLU:O	1:A:133:TRP:HB2	2.14	0.48
1:B:13:VAL:HG12	1:B:14:ASN:H	1.78	0.48
1:B:172:TRP:HB3	1:B:173:PRO:HD3	1.94	0.48
1:D:172:TRP:HB3	1:D:173:PRO:HD3	1.95	0.48
1:E:16:HIS:HA	1:E:133:TRP:HZ2	1.78	0.48
1:F:56:LEU:N	1:F:56:LEU:CD1	2.76	0.48
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.71	0.48
1:E:34:MET:HA	1:E:34:MET:HE2	1.95	0.48
1:A:137:THR:OG1	1:A:213:LEU:HD13	2.14	0.48
1:E:165:ARG:HA	1:E:185:PRO:HG2	1.95	0.48
1:F:16:HIS:HA	1:F:133:TRP:HZ2	1.78	0.48
1:F:13:VAL:HG12	1:F:14:ASN:H	1.79	0.48
1:B:136:TYR:CE2	1:B:140:ILE:HD11	2.48	0.48
1:B:32:ARG:HH12	1:B:199:SER:HA	1.79	0.48
1:B:129:GLU:O	1:B:133:TRP:HB2	2.13	0.48
1:C:65:TYR:O	1:C:69:PHE:N	2.45	0.48
1:B:63:VAL:CG1	1:B:171:ALA:HB1	2.44	0.47
1:B:65:TYR:O	1:B:69:PHE:N	2.47	0.47
1:C:144:VAL:CG2	1:C:206:ASN:HB3	2.24	0.47
1:C:32:ARG:NH2	1:C:147:GLU:OE2	2.47	0.47
1:D:56:LEU:CD1	1:D:56:LEU:N	2.77	0.47
1:E:63:VAL:CG1	1:E:171:ALA:HB1	2.44	0.47
1:A:65:TYR:O	1:A:69:PHE:N	2.48	0.47
1:B:16:HIS:HA	1:B:133:TRP:HZ2	1.80	0.47
1:B:47:GLU:O	1:B:51:PHE:HB2	2.14	0.47
1:E:181:PHE:CE2	1:F:173:PRO:HG3	2.49	0.47
1:F:32:ARG:HH12	1:F:199:SER:HA	1.78	0.47
1:C:136:TYR:CE2	1:C:140:ILE:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HA	1:A:207:VAL:HG12	1.97	0.47
1:C:183:SER:O	1:C:188:LYS:NZ	2.42	0.47
1:B:190:VAL:HG21	1:C:71:ILE:CG1	2.45	0.47
1:E:44:TRP:CH2	1:E:73:HIS:HB2	2.50	0.47
1:F:172:TRP:CE3	1:F:173:PRO:HG3	2.49	0.47
1:B:44:TRP:CH2	1:B:73:HIS:HB2	2.49	0.47
1:D:163:MET:HG3	1:D:185:PRO:HB3	1.96	0.47
1:F:193:VAL:HG12	1:F:194:PHE:N	2.28	0.47
1:F:163:MET:HG3	1:F:185:PRO:HB3	1.96	0.47
1:A:16:HIS:HA	1:A:133:TRP:HZ2	1.80	0.47
1:C:44:TRP:CH2	1:C:73:HIS:HB2	2.49	0.47
1:B:46:ASP:OD1	1:C:48:GLN:HG2	2.15	0.47
1:D:68:TYR:O	1:D:69:PHE:CD1	2.67	0.47
1:F:172:TRP:HB3	1:F:173:PRO:HD3	1.97	0.47
1:C:204:LEU:HA	1:C:207:VAL:HG12	1.96	0.47
1:D:165:ARG:HA	1:D:185:PRO:HG2	1.96	0.47
1:D:174:CYS:HB3	1:D:178:VAL:CG1	2.44	0.47
1:E:200:GLY:O	1:E:203:ILE:HB	2.15	0.47
1:A:43:VAL:HG22	1:A:44:TRP:CD1	2.50	0.47
1:C:165:ARG:HA	1:C:185:PRO:HG2	1.96	0.47
1:C:16:HIS:HA	1:C:133:TRP:HZ2	1.79	0.47
1:C:47:GLU:O	1:C:51:PHE:HB2	2.14	0.47
1:E:136:TYR:CE2	1:E:140:ILE:HD11	2.49	0.47
1:E:174:CYS:HB3	1:E:178:VAL:CG1	2.45	0.47
1:E:65:TYR:O	1:E:69:PHE:N	2.48	0.47
1:A:174:CYS:HB3	1:A:178:VAL:CG1	2.45	0.47
1:D:204:LEU:HA	1:D:207:VAL:HG12	1.96	0.47
1:D:74:ILE:HA	1:D:74:ILE:HD12	1.53	0.47
1:A:71:ILE:HG12	1:F:190:VAL:HG11	1.97	0.46
1:B:165:ARG:HA	1:B:185:PRO:HG2	1.97	0.46
1:C:172:TRP:CG	1:C:173:PRO:N	2.81	0.46
1:F:43:VAL:HG22	1:F:44:TRP:CD1	2.49	0.46
1:B:165:ARG:NH2	1:C:67:HIS:HA	2.30	0.46
1:A:189:THR:O	1:A:190:VAL:C	2.53	0.46
1:C:2:ASP:OD2	1:C:2:ASP:N	2.48	0.46
1:C:57:GLN:NE2	1:C:58:PRO:HD2	2.31	0.46
1:D:200:GLY:O	1:D:203:ILE:HB	2.15	0.46
1:D:44:TRP:CH2	1:D:73:HIS:HB2	2.51	0.46
1:F:129:GLU:O	1:F:133:TRP:HB2	2.15	0.46
1:F:174:CYS:HB3	1:F:178:VAL:CG1	2.45	0.46
1:C:71:ILE:O	1:C:158:TYR:OH	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:LEU:HA	1:D:76:LEU:HD23	1.74	0.46
1:E:172:TRP:C	1:E:172:TRP:CD1	2.85	0.46
1:E:165:ARG:HH22	1:F:67:HIS:CG	2.32	0.46
1:A:200:GLY:O	1:A:203:ILE:HB	2.16	0.46
1:B:172:TRP:CG	1:B:173:PRO:N	2.83	0.46
1:E:172:TRP:CE3	1:E:173:PRO:HG3	2.50	0.46
1:A:20:ILE:O	1:A:20:ILE:HG22	2.16	0.46
1:B:204:LEU:HA	1:B:207:VAL:HG12	1.98	0.46
1:B:2:ASP:OD2	1:B:2:ASP:N	2.48	0.46
1:A:46:ASP:OD1	1:B:48:GLN:HG2	2.15	0.46
1:C:56:LEU:N	1:C:56:LEU:CD1	2.77	0.46
1:E:172:TRP:CG	1:E:173:PRO:N	2.84	0.46
1:C:32:ARG:HA	1:C:35:ILE:HG22	1.98	0.46
1:B:183:SER:HB2	1:C:48:GLN:NE2	2.31	0.46
1:D:32:ARG:HH12	1:D:199:SER:HA	1.79	0.46
1:E:181:PHE:HE2	1:F:173:PRO:HG3	1.81	0.46
1:B:183:SER:O	1:B:188:LYS:NZ	2.44	0.46
1:E:71:ILE:O	1:E:158:TYR:OH	2.26	0.46
1:A:74:ILE:HA	1:A:74:ILE:HD12	1.55	0.46
1:B:68:TYR:CD1	1:B:167:VAL:HG21	2.40	0.46
1:C:163:MET:HG3	1:C:185:PRO:HB3	1.97	0.46
1:C:63:VAL:CG1	1:C:171:ALA:HB1	2.46	0.45
1:E:74:ILE:HD12	1:E:74:ILE:HA	1.55	0.45
1:A:48:GLN:HG2	1:F:46:ASP:OD1	2.17	0.45
1:B:200:GLY:O	1:B:203:ILE:HB	2.16	0.45
1:C:32:ARG:HH12	1:C:199:SER:HA	1.80	0.45
1:E:183:SER:O	1:E:188:LYS:NZ	2.45	0.45
1:F:32:ARG:HA	1:F:35:ILE:HG22	1.98	0.45
1:B:163:MET:HG3	1:B:185:PRO:HB3	1.99	0.45
1:D:172:TRP:CG	1:D:173:PRO:N	2.80	0.45
1:E:163:MET:HG3	1:E:185:PRO:HB3	1.99	0.45
1:A:47:GLU:O	1:A:51:PHE:HB2	2.16	0.45
1:C:32:ARG:NH1	1:C:198:VAL:HG12	2.24	0.45
1:D:57:GLN:NE2	1:D:58:PRO:HD2	2.31	0.45
1:E:204:LEU:HA	1:E:207:VAL:HG12	1.98	0.45
1:F:2:ASP:CB	1:F:6:LEU:HD11	2.46	0.45
1:E:56:LEU:CD1	1:E:56:LEU:N	2.80	0.45
1:F:16:HIS:HD2	1:F:22:LYS:HE2	1.82	0.45
1:F:65:TYR:O	1:F:69:PHE:N	2.50	0.45
1:C:68:TYR:CD1	1:C:167:VAL:HG21	2.38	0.45
1:C:66:ASP:O	1:C:68:TYR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ASP:CB	1:C:6:LEU:HD11	2.47	0.45
1:D:47:GLU:O	1:D:51:PHE:HB2	2.16	0.45
1:A:32:ARG:HA	1:A:35:ILE:HG22	1.97	0.45
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.71	0.45
1:A:16:HIS:HD2	1:A:22:LYS:HE2	1.82	0.45
1:C:50:ASP:O	1:D:62:ASN:ND2	2.36	0.45
1:E:47:GLU:O	1:E:51:PHE:HB2	2.17	0.45
1:F:57:GLN:NE2	1:F:58:PRO:HD2	2.32	0.45
1:F:68:TYR:O	1:F:69:PHE:HD1	2.00	0.45
1:A:68:TYR:O	1:A:69:PHE:HD1	2.00	0.44
1:B:172:TRP:CD1	1:B:172:TRP:C	2.85	0.44
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.74	0.44
1:C:80:GLN:HA	1:C:150:PHE:CE2	2.52	0.44
1:F:172:TRP:CG	1:F:173:PRO:N	2.83	0.44
1:F:2:ASP:OD2	1:F:2:ASP:N	2.49	0.44
1:E:31:PHE:CD2	1:E:31:PHE:C	2.90	0.44
1:A:63:VAL:CG1	1:A:171:ALA:HB1	2.47	0.44
1:A:172:TRP:HB3	1:A:173:PRO:HD3	1.98	0.44
1:B:32:ARG:NH2	1:B:147:GLU:OE2	2.50	0.44
1:B:32:ARG:NH1	1:B:198:VAL:HG12	2.24	0.44
1:C:43:VAL:HG22	1:C:44:TRP:CD1	2.52	0.44
1:D:136:TYR:CE2	1:D:140:ILE:CD1	3.00	0.44
1:A:136:TYR:CE2	1:A:140:ILE:CD1	3.01	0.44
1:B:32:ARG:HA	1:B:35:ILE:HG22	2.00	0.44
1:D:32:ARG:NH2	1:D:147:GLU:OE2	2.50	0.44
1:F:47:GLU:O	1:F:51:PHE:HB2	2.17	0.44
1:C:89:LEU:O	1:C:93:MET:HB2	2.18	0.44
1:E:2:ASP:HB2	1:E:6:LEU:HD12	1.99	0.44
1:E:32:ARG:NH2	1:E:147:GLU:OE2	2.51	0.44
1:A:32:ARG:HH12	1:A:199:SER:N	2.15	0.44
1:A:71:ILE:HG12	1:F:190:VAL:HG21	2.00	0.44
1:D:192:THR:O	1:D:196:ILE:HB	2.17	0.44
1:E:68:TYR:C	1:E:69:PHE:CD1	2.91	0.44
1:F:200:GLY:O	1:F:203:ILE:HB	2.17	0.44
1:B:10:LEU:O	1:B:13:VAL:HG22	2.17	0.44
1:B:16:HIS:HD2	1:B:22:LYS:HE2	1.83	0.44
1:B:68:TYR:O	1:B:69:PHE:HD1	2.01	0.44
1:D:185:PRO:N	1:E:66:ASP:OD1	2.50	0.44
1:E:185:PRO:N	1:F:66:ASP:OD1	2.50	0.44
1:A:32:ARG:NH1	1:A:199:SER:HA	2.33	0.44
1:D:80:GLN:HA	1:D:150:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:SER:HB2	1:F:48:GLN:NE2	2.33	0.44
1:E:10:LEU:HB3	1:E:92:ALA:HB1	1.99	0.43
1:E:10:LEU:O	1:E:13:VAL:HG22	2.18	0.43
1:A:190:VAL:HG21	1:B:71:ILE:HG12	2.00	0.43
1:A:31:PHE:C	1:A:31:PHE:CD2	2.92	0.43
1:A:166:LEU:HD13	1:B:172:TRP:HZ3	1.83	0.43
1:C:46:ASP:O	1:C:47:GLU:C	2.57	0.43
1:E:169:CYS:SG	1:E:171:ALA:HB2	2.58	0.43
1:F:20:ILE:O	1:F:20:ILE:HG22	2.18	0.43
1:F:46:ASP:O	1:F:47:GLU:C	2.55	0.43
1:C:10:LEU:O	1:C:13:VAL:HG22	2.18	0.43
1:E:40:ALA:HB2	1:E:74:ILE:HG13	2.00	0.43
1:F:204:LEU:HA	1:F:207:VAL:HG12	2.00	0.43
1:B:40:ALA:HB2	1:B:74:ILE:HG13	2.00	0.43
1:D:31:PHE:C	1:D:31:PHE:CD2	2.91	0.43
1:E:68:TYR:O	1:E:69:PHE:HD1	2.01	0.43
1:D:20:ILE:O	1:D:20:ILE:HG22	2.19	0.43
1:F:192:THR:O	1:F:196:ILE:HB	2.19	0.43
1:B:10:LEU:HB3	1:B:92:ALA:HB1	2.00	0.43
1:D:37:VAL:O	1:D:37:VAL:HG13	2.18	0.43
1:D:40:ALA:HB2	1:D:74:ILE:HG13	2.00	0.43
1:E:20:ILE:O	1:E:20:ILE:HG22	2.18	0.43
1:D:190:VAL:HG21	1:E:71:ILE:CG1	2.49	0.43
1:A:59:GLY:O	1:A:63:VAL:HG23	2.18	0.43
1:B:192:THR:O	1:B:196:ILE:HB	2.19	0.43
1:C:16:HIS:HD2	1:C:22:LYS:HE2	1.83	0.43
1:F:136:TYR:CE2	1:F:140:ILE:CD1	3.02	0.43
1:F:183:SER:O	1:F:188:LYS:NZ	2.42	0.43
1:F:66:ASP:O	1:F:68:TYR:N	2.51	0.43
1:B:143:ARG:HD3	1:B:206:ASN:OD1	2.19	0.43
1:B:95:VAL:CG1	1:B:96:ALA:N	2.82	0.43
1:D:68:TYR:C	1:D:69:PHE:CD1	2.92	0.43
1:E:192:THR:O	1:E:196:ILE:HB	2.19	0.43
1:E:16:HIS:HD2	1:E:22:LYS:HE2	1.84	0.43
1:F:40:ALA:HB2	1:F:74:ILE:HG13	2.01	0.43
1:E:165:ARG:NH1	1:F:67:HIS:HB2	2.34	0.43
1:F:74:ILE:HD12	1:F:74:ILE:HA	1.54	0.43
1:A:162:SER:HB2	1:A:189:THR:OG1	2.19	0.42
1:A:163:MET:HG3	1:A:185:PRO:HB3	2.01	0.42
1:A:80:GLN:HA	1:A:150:PHE:CE2	2.54	0.42
1:C:171:ALA:O	1:C:172:TRP:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:ILE:HG22	1:C:20:ILE:O	2.18	0.42
1:D:43:VAL:HG22	1:D:44:TRP:CD1	2.53	0.42
1:F:73:HIS:N	1:F:73:HIS:CD2	2.85	0.42
1:B:162:SER:HB2	1:B:189:THR:OG1	2.18	0.42
1:A:190:VAL:HG21	1:B:71:ILE:CG1	2.49	0.42
1:E:32:ARG:HH12	1:E:199:SER:N	2.16	0.42
1:A:32:ARG:NH2	1:A:147:GLU:OE2	2.51	0.42
1:B:2:ASP:CB	1:B:6:LEU:HD11	2.49	0.42
1:D:32:ARG:HA	1:D:35:ILE:HG22	2.01	0.42
1:B:31:PHE:CD2	1:B:31:PHE:C	2.92	0.42
1:B:32:ARG:HH12	1:B:199:SER:N	2.17	0.42
1:D:32:ARG:NH1	1:D:198:VAL:HG12	2.27	0.42
1:F:193:VAL:HG12	1:F:194:PHE:HD1	1.83	0.42
1:A:58:PRO:O	1:A:59:GLY:C	2.58	0.42
1:A:95:VAL:CG1	1:A:96:ALA:N	2.82	0.42
1:B:20:ILE:HG22	1:B:20:ILE:O	2.19	0.42
1:D:190:VAL:HG21	1:E:71:ILE:HG12	2.00	0.42
1:C:32:ARG:HH12	1:C:199:SER:N	2.18	0.42
1:D:16:HIS:HD2	1:D:22:LYS:HE2	1.83	0.42
1:F:32:ARG:NH1	1:F:199:SER:HA	2.35	0.42
1:A:68:TYR:C	1:A:69:PHE:CD1	2.91	0.42
1:C:31:PHE:CD2	1:C:31:PHE:C	2.92	0.42
1:C:37:VAL:HG13	1:C:37:VAL:O	2.19	0.42
1:E:32:ARG:HA	1:E:35:ILE:HG22	2.00	0.42
1:F:95:VAL:CG1	1:F:96:ALA:N	2.81	0.42
1:A:165:ARG:HA	1:A:185:PRO:HG2	2.01	0.42
1:B:184:ARG:N	1:B:185:PRO:HD3	2.34	0.42
1:B:193:VAL:HG12	1:B:194:PHE:HD1	1.84	0.42
1:C:66:ASP:C	1:C:68:TYR:N	2.72	0.42
1:D:89:LEU:O	1:D:93:MET:HB2	2.19	0.42
1:E:73:HIS:CD2	1:E:73:HIS:N	2.87	0.42
1:F:32:ARG:HH12	1:F:199:SER:N	2.18	0.42
1:A:71:ILE:CG1	1:F:190:VAL:HG21	2.50	0.42
1:B:43:VAL:HG12	1:C:75:ARG:NH1	2.15	0.42
1:B:58:PRO:O	1:B:59:GLY:C	2.57	0.42
1:B:89:LEU:O	1:B:93:MET:HB2	2.19	0.42
1:D:92:ALA:O	1:D:95:VAL:HG12	2.20	0.42
1:F:80:GLN:HA	1:F:150:PHE:CE2	2.55	0.42
1:A:192:THR:O	1:A:196:ILE:HB	2.20	0.42
1:B:68:TYR:C	1:B:69:PHE:CD1	2.91	0.42
1:C:74:ILE:HD12	1:C:74:ILE:HA	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:HIS:CG	1:F:165:ARG:HH22	2.36	0.42
1:A:80:GLN:HA	1:A:150:PHE:HD2	1.83	0.41
1:A:89:LEU:O	1:A:93:MET:HB2	2.19	0.41
1:B:2:ASP:HB2	1:B:6:LEU:HD12	2.00	0.41
1:C:190:VAL:HG11	1:D:71:ILE:HG12	2.01	0.41
1:D:184:ARG:N	1:D:185:PRO:HD3	2.35	0.41
1:D:193:VAL:HG12	1:D:194:PHE:HD1	1.83	0.41
1:D:165:ARG:HH22	1:E:67:HIS:CG	2.37	0.41
1:D:95:VAL:CG1	1:D:96:ALA:N	2.82	0.41
1:E:171:ALA:O	1:E:172:TRP:C	2.59	0.41
1:F:89:LEU:O	1:F:93:MET:HB2	2.19	0.41
1:B:32:ARG:NH1	1:B:199:SER:HA	2.35	0.41
1:D:169:CYS:SG	1:D:171:ALA:HB2	2.60	0.41
1:D:46:ASP:O	1:D:47:GLU:C	2.57	0.41
1:E:150:PHE:O	1:E:151:MET:C	2.58	0.41
1:F:172:TRP:C	1:F:172:TRP:CD1	2.88	0.41
1:F:63:VAL:HG12	1:F:171:ALA:HB1	2.02	0.41
1:A:172:TRP:CG	1:A:173:PRO:N	2.83	0.41
1:C:181:PHE:CE2	1:D:173:PRO:HG3	2.56	0.41
1:C:32:ARG:NH1	1:C:199:SER:HA	2.36	0.41
1:B:165:ARG:NH1	1:C:67:HIS:HB2	2.35	0.41
1:D:162:SER:HB2	1:D:189:THR:OG1	2.20	0.41
1:D:170:ASN:O	1:D:171:ALA:C	2.59	0.41
1:E:32:ARG:NH1	1:E:199:SER:HA	2.35	0.41
1:E:89:LEU:O	1:E:93:MET:HB2	2.19	0.41
1:A:183:SER:HB2	1:B:48:GLN:NE2	2.35	0.41
1:A:212:TYR:HA	1:A:215:ILE:HD12	2.03	0.41
1:A:37:VAL:HG13	1:A:37:VAL:O	2.19	0.41
1:A:46:ASP:O	1:A:47:GLU:C	2.57	0.41
1:C:200:GLY:O	1:C:203:ILE:HB	2.19	0.41
1:E:95:VAL:CG1	1:E:96:ALA:N	2.83	0.41
1:A:48:GLN:NE2	1:F:183:SER:HB2	2.36	0.41
1:C:95:VAL:CG1	1:C:96:ALA:N	2.84	0.41
1:D:181:PHE:HE2	1:E:173:PRO:HG3	1.86	0.41
1:E:46:ASP:O	1:E:47:GLU:C	2.59	0.41
1:F:143:ARG:H	1:F:143:ARG:HG3	1.74	0.41
1:B:57:GLN:HG3	1:B:173:PRO:O	2.19	0.41
1:B:80:GLN:HA	1:B:150:PHE:CE2	2.55	0.41
1:C:181:PHE:HE2	1:D:173:PRO:HG3	1.84	0.41
1:A:185:PRO:N	1:B:66:ASP:OD1	2.54	0.41
1:C:192:THR:O	1:C:196:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ALA:O	1:C:95:VAL:HG12	2.21	0.41
1:E:80:GLN:HA	1:E:150:PHE:CE2	2.55	0.41
1:D:24:TRP:CD1	1:E:90:LEU:HD21	2.55	0.41
1:E:43:VAL:HG22	1:E:44:TRP:CD1	2.55	0.41
1:B:28:LEU:HA	1:B:31:PHE:HB3	2.03	0.41
1:D:183:SER:HB2	1:E:48:GLN:NE2	2.36	0.41
1:F:143:ARG:HD3	1:F:206:ASN:OD1	2.22	0.41
1:F:31:PHE:CD2	1:F:31:PHE:C	2.93	0.41
1:E:190:VAL:HG21	1:F:71:ILE:CG1	2.51	0.41
1:A:171:ALA:O	1:A:172:TRP:C	2.59	0.40
1:C:143:ARG:HD3	1:C:206:ASN:OD1	2.21	0.40
1:F:66:ASP:C	1:F:68:TYR:N	2.74	0.40
1:C:166:LEU:HD13	1:D:172:TRP:HZ3	1.86	0.40
1:D:54:ASN:ND2	1:E:58:PRO:HG2	2.36	0.40
1:D:73:HIS:CD2	1:D:73:HIS:N	2.88	0.40
1:E:142:PHE:HA	1:E:142:PHE:HD1	1.79	0.40
1:E:84:VAL:CG2	1:E:147:GLU:HG2	2.39	0.40
1:D:181:PHE:CE2	1:E:173:PRO:HG3	2.56	0.40
1:E:28:LEU:HA	1:E:31:PHE:HB3	2.03	0.40
1:A:28:LEU:HA	1:A:31:PHE:HB3	2.04	0.40
1:C:184:ARG:N	1:C:185:PRO:HD3	2.36	0.40
1:C:28:LEU:HA	1:C:31:PHE:HB3	2.04	0.40
1:D:63:VAL:HG12	1:D:171:ALA:HB1	2.03	0.40
1:D:43:VAL:HG12	1:E:75:ARG:NH1	2.17	0.40
1:D:66:ASP:C	1:D:68:TYR:N	2.74	0.40
1:A:2:ASP:N	1:A:2:ASP:OD2	2.53	0.40
1:A:10:LEU:HB3	1:A:92:ALA:HB1	2.02	0.40
1:E:162:SER:HB2	1:E:189:THR:OG1	2.20	0.40
1:B:74:ILE:HA	1:B:74:ILE:HD12	1.58	0.40
1:C:68:TYR:C	1:C:69:PHE:CD1	2.92	0.40
1:F:32:ARG:NH1	1:F:198:VAL:HG12	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	197/226 (87%)	158 (80%)	30 (15%)	9 (5%)	2	21
1	B	197/226 (87%)	157 (80%)	31 (16%)	9 (5%)	2	21
1	C	197/226 (87%)	158 (80%)	31 (16%)	8 (4%)	3	23
1	D	197/226 (87%)	156 (79%)	33 (17%)	8 (4%)	3	23
1	E	197/226 (87%)	154 (78%)	35 (18%)	8 (4%)	3	23
1	F	197/226 (87%)	156 (79%)	32 (16%)	9 (5%)	2	21
All	All	1182/1356 (87%)	939 (79%)	192 (16%)	51 (4%)	2	22

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	49	ALA
1	B	20	ILE
1	B	49	ALA
1	C	20	ILE
1	C	49	ALA
1	D	20	ILE
1	D	49	ALA
1	E	20	ILE
1	E	49	ALA
1	F	20	ILE
1	F	49	ALA
1	A	67	HIS
1	A	154	PHE
1	B	67	HIS
1	B	154	PHE
1	B	190	VAL
1	C	67	HIS
1	C	154	PHE
1	C	190	VAL
1	D	154	PHE
1	E	154	PHE
1	F	67	HIS
1	F	154	PHE
1	A	40	ALA
1	B	40	ALA
1	C	40	ALA

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Mol	Chain	Res	Type
1	D	40	ALA
1	D	67	HIS
1	D	190	VAL
1	E	40	ALA
1	E	67	HIS
1	E	190	VAL
1	F	40	ALA
1	F	190	VAL
1	A	58	PRO
1	B	58	PRO
1	A	151	MET
1	A	190	VAL
1	C	58	PRO
1	D	58	PRO
1	F	58	PRO
1	B	172	TRP
1	C	172	TRP
1	A	172	TRP
1	E	172	TRP
1	F	172	TRP
1	B	193	VAL
1	D	172	TRP
1	E	58	PRO
1	F	70	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	177/204 (87%)	146 (82%)	31 (18%)	2 10
1	B	177/204 (87%)	148 (84%)	29 (16%)	2 13
1	C	177/204 (87%)	146 (82%)	31 (18%)	2 10
1	D	177/204 (87%)	147 (83%)	30 (17%)	2 12
1	E	177/204 (87%)	148 (84%)	29 (16%)	2 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	177/204 (87%)	147 (83%)	30 (17%)	2 12
All	All	1062/1224 (87%)	882 (83%)	180 (17%)	2 12

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	24	TRP
1	A	33	ILE
1	A	34	MET
1	A	37	VAL
1	A	43	VAL
1	A	55	THR
1	A	56	LEU
1	A	58	PRO
1	A	61	LYS
1	A	74	ILE
1	A	81	LEU
1	A	127	ARG
1	A	132	LEU
1	A	133	TRP
1	A	137	THR
1	A	138	SER
1	A	142	PHE
1	A	144	VAL
1	A	154	PHE
1	A	155	TYR
1	A	157	MET
1	A	164	GLN
1	A	166	LEU
1	A	176	ASN
1	A	182	VAL
1	A	184	ARG
1	A	207	VAL
1	A	208	THR
1	A	209	GLU
1	A	217	TYR
1	B	2	ASP
1	B	24	TRP
1	B	33	ILE
1	B	37	VAL
1	B	43	VAL

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Mol	Chain	Res	Type
1	B	55	THR
1	B	56	LEU
1	B	58	PRO
1	B	61	LYS
1	B	74	ILE
1	B	81	LEU
1	B	127	ARG
1	B	132	LEU
1	B	133	TRP
1	B	137	THR
1	B	138	SER
1	B	142	PHE
1	B	144	VAL
1	B	154	PHE
1	B	155	TYR
1	B	157	MET
1	B	164	GLN
1	B	166	LEU
1	B	176	ASN
1	B	184	ARG
1	B	207	VAL
1	B	208	THR
1	B	209	GLU
1	B	217	TYR
1	C	2	ASP
1	C	13	VAL
1	C	24	TRP
1	C	33	ILE
1	C	34	MET
1	C	37	VAL
1	C	43	VAL
1	C	55	THR
1	C	56	LEU
1	C	58	PRO
1	C	61	LYS
1	C	74	ILE
1	C	81	LEU
1	C	127	ARG
1	C	132	LEU
1	C	133	TRP
1	C	137	THR
1	C	138	SER

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Mol	Chain	Res	Type
1	C	142	PHE
1	C	144	VAL
1	C	154	PHE
1	C	155	TYR
1	C	157	MET
1	C	164	GLN
1	C	166	LEU
1	C	176	ASN
1	C	184	ARG
1	C	207	VAL
1	C	208	THR
1	C	209	GLU
1	C	217	TYR
1	D	2	ASP
1	D	24	TRP
1	D	33	ILE
1	D	34	MET
1	D	37	VAL
1	D	43	VAL
1	D	55	THR
1	D	56	LEU
1	D	58	PRO
1	D	61	LYS
1	D	74	ILE
1	D	81	LEU
1	D	127	ARG
1	D	132	LEU
1	D	133	TRP
1	D	137	THR
1	D	138	SER
1	D	142	PHE
1	D	144	VAL
1	D	154	PHE
1	D	155	TYR
1	D	157	MET
1	D	164	GLN
1	D	166	LEU
1	D	176	ASN
1	D	184	ARG
1	D	207	VAL
1	D	208	THR
1	D	209	GLU

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Mol	Chain	Res	Type
1	D	217	TYR
1	E	2	ASP
1	E	24	TRP
1	E	33	ILE
1	E	37	VAL
1	E	43	VAL
1	E	55	THR
1	E	56	LEU
1	E	58	PRO
1	E	61	LYS
1	E	74	ILE
1	E	81	LEU
1	E	127	ARG
1	E	132	LEU
1	E	133	TRP
1	E	137	THR
1	E	138	SER
1	E	142	PHE
1	E	144	VAL
1	E	154	PHE
1	E	155	TYR
1	E	157	MET
1	E	164	GLN
1	E	166	LEU
1	E	176	ASN
1	E	184	ARG
1	E	207	VAL
1	E	208	THR
1	E	209	GLU
1	E	217	TYR
1	F	2	ASP
1	F	13	VAL
1	F	24	TRP
1	F	33	ILE
1	F	37	VAL
1	F	43	VAL
1	F	55	THR
1	F	56	LEU
1	F	58	PRO
1	F	61	LYS
1	F	74	ILE
1	F	81	LEU

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Mol	Chain	Res	Type
1	F	127	ARG
1	F	132	LEU
1	F	133	TRP
1	F	137	THR
1	F	138	SER
1	F	142	PHE
1	F	144	VAL
1	F	154	PHE
1	F	155	TYR
1	F	157	MET
1	F	164	GLN
1	F	166	LEU
1	F	176	ASN
1	F	184	ARG
1	F	207	VAL
1	F	208	THR
1	F	209	GLU
1	F	217	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	80	GLN
1	A	164	GLN
1	A	170	ASN
1	B	16	HIS
1	B	57	GLN
1	B	80	GLN
1	B	164	GLN
1	B	170	ASN
1	C	16	HIS
1	C	48	GLN
1	C	57	GLN
1	C	80	GLN
1	C	164	GLN
1	C	170	ASN
1	D	57	GLN
1	D	80	GLN
1	D	164	GLN
1	D	170	ASN
1	E	16	HIS

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Mol	Chain	Res	Type
1	E	57	GLN
1	E	80	GLN
1	E	164	GLN
1	E	170	ASN
1	F	16	HIS
1	F	57	GLN
1	F	80	GLN
1	F	164	GLN
1	F	170	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	201/226 (88%)	0.34	17 (8%) 10 11	78, 126, 205, 221	0
1	B	201/226 (88%)	0.84	37 (18%) 1 1	78, 126, 205, 221	0
1	C	201/226 (88%)	0.88	36 (17%) 1 1	78, 126, 203, 221	0
1	D	201/226 (88%)	0.65	29 (14%) 2 3	78, 126, 205, 221	0
1	E	201/226 (88%)	0.94	31 (15%) 2 2	78, 126, 205, 221	0
1	F	201/226 (88%)	0.59	24 (11%) 4 5	78, 126, 203, 221	0
All	All	1206/1356 (88%)	0.71	174 (14%) 2 3	78, 127, 205, 221	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	109	GLY	16.7
1	B	4	GLY	14.7
1	C	100	HIS	11.9
1	E	4	GLY	11.7
1	E	108	LYS	11.7
1	E	7	GLN	11.1
1	B	7	GLN	10.6
1	C	97	TYR	10.3
1	C	103	LYS	9.9
1	E	107	ILE	9.6
1	E	6	LEU	9.2
1	B	5	THR	8.3
1	C	4	GLY	8.3
1	C	102	LYS	8.0
1	F	159	ASP	8.0
1	C	109	GLY	8.0
1	C	3	TRP	7.9
1	C	101	GLU	7.9
1	D	4	GLY	7.9

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Mol	Chain	Res	Type	RSRZ
1	B	3	TRP	7.4
1	D	3	TRP	7.3
1	F	105	LYS	7.2
1	F	106	PHE	7.1
1	B	215	ILE	7.1
1	E	3	TRP	6.8
1	B	109	GLY	6.7
1	B	8	THR	6.7
1	C	99	ARG	6.6
1	F	4	GLY	6.5
1	E	17	SER	6.5
1	B	106	PHE	6.4
1	E	10	LEU	6.3
1	C	96	ALA	6.3
1	E	5	THR	6.2
1	E	8	THR	6.0
1	F	7	GLN	5.6
1	B	108	LYS	5.4
1	B	213	LEU	5.4
1	E	104	ARG	5.4
1	C	107	ILE	5.3
1	F	8	THR	5.2
1	E	105	LYS	5.2
1	F	97	TYR	5.2
1	B	6	LEU	5.1
1	C	19	SER	5.1
1	E	106	PHE	5.1
1	B	101	GLU	5.1
1	D	103	LYS	4.9
1	D	102	LYS	4.8
1	A	3	TRP	4.7
1	F	3	TRP	4.7
1	D	5	THR	4.6
1	A	109	GLY	4.5
1	A	4	GLY	4.3
1	C	8	THR	4.3
1	D	14	ASN	4.2
1	C	5	THR	4.2
1	C	33	ILE	4.2
1	B	33	ILE	4.1
1	C	7	GLN	4.0
1	C	20	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	107	ILE	4.0
1	A	157	MET	4.0
1	B	105	LYS	3.9
1	A	97	TYR	3.9
1	B	214	LEU	3.9
1	B	102	LYS	3.8
1	A	42	GLU	3.8
1	B	104	ARG	3.8
1	D	40	ALA	3.8
1	B	17	SER	3.8
1	E	2	ASP	3.7
1	C	106	PHE	3.7
1	E	34	MET	3.7
1	C	9	ILE	3.7
1	F	6	LEU	3.6
1	A	106	PHE	3.6
1	B	41	LYS	3.6
1	D	41	LYS	3.6
1	C	93	MET	3.5
1	D	42	GLU	3.5
1	F	101	GLU	3.4
1	F	107	ILE	3.4
1	D	44	TRP	3.4
1	C	98	ARG	3.3
1	D	97	TYR	3.3
1	B	11	GLY	3.3
1	D	109	GLY	3.3
1	E	101	GLU	3.3
1	E	97	TYR	3.3
1	F	102	LYS	3.2
1	A	17	SER	3.2
1	E	103	LYS	3.1
1	C	10	LEU	3.1
1	F	9	ILE	3.1
1	B	34	MET	3.1
1	C	6	LEU	3.0
1	F	215	ILE	3.0
1	C	34	MET	3.0
1	C	159	ASP	3.0
1	B	30	ILE	3.0
1	A	10	LEU	3.0
1	A	7	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	12	GLY	3.0
1	F	109	GLY	2.9
1	E	102	LYS	2.9
1	D	15	LYS	2.9
1	B	158	TYR	2.9
1	C	125	LYS	2.8
1	F	177	THR	2.8
1	C	105	LYS	2.8
1	A	217	TYR	2.8
1	B	18	THR	2.8
1	E	18	THR	2.7
1	D	74	ILE	2.6
1	D	154	PHE	2.6
1	E	41	LYS	2.6
1	A	168	LYS	2.6
1	B	107	ILE	2.6
1	D	35	ILE	2.6
1	B	42	GLU	2.6
1	B	157	MET	2.6
1	C	128	ILE	2.6
1	B	177	THR	2.6
1	E	42	GLU	2.6
1	C	35	ILE	2.5
1	A	14	ASN	2.5
1	E	9	ILE	2.5
1	A	41	LYS	2.5
1	C	2	ASP	2.5
1	F	103	LYS	2.5
1	C	176	ASN	2.5
1	B	36	LEU	2.5
1	B	175	PRO	2.5
1	F	168	LYS	2.5
1	A	35	ILE	2.5
1	A	8	THR	2.4
1	C	168	LYS	2.4
1	F	10	LEU	2.4
1	D	7	GLN	2.4
1	D	96	ALA	2.4
1	B	103	LYS	2.4
1	E	31	PHE	2.4
1	E	159	ASP	2.4
1	D	34	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	9	ILE	2.4
1	B	217	TYR	2.4
1	D	33	ILE	2.3
1	F	104	ARG	2.3
1	F	11	GLY	2.3
1	F	195	MET	2.2
1	E	14	ASN	2.2
1	B	40	ALA	2.2
1	D	81	LEU	2.2
1	E	33	ILE	2.2
1	C	18	THR	2.2
1	D	16	HIS	2.2
1	E	168	LYS	2.2
1	B	176	ASN	2.2
1	D	71	ILE	2.2
1	B	10	LEU	2.1
1	D	47	GLU	2.1
1	D	2	ASP	2.1
1	F	161	PHE	2.1
1	E	30	ILE	2.1
1	D	75	ARG	2.1
1	E	11	GLY	2.1
1	C	177	THR	2.0
1	D	36	LEU	2.0
1	F	95	VAL	2.0
1	C	215	ILE	2.0
1	A	27	VAL	2.0
1	C	54	ASN	2.0
1	B	97	TYR	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.