



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 04:15 PM GMT

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 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/ValidationPDFNotes.html>

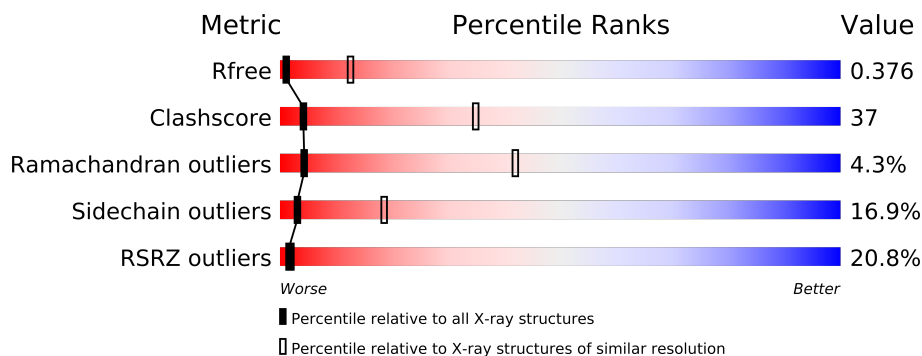
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	226	
1	B	226	
1	C	226	
1	D	226	
1	E	226	
1	F	226	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9834 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

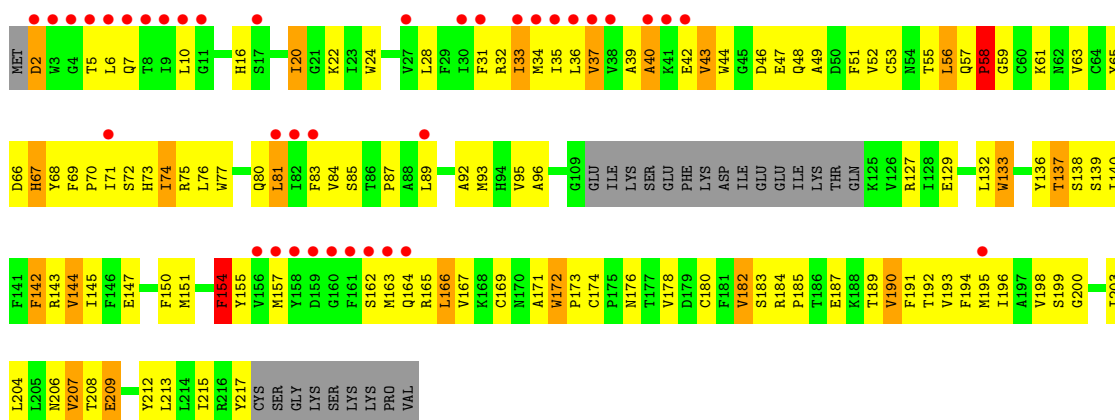
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1639	1088	269	268	14			
1	B	201	Total	C	N	O	S	0	0	0
			1639	1088	269	268	14			
1	C	201	Total	C	N	O	S	0	0	0
			1639	1088	269	268	14			
1	D	201	Total	C	N	O	S	0	0	0
			1639	1088	269	268	14			
1	E	201	Total	C	N	O	S	0	0	0
	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

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.

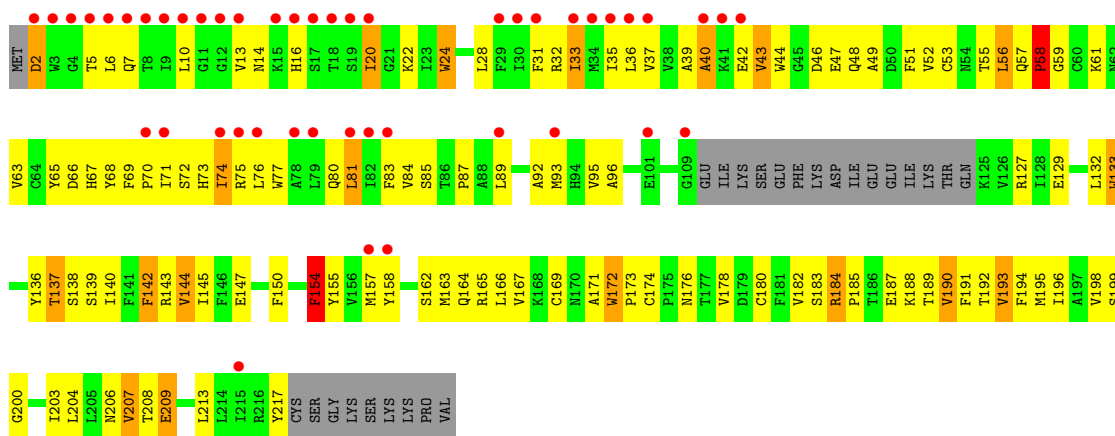
• Molecule 1: Gap junction beta-2 protein

Chain A: 



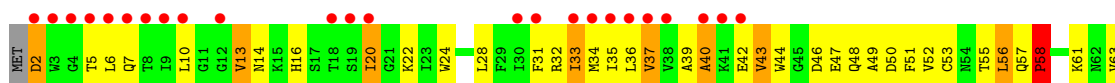
• Molecule 1: Gap junction beta-2 protein

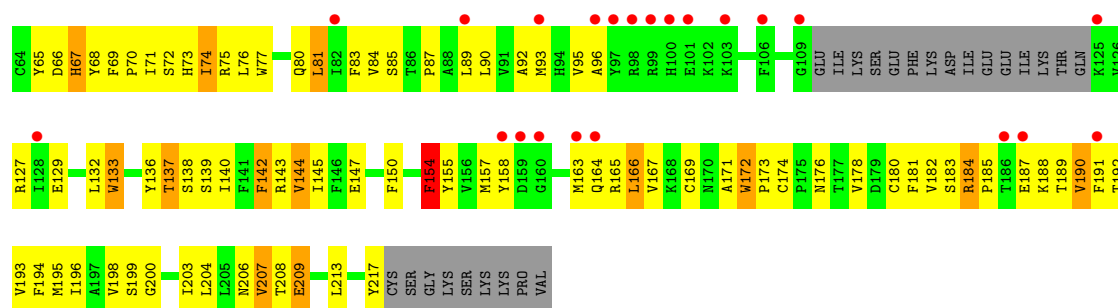
Chain B: 



• Molecule 1: Gap junction beta-2 protein

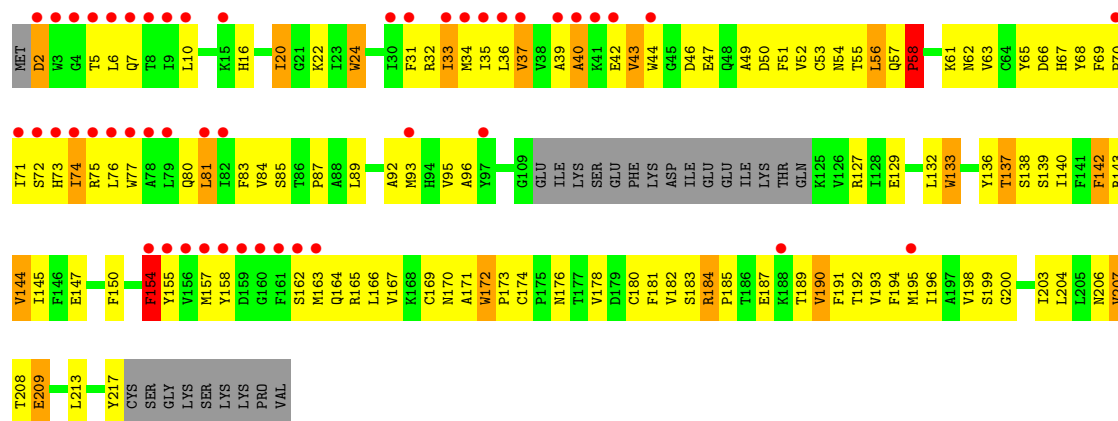
Chain C: 





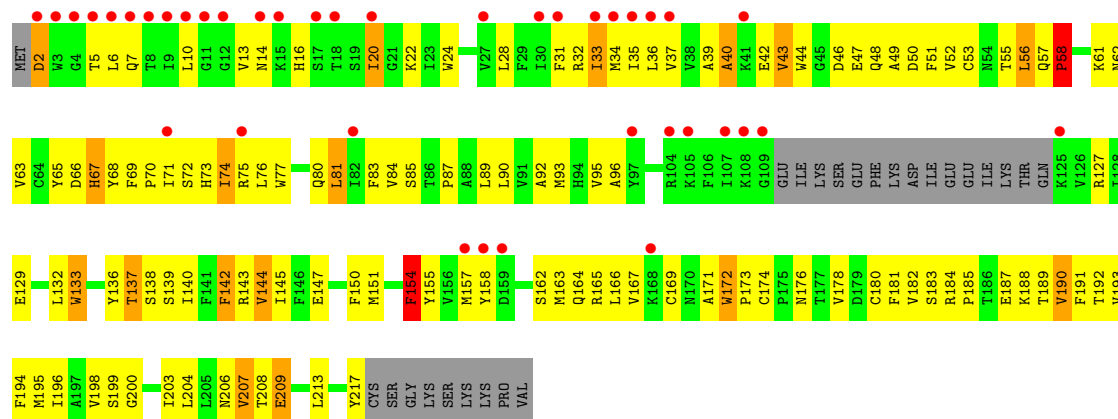
- Molecule 1: Gap junction beta-2 protein

Chain D:



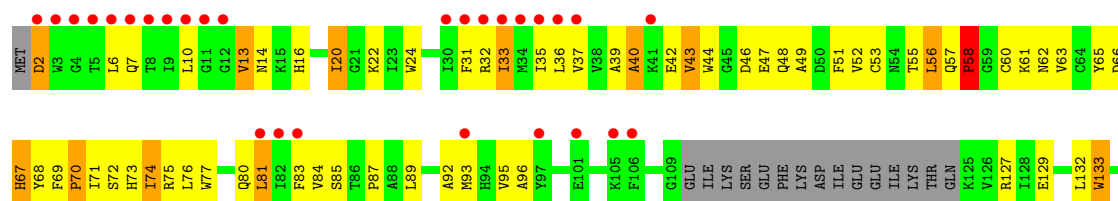
- Molecule 1: Gap junction beta-2 protein

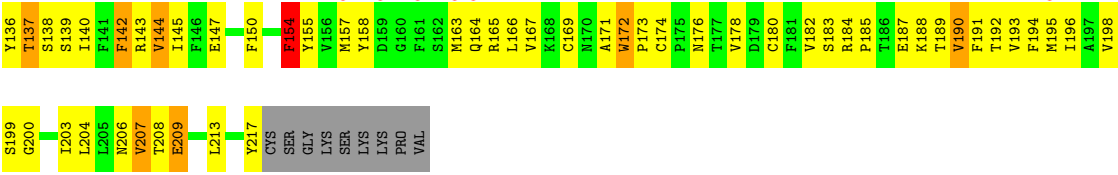
Chain E:



- Molecule 1: Gap junction beta-2 protein

Chain F: 





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.337 , 0.351 0.326 , 0.376	Depositor DCC
R_{free} test set	1578 reflections (5.05%)	DCC
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 , 40.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	6 of 31307 reflections (0.019%)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1639	0	1647	146	0
1	F	1639	0	1647	138	0
All	All	9834	0	9882	720	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

All (720) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:F:80:GLN:NE2	1:F:150:PHE:HB2	1.71	1.05
1:E:144:VAL:HG22	1:E:206:ASN:HB3	1.37	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	Distance(Å)	Clash(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:B:80:GLN:HE21	1:B:150:PHE:CB	1.78	0.94
1:A:80:GLN:HE21	1:A:150:PHE:CB	1.79	0.94
1:E:187:GLU:HB2	1:F:70:PRO:O	1.67	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:C:68:TYR:HE1	1:C:167:VAL:HG21	1.23	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: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:F:68:TYR:CE1	1:F:167:VAL:CG2	2.55	0.88
1:A:43:VAL:HG12	1:B:75:ARG:HH11	1.38	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
1:C:165:ARG:HD3	1:D:63:VAL:HG13	1.57	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:80:GLN:NE2	1:B:150:PHE:CB	2.36	0.85
1:C:80:GLN:NE2	1:C:150:PHE:CB	2.39	0.85
1:F:80:GLN:NE2	1:F:150:PHE:CB	2.35	0.85
1:A:70:PRO:O	1:F:187:GLU:HB2	1.76	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:80:GLN:NE2	1:A:150:PHE:CB	2.38	0.80
1:A:32:ARG:HH11	1:A:198:VAL:HG12	1.47	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:D:76:LEU:HB3	1:D:154:PHE:CE1	2.17	0.80
1:B:76:LEU:HB3	1:B: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:140:ILE:HA	1:C:143:ARG:HD2	1.69	0.74
1:A:140:ILE:HA	1:A:143:ARG:HD2	1.67	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:A:182:VAL:HB	1:A:185:PRO:HG3	1.73	0.69
1:C:2:ASP:HB2	1:C:6:LEU:CD1	2.23	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:C:68:TYR:HE1	1:C:167:VAL:CG2	2.01	0.68
1:B:56:LEU:HD12	1:B:56:LEU:N	2.08	0.68
1:D:187:GLU:OE1	1:E:72:SER:N	2.22	0.68
1:A:56:LEU:HD12	1:A:56:LEU:N	2.09	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:D:42:GLU:HG2	1:E:75:ARG:CZ	2.28	0.64
1:A:57:GLN:HG2	1:A:173:PRO:O	1.97	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
1:D:36:LEU:HD12	1:D:77:TRP:HB3	1.80	0.64
1:D:57:GLN:HG2	1:D:173:PRO:O	1.98	0.64
1:F:57:GLN:HG2	1:F:173:PRO:O	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:E:81:LEU:O	1:E:85:SER:HB2	1.99	0.62
1:A:57:GLN:CG	1:A:173:PRO:O	2.47	0.62
1:A:42:GLU:HG2	1:B:75:ARG:CZ	2.29	0.62
1:D:68:TYR:HE1	1:D:167:VAL:CG2	2.04	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:F:140:ILE:O	1:F:144:VAL:HG23	1.99	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:E:56:LEU:N	1:E:56:LEU:HD12	2.14	0.61
1:D:140:ILE:O	1:D:144:VAL:HG23	2.00	0.61
1:B:81:LEU:O	1:B:85:SER:HB2	2.01	0.61
1:B:187:GLU:OE1	1:C:72:SER:N	2.31	0.61
1:F:57:GLN:CG	1:F:173:PRO:O	2.49	0.61
1:A:5:THR:HB	1:B:2:ASP:OD1	2.00	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:57:GLN:CG	1:C:173:PRO:O	2.48	0.60
1:C:142:PHE:O	1:C:145:ILE:HG22	2.02	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:B:185:PRO:CD	1:C:66:ASP:OD1	2.50	0.60
1:A:139:SER:O	1:A:143:ARG:HG3	2.01	0.60
1:C:2:ASP:HB2	1:C:6:LEU:HD11	1.84	0.60
1:B:57:GLN:HG2	1:B:173:PRO:O	2.01	0.60
1:E:189:THR:O	1:E:192:THR:N	2.34	0.60
1:A:80:GLN:HA	1:A:150:PHE:CD2	2.37	0.60
1:F:81:LEU:O	1:F:85:SER:HB2	2.02	0.60
1:E:2:ASP:HB2	1:E:6:LEU:CD1	2.31	0.60
1:A:72:SER:N	1:F:187:GLU:OE1	2.29	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:57:GLN:CG	1:B:173:PRO:O	2.49	0.59
1:D:80:GLN:NE2	1:D:150:PHE:HB3	2.15	0.59
1:B:42:GLU:HG2	1:C:75:ARG:CZ	2.32	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:E:57:GLN:HG2	1:E:173:PRO:O	2.03	0.58
1:B:2:ASP:HB2	1:B:6:LEU:HD11	1.85	0.58
1:C:185:PRO:CD	1:D:66:ASP:OD1	2.49	0.58
1:A:2:ASP:HB2	1:A:6:LEU:HD11	1.84	0.58
1:F:80:GLN:HA	1:F:150:PHE:CD2	2.39	0.58
1:B:5:THR:HB	1:C:2:ASP:OD1	2.03	0.58
1:C:187:GLU:CB	1:D:70:PRO:O	2.48	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:D:2:ASP:HB2	1:D:6:LEU:CD1	2.34	0.58
1:F:68:TYR:C	1:F:69:PHE:HD1	2.07	0.58
1:C:68:TYR:C	1:C:69:PHE:HD1	2.07	0.58
1:F:80:GLN:NE2	1:F:150:PHE:HB3	2.19	0.58
1:A:80:GLN:NE2	1:A:150:PHE:HB3	2.17	0.58
1:D:57:GLN:CG	1:D:173:PRO:O	2.52	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:E:68:TYR:C	1:E:69:PHE:HD1	2.07	0.57
1:C:139:SER:O	1:C:143:ARG:HG3	2.05	0.57
1:A:2:ASP:HB2	1:A:6:LEU: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:A:39:ALA:HB2	1:A:191:PHE:CD1	2.34	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
1:B:68:TYR:C	1:B:69:PHE:HD1	2.08	0.56
1:E:80:GLN:HA	1:E:150:PHE:CD2	2.40	0.56
1:D:139:SER:O	1:D:143:ARG:HG3	2.05	0.56
1:C:182:VAL:HG12	1:C:183:SER:H	1.70	0.56
1:E:57:GLN:CG	1:E:173:PRO:O	2.53	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:174:CYS:HB3	1:C:178:VAL:HG11	1.86	0.56
1:D:68:TYR:C	1:D:69:PHE:HD1	2.08	0.56
1:B:80:GLN:HA	1:B:150:PHE:CD2	2.39	0.56
1:A:32:ARG:HH12	1:A:199:SER:CA	2.19	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:E:35:ILE:HG23	1:E:195:MET:SD	2.45	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:B:144:VAL:CG2	1:B:206:ASN:HB3	2.24	0.55
1:E:68:TYR:CD1	1:E:167:VAL:HG21	2.37	0.55
1:C:39:ALA:HB2	1:C:191:PHE:CD1	2.38	0.55
1:F:144:VAL:CG2	1:F:206:ASN:HB3	2.24	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: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:E:195:MET:O	1:E:199:SER:HB2	2.06	0.55
1:B:39:ALA:HB2	1:B:191:PHE:CD1	2.38	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:E:139:SER:O	1:E:143:ARG:HG3	2.07	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: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:D:144:VAL:CG2	1:D:206:ASN:HB3	2.23	0.54
1:B:187:GLU:CB	1:C:70:PRO:O	2.49	0.54
1:E:46:ASP:OD1	1:F:48:GLN:HG2	2.08	0.54
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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:THR:O	1:A:192:THR:N	2.40	0.54
1:B:52:VAL:O	1:B:180:CYS:HA	2.08	0.54
1:B:142:PHE:O	1:B:145:ILE:HG22	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:F:68:TYR:CD1	1:F:167:VAL:HG21	2.35	0.53
1:C:32:ARG:HH12	1:C:199:SER:CA	2.22	0.53
1:F:83:PHE:O	1:F:87:PRO:HD3	2.09	0.53
1:D:190:VAL:HG12	1:D:191:PHE:HD2	1.74	0.53
1:C:53:CYS:HA	1:C:180:CYS:HA	1.90	0.53
1:F:52:VAL:O	1:F:180:CYS:HA	2.07	0.53
1:B:95:VAL:HG13	1:B:96:ALA:N	2.24	0.53
1:D:136:TYR:CE2	1:D:140:ILE:HD11	2.44	0.53
1:B:35:ILE:HG23	1:B:195:MET:SD	2.49	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:E:80:GLN:NE2	1:E:150:PHE:HB3	2.20	0.53
1:C:80:GLN:NE2	1:C:150:PHE:HB3	2.24	0.53
1:A:53:CYS:HA	1:A:180:CYS:HA	1.91	0.53
1:D:182:VAL:HG12	1:D:183:SER:H	1.74	0.53
1:B:32:ARG:HH12	1:B:199:SER:CA	2.22	0.53
1:A:95:VAL:HG13	1:A:96:ALA:N	2.23	0.53
1:A:142:PHE:O	1:A:145:ILE:HG22	2.09	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: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:E:142:PHE:O	1:E:145:ILE:HG22	2.09	0.52
1:C:193:VAL:HG12	1:C:194:PHE:N	2.24	0.52
1:E:189:THR:O	1:E:190:VAL:C	2.47	0.52
1:D:95:VAL:HG13	1:D:96:ALA:N	2.24	0.52
1:E:95:VAL:HG13	1:E:96:ALA:N	2.25	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:C:68:TYR:O	1:C:69:PHE:CD1	2.62	0.52
1:F:182:VAL:HG12	1:F:183:SER:H	1.72	0.52
1:B:172:TRP:CE3	1:B:173:PRO:HG3	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:53:CYS:HA	1:B:180:CYS:HA	1.91	0.52
1:D:40:ALA:HA	1:D:74:ILE:HG12	1.92	0.52
1:A:68:TYR:CD1	1:A:167:VAL:HG21	2.37	0.52
1:F:10:LEU:O	1:F:13:VAL:HG22	2.10	0.52
1:E:13:VAL:HG12	1:E:14:ASN:H	1.74	0.52
1:D:83:PHE:O	1:D:87:PRO:HD3	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:F:142:PHE:O	1:F:145:ILE:HG22	2.10	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: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:187:GLU:CB	1:B:70:PRO:O	2.50	0.51
1:A:75:ARG:NE	1:F:42:GLU:HG2	2.25	0.51
1:E:32:ARG:NH1	1:E:198:VAL:HG12	2.21	0.51
1:D:195:MET:O	1:D:199:SER:HB2	2.11	0.51
1:B:189:THR:O	1:B:190:VAL:C	2.49	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:F:71:ILE:O	1:F:158:TYR:OH	2.27	0.51
1:A:52:VAL:O	1:A:180:CYS:HA	2.11	0.51
1:D:65:TYR:O	1:D:69:PHE:N	2.44	0.51
1:C:190:VAL:HG12	1:C:191:PHE:HD2	1.76	0.51
1:B:56:LEU:CD1	1:B:56:LEU:N	2.74	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:F:136:TYR:CE2	1:F:140:ILE:HD11	2.46	0.50
1:A:70:PRO:O	1:F:187:GLU:CB	2.55	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
1:C:174:CYS:HB3	1:C:178:VAL:CG1	2.41	0.50
1:D:172:TRP:CD1	1:D:172:TRP:C	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:137:THR:OG1	1:F:213:LEU:HD13	2.12	0.50
1:C:95:VAL:HG13	1:C:96:ALA:N	2.26	0.50
1:A:68:TYR:O	1:A:69:PHE:CD1	2.65	0.50
1:E:144:VAL:CG2	1:E:206:ASN:HB3	2.25	0.50
1:A:182:VAL:HG12	1:A:183:SER:H	1.76	0.50
1:F:189:THR:O	1:F:190:VAL:C	2.50	0.50
1:B:190:VAL:HG21	1:C:71:ILE:HG12	1.94	0.50
1:C:172:TRP:CD1	1:C:172:TRP:C	2.84	0.50
1:A:44:TRP:CH2	1:A:73:HIS:HB2	2.47	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:E:68:TYR:O	1:E:69:PHE:CD1	2.65	0.49
1:C:68:TYR:O	1:C:69:PHE:HD1	1.95	0.49
1:A:169:CYS:SG	1:A:171:ALA:HB2	2.52	0.49
1:E:190:VAL:HG11	1:F:71:ILE:HG12	1.93	0.49
1:C:189:THR:O	1:C:190:VAL:C	2.49	0.49
1:A:56:LEU:CD1	1:A:56:LEU:N	2.75	0.49
1:E:129:GLU:O	1:E:133:TRP:HB2	2.12	0.49
1:C:137:THR:OG1	1:C:213:LEU:HD13	2.12	0.49
1:E:182:VAL:HG12	1:E:183:SER:H	1.76	0.49
1:A:172:TRP:CD1	1:A:172:TRP:C	2.84	0.49
1:D:189:THR:O	1:D:190:VAL:C	2.51	0.49
1:F:68:TYR:O	1:F:69:PHE:CD1	2.64	0.49
1:F:44:TRP:CH2	1:F:73:HIS:HB2	2.47	0.49
1:B:24:TRP:CD1	1:C:90:LEU:HD21	2.47	0.49
1:F:2:ASP:HB2	1:F:6:LEU:HD12	1.93	0.49
1:E:40:ALA:HA	1:E:74:ILE:HG12	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:B:169:CYS:SG	1:B:171:ALA:HB2	2.53	0.49
1:A:190:VAL:HG11	1:B:71:ILE:HG12	1.94	0.49
1:C:129:GLU:O	1:C:133:TRP:HB2	2.12	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: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:B:182:VAL:HG12	1:B:183:SER:H	1.77	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:137:THR:OG1	1:B:213:LEU:HD13	2.12	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:32:ARG:HH12	1:A:199:SER:HA	1.77	0.48
1:D:172:TRP:HB3	1:D:173:PRO:HD3	1.95	0.48
1:B:172:TRP:HB3	1:B:173:PRO:HD3	1.94	0.48
1:B:13:VAL:HG12	1:B:14:ASN:H	1.78	0.48
1:A:129:GLU:O	1:A:133:TRP:HB2	2.14	0.48
1:F:56:LEU:N	1:F:56:LEU:CD1	2.76	0.48
1:E:16:HIS:HA	1:E:133:TRP:HZ2	1.78	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:E:165:ARG:HA	1:E:185:PRO:HG2	1.95	0.48
1:F:13:VAL:HG12	1:F:14:ASN:H	1.79	0.48
1:F:16:HIS:HA	1:F:133:TRP:HZ2	1.78	0.48
1:A:137:THR:OG1	1:A:213:LEU:HD13	2.14	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:C:65:TYR:O	1:C:69:PHE:N	2.45	0.48
1:B:129:GLU:O	1:B:133:TRP:HB2	2.13	0.48
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:E:63:VAL:CG1	1:E:171:ALA:HB1	2.44	0.47
1:B:63:VAL:CG1	1:B:171:ALA:HB1	2.44	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:A:65:TYR:O	1:A:69:PHE:N	2.48	0.47
1:F:32:ARG:HH12	1:F:199:SER:HA	1.78	0.47
1:E:181:PHE:CE2	1:F:173:PRO:HG3	2.49	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:C:136:TYR:CE2	1:C:140:ILE:HD11	2.49	0.47
1:C:183:SER:O	1:C:188:LYS:NZ	2.42	0.47
1:E:44:TRP:CH2	1:E:73:HIS:HB2	2.50	0.47
1:B:190:VAL:HG21	1:C:71:ILE:CG1	2.45	0.47
1:F:172:TRP:CE3	1:F:173:PRO:HG3	2.49	0.47
1:A:204:LEU:HA	1:A:207:VAL:HG12	1.97	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:B:46:ASP:OD1	1:C:48:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:68:TYR:O	1:D:69:PHE:CD1	2.67	0.47
1:D:165:ARG:HA	1:D:185:PRO:HG2	1.96	0.47
1:C:44:TRP:CH2	1:C:73:HIS:HB2	2.49	0.47
1:F:172:TRP:HB3	1:F:173:PRO:HD3	1.97	0.47
1:D:174:CYS:HB3	1:D:178:VAL:CG1	2.44	0.47
1:A:16:HIS:HA	1:A:133:TRP:HZ2	1.80	0.47
1:C:204:LEU:HA	1:C:207:VAL:HG12	1.96	0.47
1:E:200:GLY:O	1:E:203:ILE:HB	2.15	0.47
1:E:65:TYR:O	1:E:69:PHE:N	2.48	0.47
1:C:165:ARG:HA	1:C:185:PRO:HG2	1.96	0.47
1:E:136:TYR:CE2	1:E:140:ILE:HD11	2.49	0.47
1:A:43:VAL:HG22	1:A:44:TRP:CD1	2.50	0.47
1:E:174:CYS:HB3	1:E:178:VAL:CG1	2.45	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:A:174:CYS:HB3	1:A:178:VAL:CG1	2.45	0.47
1:D:74:ILE:HA	1:D:74:ILE:HD12	1.53	0.47
1:D:204:LEU:HA	1:D:207:VAL:HG12	1.96	0.47
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:A:71:ILE:HG12	1:F:190:VAL:HG11	1.97	0.46
1:B:165:ARG:NH2	1:C:67:HIS:HA	2.30	0.46
1:C:57:GLN:NE2	1:C:58:PRO:HD2	2.31	0.46
1:D:44:TRP:CH2	1:D:73:HIS:HB2	2.51	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:F:174:CYS:HB3	1:F:178:VAL:CG1	2.45	0.46
1:F:129:GLU:O	1:F:133:TRP:HB2	2.15	0.46
1:D:200:GLY:O	1:D:203:ILE:HB	2.15	0.46
1:E:165:ARG:HH22	1:F:67:HIS:CG	2.32	0.46
1:E:172:TRP:C	1:E:172:TRP:CD1	2.85	0.46
1:D:76:LEU:HA	1:D:76:LEU:HD23	1.74	0.46
1:C:71:ILE:O	1:C:158:TYR:OH	2.29	0.46
1:E:172:TRP:CE3	1:E:173:PRO:HG3	2.50	0.46
1:B:172:TRP:CG	1:B:173:PRO:N	2.83	0.46
1:A:200:GLY:O	1:A:203:ILE:HB	2.16	0.46
1:E:172:TRP:CG	1:E:173:PRO:N	2.84	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:B:2:ASP:OD2	1:B:2:ASP:N	2.48	0.46
1:A:20:ILE:O	1:A:20:ILE:HG22	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:204:LEU:HA	1:B:207:VAL:HG12	1.98	0.46
1:B:183:SER:HB2	1:C:48:GLN:NE2	2.31	0.46
1:C:32:ARG:HA	1:C:35:ILE:HG22	1.98	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: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:A:74:ILE:HA	1:A:74:ILE:HD12	1.55	0.46
1:C:63:VAL:CG1	1:C:171:ALA:HB1	2.46	0.45
1:A:48:GLN:HG2	1:F:46:ASP:OD1	2.17	0.45
1:E:74:ILE:HD12	1:E:74:ILE:HA	1.55	0.45
1:C:32:ARG:HH12	1:C:199:SER:HA	1.80	0.45
1:B:200:GLY:O	1:B:203:ILE:HB	2.16	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:E:163:MET:HG3	1:E:185:PRO:HB3	1.99	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: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:F:2:ASP:CB	1:F:6:LEU:HD11	2.46	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:65:TYR:O	1:F:69:PHE:N	2.50	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: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
1:D:47:GLU:O	1:D:51:PHE:HB2	2.16	0.45
1:C:2:ASP:CB	1:C:6:LEU:HD11	2.47	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:E:47:GLU:O	1:E:51:PHE:HB2	2.17	0.45
1:F:68:TYR:O	1:F:69:PHE:HD1	2.00	0.45
1:F:57:GLN:NE2	1:F:58:PRO:HD2	2.32	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:A:68:TYR:O	1:A:69:PHE:HD1	2.00	0.44
1:C:80:GLN:HA	1:C:150:PHE:CE2	2.52	0.44
1:C:76:LEU:HA	1:C:76:LEU:HD23	1.74	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:2:ASP:OD2	1:F:2:ASP:N	2.49	0.44
1:F:172:TRP:CG	1:F:173:PRO:N	2.83	0.44
1:B:172:TRP:CD1	1:B:172:TRP:C	2.85	0.44
1:E:31:PHE:CD2	1:E:31:PHE:C	2.90	0.44
1:D:136:TYR:CE2	1:D:140:ILE:CD1	3.00	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: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:C:43:VAL:HG22	1:C:44:TRP:CD1	2.52	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:F:47:GLU:O	1:F:51:PHE:HB2	2.17	0.44
1:D:32:ARG:NH2	1:D:147:GLU:OE2	2.50	0.44
1:C:89:LEU:O	1:C:93:MET:HB2	2.18	0.44
1:E:32:ARG:NH2	1:E:147:GLU:OE2	2.51	0.44
1:E:2:ASP:HB2	1:E:6:LEU:HD12	1.99	0.44
1:A:32:ARG:HH12	1:A:199:SER:N	2.15	0.44
1:E:68:TYR:C	1:E:69:PHE:CD1	2.91	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:F:200:GLY:O	1:F:203:ILE:HB	2.17	0.44
1:E:185:PRO:N	1:F:66:ASP:OD1	2.50	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: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:E:183:SER:HB2	1:F:48:GLN:NE2	2.33	0.44
1:D:80:GLN:HA	1:D:150:PHE:CE2	2.52	0.44
1:A:32:ARG:NH1	1:A:199:SER:HA	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:E:169:CYS:SG	1:E:171:ALA:HB2	2.58	0.43
1:F:46:ASP:O	1:F:47:GLU:C	2.55	0.43
1:A:190:VAL:HG21	1:B:71:ILE:HG12	2.00	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:A:31:PHE:C	1:A:31:PHE:CD2	2.92	0.43
1:F:20:ILE:O	1:F:20:ILE:HG22	2.18	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:68:TYR:O	1:E:69:PHE:HD1	2.01	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:F:192:THR:O	1:F:196:ILE:HB	2.19	0.43
1:D:20:ILE:O	1:D:20:ILE:HG22	2.19	0.43
1:D:40:ALA:HB2	1:D:74:ILE:HG13	2.00	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:190:VAL:HG21	1:E:71:ILE:CG1	2.49	0.43
1:E:20:ILE:O	1:E:20:ILE:HG22	2.18	0.43
1:F:66:ASP:O	1:F:68:TYR:N	2.51	0.43
1:F:136:TYR:CE2	1:F:140:ILE:CD1	3.02	0.43
1:A:59:GLY:O	1:A:63:VAL:HG23	2.18	0.43
1:F:183:SER:O	1:F:188:LYS:NZ	2.42	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:E:165:ARG:NH1	1:F:67:HIS:HB2	2.34	0.43
1:D:68:TYR:C	1:D:69:PHE:CD1	2.92	0.43
1:B:143:ARG:HD3	1:B:206:ASN:OD1	2.19	0.43
1:E:192:THR:O	1:E:196:ILE:HB	2.19	0.43
1:B:95:VAL:CG1	1:B:96:ALA:N	2.82	0.43
1:F:40:ALA:HB2	1:F:74:ILE:HG13	2.01	0.43
1:F:74:ILE:HD12	1:F:74:ILE:HA	1.54	0.43
1:E:16:HIS:HD2	1:E:22:LYS:HE2	1.84	0.43
1:C:171:ALA:O	1:C:172:TRP:C	2.57	0.42
1:A:80:GLN:HA	1:A:150:PHE:CE2	2.54	0.42
1:D:43:VAL:HG22	1:D:44:TRP:CD1	2.53	0.42
1:A:163:MET:HG3	1:A:185:PRO:HB3	2.01	0.42
1:F:73:HIS:N	1:F:73:HIS:CD2	2.85	0.42
1:A:162:SER:HB2	1:A:189:THR:OG1	2.19	0.42
1:C:20:ILE:HG22	1:C:20:ILE:O	2.18	0.42
1:E:32:ARG:HH12	1:E:199:SER:N	2.16	0.42
1:A:190:VAL:HG21	1:B:71:ILE:CG1	2.49	0.42
1:B:162:SER:HB2	1:B:189:THR:OG1	2.18	0.42
1:A:32:ARG:NH2	1:A:147:GLU:OE2	2.51	0.42
1:D:32:ARG:HA	1:D:35:ILE:HG22	2.01	0.42
1:B:2:ASP:CB	1:B:6:LEU:HD11	2.49	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:B:31:PHE:CD2	1:B:31:PHE:C	2.92	0.42
1:A:58:PRO:O	1:A:59:GLY:C	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:190:VAL:HG21	1:E:71:ILE:HG12	2.00	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:C:32:ARG:HH12	1:C:199:SER:N	2.18	0.42
1:F:32:ARG:NH1	1:F:199:SER:HA	2.35	0.42
1:D:16:HIS:HD2	1:D:22:LYS:HE2	1.83	0.42
1:A:68:TYR:C	1:A:69:PHE:CD1	2.91	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:C:31:PHE:C	1:C:31:PHE:CD2	2.92	0.42
1:C:37:VAL:O	1:C:37:VAL:HG13	2.19	0.42
1:B:184:ARG:N	1:B:185:PRO:HD3	2.34	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:A:165:ARG:HA	1:A:185:PRO:HG2	2.01	0.42
1:F:32:ARG:HH12	1:F:199:SER:N	2.18	0.42
1:B:193:VAL:HG12	1:B:194:PHE:HD1	1.84	0.42
1:F:80:GLN:HA	1:F:150:PHE:CE2	2.55	0.42
1:B:89:LEU:O	1:B:93:MET:HB2	2.19	0.42
1:B:43:VAL:HG12	1:C:75:ARG:NH1	2.15	0.42
1:A:71:ILE:CG1	1:F:190:VAL:HG21	2.50	0.42
1:D:92:ALA:O	1:D:95:VAL:HG12	2.20	0.42
1:B:58:PRO:O	1:B:59:GLY:C	2.57	0.42
1:B:68:TYR:C	1:B:69:PHE:CD1	2.91	0.42
1:A:67:HIS:CG	1:F:165:ARG:HH22	2.36	0.42
1:A:192:THR:O	1:A:196:ILE:HB	2.20	0.42
1:C:74:ILE:HD12	1:C:74:ILE:HA	1.57	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:D:184:ARG:N	1:D:185:PRO:HD3	2.35	0.41
1:C:190:VAL:HG11	1:D:71:ILE:HG12	2.01	0.41
1:B:2:ASP:HB2	1:B:6:LEU:HD12	2.00	0.41
1:D:193:VAL:HG12	1:D:194:PHE:HD1	1.83	0.41
1:F:89:LEU:O	1:F:93:MET:HB2	2.19	0.41
1:D:165:ARG:HH22	1:E:67:HIS:CG	2.37	0.41
1:E:171:ALA:O	1:E:172:TRP:C	2.59	0.41
1:D:95:VAL:CG1	1:D:96:ALA:N	2.82	0.41
1:F:63:VAL:HG12	1:F:171:ALA:HB1	2.02	0.41
1:D:169:CYS:SG	1:D:171:ALA:HB2	2.60	0.41
1:E:150:PHE:O	1:E:151:MET:C	2.58	0.41
1:D:46:ASP:O	1:D:47:GLU:C	2.57	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:32:ARG:NH1	1:B:199:SER:HA	2.35	0.41
1:F:172:TRP:C	1:F:172:TRP:CD1	2.88	0.41
1:B:165:ARG:NH1	1:C:67:HIS:HB2	2.35	0.41
1:D:170:ASN:O	1:D:171:ALA:C	2.59	0.41
1:E:89:LEU:O	1:E:93:MET:HB2	2.19	0.41
1:E:32:ARG:NH1	1:E:199:SER:HA	2.35	0.41
1:C:32:ARG:NH1	1:C:199:SER:HA	2.36	0.41
1:A:172:TRP:CG	1:A:173:PRO:N	2.83	0.41
1:D:162:SER:HB2	1:D:189:THR:OG1	2.20	0.41
1:C:181:PHE:CE2	1:D:173:PRO:HG3	2.56	0.41
1:A:183:SER:HB2	1:B:48:GLN:NE2	2.35	0.41
1:A:46:ASP:O	1:A:47:GLU:C	2.57	0.41
1:E:95:VAL:CG1	1:E:96:ALA:N	2.83	0.41
1:A:37:VAL:HG13	1:A:37:VAL:O	2.19	0.41
1:C:200:GLY:O	1:C:203:ILE:HB	2.19	0.41
1:A:212:TYR:HA	1:A:215:ILE:HD12	2.03	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: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:D:181:PHE:HE2	1:E:173:PRO:HG3	1.86	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:B:57:GLN:HG3	1:B:173:PRO:O	2.19	0.41
1:E:80:GLN:HA	1:E:150:PHE:CE2	2.55	0.41
1:E:43:VAL:HG22	1:E:44:TRP:CD1	2.55	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
1:C:92:ALA:O	1:C:95:VAL:HG12	2.21	0.41
1:D:24:TRP:CD1	1:E:90:LEU:HD21	2.55	0.41
1:F:143:ARG:HD3	1:F:206:ASN:OD1	2.22	0.41
1:D:183:SER:HB2	1:E:48:GLN:NE2	2.36	0.41
1:E:190:VAL:HG21	1:F:71:ILE:CG1	2.51	0.41
1:B:28:LEU:HA	1:B:31:PHE:HB3	2.03	0.41
1:F:31:PHE:CD2	1:F:31:PHE:C	2.93	0.41
1:F:66:ASP:C	1:F:68:TYR:N	2.74	0.40
1:C:143:ARG:HD3	1:C:206:ASN:OD1	2.21	0.40
1:A:171:ALA:O	1:A:172:TRP:C	2.59	0.40
1:D:54:ASN:ND2	1:E:58:PRO:HG2	2.36	0.40
1:D:181:PHE:CE2	1:E:173:PRO:HG3	2.56	0.40
1:D:73:HIS:N	1:D:73:HIS:CD2	2.88	0.40
1:E:84:VAL:CG2	1:E:147:GLU:HG2	2.39	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:166:LEU:HD13	1:D:172:TRP:HZ3	1.86	0.40
1:E:142:PHE:HA	1:E:142:PHE:HD1	1.79	0.40
1:E:28:LEU:HA	1:E:31:PHE:HB3	2.03	0.40
1:C:184:ARG:N	1:C:185:PRO:HD3	2.36	0.40
1:D:63:VAL:HG12	1:D:171:ALA:HB1	2.03	0.40
1:D:66:ASP:C	1:D:68:TYR:N	2.74	0.40
1:D:43:VAL:HG12	1:E:75:ARG:NH1	2.17	0.40
1:A:28:LEU:HA	1:A:31:PHE:HB3	2.04	0.40
1:C:28:LEU:HA	1:C:31:PHE:HB3	2.04	0.40
1:E:162:SER:HB2	1:E:189:THR:OG1	2.20	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: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
1:B:74:ILE:HA	1:B:74:ILE:HD12	1.58	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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%)	4	39
1	B	197/226 (87%)	157 (80%)	31 (16%)	9 (5%)	4	39
1	C	197/226 (87%)	158 (80%)	31 (16%)	8 (4%)	4	44
1	D	197/226 (87%)	156 (79%)	33 (17%)	8 (4%)	4	44
1	E	197/226 (87%)	154 (78%)	35 (18%)	8 (4%)	4	44
1	F	197/226 (87%)	156 (79%)	32 (16%)	9 (5%)	4	39
All	All	1182/1356 (87%)	939 (79%)	192 (16%)	51 (4%)	4	42

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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	3	17
1	B	177/204 (87%)	148 (84%)	29 (16%)	3	20
1	C	177/204 (87%)	146 (82%)	31 (18%)	3	17
1	D	177/204 (87%)	147 (83%)	30 (17%)	3	18
1	E	177/204 (87%)	148 (84%)	29 (16%)	3	20
1	F	177/204 (87%)	147 (83%)	30 (17%)	3	18
All	All	1062/1224 (87%)	882 (83%)	180 (17%)	3	18

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 ⓘ

There are no RNA chains 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, 95th 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%)	1.12	38 (18%) 2 2	78, 126, 205, 221	0
1	B	201/226 (88%)	1.30	46 (22%) 1 2	78, 126, 205, 221	0
1	C	201/226 (88%)	1.40	46 (22%) 1 2	78, 126, 203, 221	0
1	D	201/226 (88%)	1.42	48 (23%) 1 2	78, 126, 205, 221	0
1	E	201/226 (88%)	1.20	39 (19%) 2 2	78, 126, 205, 221	0
1	F	201/226 (88%)	1.05	34 (16%) 2 2	78, 126, 203, 221	0
All	All	1206/1356 (88%)	1.25	251 (20%) 1 2	78, 127, 205, 221	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	THR	24.1
1	B	4	GLY	20.1
1	B	6	LEU	18.3
1	E	4	GLY	18.0
1	E	5	THR	17.8
1	B	7	GLN	16.7
1	C	2	ASP	16.0
1	D	2	ASP	15.3
1	E	6	LEU	15.2
1	C	5	THR	15.2
1	C	4	GLY	14.8
1	E	7	GLN	14.3
1	E	2	ASP	14.1
1	A	4	GLY	13.5
1	F	4	GLY	13.1
1	E	3	TRP	12.8
1	B	3	TRP	12.3
1	F	7	GLN	12.2
1	D	4	GLY	12.1

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Mol	Chain	Res	Type	RSRZ
1	F	6	LEU	12.1
1	B	2	ASP	12.1
1	C	6	LEU	11.7
1	D	3	TRP	11.5
1	A	3	TRP	11.4
1	A	5	THR	11.3
1	C	3	TRP	11.1
1	A	7	GLN	10.9
1	C	9	ILE	10.8
1	C	7	GLN	10.4
1	F	3	TRP	10.3
1	F	5	THR	10.3
1	D	5	THR	10.2
1	D	158	TYR	9.8
1	F	2	ASP	9.6
1	B	8	THR	9.5
1	D	157	MET	9.1
1	F	8	THR	8.9
1	E	10	LEU	8.8
1	B	34	MET	8.8
1	A	6	LEU	8.7
1	F	9	ILE	8.6
1	C	8	THR	8.5
1	C	97	TYR	8.2
1	C	34	MET	8.1
1	A	34	MET	8.1
1	D	159	ASP	8.0
1	C	20	ILE	8.0
1	A	157	MET	8.0
1	E	8	THR	7.8
1	D	75	ARG	7.8
1	E	34	MET	7.6
1	A	159	ASP	7.5
1	A	10	LEU	7.4
1	C	33	ILE	7.4
1	A	2	ASP	7.3
1	C	10	LEU	7.3
1	A	8	THR	7.2
1	D	6	LEU	7.1
1	D	41	LYS	7.1
1	D	34	MET	7.0
1	B	11	GLY	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	33	ILE	6.8
1	C	159	ASP	6.7
1	A	9	ILE	6.6
1	F	10	LEU	6.5
1	F	34	MET	6.4
1	F	159	ASP	6.4
1	E	9	ILE	6.2
1	D	74	ILE	6.2
1	B	12	GLY	6.2
1	A	35	ILE	5.9
1	C	35	ILE	5.8
1	D	71	ILE	5.7
1	A	41	LYS	5.7
1	A	158	TYR	5.7
1	F	11	GLY	5.6
1	D	35	ILE	5.6
1	D	154	PHE	5.5
1	A	33	ILE	5.5
1	B	10	LEU	5.5
1	D	36	LEU	5.4
1	B	75	ARG	5.4
1	C	12	GLY	5.4
1	D	40	ALA	5.4
1	A	163	MET	5.3
1	A	42	GLU	5.3
1	D	163	MET	5.3
1	B	9	ILE	5.3
1	C	41	LYS	5.2
1	D	9	ILE	5.2
1	B	36	LEU	5.2
1	B	30	ILE	5.1
1	B	35	ILE	5.0
1	D	7	GLN	4.9
1	E	157	MET	4.9
1	E	159	ASP	4.9
1	D	78	ALA	4.8
1	D	33	ILE	4.8
1	E	33	ILE	4.8
1	D	70	PRO	4.8
1	B	41	LYS	4.8
1	B	157	MET	4.8
1	D	73	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	31	PHE	4.7
1	F	12	GLY	4.7
1	F	31	PHE	4.7
1	E	17	SER	4.7
1	A	36	LEU	4.6
1	C	19	SER	4.6
1	A	160	GLY	4.6
1	F	35	ILE	4.6
1	E	108	LYS	4.5
1	C	18	THR	4.4
1	D	76	LEU	4.4
1	D	42	GLU	4.3
1	E	109	GLY	4.3
1	D	72	SER	4.3
1	D	97	TYR	4.3
1	E	107	ILE	4.3
1	F	33	ILE	4.2
1	C	36	LEU	4.2
1	B	18	THR	4.2
1	C	109	GLY	4.1
1	D	162	SER	4.1
1	C	125	LYS	4.0
1	D	77	TRP	4.0
1	A	31	PHE	3.9
1	B	158	TYR	3.9
1	B	37	VAL	3.9
1	C	42	GLU	3.9
1	C	96	ALA	3.9
1	E	158	TYR	3.8
1	E	41	LYS	3.8
1	B	20	ILE	3.8
1	C	37	VAL	3.8
1	A	30	ILE	3.8
1	B	82	ILE	3.7
1	D	156	VAL	3.7
1	F	36	LEU	3.7
1	C	99	ARG	3.7
1	D	44	TRP	3.7
1	B	79	LEU	3.7
1	C	93	MET	3.6
1	E	15	LYS	3.6
1	C	30	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	78	ALA	3.6
1	A	40	ALA	3.6
1	B	31	PHE	3.6
1	E	35	ILE	3.6
1	E	11	GLY	3.5
1	E	30	ILE	3.5
1	C	31	PHE	3.5
1	F	82	ILE	3.5
1	C	187	GLU	3.4
1	F	41	LYS	3.4
1	C	100	HIS	3.4
1	D	37	VAL	3.4
1	F	97	TYR	3.4
1	B	71	ILE	3.4
1	B	42	GLU	3.4
1	A	162	SER	3.4
1	E	36	LEU	3.3
1	A	161	PHE	3.2
1	B	109	GLY	3.2
1	B	17	SER	3.2
1	F	195	MET	3.1
1	B	215	ILE	3.1
1	E	20	ILE	3.1
1	C	163	MET	3.1
1	D	195	MET	3.1
1	C	158	TYR	3.1
1	A	81	LEU	3.1
1	D	160	GLY	3.1
1	A	27	VAL	3.0
1	B	40	ALA	3.0
1	D	82	ILE	3.0
1	D	8	THR	3.0
1	F	30	ILE	3.0
1	D	30	ILE	3.0
1	D	155	TYR	3.0
1	D	31	PHE	2.9
1	C	191	PHE	2.9
1	B	74	ILE	2.9
1	D	10	LEU	2.9
1	F	93	MET	2.9
1	D	81	LEU	2.8
1	F	161	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	79	LEU	2.8
1	A	11	GLY	2.8
1	A	17	SER	2.8
1	F	105	LYS	2.8
1	A	164	GLN	2.8
1	A	71	ILE	2.8
1	A	37	VAL	2.8
1	E	104	ARG	2.7
1	C	128	ILE	2.7
1	C	101	GLU	2.7
1	B	13	VAL	2.7
1	B	81	LEU	2.7
1	B	89	LEU	2.7
1	A	38	VAL	2.6
1	D	15	LYS	2.6
1	C	40	ALA	2.6
1	E	12	GLY	2.5
1	A	89	LEU	2.5
1	D	188	LYS	2.5
1	E	37	VAL	2.5
1	B	19	SER	2.5
1	E	18	THR	2.5
1	F	37	VAL	2.5
1	C	38	VAL	2.5
1	E	71	ILE	2.4
1	C	160	GLY	2.4
1	F	83	PHE	2.4
1	E	27	VAL	2.4
1	E	14	ASN	2.4
1	B	70	PRO	2.4
1	C	82	ILE	2.4
1	E	125	LYS	2.4
1	B	101	GLU	2.4
1	F	81	LEU	2.3
1	F	164	GLN	2.3
1	C	98	ARG	2.3
1	C	103	LYS	2.3
1	A	195	MET	2.3
1	D	39	ALA	2.3
1	A	82	ILE	2.3
1	F	163	MET	2.3
1	A	83	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	105	LYS	2.2
1	F	32	ARG	2.2
1	E	168	LYS	2.2
1	B	93	MET	2.2
1	C	106	PHE	2.2
1	B	16	HIS	2.2
1	F	157	MET	2.2
1	A	156	VAL	2.2
1	B	76	LEU	2.1
1	B	83	PHE	2.1
1	E	82	ILE	2.1
1	E	75	ARG	2.1
1	F	101	GLU	2.1
1	C	186	THR	2.1
1	C	164	GLN	2.1
1	D	93	MET	2.0
1	C	89	LEU	2.0
1	B	29	PHE	2.0
1	B	15	LYS	2.0
1	E	97	TYR	2.0
1	D	161	PHE	2.0
1	F	106	PHE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.