Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2023 – 07:00 PM EDT

PDB ID	:	8SV6
Title	:	Structure of the M. smegmatis DarR protein
Authors	:	Schumacher, M.A.
Deposited on	:	2023-05-15
Resolution	:	3.56 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

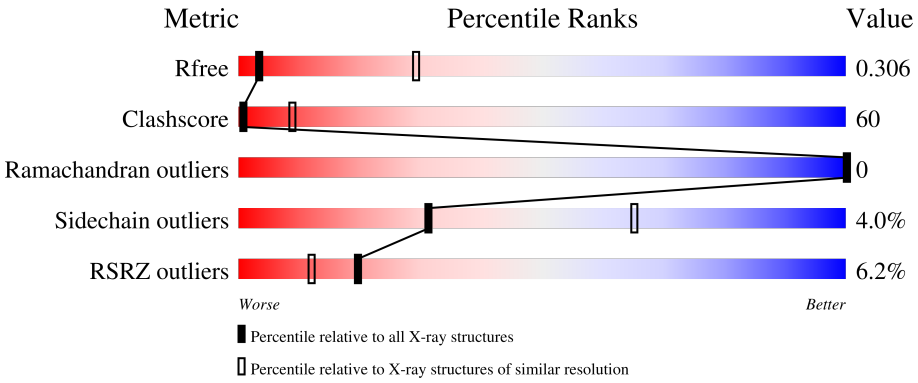
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.56 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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 of 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	213	3% 39% 50% · 9%
1	B	213	3% 36% 57% · 6%
1	C	213	8% 34% 53% · 9%
1	D	213	8% 32% 60% · 8%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5864 atoms, of which 13 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 Fatty acid metabolism regulator protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1469	920	263	279	7			
1	B	200	Total	C	N	O	S	0	0	0
			1514	950	274	283	7			
1	C	193	Total	C	N	O	S	0	0	0
			1422	900	250	269	3			
1	D	197	Total	C	H	N	O	S	0	0	0
			1459	910	13	254	277	5			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A653FFT2
A	-1	SER	-	expression tag	UNP A0A653FFT2
A	0	HIS	-	expression tag	UNP A0A653FFT2
A	1	MET	-	expression tag	UNP A0A653FFT2
A	2	SER	-	expression tag	UNP A0A653FFT2
A	3	ALA	-	expression tag	UNP A0A653FFT2
A	4	GLU	-	expression tag	UNP A0A653FFT2
A	5	LEU	-	expression tag	UNP A0A653FFT2
B	-2	GLY	-	expression tag	UNP A0A653FFT2
B	-1	SER	-	expression tag	UNP A0A653FFT2
B	0	HIS	-	expression tag	UNP A0A653FFT2
B	1	MET	-	expression tag	UNP A0A653FFT2
B	2	SER	-	expression tag	UNP A0A653FFT2
B	3	ALA	-	expression tag	UNP A0A653FFT2
B	4	GLU	-	expression tag	UNP A0A653FFT2
B	5	LEU	-	expression tag	UNP A0A653FFT2
C	-2	GLY	-	expression tag	UNP A0A653FFT2
C	-1	SER	-	expression tag	UNP A0A653FFT2
C	0	HIS	-	expression tag	UNP A0A653FFT2
C	1	MET	-	expression tag	UNP A0A653FFT2
C	2	SER	-	expression tag	UNP A0A653FFT2

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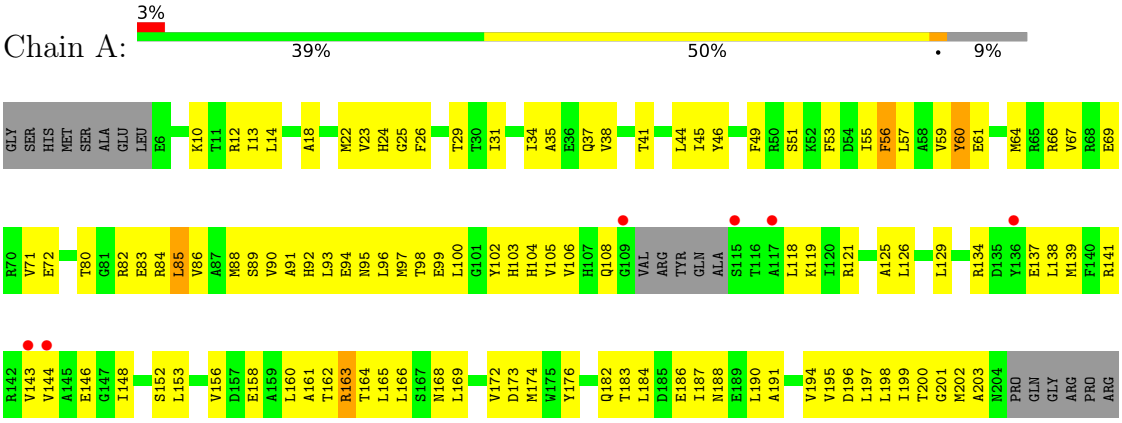
Chain	Residue	Modelled	Actual	Comment	Reference
C	3	ALA	-	expression tag	UNP A0A653FFT2
C	4	GLU	-	expression tag	UNP A0A653FFT2
C	5	LEU	-	expression tag	UNP A0A653FFT2
D	-2	GLY	-	expression tag	UNP A0A653FFT2
D	-1	SER	-	expression tag	UNP A0A653FFT2
D	0	HIS	-	expression tag	UNP A0A653FFT2
D	1	MET	-	expression tag	UNP A0A653FFT2
D	2	SER	-	expression tag	UNP A0A653FFT2
D	3	ALA	-	expression tag	UNP A0A653FFT2
D	4	GLU	-	expression tag	UNP A0A653FFT2
D	5	LEU	-	expression tag	UNP A0A653FFT2

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

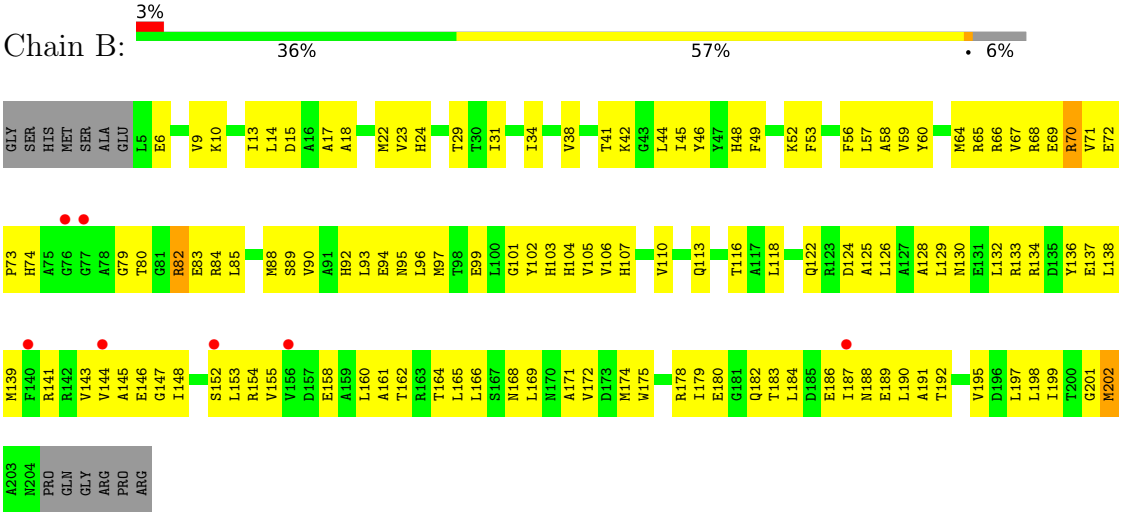
• Molecule 1: Fatty acid metabolism regulator protein

Chain A:



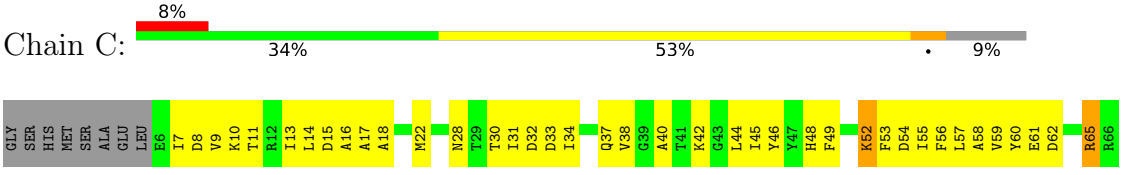
• Molecule 1: Fatty acid metabolism regulator protein

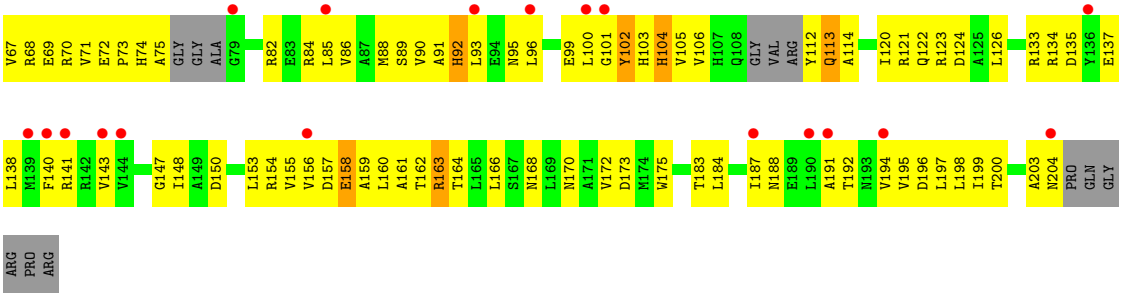
Chain B:



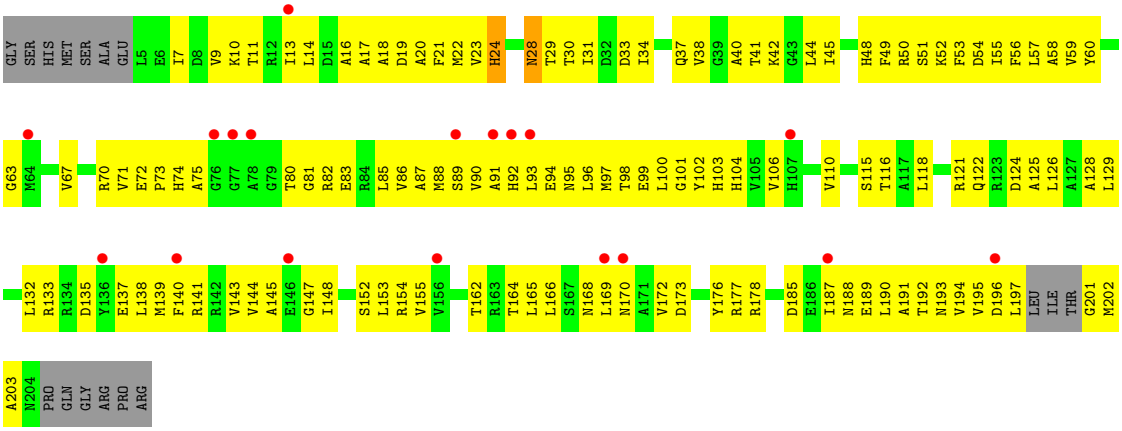
• Molecule 1: Fatty acid metabolism regulator protein

Chain C:





• Molecule 1: Fatty acid metabolism regulator protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.42Å 94.42Å 215.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.21 – 3.56 47.21 – 3.56	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.21-3.56) 99.8 (47.21-3.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.275 , 0.305 0.276 , 0.306	Depositor DCC
R_{free} test set	1230 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	144.7	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 148.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5864	wwPDB-VP
Average B, all atoms (Å^2)	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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	0.26	0/1489	0.52	0/2019
1	B	0.26	0/1535	0.51	0/2081
1	C	0.25	0/1441	0.52	0/1960
1	D	0.26	0/1467	0.52	0/1995
All	All	0.26	0/5932	0.52	0/8055

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1469	0	1412	154	0
1	B	1514	0	1467	185	0
1	C	1422	0	1327	174	0
1	D	1446	13	1343	207	0
All	All	5851	13	5549	689	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 60.

All (689) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:HG13	1:B:139:MET:HE1	1.26	1.12
1:A:137:GLU:HG2	1:A:166:LEU:HD13	1.29	1.11
1:C:40:ALA:HB1	1:C:44:LEU:HD12	1.25	1.08
1:D:190:LEU:HA	1:D:193:ASN:HB2	1.36	1.06
1:B:82:ARG:H	1:B:153:LEU:HD21	1.23	1.03
1:C:84:ARG:HH21	1:C:143:VAL:HG22	1.23	1.02
1:A:86:VAL:HG23	1:A:195:VAL:HG11	1.37	1.02
1:D:57:LEU:HD11	1:D:125:ALA:HB1	1.44	0.98
1:D:82:ARG:HA	1:D:85:LEU:HD13	1.44	0.97
1:B:80:THR:HG21	1:B:152:SER:HB3	1.43	0.97
1:C:52:LYS:H	1:C:52:LYS:HD2	1.29	0.96
1:B:17:ALA:HA	1:B:34:ILE:HD11	1.49	0.95
1:C:71:VAL:HG21	1:C:92:HIS:HB2	1.50	0.94
1:A:93:LEU:HB3	1:A:97:MET:HE3	1.48	0.93
1:B:141:ARG:HB2	1:B:162:THR:HG21	1.51	0.91
1:D:18:ALA:HB2	1:D:59:VAL:HG21	1.54	0.90
1:C:183:THR:HG22	1:C:184:LEU:H	1.38	0.88
1:B:130:ASN:HA	1:B:133:ARG:HG3	1.55	0.88
1:D:49:PHE:HB3	1:D:55:ILE:HG22	1.54	0.87
1:D:71:VAL:HG22	1:D:91:ALA:HB3	1.56	0.87
1:B:64:MET:O	1:B:68:ARG:N	2.08	0.86
1:D:82:ARG:H	1:D:152:SER:HB3	1.40	0.86
1:B:24:HIS:HB2	1:B:29:THR:HG23	1.57	0.85
1:A:168:ASN:HB3	1:A:198:LEU:HD11	1.58	0.85
1:C:196:ASP:HA	1:C:199:ILE:HG22	1.59	0.84
1:A:137:GLU:CG	1:A:166:LEU:HD13	2.06	0.84
1:C:40:ALA:CB	1:C:44:LEU:HD12	2.07	0.83
1:C:102:TYR:O	1:C:106:VAL:HG13	1.77	0.83
1:D:16:ALA:HB1	1:D:37:GLN:HG3	1.61	0.83
1:C:67:VAL:HG22	1:C:95:ASN:CB	2.08	0.83
1:B:31:ILE:HG12	1:B:52:LYS:HG2	1.61	0.82
1:A:93:LEU:HD22	1:A:172:VAL:HG21	1.61	0.82
1:A:13:ILE:HD12	1:A:45:ILE:CD1	2.10	0.81
1:B:31:ILE:HG21	1:B:46:TYR:CE1	2.16	0.81
1:B:90:VAL:HG23	1:B:195:VAL:HG21	1.63	0.80
1:D:139:MET:O	1:D:143:VAL:HG23	1.83	0.79
1:A:80:THR:CG2	1:A:83:GLU:HG3	2.13	0.79
1:D:22:MET:HE3	1:D:101:GLY:HA2	1.63	0.79
1:C:141:ARG:NH2	1:C:159:ALA:HB2	1.98	0.79
1:B:134:ARG:O	1:B:138:LEU:HD23	1.82	0.79
1:D:85:LEU:CD1	1:D:143:VAL:HG12	2.14	0.78
1:A:160:LEU:HD23	1:B:197:LEU:HD22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:PHE:HZ	1:D:126:LEU:HD12	1.49	0.78
1:C:99:GLU:HB3	1:C:102:TYR:HB2	1.66	0.78
1:A:13:ILE:HD13	1:A:38:VAL:HG21	1.66	0.77
1:C:53:PHE:CZ	1:C:57:LEU:HD11	2.20	0.76
1:C:141:ARG:HG3	1:C:162:THR:HG21	1.66	0.76
1:A:202:MET:HG2	1:B:199:ILE:O	1.85	0.76
1:B:82:ARG:N	1:B:153:LEU:HD21	1.99	0.76
1:A:26:PHE:HB2	1:A:108:GLN:HE22	1.49	0.76
1:D:148:ILE:HB	1:D:155:VAL:HG12	1.68	0.76
1:A:103:HIS:O	1:A:106:VAL:HG22	1.86	0.76
1:C:133:ARG:O	1:C:137:GLU:HG2	1.86	0.76
1:A:13:ILE:CD1	1:A:38:VAL:HG21	2.17	0.75
1:A:90:VAL:O	1:A:94:GLU:HG3	1.87	0.75
1:C:70:ARG:O	1:C:91:ALA:HB1	1.87	0.75
1:C:74:HIS:CD2	1:C:88:MET:HG2	2.21	0.75
1:D:22:MET:HG2	1:D:104:HIS:ND1	2.00	0.75
1:C:103:HIS:O	1:C:106:VAL:HG22	1.87	0.75
1:C:71:VAL:HG13	1:C:88:MET:O	1.87	0.75
1:D:85:LEU:HG	1:D:143:VAL:HG12	1.67	0.75
1:C:74:HIS:HB2	1:C:88:MET:SD	2.26	0.74
1:B:23:VAL:HG23	1:B:24:HIS:CD2	2.22	0.74
1:A:190:LEU:O	1:A:194:VAL:HG23	1.88	0.74
1:B:71:VAL:CG1	1:B:139:MET:HE1	2.12	0.74
1:C:74:HIS:HD2	1:C:88:MET:HG2	1.53	0.74
1:D:140:PHE:O	1:D:144:VAL:HG23	1.88	0.74
1:A:168:ASN:HB3	1:A:198:LEU:CD1	2.16	0.73
1:C:84:ARG:NH2	1:C:143:VAL:HG22	2.02	0.73
1:B:17:ALA:CA	1:B:34:ILE:HD11	2.18	0.73
1:B:67:VAL:HG23	1:B:95:ASN:HD22	1.53	0.73
1:B:161:ALA:O	1:B:165:LEU:N	2.19	0.73
1:A:13:ILE:HD12	1:A:45:ILE:HD11	1.71	0.73
1:C:93:LEU:HB3	1:C:191:ALA:HB1	1.71	0.72
1:A:184:LEU:HA	1:A:187:ILE:HG12	1.71	0.72
1:D:21:PHE:CE1	1:D:29:THR:HG21	2.25	0.72
1:C:22:MET:HG3	1:C:104:HIS:CG	2.25	0.72
1:D:60:TYR:CE1	1:D:129:LEU:HB3	2.25	0.71
1:B:179:ILE:O	1:B:182:GLN:NE2	2.23	0.71
1:D:85:LEU:HD11	1:D:143:VAL:O	1.89	0.71
1:A:84:ARG:NH2	1:A:146:GLU:OE1	2.23	0.71
1:C:141:ARG:HH21	1:C:159:ALA:HB2	1.55	0.71
1:B:71:VAL:HG11	1:B:136:TYR:CZ	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:O	1:A:86:VAL:HG12	1.90	0.71
1:C:52:LYS:HD2	1:C:52:LYS:N	2.04	0.71
1:B:67:VAL:HG23	1:B:95:ASN:ND2	2.05	0.71
1:B:145:ALA:HA	1:B:148:ILE:HG12	1.71	0.71
1:C:88:MET:HB3	1:C:140:PHE:HZ	1.55	0.71
1:C:90:VAL:HA	1:C:93:LEU:HB2	1.71	0.71
1:D:86:VAL:O	1:D:90:VAL:HG13	1.91	0.70
1:A:41:THR:OG1	1:A:44:LEU:HB2	1.89	0.70
1:B:184:LEU:HD23	1:B:184:LEU:O	1.92	0.70
1:A:84:ARG:O	1:A:88:MET:HG3	1.90	0.70
1:D:49:PHE:CB	1:D:55:ILE:HG22	2.21	0.70
1:A:141:ARG:O	1:A:144:VAL:HG22	1.91	0.70
1:C:159:ALA:O	1:C:163:ARG:HG2	1.91	0.70
1:D:57:LEU:HD11	1:D:125:ALA:CB	2.19	0.70
1:A:173:ASP:OD1	1:A:174:MET:N	2.25	0.69
1:C:96:LEU:HD21	1:C:173:ASP:HB3	1.72	0.69
1:C:148:ILE:HG12	1:C:155:VAL:HG22	1.72	0.69
1:D:191:ALA:O	1:D:195:VAL:HG23	1.92	0.69
1:D:128:ALA:O	1:D:132:LEU:HD13	1.92	0.69
1:A:93:LEU:HB3	1:A:97:MET:CE	2.21	0.69
1:D:60:TYR:HE1	1:D:129:LEU:HB3	1.57	0.69
1:A:183:THR:O	1:A:187:ILE:HG23	1.93	0.69
1:B:31:ILE:CG1	1:B:52:LYS:HG2	2.22	0.69
1:B:70:ARG:HD3	1:B:95:ASN:HB2	1.74	0.69
1:C:156:VAL:HG12	1:C:157:ASP:H	1.58	0.69
1:C:55:ILE:O	1:C:59:VAL:HG12	1.92	0.69
1:B:80:THR:HG21	1:B:152:SER:CB	2.21	0.69
1:D:145:ALA:O	1:D:148:ILE:HG12	1.93	0.69
1:B:10:LYS:HE2	1:B:48:HIS:HD2	1.57	0.68
1:B:74:HIS:HB2	1:B:88:MET:HB3	1.76	0.68
1:B:141:ARG:NH1	1:B:158:GLU:O	2.24	0.68
1:A:94:GLU:O	1:A:98:THR:HG23	1.94	0.68
1:D:82:ARG:HB3	1:D:152:SER:CB	2.24	0.68
1:D:88:MET:SD	1:D:143:VAL:HG21	2.34	0.68
1:C:199:ILE:HG23	1:C:200:THR:HG23	1.74	0.67
1:C:103:HIS:HA	1:C:106:VAL:HG22	1.74	0.67
1:D:22:MET:CE	1:D:101:GLY:HA2	2.24	0.67
1:D:197:LEU:HD23	1:D:197:LEU:O	1.94	0.67
1:B:59:VAL:CG2	1:B:105:VAL:HG21	2.25	0.67
1:C:120:ILE:HG23	1:C:121:ARG:H	1.59	0.67
1:D:96:LEU:HD21	1:D:170:ASN:HA	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ALA:HB2	1:B:82:ARG:HG3	1.76	0.67
1:B:128:ALA:O	1:B:132:LEU:HG	1.94	0.67
1:D:122:GLN:O	1:D:126:LEU:HB3	1.95	0.67
1:A:96:LEU:HD12	1:A:103:HIS:CE1	2.30	0.67
1:B:103:HIS:O	1:B:106:VAL:HG22	1.95	0.67
1:D:97:MET:SD	1:D:187:ILE:HG23	2.34	0.67
1:A:88:MET:SD	1:A:143:VAL:HG21	2.36	0.66
1:B:184:LEU:O	1:B:187:ILE:HG12	1.95	0.66
1:D:21:PHE:CE2	1:D:56:PHE:HB2	2.30	0.66
1:D:85:LEU:CG	1:D:143:VAL:HG12	2.25	0.66
1:C:85:LEU:HD23	1:C:199:ILE:HD11	1.76	0.66
1:C:112:TYR:C	1:C:113:GLN:HG3	2.16	0.66
1:D:71:VAL:O	1:D:74:HIS:HB2	1.95	0.66
1:B:71:VAL:HG11	1:B:136:TYR:OH	1.94	0.66
1:B:89:SER:O	1:B:93:LEU:HD23	1.96	0.66
1:C:101:GLY:O	1:C:105:VAL:HG22	1.94	0.66
1:C:161:ALA:HA	1:C:164:THR:HG22	1.78	0.66
1:A:71:VAL:CG1	1:A:88:MET:HB3	2.26	0.66
1:C:13:ILE:HG21	1:C:45:ILE:HD13	1.78	0.66
1:C:62:ASP:OD1	1:C:65:ARG:HD3	1.95	0.66
1:D:97:MET:HB3	1:D:176:TYR:CE2	2.31	0.66
1:B:183:THR:O	1:B:187:ILE:HG23	1.95	0.66
1:D:56:PHE:HA	1:D:59:VAL:HG12	1.77	0.66
1:A:166:LEU:HA	1:A:169:LEU:HD12	1.78	0.65
1:D:116:THR:HG23	1:D:116:THR:O	1.95	0.65
1:C:99:GLU:O	1:C:102:TYR:N	2.30	0.65
1:D:40:ALA:HB1	1:D:44:LEU:HD21	1.77	0.65
1:D:90:VAL:HG13	1:D:195:VAL:HG11	1.78	0.65
1:B:125:ALA:O	1:B:129:LEU:HD12	1.96	0.65
1:C:84:ARG:O	1:C:88:MET:HG3	1.96	0.65
1:D:82:ARG:CA	1:D:85:LEU:HD13	2.24	0.65
1:B:34:ILE:O	1:B:38:VAL:HG22	1.96	0.65
1:A:55:ILE:O	1:A:59:VAL:HG12	1.96	0.65
1:B:145:ALA:HA	1:B:148:ILE:CG1	2.27	0.65
1:D:53:PHE:CZ	1:D:126:LEU:HD12	2.31	0.65
1:D:82:ARG:HB2	1:D:153:LEU:HB3	1.79	0.65
1:C:184:LEU:HD23	1:C:184:LEU:O	1.97	0.65
1:A:93:LEU:CD2	1:A:172:VAL:HG21	2.26	0.65
1:D:118:LEU:HA	1:D:122:GLN:CB	2.26	0.64
1:B:90:VAL:HG22	1:B:191:ALA:O	1.98	0.64
1:C:14:LEU:HD11	1:C:49:PHE:HZ	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:MET:HG2	1:B:104:HIS:CG	2.32	0.64
1:B:60:TYR:CD1	1:B:106:VAL:HA	2.32	0.64
1:C:84:ARG:HB3	1:C:143:VAL:HG11	1.80	0.64
1:A:85:LEU:HD21	1:A:165:LEU:HD22	1.80	0.64
1:D:75:ALA:HB2	1:D:88:MET:SD	2.38	0.64
1:B:14:LEU:HD11	1:B:49:PHE:HZ	1.63	0.64
1:B:69:GLU:O	1:B:73:PRO:HD3	1.98	0.64
1:C:200:THR:HA	1:D:203:ALA:HB3	1.80	0.64
1:A:201:GLY:HA3	1:B:201:GLY:CA	2.27	0.64
1:B:59:VAL:HG22	1:B:105:VAL:HG21	1.79	0.63
1:B:85:LEU:HG	1:B:143:VAL:HG22	1.80	0.63
1:D:18:ALA:CB	1:D:59:VAL:HG21	2.27	0.63
1:B:60:TYR:CD2	1:B:129:LEU:HD22	2.34	0.63
1:D:137:GLU:HA	1:D:166:LEU:HD11	1.80	0.63
1:D:177:ARG:HB2	1:D:177:ARG:NH1	2.14	0.63
1:B:14:LEU:HD21	1:B:58:ALA:HB1	1.81	0.62
1:B:145:ALA:O	1:B:148:ILE:HG13	1.99	0.62
1:C:134:ARG:O	1:C:137:GLU:HB2	1.99	0.62
1:A:85:LEU:HD21	1:A:165:LEU:CD2	2.29	0.62
1:D:141:ARG:CB	1:D:162:THR:HG21	2.30	0.62
1:D:21:PHE:HE1	1:D:29:THR:HG21	1.64	0.62
1:B:82:ARG:HB2	1:B:153:LEU:CD1	2.28	0.62
1:B:166:LEU:HA	1:B:169:LEU:HD12	1.81	0.62
1:A:64:MET:O	1:A:67:VAL:HG12	2.00	0.62
1:A:18:ALA:HB2	1:A:59:VAL:HG21	1.82	0.62
1:B:59:VAL:HG23	1:B:102:TYR:CD2	2.34	0.62
1:D:71:VAL:HG22	1:D:91:ALA:CB	2.30	0.61
1:A:86:VAL:HG23	1:A:195:VAL:CG1	2.21	0.61
1:C:15:ASP:OD1	1:C:16:ALA:N	2.33	0.61
1:B:31:ILE:HG21	1:B:46:TYR:HE1	1.61	0.61
1:A:60:TYR:CE2	1:A:129:LEU:HB3	2.35	0.61
1:B:96:LEU:HG	1:B:103:HIS:CG	2.35	0.61
1:C:148:ILE:HG23	1:C:155:VAL:HG21	1.82	0.61
1:D:129:LEU:HD22	1:D:132:LEU:HD22	1.82	0.61
1:B:178:ARG:O	1:B:178:ARG:HG2	2.00	0.61
1:C:112:TYR:O	1:C:113:GLN:HG3	2.01	0.61
1:D:92:HIS:CD2	1:D:169:LEU:HB3	2.35	0.61
1:A:22:MET:SD	1:A:100:LEU:HD22	2.41	0.61
1:B:18:ALA:HB1	1:B:101:GLY:C	2.21	0.61
1:C:183:THR:O	1:C:187:ILE:N	2.34	0.61
1:D:82:ARG:HB3	1:D:152:SER:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MET:SD	1:A:190:LEU:HD22	2.41	0.60
1:A:199:ILE:O	1:B:202:MET:N	2.28	0.60
1:B:172:VAL:HA	1:B:175:TRP:CD1	2.36	0.60
1:D:96:LEU:O	1:D:100:LEU:HD13	2.01	0.60
1:C:14:LEU:HD11	1:C:49:PHE:CZ	2.37	0.60
1:A:165:LEU:O	1:A:169:LEU:HD12	2.01	0.60
1:D:63:GLY:HA3	1:D:102:TYR:HB3	1.83	0.60
1:C:104:HIS:ND1	1:C:173:ASP:OD2	2.35	0.60
1:B:85:LEU:HD11	1:B:144:VAL:CG2	2.31	0.60
1:C:88:MET:HB3	1:C:140:PHE:CZ	2.35	0.60
1:C:160:LEU:HD21	1:D:197:LEU:HD13	1.84	0.60
1:D:147:GLY:HA3	1:D:153:LEU:CD2	2.31	0.60
1:C:154:ARG:HE	1:C:156:VAL:HG22	1.67	0.60
1:C:184:LEU:HD23	1:C:188:ASN:HB2	1.84	0.60
1:C:53:PHE:HE2	1:C:122:GLN:CB	2.15	0.60
1:D:49:PHE:CG	1:D:55:ILE:HG22	2.37	0.60
1:D:164:THR:O	1:D:168:ASN:ND2	2.35	0.60
1:C:62:ASP:HB3	1:C:102:TYR:HE1	1.67	0.60
1:C:71:VAL:HG12	1:C:140:PHE:CZ	2.37	0.60
1:A:199:ILE:HG22	1:B:202:MET:HE3	1.84	0.60
1:C:148:ILE:HG23	1:C:155:VAL:CG2	2.32	0.60
1:A:66:ARG:O	1:A:69:GLU:HG2	2.02	0.59
1:C:52:LYS:H	1:C:52:LYS:CD	2.09	0.59
1:C:126:LEU:HD23	1:C:126:LEU:O	2.02	0.59
1:A:25:GLY:O	1:A:29:THR:HG22	2.03	0.59
1:A:160:LEU:O	1:A:164:THR:HG22	2.00	0.59
1:B:82:ARG:HB2	1:B:153:LEU:CD2	2.32	0.59
1:C:22:MET:HB2	1:C:105:VAL:HG13	1.83	0.59
1:D:103:HIS:HA	1:D:106:VAL:CB	2.32	0.59
1:D:147:GLY:HA3	1:D:153:LEU:HD23	1.83	0.59
1:B:82:ARG:CA	1:B:153:LEU:HD11	2.32	0.59
1:D:95:ASN:O	1:D:99:GLU:N	2.32	0.59
1:A:26:PHE:HA	1:A:29:THR:HG22	1.83	0.59
1:C:13:ILE:HA	1:C:38:VAL:HG11	1.85	0.59
1:D:30:THR:O	1:D:33:ASP:N	2.34	0.59
1:A:203:ALA:H	1:B:154:ARG:H	1.51	0.59
1:C:71:VAL:HG12	1:C:140:PHE:HZ	1.66	0.59
1:B:82:ARG:HA	1:B:153:LEU:HD11	1.84	0.59
1:B:93:LEU:HB3	1:B:97:MET:HE3	1.85	0.59
1:A:169:LEU:O	1:A:172:VAL:HG22	2.03	0.59
1:C:71:VAL:HG22	1:C:92:HIS:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:THR:HG22	1:C:184:LEU:N	2.11	0.59
1:D:18:ALA:HB2	1:D:59:VAL:CG2	2.32	0.58
1:C:67:VAL:HG21	1:C:92:HIS:CE1	2.38	0.58
1:C:84:ARG:HB3	1:C:143:VAL:CG1	2.33	0.58
1:C:160:LEU:O	1:C:164:THR:HB	2.04	0.58
1:A:53:PHE:CE1	1:A:57:LEU:HD21	2.37	0.58
1:D:22:MET:CE	1:D:100:LEU:HG	2.33	0.58
1:B:60:TYR:HD1	1:B:106:VAL:HA	1.67	0.58
1:C:18:ALA:HB2	1:C:59:VAL:HG21	1.86	0.58
1:B:66:ARG:HB3	1:B:99:GLU:OE1	2.04	0.58
1:B:192:THR:O	1:B:195:VAL:HG22	2.02	0.58
1:B:93:LEU:HB3	1:B:97:MET:CE	2.34	0.58
1:C:45:ILE:CG2	1:C:55:ILE:HD11	2.33	0.58
1:D:82:ARG:NH1	1:D:83:GLU:HG2	2.19	0.58
1:D:100:LEU:HD11	1:D:173:ASP:HB2	1.85	0.58
1:C:200:THR:C	1:D:201:GLY:HA3	2.24	0.57
1:D:21:PHE:HE2	1:D:56:PHE:HB2	1.68	0.57
1:A:35:ALA:HA	1:A:38:VAL:CG1	2.34	0.57
1:A:72:GLU:HA	1:A:139:MET:HE2	1.86	0.57
1:C:22:MET:HG3	1:C:104:HIS:HB3	1.86	0.57
1:C:198:LEU:HD11	1:D:168:ASN:HD21	1.67	0.57
1:D:110:VAL:HG12	1:D:110:VAL:O	2.04	0.57
1:A:184:LEU:HD12	1:A:184:LEU:H	1.70	0.57
1:C:22:MET:HG3	1:C:104:HIS:CD2	2.39	0.57
1:B:66:ARG:HD3	1:B:99:GLU:OE1	2.04	0.57
1:C:7:ILE:HB	1:C:11:THR:HG23	1.87	0.57
1:C:17:ALA:HB2	1:C:34:ILE:HD13	1.86	0.57
1:B:24:HIS:HB2	1:B:29:THR:CG2	2.32	0.57
1:A:156:VAL:HG21	1:B:197:LEU:HG	1.86	0.57
1:C:99:GLU:CB	1:C:102:TYR:HB2	2.34	0.57
1:A:35:ALA:HA	1:A:38:VAL:HG12	1.86	0.57
1:A:196:ASP:O	1:A:200:THR:HG23	2.05	0.57
1:C:88:MET:O	1:C:91:ALA:HB3	2.05	0.57
1:D:140:PHE:CE1	1:D:165:LEU:HG	2.39	0.57
1:B:147:GLY:HA3	1:B:153:LEU:CD2	2.35	0.56
1:D:7:ILE:O	1:D:11:THR:HG22	2.05	0.56
1:B:84:ARG:O	1:B:88:MET:HG2	2.05	0.56
1:D:49:PHE:HB3	1:D:55:ILE:CG2	2.32	0.56
1:D:72:GLU:HB3	1:D:73:PRO:HD3	1.87	0.56
1:D:54:ASP:O	1:D:58:ALA:N	2.38	0.56
1:A:53:PHE:O	1:A:56:PHE:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ALA:O	1:C:61:GLU:HB3	2.04	0.56
1:D:81:GLY:O	1:D:85:LEU:HD12	2.05	0.56
1:D:82:ARG:O	1:D:85:LEU:HB2	2.06	0.56
1:B:31:ILE:HD11	1:B:52:LYS:HA	1.87	0.56
1:C:17:ALA:CB	1:C:34:ILE:HD13	2.36	0.56
1:A:104:HIS:NE2	1:A:108:GLN:HG3	2.21	0.56
1:B:53:PHE:CE2	1:B:118:LEU:HD11	2.41	0.56
1:C:82:ARG:CB	1:C:153:LEU:HG	2.36	0.56
1:B:137:GLU:HB2	1:B:166:LEU:CD1	2.35	0.56
1:D:75:ALA:HB2	1:D:88:MET:CE	2.35	0.56
1:D:82:ARG:HB3	1:D:152:SER:OG	2.05	0.56
1:D:63:GLY:O	1:D:67:VAL:HG22	2.06	0.55
1:A:13:ILE:HD12	1:A:45:ILE:HD12	1.86	0.55
1:A:53:PHE:HE1	1:A:57:LEU:HD21	1.71	0.55
1:D:37:GLN:OE1	1:D:37:GLN:HA	2.05	0.55
1:C:31:ILE:CG2	1:C:42:LYS:HG2	2.37	0.55
1:D:97:MET:HB3	1:D:176:TYR:CZ	2.41	0.55
1:D:148:ILE:CB	1:D:155:VAL:HG12	2.36	0.55
1:A:160:LEU:CD2	1:B:197:LEU:HD22	2.35	0.55
1:C:154:ARG:HB3	1:D:202:MET:HA	1.88	0.55
1:D:14:LEU:HD21	1:D:49:PHE:CZ	2.42	0.55
1:C:11:THR:HA	1:C:14:LEU:HD22	1.88	0.55
1:D:96:LEU:HD11	1:D:170:ASN:OD1	2.07	0.55
1:C:96:LEU:HD21	1:C:173:ASP:CB	2.35	0.55
1:A:56:PHE:HA	1:A:59:VAL:CG1	2.37	0.55
1:A:152:SER:O	1:A:153:LEU:HD23	2.07	0.55
1:B:14:LEU:HD21	1:B:58:ALA:CB	2.36	0.55
1:B:60:TYR:OH	1:B:133:ARG:HD2	2.07	0.55
1:C:62:ASP:HB3	1:C:102:TYR:CE1	2.41	0.54
1:D:22:MET:HE2	1:D:100:LEU:HG	1.88	0.54
1:C:120:ILE:HG23	1:C:121:ARG:N	2.22	0.54
1:C:147:GLY:HA2	1:C:150:ASP:OD2	2.07	0.54
1:B:59:VAL:HG22	1:B:105:VAL:CG2	2.38	0.54
1:C:69:GLU:OE1	1:C:69:GLU:HA	2.07	0.54
1:D:83:GLU:HA	1:D:86:VAL:HG22	1.89	0.54
1:B:94:GLU:HA	1:B:97:MET:HG3	1.89	0.54
1:C:200:THR:O	1:D:201:GLY:HA3	2.06	0.54
1:D:70:ARG:O	1:D:70:ARG:HG3	2.06	0.54
1:A:31:ILE:HD12	1:A:31:ILE:H	1.72	0.54
1:D:60:TYR:CD2	1:D:106:VAL:HA	2.43	0.54
1:D:97:MET:HE2	1:D:187:ILE:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:GLU:HG3	1:D:190:LEU:CD1	2.37	0.54
1:A:134:ARG:O	1:A:138:LEU:HD13	2.07	0.54
1:A:22:MET:HG3	1:A:104:HIS:CD2	2.43	0.54
1:B:141:ARG:HH11	1:B:158:GLU:HG2	1.72	0.54
1:C:13:ILE:HG21	1:C:45:ILE:CD1	2.37	0.54
1:C:85:LEU:HD23	1:C:153:LEU:HD11	1.89	0.53
1:A:85:LEU:HD13	1:A:144:VAL:HG12	1.89	0.53
1:B:130:ASN:CA	1:B:133:ARG:HG3	2.34	0.53
1:A:60:TYR:CG	1:A:129:LEU:HD12	2.44	0.53
1:B:10:LYS:HA	1:B:13:ILE:HD12	1.89	0.53
1:B:166:LEU:HD23	1:B:169:LEU:HD12	1.91	0.53
1:C:158:GLU:O	1:C:162:THR:N	2.31	0.53
1:D:96:LEU:CD2	1:D:170:ASN:HA	2.37	0.53
1:A:160:LEU:HD23	1:B:197:LEU:CD2	2.37	0.53
1:B:85:LEU:HD11	1:B:144:VAL:HG22	1.89	0.53
1:C:96:LEU:C	1:C:96:LEU:HD23	2.29	0.53
1:C:160:LEU:HD11	1:D:194:VAL:HG13	1.90	0.53
1:D:90:VAL:HG12	1:D:195:VAL:HG21	1.90	0.53
1:D:177:ARG:HB2	1:D:177:ARG:HH11	1.73	0.53
1:A:23:VAL:HG13	1:A:24:HIS:H	1.72	0.53
1:B:96:LEU:HD21	1:B:103:HIS:CD2	2.43	0.53
1:C:40:ALA:HB1	1:C:44:LEU:CD1	2.18	0.53
1:C:200:THR:HG22	1:D:203:ALA:CB	2.39	0.53
1:D:41:THR:HG22	1:D:44:LEU:HD23	1.90	0.53
1:D:82:ARG:H	1:D:152:SER:CB	2.16	0.53
1:D:90:VAL:CG1	1:D:195:VAL:HG11	2.38	0.53
1:B:85:LEU:HG	1:B:143:VAL:CG2	2.38	0.53
1:A:126:LEU:HD23	1:A:126:LEU:O	2.09	0.53
1:B:99:GLU:CG	1:B:99:GLU:O	2.57	0.53
1:B:24:HIS:CB	1:B:29:THR:HG23	2.36	0.52
1:B:175:TRP:HH2	1:B:190:LEU:HD21	1.74	0.52
1:C:61:GLU:O	1:C:65:ARG:HB3	2.09	0.52
1:C:204:ASN:CB	1:D:154:ARG:HE	2.22	0.52
1:B:171:ALA:O	1:B:174:MET:HG2	2.08	0.52
1:B:90:VAL:CG2	1:B:192:THR:HA	2.39	0.52
1:A:191:ALA:O	1:A:195:VAL:HG23	2.09	0.52
1:D:21:PHE:CD1	1:D:29:THR:HG21	2.44	0.52
1:D:115:SER:O	1:D:116:THR:HG22	2.09	0.52
1:A:199:ILE:HG22	1:B:202:MET:CE	2.40	0.52
1:B:14:LEU:HD11	1:B:49:PHE:CZ	2.44	0.52
1:D:55:ILE:HG13	1:D:56:PHE:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SER:HB2	1:A:169:LEU:HD21	1.92	0.52
1:C:53:PHE:CE1	1:C:57:LEU:HD21	2.45	0.52
1:C:166:LEU:O	1:C:170:ASN:HB2	2.10	0.52
1:C:172:VAL:HG13	1:C:175:TRP:NE1	2.25	0.52
1:C:161:ALA:HA	1:C:164:THR:CG2	2.39	0.52
1:A:71:VAL:HG13	1:A:88:MET:HB3	1.91	0.52
1:B:60:TYR:CD1	1:B:106:VAL:HG12	2.45	0.52
1:B:64:MET:HA	1:B:67:VAL:HG12	1.92	0.51
1:B:90:VAL:CG2	1:B:195:VAL:HG21	2.38	0.51
1:C:9:VAL:HG22	1:C:48:HIS:NE2	2.25	0.51
1:A:201:GLY:HA3	1:B:201:GLY:HA2	1.92	0.51
1:C:30:THR:HG23	1:C:32:ASP:HB2	1.91	0.51
1:C:60:TYR:CE1	1:C:106:VAL:HB	2.45	0.51
1:A:195:VAL:O	1:A:198:LEU:HB2	2.11	0.51
1:C:62:ASP:O	1:C:65:ARG:HG2	2.10	0.51
1:D:192:THR:HA	1:D:195:VAL:HB	1.92	0.51
1:A:10:LYS:HB2	1:A:10:LYS:NZ	2.25	0.51
1:B:88:MET:SD	1:B:143:VAL:HG11	2.51	0.51
1:B:93:LEU:O	1:B:97:MET:HG3	2.10	0.51
1:D:80:THR:CG2	1:D:83:GLU:HB2	2.40	0.51
1:D:34:ILE:CD1	1:D:55:ILE:HD11	2.41	0.51
1:D:67:VAL:CG1	1:D:95:ASN:HD22	2.23	0.51
1:B:96:LEU:HD21	1:B:103:HIS:NE2	2.26	0.51
1:C:137:GLU:OE1	1:C:166:LEU:HD11	2.10	0.51
1:D:135:ASP:O	1:D:138:LEU:HB3	2.10	0.51
1:A:61:GLU:CA	1:A:129:LEU:HD11	2.40	0.51
1:B:64:MET:O	1:B:67:VAL:HG12	2.10	0.51
1:C:22:MET:HG3	1:C:104:HIS:CB	2.41	0.51
1:C:135:ASP:OD1	1:C:138:LEU:HD12	2.11	0.51
1:D:86:VAL:HG11	1:D:196:ASP:OD1	2.10	0.51
1:D:104:HIS:CD2	1:D:173:ASP:HB2	2.46	0.51
1:B:90:VAL:HG22	1:B:192:THR:HA	1.92	0.51
1:C:75:ALA:HB2	1:C:88:MET:HE1	1.91	0.51
1:A:92:HIS:HE1	1:A:103:HIS:NE2	2.09	0.51
1:C:93:LEU:HB3	1:C:191:ALA:CB	2.40	0.51
1:D:148:ILE:HB	1:D:155:VAL:CG1	2.40	0.51
1:D:133:ARG:HG2	1:D:133:ARG:HH11	1.74	0.51
1:A:158:GLU:O	1:A:162:THR:HG22	2.11	0.50
1:A:187:ILE:HG13	1:A:188:ASN:N	2.26	0.50
1:B:10:LYS:HE2	1:B:48:HIS:CD2	2.44	0.50
1:B:137:GLU:HB2	1:B:166:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:ARG:HE	1:C:156:VAL:CG2	2.23	0.50
1:C:161:ALA:O	1:C:164:THR:HG22	2.10	0.50
1:D:104:HIS:NE2	1:D:173:ASP:HB2	2.26	0.50
1:A:71:VAL:HG22	1:A:91:ALA:HB3	1.93	0.50
1:A:102:TYR:O	1:A:106:VAL:HG13	2.10	0.50
1:B:10:LYS:O	1:B:14:LEU:HD12	2.11	0.50
1:C:121:ARG:HD2	1:C:124:ASP:HB3	1.93	0.50
1:C:204:ASN:N	1:D:154:ARG:HG3	2.25	0.50
1:D:97:MET:CE	1:D:187:ILE:HG13	2.41	0.50
1:B:180:GLU:OE1	1:B:180:GLU:N	2.45	0.50
1:C:16:ALA:HB1	1:C:37:GLN:CG	2.42	0.50
1:A:166:LEU:HA	1:A:169:LEU:CD1	2.42	0.50
1:C:148:ILE:HA	1:C:155:VAL:HG22	1.92	0.50
1:A:182:GLN:OE1	1:A:187:ILE:HG22	2.11	0.50
1:C:96:LEU:HD23	1:C:96:LEU:O	2.12	0.50
1:A:10:LYS:HG3	1:A:49:PHE:CZ	2.46	0.50
1:C:10:LYS:O	1:C:14:LEU:HD13	2.12	0.50
1:A:86:VAL:HA	1:A:89:SER:OG	2.10	0.50
1:D:22:MET:HG2	1:D:104:HIS:CG	2.46	0.50
1:D:100:LEU:HD11	1:D:173:ASP:CB	2.42	0.50
1:A:95:ASN:ND2	1:A:99:GLU:HB2	2.27	0.49
1:D:28:ASN:HD22	1:D:28:ASN:C	2.15	0.49
1:B:80:THR:HG23	1:B:153:LEU:HD21	1.94	0.49
1:D:148:ILE:CA	1:D:155:VAL:HG12	2.41	0.49
1:B:31:ILE:CD1	1:B:52:LYS:HG2	2.41	0.49
1:D:95:ASN:OD1	1:D:96:LEU:N	2.45	0.49
1:A:10:LYS:HG3	1:A:49:PHE:HZ	1.76	0.49
1:A:89:SER:CB	1:A:169:LEU:HD21	2.43	0.49
1:A:194:VAL:O	1:A:198:LEU:HD23	2.12	0.49
1:D:67:VAL:HG11	1:D:95:ASN:HD22	1.78	0.49
1:D:82:ARG:HH11	1:D:82:ARG:HG2	1.78	0.49
1:C:103:HIS:CA	1:C:106:VAL:HG22	2.40	0.49
1:D:67:VAL:HB	1:D:95:ASN:HD22	1.78	0.49
1:B:15:ASP:OD1	1:B:102:TYR:HE1	1.95	0.49
1:B:59:VAL:HG23	1:B:102:TYR:CE2	2.48	0.49
1:B:126:LEU:HA	1:B:129:LEU:HD12	1.94	0.49
1:C:192:THR:O	1:C:195:VAL:HG12	2.13	0.49
1:D:72:GLU:O	1:D:75:ALA:N	2.46	0.49
1:B:85:LEU:HD11	1:B:144:VAL:HG23	1.94	0.49
1:A:60:TYR:O	1:A:64:MET:HB3	2.12	0.49
1:A:172:VAL:O	1:A:176:TYR:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:PHE:HA	1:C:59:VAL:CG1	2.43	0.49
1:A:53:PHE:CE2	1:A:118:LEU:HD13	2.48	0.48
1:A:105:VAL:HA	1:A:108:GLN:HB2	1.94	0.48
1:B:22:MET:HA	1:B:104:HIS:CE1	2.48	0.48
1:B:95:ASN:OD1	1:B:99:GLU:HB3	2.12	0.48
1:C:194:VAL:HA	1:C:197:LEU:HB3	1.95	0.48
1:D:176:TYR:CZ	1:D:178:ARG:HA	2.48	0.48
1:D:30:THR:O	1:D:33:ASP:HB2	2.13	0.48
1:A:53:PHE:O	1:A:56:PHE:N	2.47	0.48
1:B:92:HIS:HD2	1:B:96:LEU:HD22	1.78	0.48
1:B:107:HIS:O	1:B:110:VAL:HG22	2.13	0.48
1:D:104:HIS:HE2	1:D:173:ASP:HB2	1.78	0.48
1:D:140:PHE:HE1	1:D:165:LEU:HD21	1.78	0.48
1:A:26:PHE:HA	1:A:29:THR:CG2	2.43	0.48
1:A:72:GLU:HA	1:A:139:MET:CE	2.43	0.48
1:B:59:VAL:HG21	1:B:105:VAL:HG21	1.96	0.48
1:B:60:TYR:HD2	1:B:129:LEU:HD22	1.75	0.48
1:B:67:VAL:HG22	1:B:136:TYR:HE2	1.77	0.48
1:B:67:VAL:HB	1:B:95:ASN:HD21	1.79	0.48
1:B:147:GLY:HA3	1:B:153:LEU:HD23	1.95	0.48
1:C:74:HIS:HB2	1:C:88:MET:CE	2.44	0.48
1:B:198:LEU:HD23	1:B:198:LEU:O	2.13	0.47
1:C:154:ARG:N	1:D:202:MET:O	2.47	0.47
1:A:197:LEU:HD23	1:A:197:LEU:H	1.78	0.47
1:D:140:PHE:HE1	1:D:165:LEU:CD2	2.27	0.47
1:D:140:PHE:HE1	1:D:165:LEU:CG	2.27	0.47
1:D:17:ALA:HB2	1:D:34:ILE:HD13	1.97	0.47
1:D:85:LEU:HG	1:D:143:VAL:CG1	2.40	0.47
1:B:144:VAL:O	1:B:148:ILE:HG23	2.15	0.47
1:D:67:VAL:CB	1:D:95:ASN:HD22	2.27	0.47
1:A:31:ILE:HG21	1:A:46:TYR:CE2	2.49	0.47
1:A:121:ARG:O	1:A:121:ARG:NH1	2.47	0.47
1:C:120:ILE:O	1:C:123:ARG:N	2.47	0.47
1:C:156:VAL:HG12	1:C:157:ASP:N	2.27	0.47
1:D:74:HIS:NE2	1:D:91:ALA:HB2	2.29	0.47
1:A:161:ALA:HA	1:B:197:LEU:HD23	1.96	0.47
1:C:22:MET:HB2	1:C:105:VAL:CG1	2.44	0.47
1:D:104:HIS:NE2	1:D:173:ASP:O	2.44	0.47
1:D:190:LEU:HA	1:D:193:ASN:CB	2.25	0.47
1:A:13:ILE:CD1	1:A:45:ILE:CD1	2.88	0.47
1:A:23:VAL:HG13	1:A:24:HIS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:LEU:O	1:C:104:HIS:HB2	2.15	0.47
1:A:105:VAL:HA	1:A:108:GLN:CB	2.45	0.47
1:D:60:TYR:HE2	1:D:106:VAL:O	1.97	0.47
1:A:163:ARG:HD3	1:A:163:ARG:HA	1.67	0.47
1:B:165:LEU:CD1	1:B:198:LEU:HD22	2.45	0.47
1:B:175:TRP:HE3	1:B:175:TRP:O	1.98	0.47
1:D:103:HIS:HA	1:D:106:VAL:H	1.80	0.47
1:C:158:GLU:HG3	1:C:159:ALA:H	1.80	0.46
1:D:19:ASP:OD1	1:D:101:GLY:HA3	2.15	0.46
1:D:106:VAL:O	1:D:133:ARG:HD3	2.15	0.46
1:A:53:PHE:CD1	1:A:53:PHE:C	2.88	0.46
1:A:67:VAL:HB	1:A:95:ASN:OD1	2.14	0.46
1:C:60:TYR:CD1	1:C:106:VAL:HG12	2.50	0.46
1:C:112:TYR:C	1:C:114:ALA:H	2.19	0.46
1:B:168:ASN:CB	1:B:198:LEU:HD11	2.46	0.46
1:C:72:GLU:N	1:C:73:PRO:CD	2.78	0.46
1:A:105:VAL:O	1:A:105:VAL:CG1	2.64	0.46
1:A:125:ALA:O	1:A:129:LEU:HD23	2.16	0.46
1:A:203:ALA:HA	1:B:153:LEU:HA	1.98	0.46
1:D:80:THR:HG23	1:D:80:THR:O	2.15	0.46
1:A:26:PHE:CA	1:A:29:THR:HG22	2.45	0.46
1:A:118:LEU:HD12	1:A:119:LYS:H	1.80	0.46
1:B:56:PHE:CD2	1:B:57:LEU:HD23	2.50	0.46
1:B:118:LEU:HD21	1:B:122:GLN:HB3	1.95	0.46
1:C:67:VAL:HG11	1:C:92:HIS:CE1	2.50	0.46
1:D:85:LEU:O	1:D:88:MET:HB2	2.16	0.46
1:A:86:VAL:HB	1:A:199:ILE:CD1	2.46	0.46
1:B:80:THR:OG1	1:B:147:GLY:HA2	2.15	0.46
1:B:147:GLY:CA	1:B:153:LEU:HD23	2.46	0.46
1:B:154:ARG:HG2	1:B:155:VAL:H	1.80	0.46
1:D:148:ILE:HB	1:D:155:VAL:HA	1.97	0.46
1:D:57:LEU:C	1:D:57:LEU:HD23	2.36	0.46
1:C:31:ILE:HG22	1:C:42:LYS:HG2	1.98	0.46
1:D:13:ILE:HD11	1:D:44:LEU:HD12	1.98	0.46
1:A:37:GLN:O	1:A:37:GLN:HG2	2.16	0.45
1:C:70:ARG:O	1:C:70:ARG:HG3	2.16	0.45
1:C:200:THR:HA	1:D:203:ALA:CB	2.44	0.45
1:D:85:LEU:HD12	1:D:143:VAL:HG12	1.95	0.45
1:D:140:PHE:HE1	1:D:165:LEU:HG	1.80	0.45
1:B:53:PHE:CE1	1:B:57:LEU:HD21	2.52	0.45
1:B:143:VAL:HG22	1:B:143:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ASP:HA	1:D:188:ASN:CB	2.46	0.45
1:B:160:LEU:HD23	1:B:160:LEU:C	2.37	0.45
1:C:70:ARG:HE	1:C:70:ARG:HB2	1.62	0.45
1:D:71:VAL:O	1:D:71:VAL:CG1	2.64	0.45
1:A:96:LEU:HD13	1:A:172:VAL:HG22	1.99	0.45
1:D:80:THR:HG21	1:D:83:GLU:HB2	1.99	0.45
1:B:84:ARG:NE	1:B:146:GLU:OE1	2.48	0.45
1:D:54:ASP:O	1:D:57:LEU:HB3	2.16	0.45
1:D:67:VAL:HG11	1:D:95:ASN:ND2	2.32	0.45
1:D:74:HIS:ND1	1:D:87:ALA:O	2.50	0.45
1:B:60:TYR:HE2	1:B:129:LEU:HB2	1.82	0.45
1:B:161:ALA:HA	1:B:164:THR:HB	1.98	0.45
1:B:82:ARG:HB2	1:B:153:LEU:HD13	1.97	0.45
1:C:168:ASN:HB3	1:C:198:LEU:HD21	1.99	0.45
1:D:71:VAL:O	1:D:71:VAL:HG12	2.16	0.45
1:A:56:PHE:HE2	1:A:108:GLN:OE1	2.00	0.45
1:B:79:GLY:HA3	1:B:83:GLU:CD	2.38	0.45
1:B:154:ARG:HG2	1:B:155:VAL:N	2.31	0.45
1:A:80:THR:HG23	1:A:83:GLU:HG3	1.95	0.45
1:B:92:HIS:CD2	1:B:96:LEU:HD22	2.51	0.45
1:C:96:LEU:HD23	1:C:100:LEU:HD12	1.98	0.45
1:A:22:MET:SD	1:A:100:LEU:CD2	3.05	0.45
1:A:56:PHE:HA	1:A:59:VAL:HG12	1.99	0.45
1:B:103:HIS:O	1:B:106:VAL:CG2	2.65	0.45
1:D:71:VAL:HA	1:D:74:HIS:HD2	1.83	0.45
1:A:96:LEU:C	1:A:96:LEU:HD23	2.37	0.44
1:D:14:LEU:O	1:D:18:ALA:N	2.35	0.44
1:A:31:ILE:HD13	1:A:46:TYR:OH	2.17	0.44
1:A:183:THR:HG23	1:A:186:GLU:H	1.81	0.44
1:B:99:GLU:HG3	1:B:102:TYR:HB2	1.99	0.44
1:B:186:GLU:HA	1:B:189:GLU:HG3	2.00	0.44
1:C:172:VAL:HG13	1:C:175:TRP:HE1	1.81	0.44
1:A:190:LEU:HD23	1:A:190:LEU:C	2.37	0.44
1:B:31:ILE:HG13	1:B:46:TYR:CZ	2.52	0.44
1:D:38:VAL:HG12	1:D:38:VAL:O	2.17	0.44
1:D:49:PHE:CD1	1:D:55:ILE:HG22	2.52	0.44
1:D:67:VAL:HG21	1:D:103:HIS:NE2	2.32	0.44
1:C:85:LEU:HD23	1:C:153:LEU:CD1	2.48	0.44
1:A:10:LYS:O	1:A:14:LEU:HG	2.18	0.44
1:A:60:TYR:CD1	1:A:129:LEU:HD12	2.53	0.44
1:B:191:ALA:O	1:B:195:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:LEU:CD2	1:C:199:ILE:HD11	2.47	0.44
1:B:6:GLU:O	1:B:9:VAL:HG22	2.17	0.44
1:D:148:ILE:O	1:D:155:VAL:HG12	2.18	0.44
1:A:72:GLU:HB2	1:A:139:MET:HE1	1.99	0.44
1:A:83:GLU:HA	1:A:86:VAL:CG1	2.47	0.44
1:B:160:LEU:HD23	1:B:164:THR:OG1	2.17	0.43
1:C:33:ASP:OD1	1:C:33:ASP:N	2.49	0.43
1:C:183:THR:CG2	1:C:184:LEU:H	2.18	0.43
1:D:50:ARG:HD2	1:D:50:ARG:N	2.33	0.43
1:D:74:HIS:HB3	1:D:88:MET:HA	2.00	0.43
1:B:65:ARG:HA	1:B:68:ARG:HB3	1.98	0.43
1:C:31:ILE:HG21	1:C:42:LYS:HG2	1.99	0.43
1:C:53:PHE:O	1:C:57:LEU:HG	2.18	0.43
1:C:86:VAL:HG23	1:C:195:VAL:O	2.18	0.43
1:C:112:TYR:O	1:C:114:ALA:N	2.51	0.43
1:A:18:ALA:HB2	1:A:59:VAL:CG2	2.46	0.43
1:A:96:LEU:HD22	1:A:172:VAL:HG23	2.00	0.43
1:A:97:MET:HB3	1:A:176:TYR:CZ	2.53	0.43
1:B:71:VAL:HG23	1:B:88:MET:O	2.17	0.43
1:B:67:VAL:CG2	1:B:95:ASN:ND2	2.78	0.43
1:C:53:PHE:CE1	1:C:57:LEU:HD11	2.53	0.43
1:A:29:THR:HG23	1:A:29:THR:O	2.19	0.43
1:B:113:GLN:O	1:B:116:THR:HB	2.18	0.43
1:A:57:LEU:HD13	1:A:125:ALA:HB3	2.01	0.43
1:C:38:VAL:HG23	1:C:40:ALA:H	1.83	0.43
1:D:80:THR:OG1	1:D:83:GLU:HB2	2.19	0.43
1:A:97:MET:HG2	1:A:176:TYR:CE2	2.53	0.43
1:A:200:THR:O	1:B:201:GLY:HA3	2.18	0.43
1:B:187:ILE:HG13	1:B:188:ASN:N	2.33	0.43
1:C:56:PHE:CD1	1:C:56:PHE:C	2.92	0.43
1:D:129:LEU:HD13	1:D:132:LEU:CD2	2.48	0.43
1:A:80:THR:HG23	1:A:83:GLU:H	1.84	0.43
1:B:67:VAL:HG22	1:B:136:TYR:CE2	2.53	0.43
1:C:68:ARG:NH1	1:C:69:GLU:OE2	2.51	0.43
1:D:42:LYS:HE3	1:D:42:LYS:HB2	1.68	0.43
1:A:121:ARG:HA	1:A:121:ARG:HH11	1.84	0.43
1:A:166:LEU:CA	1:A:169:LEU:HD12	2.48	0.43
1:C:7:ILE:HG22	1:C:8:ASP:H	1.84	0.43
1:D:94:GLU:HA	1:D:94:GLU:OE1	2.18	0.43
1:B:53:PHE:CZ	1:B:118:LEU:HD11	2.54	0.42
1:A:165:LEU:O	1:A:168:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:THR:CG2	1:C:32:ASP:HB2	2.49	0.42
1:C:147:GLY:HA2	1:C:150:ASP:CG	2.39	0.42
1:D:94:GLU:OE1	1:D:187:ILE:HG22	2.19	0.42
1:A:34:ILE:O	1:A:38:VAL:HG12	2.19	0.42
1:A:196:ASP:OD1	1:A:200:THR:HG21	2.19	0.42
1:B:60:TYR:HE1	1:B:106:VAL:O	2.02	0.42
1:D:93:LEU:HD12	1:D:93:LEU:O	2.19	0.42
1:B:116:THR:HG23	1:B:116:THR:O	2.17	0.42
1:C:133:ARG:O	1:C:137:GLU:N	2.52	0.42
1:D:34:ILE:CD1	1:D:55:ILE:CD1	2.98	0.42
1:D:60:TYR:HD2	1:D:106:VAL:HA	1.83	0.42
1:B:126:LEU:HD23	1:B:130:ASN:OD1	2.19	0.42
1:D:9:VAL:HG11	1:D:48:HIS:NE2	2.35	0.42
1:D:95:ASN:OD1	1:D:95:ASN:C	2.58	0.42
1:B:141:ARG:HH11	1:B:141:ARG:HG3	1.84	0.42
1:D:52:LYS:O	1:D:55:ILE:HG12	2.20	0.42
1:D:82:ARG:HH12	1:D:83:GLU:HG2	1.84	0.42
1:B:31:ILE:HD11	1:B:52:LYS:HG2	2.02	0.42
1:D:23:VAL:HG22	1:D:24:HIS:ND1	2.34	0.42
1:B:56:PHE:HA	1:B:59:VAL:HG12	2.01	0.42
1:B:72:GLU:N	1:B:73:PRO:CD	2.83	0.42
1:B:168:ASN:HB2	1:B:198:LEU:HD11	2.01	0.42
1:C:31:ILE:HG13	1:C:46:TYR:OH	2.20	0.42
1:D:31:ILE:HG23	1:D:45:ILE:HG21	2.02	0.42
1:D:74:HIS:CB	1:D:88:MET:HA	2.50	0.42
1:A:105:VAL:O	1:A:105:VAL:HG12	2.20	0.42
1:A:161:ALA:HA	1:B:197:LEU:CD2	2.50	0.42
1:B:95:ASN:OD1	1:B:95:ASN:C	2.57	0.42
1:D:172:VAL:HG12	1:D:172:VAL:O	2.19	0.42
1:B:41:THR:OG1	1:B:44:LEU:HD22	2.20	0.41
1:D:67:VAL:HG21	1:D:103:HIS:CE1	2.55	0.41
1:D:133:ARG:HG2	1:D:133:ARG:NH1	2.36	0.41
1:D:173:ASP:N	1:D:173:ASP:OD1	2.53	0.41
1:A:190:LEU:CD2	1:A:194:VAL:HG21	2.50	0.41
1:B:85:LEU:HG	1:B:143:VAL:HG13	2.02	0.41
1:C:89:SER:OG	1:C:195:VAL:CG2	2.69	0.41
1:C:95:ASN:HA	1:C:99:GLU:OE1	2.21	0.41
1:C:168:ASN:OD1	1:D:168:ASN:HB3	2.19	0.41
1:D:23:VAL:HG22	1:D:24:HIS:CE1	2.56	0.41
1:D:121:ARG:HA	1:D:124:ASP:OD1	2.20	0.41
1:C:56:PHE:HA	1:C:59:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:PHE:HA	1:D:59:VAL:CG1	2.46	0.41
1:B:42:LYS:O	1:B:46:TYR:HD1	2.04	0.41
1:C:141:ARG:HG3	1:C:162:THR:CG2	2.42	0.41
1:C:203:ALA:H	1:D:154:ARG:H	1.67	0.41
1:D:145:ALA:HA	1:D:148:ILE:HG12	2.02	0.41
1:C:96:LEU:HD23	1:C:100:LEU:CD1	2.51	0.41
1:A:12:ARG:NH2	1:A:38:VAL:O	2.53	0.41
1:B:15:ASP:OD1	1:B:102:TYR:CE1	2.73	0.41
1:B:85:LEU:CD1	1:B:144:VAL:HG22	2.51	0.41
1:C:7:ILE:HG22	1:C:8:ASP:N	2.35	0.41
1:D:95:ASN:HA	1:D:98:THR:OG1	2.21	0.41
1:A:35:ALA:CA	1:A:38:VAL:HG12	2.49	0.41
1:B:56:PHE:O	1:B:59:VAL:HG12	2.21	0.41
1:B:178:ARG:O	1:B:178:ARG:CG	2.66	0.41
1:D:80:THR:HG21	1:D:83:GLU:CB	2.51	0.41
1:B:172:VAL:HG12	1:B:175:TRP:HE1	1.86	0.41
1:D:16:ALA:O	1:D:20:ALA:HB2	2.20	0.41
1:D:72:GLU:OE1	1:D:139:MET:SD	2.79	0.41
1:D:138:LEU:HD23	1:D:139:MET:N	2.36	0.41
1:D:189:GLU:HG3	1:D:190:LEU:HD12	2.02	0.41
1:A:26:PHE:CD1	1:A:26:PHE:C	2.94	0.41
1:A:195:VAL:O	1:A:199:ILE:HG12	2.21	0.41
1:B:31:ILE:HG23	1:B:45:ILE:HG21	2.01	0.40
1:C:162:THR:HB	1:C:163:ARG:HH12	1.86	0.40
1:A:148:ILE:HG22	1:A:153:LEU:HB2	2.03	0.40
1:D:89:SER:HB3	1:D:140:PHE:HZ	1.86	0.40
1:C:200:THR:HG22	1:D:203:ALA:HB3	2.02	0.40
1:D:41:THR:CG2	1:D:44:LEU:HD23	2.50	0.40
1:D:143:VAL:HG12	1:D:143:VAL:O	2.20	0.40
1:C:93:LEU:CB	1:C:191:ALA:HB1	2.47	0.40
1:D:51:SER:O	1:D:55:ILE:HG23	2.22	0.40
1:D:190:LEU:CA	1:D:193:ASN:HB2	2.27	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	190/213 (89%)	179 (94%)	11 (6%)	0	100	100
1	B	198/213 (93%)	185 (93%)	13 (7%)	0	100	100
1	C	187/213 (88%)	163 (87%)	24 (13%)	0	100	100
1	D	193/213 (91%)	176 (91%)	17 (9%)	0	100	100
All	All	768/852 (90%)	703 (92%)	65 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	144/172 (84%)	139 (96%)	5 (4%)	36	68
1	B	147/172 (86%)	143 (97%)	4 (3%)	44	74
1	C	130/172 (76%)	120 (92%)	10 (8%)	13	44
1	D	133/172 (77%)	130 (98%)	3 (2%)	50	77
All	All	554/688 (80%)	532 (96%)	22 (4%)	31	65

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	56	PHE
1	A	60	TYR
1	A	85	LEU
1	A	163	ARG
1	B	70	ARG
1	B	82	ARG
1	B	124	ASP

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Mol	Chain	Res	Type
1	B	202	MET
1	C	28	ASN
1	C	52	LYS
1	C	54	ASP
1	C	65	ARG
1	C	92	HIS
1	C	102	TYR
1	C	104	HIS
1	C	113	GLN
1	C	158	GLU
1	C	163	ARG
1	D	10	LYS
1	D	24	HIS
1	D	28	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	C	74	HIS
1	C	107	HIS
1	D	92	HIS
1	D	168	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	194/213 (91%)	0.03	6 (3%) 49 33	78, 120, 180, 252	0
1	B	200/213 (93%)	0.14	7 (3%) 44 29	89, 137, 224, 294	0
1	C	193/213 (90%)	0.25	18 (9%) 8 5	109, 195, 265, 322	0
1	D	197/213 (92%)	0.39	18 (9%) 9 5	101, 192, 262, 352	0
All	All	784/852 (92%)	0.20	49 (6%) 20 12	78, 153, 249, 352	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	77	GLY	7.9
1	B	76	GLY	7.3
1	C	191	ALA	6.6
1	D	196	ASP	5.7
1	A	115	SER	5.3
1	C	190	LEU	5.3
1	D	92	HIS	4.6
1	D	187	ILE	4.3
1	C	187	ILE	4.2
1	D	107	HIS	4.1
1	C	156	VAL	4.0
1	D	170	ASN	3.9
1	C	140	PHE	3.7
1	D	140	PHE	3.5
1	C	85	LEU	3.5
1	A	109	GLY	3.3
1	D	89	SER	3.3
1	C	144	VAL	3.2
1	D	146	GLU	2.9
1	C	136	TYR	2.9
1	A	144	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	156	VAL	2.8
1	B	140	PHE	2.7
1	C	204	ASN	2.7
1	B	152	SER	2.7
1	B	77	GLY	2.7
1	D	76	GLY	2.7
1	C	100	LEU	2.6
1	C	194	VAL	2.6
1	D	136	TYR	2.5
1	D	91	ALA	2.5
1	C	139	MET	2.5
1	C	143	VAL	2.5
1	A	117	ALA	2.4
1	C	101	GLY	2.4
1	D	156	VAL	2.4
1	C	93	LEU	2.4
1	C	96	LEU	2.2
1	B	144	VAL	2.2
1	D	78	ALA	2.2
1	C	141	ARG	2.2
1	A	143	VAL	2.1
1	D	169	LEU	2.1
1	C	79	GLY	2.1
1	B	187	ILE	2.1
1	D	64	MET	2.1
1	A	136	TYR	2.1
1	D	93	LEU	2.0
1	D	13	ILE	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 monosaccharides 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.