Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 03:21 AM EDT

PDB ID	:	4DWZ
Title	:	Crystal Structure of Ton_0340
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Deposited on	:	2012-02-27
Resolution	:	2.70 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:

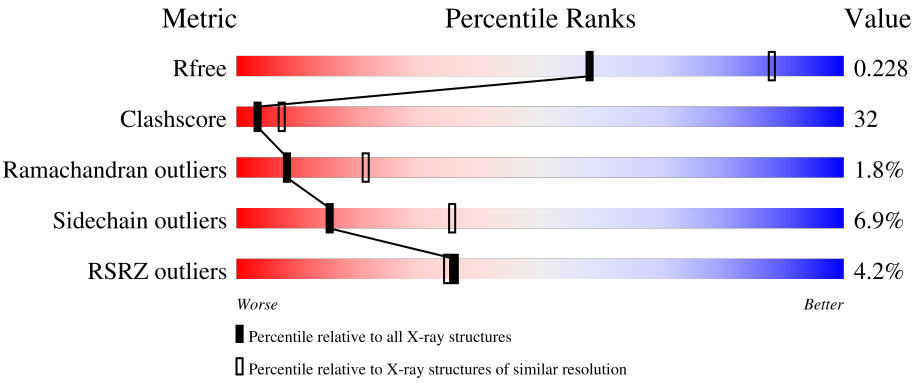
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	269	63% 30%
1	B	269	62% 32% 5%
1	C	269	7% 41% 51% 7%
1	D	269	55% 41%
1	E	269	16% 43% 47% 5%

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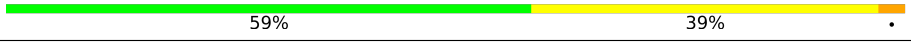
Mol	Chain	Length	Quality of chain
1	F	269	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12201 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hypothetical protein TON_0340.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1963	1251	333	372	7			
1	B	265	Total	C	N	O	S	0	0	0
			2002	1276	337	382	7			
1	C	269	Total	C	N	O	S	0	0	0
			2045	1303	347	387	8			
1	D	269	Total	C	N	O	S	0	0	0
			2045	1303	347	387	8			
1	E	256	Total	C	N	O	S	0	0	0
			1944	1241	327	369	7			
1	F	269	Total	C	N	O	S	0	0	0
			2045	1303	347	387	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	269	LEU	-	expression tag	UNP B6YTD8
B	269	LEU	-	expression tag	UNP B6YTD8
C	269	LEU	-	expression tag	UNP B6YTD8
D	269	LEU	-	expression tag	UNP B6YTD8
E	269	LEU	-	expression tag	UNP B6YTD8
F	269	LEU	-	expression tag	UNP B6YTD8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total	Zn	0	0
			7	7		
2	B	7	Total	Zn	0	0
			7	7		
2	C	4	Total	Zn	0	0
			4	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	5	Total Zn 5 5	0	0
2	E	8	Total Zn 8 8	0	0
2	F	7	Total Zn 7 7	0	0

- Molecule 3 is water.

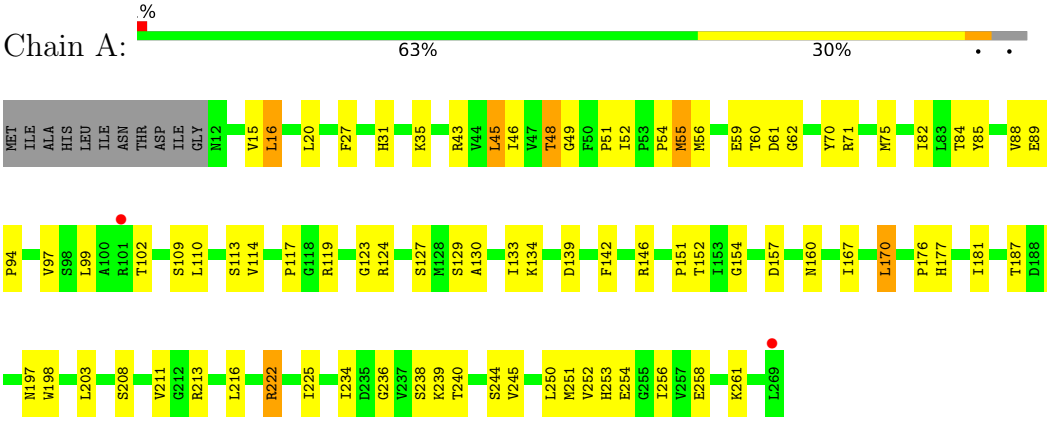
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	15	Total O 15 15	0	0
3	B	14	Total O 14 14	0	0
3	C	13	Total O 13 13	0	0
3	D	23	Total O 23 23	0	0
3	E	19	Total O 19 19	0	0
3	F	35	Total O 35 35	0	0

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.

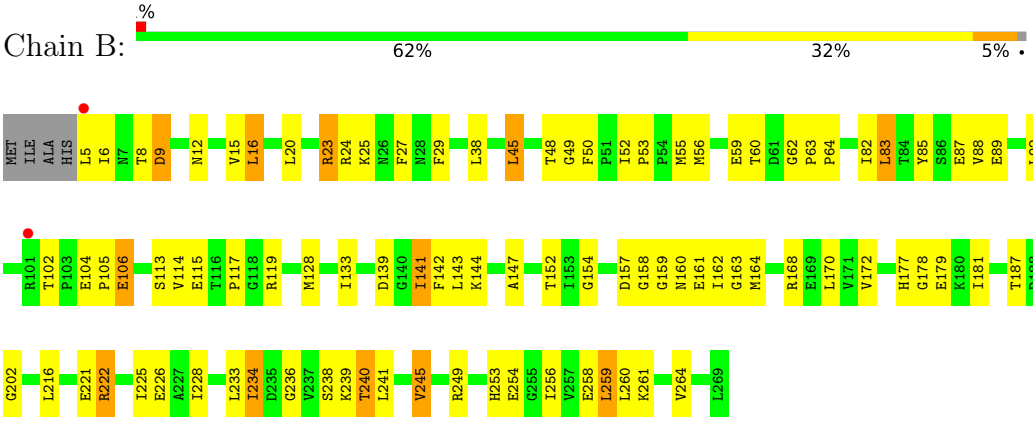
• Molecule 1: Hypothetical protein TON_0340

Chain A:



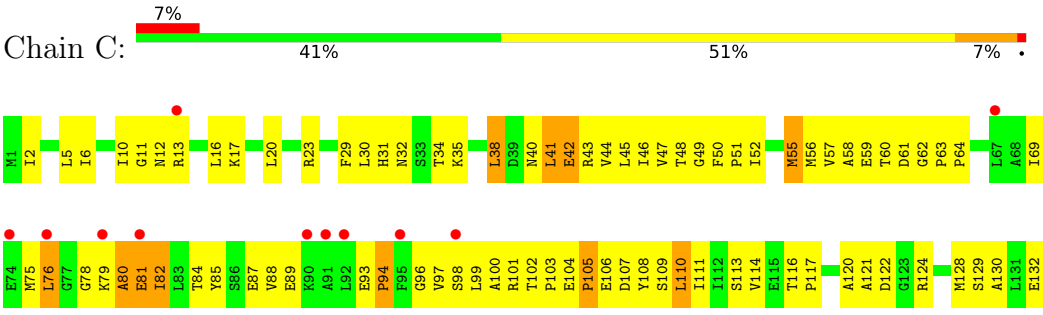
• Molecule 1: Hypothetical protein TON_0340

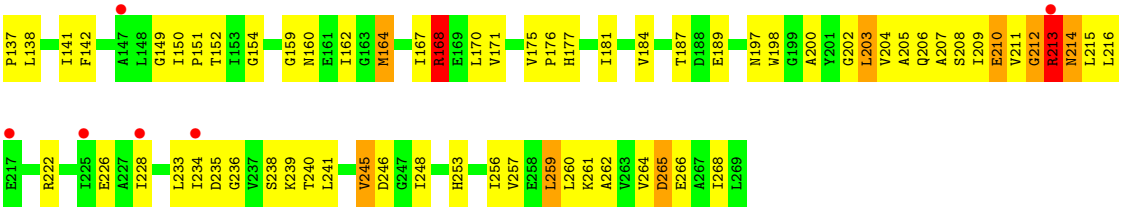
Chain B:



• Molecule 1: Hypothetical protein TON_0340

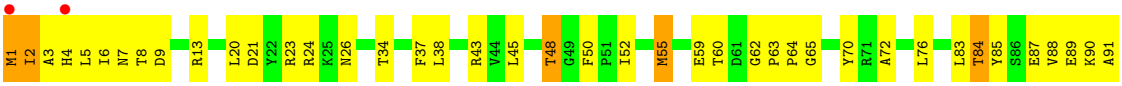
Chain C:

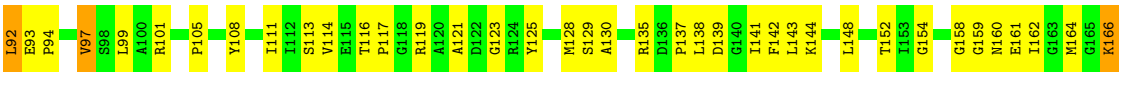




• Molecule 1: Hypothetical protein TON_0340

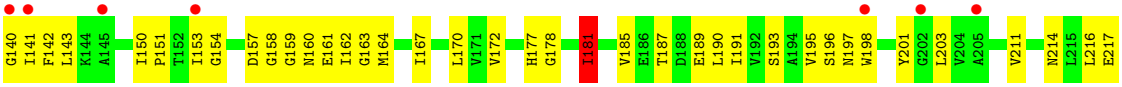
Chain D:

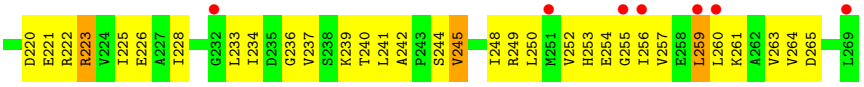




• Molecule 1: Hypothetical protein TON_0340

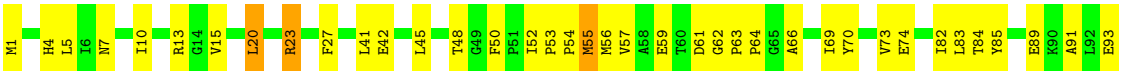
Chain E:

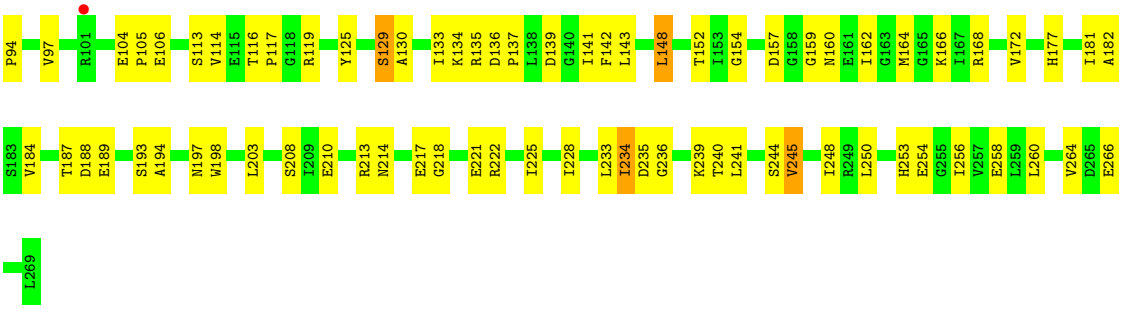




• Molecule 1: Hypothetical protein TON_0340

Chain F:




P94
V97
R101
E104
P105
E106
S113
V114
E115
T116
P117
G118
R119
Y125
S129
A130
I133
K134
R135
D136
P137
L138
D139
G140
I141
F142
L143
L148
T152
I153
G154
D157
G158
G159
N160
E161
I162
G163
M164
G165
K166
I167
R168
V172
H177
I181
A182
S183
V184
T187
D188
E189
S193
A194
N197
W198
L203
S208
I209
E210
R213
N214
E217
G218
E221
R222
I225
I228
L233
T234
D235
G236
K239
T240
L241
S244
V245
I248
R249
L250
H253
E254
G255
I256
V257
E258
L259
L260
V264
D265
E266
L269

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.44Å 107.44Å 355.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.70 48.92 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.6 (48.92-2.70) 99.5 (48.92-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.72 (at 2.69Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.223 , 0.270 0.229 , 0.228	Depositor DCC
R_{free} test set	2949 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	49.2	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12201	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.41	0/1997	0.68	1/2706 (0.0%)
1	B	0.37	0/2036	0.65	0/2761
1	C	0.40	0/2080	0.64	0/2819
1	D	0.42	0/2080	0.67	0/2819
1	E	0.36	0/1978	0.63	0/2681
1	F	0.40	0/2080	0.64	0/2819
All	All	0.39	0/12251	0.65	1/16605 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	123	GLY	N-CA-C	-5.65	98.96	113.10

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	1963	0	2002	74	0
1	B	2002	0	2031	112	0
1	C	2045	0	2090	228	0
1	D	2045	0	2090	152	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1944	0	1983	140	0
1	F	2045	0	2090	113	0
2	A	7	0	0	0	0
2	B	7	0	0	0	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0
2	E	8	0	0	0	0
2	F	7	0	0	0	0
3	A	15	0	0	2	0
3	B	14	0	0	1	0
3	C	13	0	0	1	0
3	D	23	0	0	3	0
3	E	19	0	0	3	0
3	F	35	0	0	2	0
All	All	12201	0	12286	785	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 32.

All (785) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:SD	1:D:205:ALA:HB1	1.65	1.34
1:B:16:LEU:HD21	1:D:4:HIS:NE2	1.51	1.23
1:C:45:LEU:HA	1:C:81:GLU:OE1	1.40	1.20
1:C:44:VAL:HB	1:C:79:LYS:CD	1.75	1.15
1:B:152:THR:HG22	1:B:187:THR:HG23	1.17	1.13
1:B:8:THR:HG23	1:D:2:ILE:HD13	1.16	1.08
1:C:159:GLY:HA2	1:C:164:MET:HG2	1.35	1.05
1:D:159:GLY:HA2	1:D:164:MET:HG2	1.39	1.05
1:C:44:VAL:HB	1:C:79:LYS:HD3	1.06	1.04
1:C:45:LEU:HB3	1:C:111:ILE:HG23	1.39	1.03
1:D:1:MET:SD	1:D:205:ALA:CB	2.47	1.02
1:D:52:ILE:HD13	1:D:236:GLY:HA2	1.43	1.00
1:E:52:ILE:HD11	1:E:59:GLU:HB3	1.44	0.99
1:F:10:ILE:HG21	1:F:248:ILE:HD11	1.44	0.98
1:C:124:ARG:HD2	1:C:132:GLU:OE2	1.64	0.98
1:F:53:PRO:HA	1:F:56:MET:HE2	1.46	0.97
1:C:73:VAL:HG21	1:C:79:LYS:HD2	1.47	0.96
1:B:8:THR:CG2	1:D:2:ILE:HD13	1.94	0.96
1:C:6:ILE:HD11	1:C:202:GLY:HA3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:VAL:CB	1:C:79:LYS:HD3	1.94	0.96
1:C:104:GLU:HG2	1:C:105:PRO:HD2	1.48	0.96
1:B:159:GLY:HA2	1:B:164:MET:HG2	1.47	0.94
1:C:41:LEU:HD13	1:C:76:LEU:HD13	1.47	0.94
1:C:56:MET:HE3	1:C:134:LYS:H	1.33	0.93
1:E:159:GLY:HA2	1:E:164:MET:HG2	1.48	0.93
1:B:53:PRO:HA	1:B:56:MET:HE2	1.49	0.91
1:A:82:ILE:HD12	1:A:97:VAL:HG11	1.50	0.91
1:F:240:THR:HG22	1:F:241:LEU:H	1.36	0.91
1:F:159:GLY:HA2	1:F:164:MET:HG2	1.53	0.91
1:C:62:GLY:N	1:C:197:ASN:HD21	1.67	0.90
1:B:52:ILE:CD1	1:B:236:GLY:HA2	2.03	0.89
1:C:43:ARG:HH12	1:C:107:ASP:HB3	1.39	0.88
1:D:52:ILE:CD1	1:D:236:GLY:HA2	2.03	0.87
1:B:62:GLY:H	1:B:197:ASN:HD21	1.18	0.87
1:C:73:VAL:HG11	1:C:79:LYS:HG3	1.54	0.87
1:D:65:GLY:H	1:D:197:ASN:ND2	1.72	0.87
1:C:82:ILE:HD12	1:C:97:VAL:HG11	1.54	0.87
1:F:52:ILE:HD13	1:F:236:GLY:HA2	1.56	0.86
1:C:234:ILE:HG22	1:C:235:ASP:H	1.39	0.86
1:C:62:GLY:H	1:C:197:ASN:HD21	0.91	0.86
1:C:41:LEU:HA	1:C:79:LYS:CE	2.07	0.85
1:B:6:ILE:HD11	1:B:202:GLY:HA3	1.56	0.84
1:C:56:MET:CE	1:C:134:LYS:H	1.90	0.84
1:B:9:ASP:HB3	1:D:2:ILE:HG12	1.56	0.84
1:D:105:PRO:HG3	1:D:141:ILE:HG13	1.59	0.84
1:D:152:THR:HG22	1:D:187:THR:HG23	1.58	0.84
1:C:41:LEU:HA	1:C:79:LYS:HE3	1.60	0.84
1:C:51:PRO:HA	1:C:57:VAL:O	1.79	0.83
1:C:44:VAL:O	1:C:79:LYS:HB3	1.78	0.83
1:A:84:THR:HG22	1:A:85:TYR:H	1.43	0.82
1:C:63:PRO:HG2	1:C:64:PRO:HD3	1.61	0.82
1:B:60:THR:HG22	1:B:245:VAL:HB	1.60	0.81
1:A:31:HIS:CE1	1:A:35:LYS:HE3	2.16	0.81
1:B:9:ASP:HB3	1:D:2:ILE:CG1	2.09	0.81
1:C:81:GLU:OE2	1:C:108:TYR:CE1	2.33	0.81
1:E:164:MET:HE3	1:E:167:ILE:HD11	1.61	0.80
1:A:238:SER:OG	1:A:240:THR:HG22	1.80	0.80
1:A:52:ILE:HD13	1:A:236:GLY:HA2	1.64	0.80
1:F:10:ILE:HD11	1:F:198:TRP:CH2	2.17	0.80
1:F:52:ILE:CD1	1:F:236:GLY:HA2	2.12	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:ILE:HD12	1:F:97:VAL:HG11	1.64	0.79
1:C:234:ILE:HG22	1:C:235:ASP:N	1.94	0.79
1:F:62:GLY:H	1:F:197:ASN:HD21	1.31	0.79
1:C:44:VAL:HG21	1:C:110:LEU:HD23	1.65	0.79
1:B:216:LEU:O	1:B:261:LYS:HE2	1.82	0.79
1:E:222:ARG:HG3	1:E:250:LEU:HD13	1.65	0.79
1:C:44:VAL:H	1:C:79:LYS:HG2	1.47	0.78
1:C:69:ILE:O	1:C:72:ALA:HB3	1.84	0.78
1:D:70:TYR:CE2	1:D:97:VAL:HG12	2.17	0.78
1:C:73:VAL:CG2	1:C:79:LYS:HD2	2.13	0.78
1:E:82:ILE:HD12	1:E:97:VAL:HG11	1.66	0.78
1:D:72:ALA:HB1	1:D:215:LEU:HD23	1.67	0.77
1:C:40:ASN:ND2	1:C:151:PRO:HG2	1.98	0.77
1:E:154:GLY:H	1:E:187:THR:HG21	1.46	0.77
1:F:54:PRO:HD2	1:F:55:MET:HE1	1.66	0.77
1:C:89:GLU:OE2	1:C:99:LEU:HD23	1.85	0.77
1:B:159:GLY:CA	1:B:164:MET:HG2	2.15	0.77
1:D:159:GLY:HA2	1:D:164:MET:CG	2.13	0.77
1:D:159:GLY:CA	1:D:164:MET:HG2	2.14	0.77
1:F:10:ILE:HD11	1:F:198:TRP:CZ3	2.20	0.77
1:C:259:LEU:HD12	1:E:259:LEU:HD12	1.67	0.77
1:B:52:ILE:HD13	1:B:236:GLY:HA2	1.66	0.76
1:D:7:ASN:ND2	1:D:193:SER:HA	2.00	0.76
1:E:164:MET:CE	1:E:167:ILE:HD11	2.16	0.76
1:E:234:ILE:HG22	1:E:241:LEU:HD12	1.67	0.75
1:C:81:GLU:HA	1:C:98:SER:O	1.85	0.75
1:E:63:PRO:HG2	1:E:64:PRO:HD3	1.69	0.75
1:A:60:THR:HB	1:A:234:ILE:O	1.87	0.75
1:C:228:ILE:HG23	1:C:233:LEU:HD22	1.68	0.75
1:C:62:GLY:H	1:C:197:ASN:ND2	1.76	0.75
1:F:10:ILE:O	1:F:10:ILE:HG22	1.87	0.75
1:C:207:ALA:O	1:C:211:VAL:HB	1.87	0.74
1:B:62:GLY:H	1:B:197:ASN:ND2	1.85	0.74
1:F:152:THR:HG23	1:F:187:THR:HG23	1.69	0.74
1:D:48:THR:HG22	1:D:114:VAL:O	1.86	0.74
1:B:24:ARG:HH12	1:B:25:LYS:HE2	1.52	0.74
1:C:167:ILE:CG2	1:C:170:LEU:HB2	2.17	0.74
1:D:2:ILE:CG2	1:D:4:HIS:HB2	2.17	0.74
1:F:48:THR:HG22	1:F:114:VAL:O	1.87	0.74
1:D:1:MET:SD	1:D:205:ALA:CA	2.76	0.73
1:B:9:ASP:CB	1:D:2:ILE:HG12	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:LEU:O	1:E:264:VAL:HG23	1.88	0.73
1:D:85:TYR:HB3	1:D:135:ARG:NH2	2.03	0.73
1:C:43:ARG:NH1	1:C:107:ASP:HB3	2.03	0.72
1:D:55:MET:HE1	1:D:239:LYS:HD3	1.71	0.72
1:E:245:VAL:HG13	1:E:253:HIS:NE2	2.04	0.72
1:B:5:LEU:HD22	1:D:8:THR:HG23	1.70	0.72
1:D:152:THR:CG2	1:D:187:THR:HG23	2.19	0.72
1:C:152:THR:HG22	1:C:187:THR:HG23	1.72	0.72
1:C:167:ILE:HG23	1:C:170:LEU:HB2	1.71	0.72
1:C:75:MET:O	1:C:76:LEU:HG	1.90	0.71
1:C:137:PRO:O	1:C:138:LEU:HD12	1.90	0.71
1:F:159:GLY:HA2	1:F:164:MET:CG	2.21	0.71
1:D:48:THR:O	1:D:84:THR:HG23	1.91	0.70
1:F:119:ARG:HH21	1:F:143:LEU:HD22	1.56	0.70
1:C:10:ILE:O	1:C:10:ILE:HG22	1.92	0.70
1:B:159:GLY:HA2	1:B:164:MET:CG	2.22	0.70
1:F:160:ASN:HB3	1:F:181:ILE:HG23	1.72	0.70
1:E:60:THR:HG22	1:E:245:VAL:HB	1.74	0.70
1:C:73:VAL:HG11	1:C:79:LYS:CG	2.21	0.70
1:D:1:MET:HE3	1:D:1:MET:HA	1.72	0.69
1:F:15:VAL:HG21	1:F:157:ASP:O	1.92	0.69
1:F:119:ARG:HE	1:F:143:LEU:HD21	1.57	0.69
1:B:105:PRO:HG3	1:B:141:ILE:HG13	1.73	0.69
1:B:234:ILE:HG12	1:B:240:THR:O	1.93	0.69
1:E:134:LYS:O	1:E:135:ARG:HB2	1.91	0.69
1:A:51:PRO:HD2	1:A:117:PRO:HG2	1.74	0.69
1:D:240:THR:HG22	1:D:241:LEU:H	1.56	0.69
1:B:9:ASP:CA	1:D:2:ILE:HG12	2.23	0.69
1:F:159:GLY:CA	1:F:164:MET:HG2	2.23	0.69
1:A:93:GLU:HB2	1:A:94:PRO:HD3	1.75	0.68
1:D:1:MET:HB2	1:D:206:GLN:NE2	2.08	0.68
1:E:228:ILE:HG12	1:E:233:LEU:HD22	1.74	0.68
1:C:176:PRO:HA	1:F:106:GLU:HG2	1.76	0.68
1:F:152:THR:CG2	1:F:188:ASP:H	2.06	0.68
1:F:54:PRO:HA	1:F:56:MET:HE2	1.76	0.68
1:C:171:VAL:HG13	1:C:175:VAL:HG21	1.75	0.68
1:D:2:ILE:HG22	1:D:5:LEU:H	1.58	0.68
1:A:48:THR:O	1:A:84:THR:HG23	1.94	0.68
1:D:90:LYS:O	1:D:93:GLU:HG2	1.94	0.68
1:E:216:LEU:O	1:E:261:LYS:HE2	1.94	0.68
1:C:81:GLU:O	1:C:82:ILE:HB	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:THR:CG2	1:F:114:VAL:HB	2.25	0.67
1:D:160:ASN:HB3	1:D:181:ILE:HG23	1.76	0.67
1:A:31:HIS:HE1	1:A:35:LYS:HE3	1.57	0.67
1:A:187:THR:HG22	1:A:189:GLU:O	1.95	0.67
1:A:154:GLY:N	1:A:187:THR:HG21	2.10	0.67
1:D:1:MET:HA	1:D:1:MET:CE	2.25	0.67
1:C:45:LEU:CA	1:C:81:GLU:OE1	2.32	0.67
1:D:1:MET:HG3	1:D:205:ALA:C	2.14	0.67
1:C:257:VAL:HG12	1:C:261:LYS:HE3	1.76	0.67
1:E:119:ARG:NH1	1:E:143:LEU:HD21	2.10	0.67
1:B:9:ASP:HB2	1:D:2:ILE:HG23	1.77	0.67
1:D:1:MET:HG3	1:D:205:ALA:O	1.94	0.67
1:F:52:ILE:HD12	1:F:59:GLU:HB3	1.76	0.67
1:F:119:ARG:HE	1:F:143:LEU:CD2	2.08	0.66
1:A:152:THR:HG22	1:A:187:THR:HG23	1.76	0.66
1:F:62:GLY:H	1:F:197:ASN:ND2	1.93	0.66
1:F:93:GLU:HB3	1:F:94:PRO:HD3	1.78	0.66
1:A:52:ILE:CD1	1:A:236:GLY:HA2	2.25	0.66
1:C:228:ILE:HG22	1:C:233:LEU:HB2	1.76	0.66
1:C:40:ASN:HD21	1:C:151:PRO:HG2	1.60	0.66
1:F:160:ASN:HB3	1:F:181:ILE:CG2	2.26	0.66
1:C:57:VAL:HG12	1:C:58:ALA:N	2.11	0.66
1:F:53:PRO:HA	1:F:56:MET:CE	2.24	0.66
1:B:48:THR:HG23	1:B:114:VAL:O	1.96	0.65
1:B:119:ARG:HG3	1:B:139:ASP:OD1	1.96	0.65
1:C:57:VAL:HG12	1:C:58:ALA:H	1.62	0.65
1:A:119:ARG:HB2	1:A:139:ASP:OD1	1.96	0.65
1:C:257:VAL:O	1:C:261:LYS:HG3	1.97	0.65
1:E:119:ARG:CZ	1:E:143:LEU:HD21	2.27	0.65
1:E:216:LEU:O	1:E:216:LEU:HD23	1.97	0.65
1:B:8:THR:OG1	1:D:5:LEU:CD2	2.44	0.65
1:D:84:THR:HG21	1:D:88:VAL:HG11	1.79	0.65
1:D:202:GLY:O	1:D:205:ALA:HB3	1.97	0.65
1:E:214:ASN:CG	1:E:217:GLU:HG3	2.17	0.64
1:E:160:ASN:OD1	3:E:401:HOH:O	2.15	0.64
1:C:64:PRO:HG3	1:C:228:ILE:HD12	1.78	0.64
1:B:24:ARG:NH1	1:B:25:LYS:HE2	2.12	0.64
1:C:52:ILE:CD1	1:C:236:GLY:HA2	2.27	0.64
1:D:1:MET:SD	1:D:264:VAL:CG2	2.86	0.64
1:B:245:VAL:HG13	1:B:253:HIS:NE2	2.13	0.64
1:E:163:GLY:O	1:E:190:LEU:HD22	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:VAL:HG22	1:D:253:HIS:CE1	2.33	0.64
1:C:104:GLU:HG2	1:C:105:PRO:CD	2.25	0.63
1:C:41:LEU:HA	1:C:79:LYS:NZ	2.13	0.63
1:F:48:THR:HG22	1:F:114:VAL:HB	1.80	0.63
1:E:60:THR:CG2	1:E:245:VAL:HB	2.29	0.63
1:B:5:LEU:HD23	1:B:5:LEU:N	2.14	0.63
1:B:9:ASP:CB	1:D:2:ILE:HG23	2.28	0.63
1:D:265:ASP:O	1:D:269:LEU:HG	1.97	0.63
1:E:55:MET:CE	1:E:239:LYS:HD3	2.29	0.63
1:E:127:SER:O	1:E:181:ILE:HD11	1.98	0.63
1:A:254:GLU:O	1:A:258:GLU:HG3	1.98	0.63
1:E:84:THR:HG21	1:E:88:VAL:HG11	1.80	0.63
1:E:162:ILE:HG23	1:E:185:VAL:HG11	1.81	0.63
1:A:59:GLU:HG2	1:A:60:THR:N	2.14	0.63
1:A:60:THR:HG21	1:A:244:SER:O	1.98	0.63
1:B:160:ASN:HB3	1:B:181:ILE:CG2	2.28	0.63
1:D:119:ARG:HG3	1:D:139:ASP:OD2	1.99	0.63
1:C:44:VAL:H	1:C:79:LYS:CG	2.12	0.62
1:C:52:ILE:HD13	1:C:236:GLY:HA2	1.81	0.62
1:D:142:PHE:CD1	1:D:162:ILE:HD13	2.34	0.62
1:E:113:SER:HB2	1:E:142:PHE:CZ	2.34	0.62
1:A:48:THR:HG23	1:A:114:VAL:O	1.99	0.62
1:D:221:GLU:OE2	1:D:225:ILE:HD11	1.99	0.62
1:C:46:ILE:O	1:C:82:ILE:HA	2.00	0.62
1:A:70:TYR:CE2	1:A:97:VAL:HG13	2.34	0.62
1:F:152:THR:HG23	1:F:188:ASP:H	1.65	0.62
1:D:128:MET:HE1	1:D:158:GLY:HA3	1.80	0.62
1:A:124:ARG:NH2	3:A:411:HOH:O	2.27	0.62
1:B:8:THR:HG22	1:B:8:THR:O	2.00	0.62
1:D:187:THR:HG22	1:D:189:GLU:H	1.65	0.62
1:E:48:THR:HG21	1:E:63:PRO:HA	1.82	0.62
1:D:2:ILE:HG22	1:D:4:HIS:H	1.65	0.62
1:B:241:LEU:HD12	1:B:241:LEU:N	2.15	0.61
1:C:159:GLY:CA	1:C:164:MET:HG2	2.22	0.61
1:D:70:TYR:CZ	1:D:97:VAL:HG12	2.36	0.61
1:E:23:ARG:HG3	1:E:23:ARG:HH11	1.64	0.61
1:A:154:GLY:O	1:A:190:LEU:HD12	2.01	0.61
1:D:2:ILE:HG22	1:D:4:HIS:N	2.14	0.61
1:A:48:THR:HG22	1:A:49:GLY:H	1.65	0.61
1:F:119:ARG:HG3	1:F:139:ASP:OD1	2.01	0.61
1:A:113:SER:HB2	1:A:142:PHE:CZ	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:HIS:HB2	1:A:181:ILE:HD12	1.82	0.61
1:C:75:MET:HG3	1:C:215:LEU:HD22	1.83	0.61
1:E:119:ARG:HH21	1:E:139:ASP:HB3	1.66	0.61
1:A:82:ILE:CD1	1:A:97:VAL:HG11	2.28	0.60
1:C:52:ILE:HD11	1:C:59:GLU:HB3	1.82	0.60
1:E:164:MET:HE1	1:E:190:LEU:HD21	1.82	0.60
1:C:10:ILE:CD1	1:C:198:TRP:HH2	2.14	0.60
1:B:45:LEU:HD21	1:B:83:LEU:HB2	1.83	0.60
1:B:85:TYR:O	1:B:89:GLU:HG3	2.00	0.60
1:C:52:ILE:HD11	1:C:59:GLU:CB	2.31	0.60
1:B:113:SER:HB2	1:B:142:PHE:CZ	2.36	0.60
1:B:254:GLU:O	1:B:258:GLU:HG3	2.02	0.60
1:E:154:GLY:N	1:E:187:THR:HG21	2.16	0.60
1:B:48:THR:HG22	1:B:49:GLY:N	2.17	0.60
1:C:34:THR:OG1	1:C:206:GLN:HB2	2.02	0.60
1:C:44:VAL:O	1:C:81:GLU:OE1	2.19	0.60
1:C:99:LEU:HD12	1:C:99:LEU:H	1.66	0.60
1:C:228:ILE:CG2	1:C:233:LEU:HD22	2.31	0.60
1:D:113:SER:HB2	1:D:142:PHE:CZ	2.35	0.60
1:C:5:LEU:HD11	1:C:259:LEU:HD13	1.83	0.60
1:D:93:GLU:CG	1:D:94:PRO:HD3	2.32	0.60
1:D:60:THR:HB	3:D:417:HOH:O	2.01	0.60
1:D:6:ILE:HG22	1:D:193:SER:CB	2.32	0.60
1:D:65:GLY:H	1:D:197:ASN:HD22	1.49	0.60
1:E:65:GLY:HA2	1:E:201:TYR:HE1	1.65	0.60
1:C:82:ILE:HD12	1:C:97:VAL:CG1	2.32	0.59
1:C:234:ILE:CG2	1:C:235:ASP:H	2.10	0.59
1:C:87:GLU:OE2	1:C:135:ARG:NH2	2.35	0.59
1:C:99:LEU:H	1:C:99:LEU:CD1	2.14	0.59
1:A:48:THR:HG21	1:A:62:GLY:C	2.23	0.59
1:C:234:ILE:CG2	1:C:235:ASP:N	2.65	0.59
1:D:1:MET:HG2	1:D:209:ILE:HD11	1.85	0.59
1:B:87:GLU:HG2	1:B:88:VAL:H	1.67	0.59
1:D:1:MET:HG3	1:D:206:GLN:HA	1.85	0.59
1:E:112:ILE:HG12	1:E:153:ILE:HB	1.84	0.59
1:E:105:PRO:HG3	1:E:141:ILE:HG23	1.85	0.59
1:F:54:PRO:HD2	1:F:55:MET:CE	2.31	0.59
1:C:93:GLU:HB3	1:C:94:PRO:HD3	1.84	0.59
1:C:128:MET:HE2	1:C:128:MET:HA	1.85	0.59
1:E:23:ARG:O	1:E:23:ARG:HD3	2.03	0.59
1:B:119:ARG:HH12	1:B:139:ASP:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ILE:HD12	1:B:97:VAL:HG21	1.85	0.58
1:F:240:THR:HG22	1:F:241:LEU:N	2.15	0.58
1:D:1:MET:SD	1:D:205:ALA:C	2.81	0.58
1:B:168:ARG:O	1:B:172:VAL:HG23	2.03	0.58
1:B:48:THR:HG21	1:B:62:GLY:C	2.24	0.58
1:F:48:THR:HG21	1:F:66:ALA:HB2	1.85	0.58
1:C:70:TYR:CE2	1:C:80:ALA:HA	2.38	0.58
1:C:99:LEU:HD12	1:C:99:LEU:N	2.19	0.58
1:E:220:ASP:OD1	1:E:223:ARG:CZ	2.52	0.58
1:E:15:VAL:HG23	3:E:413:HOH:O	2.02	0.58
1:C:44:VAL:HG22	1:C:110:LEU:CB	2.34	0.57
1:B:15:VAL:HG21	1:B:157:ASP:O	2.04	0.57
1:C:215:LEU:C	1:C:216:LEU:HD12	2.25	0.57
1:E:34:THR:O	1:E:37:PHE:HB3	2.04	0.57
1:D:116:THR:HB	1:D:162:ILE:HD12	1.85	0.57
1:D:222:ARG:O	1:D:226:GLU:HG3	2.05	0.57
1:E:52:ILE:HD13	1:E:236:GLY:HA2	1.85	0.57
1:E:245:VAL:HG13	1:E:253:HIS:CE1	2.38	0.57
1:F:50:PHE:CE1	1:F:117:PRO:HG3	2.40	0.57
1:C:44:VAL:HG22	1:C:110:LEU:HB3	1.87	0.57
1:C:124:ARG:CD	1:C:132:GLU:OE2	2.46	0.57
1:A:216:LEU:O	1:A:261:LYS:HE2	2.04	0.57
1:B:8:THR:OG1	1:D:5:LEU:HD21	2.05	0.57
1:D:236:GLY:HA3	3:D:414:HOH:O	2.04	0.57
1:A:60:THR:HG21	1:A:245:VAL:HA	1.85	0.57
1:A:177:HIS:CB	1:A:181:ILE:HD12	2.34	0.57
1:C:260:LEU:O	1:C:264:VAL:HG23	2.04	0.56
1:E:161:GLU:OE1	1:E:161:GLU:N	2.36	0.56
1:B:87:GLU:HG2	1:B:88:VAL:N	2.20	0.56
1:C:113:SER:OG	1:C:162:ILE:HB	2.05	0.56
1:D:48:THR:CG2	1:D:114:VAL:HB	2.35	0.56
1:F:245:VAL:HG13	1:F:253:HIS:CE1	2.40	0.56
1:C:209:ILE:C	1:C:211:VAL:H	2.09	0.56
1:C:245:VAL:HG13	1:C:253:HIS:CE1	2.40	0.56
1:B:119:ARG:HG3	1:B:119:ARG:HH11	1.70	0.56
1:C:81:GLU:HG2	1:C:108:TYR:OH	2.04	0.56
1:C:234:ILE:HG21	1:C:239:LYS:HA	1.87	0.56
1:C:34:THR:HG21	1:C:207:ALA:N	2.21	0.56
1:A:160:ASN:HB3	1:A:181:ILE:CG2	2.36	0.56
1:B:187:THR:CG2	1:B:189:GLU:O	2.54	0.56
1:F:10:ILE:HD12	1:F:194:ALA:HB1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:MET:HE1	1:E:239:LYS:HD3	1.87	0.56
1:F:52:ILE:HD13	1:F:236:GLY:CA	2.34	0.56
1:A:60:THR:CG2	1:A:245:VAL:HA	2.35	0.56
1:B:48:THR:HG22	1:B:49:GLY:H	1.71	0.56
1:D:201:TYR:O	1:D:205:ALA:HB2	2.06	0.56
1:F:166:LYS:HD2	3:F:433:HOH:O	2.06	0.56
1:A:59:GLU:OE2	1:A:61:ASP:HB3	2.06	0.55
1:A:15:VAL:HG21	1:A:157:ASP:O	2.05	0.55
1:B:221:GLU:OE2	1:B:225:ILE:HD11	2.07	0.55
1:C:152:THR:O	1:C:187:THR:HG23	2.06	0.55
1:D:202:GLY:C	1:D:205:ALA:HB3	2.27	0.55
1:E:48:THR:HG21	1:E:63:PRO:CA	2.36	0.55
1:D:2:ILE:O	1:D:6:ILE:HG13	2.07	0.55
1:F:129:SER:O	1:F:130:ALA:HB3	2.07	0.55
1:B:142:PHE:CD1	1:B:162:ILE:HD13	2.42	0.55
1:C:208:SER:O	1:C:212:GLY:N	2.40	0.55
1:E:211:VAL:HG12	1:E:211:VAL:O	2.06	0.55
1:F:172:VAL:O	3:F:408:HOH:O	2.18	0.55
1:F:187:THR:HG22	1:F:189:GLU:H	1.72	0.55
1:C:81:GLU:OE2	1:C:108:TYR:CD1	2.59	0.55
1:C:109:SER:O	1:C:151:PRO:HD2	2.07	0.55
1:F:63:PRO:HB2	1:F:64:PRO:HD3	1.88	0.55
1:A:252:VAL:HG21	1:F:266:GLU:HG3	1.89	0.55
1:B:50:PHE:CD1	1:B:117:PRO:HG3	2.42	0.54
1:B:9:ASP:O	1:D:2:ILE:CG1	2.55	0.54
1:B:23:ARG:O	1:B:27:PHE:HA	2.08	0.54
1:C:89:GLU:CD	1:C:99:LEU:HD23	2.27	0.54
1:D:52:ILE:O	1:D:55:MET:HE2	2.06	0.54
1:C:17:LYS:HE2	1:E:27:PHE:CD2	2.41	0.54
1:A:88:VAL:HG12	1:A:92:LEU:HD22	1.89	0.54
1:A:51:PRO:HG2	1:A:133:ILE:HG21	1.88	0.54
1:C:56:MET:HE3	1:C:134:LYS:N	2.13	0.54
1:C:233:LEU:N	1:C:233:LEU:HD12	2.22	0.54
1:E:253:HIS:O	1:E:257:VAL:HG23	2.06	0.54
1:B:50:PHE:CE1	1:B:117:PRO:HG3	2.43	0.54
1:C:104:GLU:CG	1:C:105:PRO:HD2	2.31	0.54
1:E:198:TRP:HE1	1:E:253:HIS:CD2	2.25	0.54
1:F:198:TRP:HE1	1:F:253:HIS:HD2	1.56	0.54
1:C:167:ILE:O	1:C:167:ILE:HG22	2.08	0.54
1:E:35:LYS:O	1:E:37:PHE:N	2.41	0.54
1:F:55:MET:CB	1:F:57:VAL:HG23	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:THR:HG23	1:D:114:VAL:HB	1.88	0.54
1:E:102:THR:HG22	1:E:102:THR:O	2.08	0.54
1:A:187:THR:CG2	1:A:189:GLU:O	2.56	0.54
1:B:23:ARG:HG3	1:B:23:ARG:HH11	1.73	0.54
1:F:113:SER:HB2	1:F:142:PHE:CZ	2.43	0.54
1:F:7:ASN:OD1	1:F:193:SER:HA	2.07	0.53
1:E:256:ILE:O	1:E:260:LEU:HG	2.08	0.53
1:C:44:VAL:CG2	1:C:110:LEU:HB3	2.38	0.53
1:C:82:ILE:HG23	1:C:84:THR:HG23	1.90	0.53
1:C:167:ILE:HG23	1:C:170:LEU:HD22	1.90	0.53
1:E:222:ARG:O	1:E:226:GLU:HG3	2.08	0.53
1:D:70:TYR:CD2	1:D:97:VAL:HG12	2.44	0.53
1:D:93:GLU:HG3	1:D:94:PRO:HD3	1.89	0.53
1:E:48:THR:OG1	1:E:66:ALA:HB2	2.09	0.53
1:F:260:LEU:O	1:F:264:VAL:HG23	2.08	0.53
1:B:249:ARG:HH12	1:D:269:LEU:HD13	1.73	0.53
1:C:20:LEU:HD23	1:E:24:ARG:HA	1.91	0.53
1:F:10:ILE:CG2	1:F:248:ILE:HD11	2.29	0.53
1:F:1:MET:O	1:F:5:LEU:HG	2.08	0.53
1:B:143:LEU:HD12	1:B:143:LEU:N	2.24	0.53
1:E:52:ILE:HD12	1:E:234:ILE:HG13	1.90	0.53
1:F:54:PRO:HA	1:F:56:MET:CE	2.39	0.53
1:B:160:ASN:HB3	1:B:181:ILE:HG23	1.90	0.53
1:C:167:ILE:O	1:C:168:ARG:C	2.47	0.53
1:D:50:PHE:CD1	1:D:117:PRO:HG3	2.43	0.52
1:D:1:MET:CG	1:D:205:ALA:C	2.77	0.52
1:B:93:GLU:HB3	1:B:94:PRO:HD3	1.90	0.52
1:B:115:GLU:OE1	1:B:161:GLU:HG2	2.09	0.52
1:D:52:ILE:CD1	1:D:59:GLU:HB3	2.39	0.52
1:D:152:THR:HG22	1:D:187:THR:CG2	2.37	0.52
1:D:6:ILE:HG22	1:D:193:SER:HB3	1.91	0.52
1:A:110:LEU:HD12	1:A:151:PRO:O	2.10	0.52
1:D:1:MET:HG2	1:D:209:ILE:CD1	2.39	0.52
1:E:37:PHE:HA	1:E:110:LEU:HD22	1.91	0.52
1:B:102:THR:HG22	1:B:102:THR:O	2.08	0.52
1:C:47:VAL:HG21	1:C:142:PHE:HE1	1.73	0.52
1:D:129:SER:O	1:D:130:ALA:HB3	2.08	0.52
1:E:248:ILE:HB	1:E:253:HIS:CE1	2.45	0.52
1:F:154:GLY:N	1:F:187:THR:HG21	2.25	0.52
1:D:48:THR:O	1:D:84:THR:CG2	2.58	0.52
1:F:85:TYR:O	1:F:89:GLU:HG3	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LEU:HD23	1:C:79:LYS:HZ2	1.74	0.52
1:E:34:THR:HG22	1:E:38:LEU:HD22	1.92	0.52
1:E:177:HIS:CD2	3:E:405:HOH:O	2.61	0.52
1:C:48:THR:HG22	1:C:49:GLY:N	2.25	0.52
1:C:137:PRO:C	1:C:138:LEU:HD12	2.29	0.52
1:C:41:LEU:CA	1:C:79:LYS:HE3	2.37	0.51
1:C:55:MET:CE	1:C:239:LYS:HB3	2.39	0.51
1:E:190:LEU:HD12	1:E:191:ILE:N	2.25	0.51
1:C:110:LEU:HB2	1:C:151:PRO:HB2	1.92	0.51
1:E:220:ASP:OD1	1:E:223:ARG:NE	2.43	0.51
1:E:228:ILE:CG1	1:E:233:LEU:HD22	2.39	0.51
1:C:85:TYR:O	1:C:89:GLU:HG3	2.10	0.51
1:A:250:LEU:O	1:A:254:GLU:HG3	2.10	0.51
1:B:260:LEU:O	1:B:264:VAL:HG23	2.10	0.51
1:C:257:VAL:CG1	1:C:261:LYS:HE3	2.39	0.51
1:D:2:ILE:CG2	1:D:5:LEU:H	2.24	0.51
1:D:6:ILE:HG22	1:D:193:SER:HB2	1.92	0.51
1:F:134:LYS:O	1:F:135:ARG:HB2	2.10	0.51
1:C:44:VAL:HB	1:C:79:LYS:CG	2.40	0.51
1:C:102:THR:O	1:C:102:THR:HG22	2.11	0.51
1:E:164:MET:CE	1:E:190:LEU:HD21	2.40	0.51
1:C:160:ASN:HB3	1:C:181:ILE:HG23	1.91	0.51
1:E:132:GLU:HG2	1:E:134:LYS:HZ3	1.75	0.51
1:A:59:GLU:HG2	1:A:60:THR:H	1.75	0.51
1:C:70:TYR:HD1	1:C:71:ARG:N	2.08	0.51
1:F:61:ASP:HB2	1:F:245:VAL:HG23	1.92	0.51
1:F:187:THR:CG2	1:F:189:GLU:O	2.59	0.51
1:C:154:GLY:N	1:C:187:THR:HG21	2.26	0.51
1:C:213:ARG:O	1:C:213:ARG:HG3	2.11	0.51
1:F:116:THR:O	1:F:162:ILE:HG13	2.11	0.51
1:A:129:SER:O	1:A:130:ALA:HB3	2.11	0.51
1:C:198:TRP:CH2	1:C:256:ILE:HD12	2.46	0.51
1:C:264:VAL:C	1:C:266:GLU:H	2.15	0.51
1:F:221:GLU:OE2	1:F:225:ILE:HD11	2.10	0.51
1:E:221:GLU:OE2	1:E:225:ILE:HD11	2.11	0.50
1:D:89:GLU:OE2	1:D:101:ARG:NH1	2.44	0.50
1:C:59:GLU:HG3	1:C:61:ASP:H	1.77	0.50
1:D:228:ILE:HG23	1:D:233:LEU:CD2	2.41	0.50
1:E:84:THR:HG21	1:E:88:VAL:CG1	2.41	0.50
1:C:10:ILE:CD1	1:C:198:TRP:CH2	2.94	0.50
1:C:89:GLU:HB3	1:C:99:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:THR:HG22	1:C:241:LEU:N	2.26	0.50
1:D:3:ALA:HA	1:D:6:ILE:HD12	1.92	0.50
1:E:53:PRO:HG3	1:E:133:ILE:HA	1.93	0.50
1:B:222:ARG:HG3	1:F:218:GLY:HA3	1.93	0.50
1:F:82:ILE:HD12	1:F:97:VAL:CG1	2.38	0.50
1:A:71:ARG:O	1:A:75:MET:HG3	2.12	0.50
1:C:30:LEU:HG	1:C:206:GLN:HG3	1.93	0.50
1:C:206:GLN:HA	1:C:206:GLN:OE1	2.11	0.50
1:E:48:THR:HG22	1:E:49:GLY:N	2.27	0.50
1:B:154:GLY:N	1:B:187:THR:HG21	2.26	0.50
1:C:45:LEU:HD23	1:C:141:ILE:HD13	1.93	0.50
1:C:63:PRO:CG	1:C:64:PRO:HD3	2.35	0.50
1:C:160:ASN:HB3	1:C:181:ILE:CG2	2.42	0.50
1:C:204:VAL:HG12	1:C:216:LEU:HD11	1.92	0.50
1:C:234:ILE:CG2	1:C:239:LYS:HA	2.41	0.50
1:D:1:MET:SD	1:D:264:VAL:HG23	2.52	0.50
1:E:118:GLY:HA2	1:E:162:ILE:HG12	1.93	0.50
1:D:88:VAL:O	1:D:92:LEU:HB2	2.12	0.49
1:E:93:GLU:HB3	1:E:94:PRO:HD3	1.94	0.49
1:B:119:ARG:NH1	1:B:139:ASP:CG	2.66	0.49
1:B:187:THR:HG22	1:B:189:GLU:H	1.78	0.49
1:C:222:ARG:O	1:C:226:GLU:HG2	2.13	0.49
1:D:1:MET:HB2	1:D:206:GLN:HE21	1.76	0.49
1:D:34:THR:O	1:D:37:PHE:HB3	2.12	0.49
1:D:201:TYR:O	1:D:205:ALA:CB	2.60	0.49
1:E:45:LEU:HG	1:E:108:TYR:CE2	2.47	0.49
1:A:160:ASN:HB3	1:A:181:ILE:HG22	1.94	0.49
1:F:55:MET:HB2	1:F:57:VAL:HG23	1.93	0.49
1:A:89:GLU:OE1	3:A:409:HOH:O	2.19	0.49
1:E:242:ALA:O	1:E:244:SER:N	2.45	0.49
1:B:23:ARG:O	1:B:23:ARG:HD3	2.12	0.49
1:D:198:TRP:CD2	1:D:256:ILE:HD13	2.48	0.49
1:E:198:TRP:HE1	1:E:253:HIS:HD2	1.61	0.49
1:A:51:PRO:HG2	1:A:133:ILE:CG2	2.41	0.49
1:B:52:ILE:CD1	1:B:59:GLU:HB3	2.42	0.49
1:E:132:GLU:HB3	1:E:134:LYS:HZ3	1.77	0.49
1:A:56:MET:CE	1:A:134:LYS:H	2.25	0.49
1:C:149:GLY:C	1:C:150:ILE:HG13	2.33	0.49
1:D:52:ILE:HD11	1:D:59:GLU:HB3	1.94	0.49
1:C:70:TYR:CD1	1:C:71:ARG:N	2.81	0.49
1:E:214:ASN:ND2	1:E:264:VAL:HB	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:THR:HG22	1:D:38:LEU:CD2	2.42	0.48
1:E:62:GLY:H	1:E:197:ASN:ND2	2.11	0.48
1:E:115:GLU:OE1	1:E:115:GLU:HA	2.13	0.48
1:F:248:ILE:O	1:F:253:HIS:HE1	1.96	0.48
1:B:9:ASP:O	1:D:2:ILE:HG12	2.13	0.48
1:C:213:ARG:O	1:C:214:ASN:HB3	2.13	0.48
1:E:52:ILE:CD1	1:E:236:GLY:HA2	2.43	0.48
1:E:132:GLU:CG	1:E:134:LYS:HZ3	2.26	0.48
1:E:259:LEU:O	1:E:263:VAL:HG23	2.13	0.48
1:D:228:ILE:HG23	1:D:233:LEU:HD23	1.94	0.48
1:F:222:ARG:HG3	1:F:250:LEU:HD13	1.94	0.48
1:A:208:SER:HB3	1:A:213:ARG:O	2.14	0.48
1:B:60:THR:CG2	1:B:245:VAL:HB	2.38	0.48
1:C:16:LEU:HD23	1:C:16:LEU:O	2.13	0.48
1:C:79:LYS:O	1:C:80:ALA:C	2.52	0.48
1:C:110:LEU:HA	1:C:151:PRO:HB2	1.94	0.48
1:E:65:GLY:HA2	1:E:201:TYR:CE1	2.46	0.48
1:F:10:ILE:O	1:F:10:ILE:CG2	2.56	0.48
1:D:34:THR:HG22	1:D:38:LEU:HD23	1.96	0.48
1:A:222:ARG:HG3	1:A:250:LEU:HD13	1.94	0.48
1:B:82:ILE:CD1	1:B:97:VAL:HG21	2.43	0.48
1:B:170:LEU:HD12	1:B:170:LEU:N	2.29	0.48
1:C:208:SER:HB3	1:C:214:ASN:HA	1.95	0.48
1:D:240:THR:HG22	1:D:241:LEU:N	2.27	0.48
1:E:23:ARG:HG3	1:E:23:ARG:NH1	2.28	0.48
1:E:52:ILE:O	1:E:55:MET:HG2	2.13	0.48
1:D:187:THR:CG2	1:D:189:GLU:O	2.62	0.48
1:A:52:ILE:HD11	1:A:59:GLU:HB2	1.95	0.48
1:C:10:ILE:HD11	1:C:198:TRP:CH2	2.49	0.48
1:C:200:ALA:O	1:C:204:VAL:HG23	2.14	0.48
1:D:6:ILE:HG21	1:D:199:GLY:HA2	1.95	0.48
1:A:51:PRO:HD2	1:A:117:PRO:CG	2.43	0.47
1:C:124:ARG:HD2	1:C:132:GLU:CD	2.34	0.47
1:C:198:TRP:CZ2	1:C:256:ILE:HD12	2.48	0.47
1:A:176:PRO:O	1:A:177:HIS:HB2	2.14	0.47
1:C:44:VAL:HB	1:C:79:LYS:CE	2.41	0.47
1:F:250:LEU:O	1:F:254:GLU:HG3	2.14	0.47
1:B:8:THR:OG1	1:D:5:LEU:HD23	2.14	0.47
1:A:167:ILE:HB	1:A:170:LEU:HD22	1.97	0.47
1:C:10:ILE:HD11	1:C:198:TRP:HH2	1.77	0.47
1:C:55:MET:HE1	1:C:239:LYS:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:GLU:CA	1:C:98:SER:O	2.58	0.47
1:E:52:ILE:HD12	1:E:234:ILE:CD1	2.44	0.47
1:A:61:ASP:HA	1:A:197:ASN:HD21	1.79	0.47
1:B:170:LEU:H	1:B:170:LEU:CD1	2.28	0.47
1:E:45:LEU:HG	1:E:108:TYR:CZ	2.49	0.47
1:A:27:PHE:CE1	1:F:13:ARG:HG3	2.50	0.47
1:C:56:MET:HE1	1:C:133:ILE:HA	1.96	0.47
1:C:213:ARG:N	1:C:268:ILE:HD13	2.29	0.47
1:C:248:ILE:O	1:C:253:HIS:HE1	1.98	0.47
1:D:128:MET:CE	1:D:158:GLY:HA3	2.44	0.47
1:E:198:TRP:CZ2	1:E:256:ILE:HD12	2.50	0.47
1:B:52:ILE:HD12	1:B:59:GLU:HB3	1.97	0.47
1:C:152:THR:HG22	1:C:187:THR:CG2	2.44	0.47
1:D:2:ILE:HG22	1:D:4:HIS:HB2	1.94	0.47
1:D:63:PRO:HB2	1:D:64:PRO:HD3	1.96	0.47
1:D:105:PRO:HG3	1:D:141:ILE:CG1	2.40	0.47
1:D:161:GLU:O	1:D:164:MET:HB2	2.14	0.47
1:B:119:ARG:NH1	1:B:139:ASP:HB3	2.29	0.47
1:C:2:ILE:HD13	1:C:205:ALA:HB1	1.97	0.47
1:D:121:ALA:C	1:D:123:GLY:H	2.19	0.47
1:E:124:ARG:HD3	1:E:132:GLU:OE1	2.15	0.47
1:E:150:ILE:HA	1:E:151:PRO:HD3	1.82	0.47
1:E:233:LEU:N	1:E:233:LEU:HD12	2.30	0.47
1:B:238:SER:O	1:B:239:LYS:HB2	2.15	0.46
1:C:70:TYR:CD2	1:C:80:ALA:HA	2.50	0.46
1:C:214:ASN:OD1	1:C:214:ASN:O	2.33	0.46
1:D:5:LEU:HD22	1:D:259:LEU:HD23	1.97	0.46
1:F:55:MET:HE1	1:F:239:LYS:HD3	1.97	0.46
1:F:208:SER:HB3	1:F:213:ARG:O	2.15	0.46
1:B:178:GLY:O	1:B:179:GLU:C	2.54	0.46
1:C:42:GLU:O	1:C:78:GLY:O	2.33	0.46
1:E:35:LYS:C	1:E:37:PHE:N	2.69	0.46
1:E:61:ASP:O	1:E:115:GLU:HG2	2.14	0.46
1:E:248:ILE:HB	1:E:253:HIS:HE1	1.81	0.46
1:F:23:ARG:O	1:F:27:PHE:HA	2.16	0.46
1:D:87:GLU:HG2	1:D:88:VAL:N	2.31	0.46
1:F:48:THR:O	1:F:84:THR:HG22	2.16	0.46
1:D:152:THR:CB	1:D:187:THR:HG23	2.44	0.46
1:C:48:THR:HG23	1:C:114:VAL:O	2.15	0.46
1:C:266:GLU:HG3	1:E:249:ARG:CD	2.45	0.46
1:D:144:LYS:O	1:D:148:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:THR:CG2	1:E:49:GLY:N	2.78	0.46
1:F:214:ASN:HB3	1:F:217:GLU:HG2	1.97	0.46
1:F:228:ILE:HG23	1:F:233:LEU:HD22	1.98	0.46
1:F:244:SER:HB2	1:F:248:ILE:O	2.16	0.46
1:F:52:ILE:CD1	1:F:236:GLY:CA	2.89	0.46
1:A:222:ARG:HB2	1:A:254:GLU:OE2	2.16	0.46
1:B:226:GLU:OE2	1:F:213:ARG:NH2	2.49	0.46
1:C:44:VAL:HG21	1:C:79:LYS:NZ	2.30	0.46
1:C:44:VAL:HG22	1:C:110:LEU:O	2.16	0.46
1:C:213:ARG:H	1:C:268:ILE:HD13	1.80	0.46
1:D:154:GLY:N	1:D:187:THR:HG21	2.30	0.46
1:F:222:ARG:HB2	1:F:254:GLU:OE2	2.15	0.46
1:F:245:VAL:HG13	1:F:253:HIS:NE2	2.31	0.46
1:B:48:THR:HG21	1:B:63:PRO:N	2.31	0.46
1:C:80:ALA:HB3	1:C:98:SER:HB2	1.98	0.46
1:C:104:GLU:CG	1:C:105:PRO:CD	2.92	0.46
1:E:51:PRO:O	1:E:53:PRO:HD3	2.15	0.46
1:B:9:ASP:N	1:D:2:ILE:HG12	2.31	0.46
1:D:43:ARG:HG2	1:D:108:TYR:CD1	2.51	0.46
1:E:39:ASP:O	1:E:40:ASN:OD1	2.34	0.46
1:E:129:SER:O	1:E:130:ALA:HB3	2.16	0.46
1:E:222:ARG:NH2	1:E:254:GLU:OE2	2.49	0.46
1:E:154:GLY:O	1:E:190:LEU:HD12	2.15	0.46
1:A:84:THR:HG21	1:A:88:VAL:HG11	1.98	0.45
1:B:104:GLU:HB3	1:B:106:GLU:OE2	2.15	0.45
1:C:56:MET:HE1	1:C:134:LYS:H	1.78	0.45
1:E:23:ARG:HG2	1:E:29:PHE:HE2	1.82	0.45
1:E:43:ARG:O	1:E:108:TYR:HD1	1.99	0.45
1:B:9:ASP:C	1:D:2:ILE:HG12	2.37	0.45
1:B:228:ILE:O	1:B:233:LEU:HB2	2.16	0.45
1:C:45:LEU:CD2	1:C:141:ILE:HD13	2.47	0.45
1:B:160:ASN:HB3	1:B:181:ILE:HG22	1.96	0.45
1:E:225:ILE:HD12	1:E:250:LEU:CD2	2.47	0.45
1:F:62:GLY:HA2	1:F:114:VAL:HG12	1.97	0.45
1:F:105:PRO:HG3	1:F:141:ILE:HG13	1.98	0.45
1:F:168:ARG:HG3	1:F:182:ALA:HB1	1.99	0.45
1:B:20:LEU:O	1:B:24:ARG:HB2	2.17	0.45
1:E:18:VAL:HG13	1:E:170:LEU:HB3	1.99	0.45
1:B:177:HIS:HB2	1:B:181:ILE:HD12	1.99	0.45
1:C:10:ILE:HG21	1:C:248:ILE:HD13	1.98	0.45
1:C:100:ALA:C	1:C:101:ARG:HG3	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:ASP:CB	1:E:193:SER:O	2.64	0.45
1:F:142:PHE:CD1	1:F:162:ILE:HD13	2.52	0.45
1:F:228:ILE:HG23	1:F:233:LEU:CD2	2.46	0.45
1:A:245:VAL:HB	1:A:253:HIS:CE1	2.51	0.45
1:F:23:ARG:HD3	1:F:27:PHE:HA	1.97	0.45
1:F:125:TYR:HB2	1:F:133:ILE:HB	1.99	0.45
1:F:234:ILE:HG12	1:F:240:THR:O	2.17	0.45
1:C:47:VAL:HG21	1:C:142:PHE:CE1	2.50	0.45
1:C:70:TYR:CE2	1:C:97:VAL:HG13	2.52	0.45
1:C:168:ARG:HG2	1:C:168:ARG:HH11	1.82	0.45
1:D:187:THR:HG22	1:D:188:ASP:N	2.31	0.45
1:E:63:PRO:CG	1:E:64:PRO:HD3	2.45	0.45
1:B:119:ARG:HH11	1:B:139:ASP:CG	2.18	0.45
1:C:38:LEU:HA	1:C:41:LEU:HD11	1.99	0.45
1:C:48:THR:O	1:C:84:THR:HG22	2.16	0.45
1:C:167:ILE:HG22	1:C:171:VAL:HG23	1.99	0.45
1:F:104:GLU:O	1:F:105:PRO:C	2.55	0.45
1:A:102:THR:O	1:A:102:THR:HG22	2.17	0.45
1:C:240:THR:HG22	1:C:241:LEU:H	1.81	0.45
1:C:57:VAL:CG1	1:C:58:ALA:N	2.80	0.44
1:C:80:ALA:CB	1:C:98:SER:HB2	2.47	0.44
1:F:222:ARG:HD2	1:F:254:GLU:OE2	2.17	0.44
1:A:84:THR:HG21	1:A:88:VAL:HG21	1.99	0.44
1:B:62:GLY:N	1:B:197:ASN:HD21	1.99	0.44
1:B:177:HIS:HB2	1:B:181:ILE:CD1	2.48	0.44
1:E:116:THR:O	1:E:162:ILE:HG13	2.17	0.44
1:B:228:ILE:HB	1:B:233:LEU:HD22	1.99	0.44
1:E:35:LYS:O	1:E:36:MET:C	2.55	0.44
1:B:163:GLY:CA	1:B:187:THR:OG1	2.65	0.44
1:C:212:GLY:O	1:C:213:ARG:HB2	2.16	0.44
1:D:6:ILE:CG2	1:D:199:GLY:HA2	2.47	0.44
1:D:43:ARG:HG2	1:D:108:TYR:HD1	1.82	0.44
1:D:60:THR:HG21	1:D:244:SER:O	2.17	0.44
1:E:52:ILE:CD1	1:E:59:GLU:HB3	2.33	0.44
1:F:198:TRP:CE3	1:F:256:ILE:HD13	2.52	0.44
1:B:159:GLY:C	1:B:164:MET:HG2	2.37	0.44
1:C:52:ILE:HD11	1:C:236:GLY:HA2	1.97	0.44
1:F:10:ILE:HD13	1:F:248:ILE:CD1	2.47	0.44
1:A:56:MET:HE1	1:A:134:LYS:H	1.81	0.44
1:C:52:ILE:HD11	1:C:59:GLU:HB2	2.00	0.44
1:B:23:ARG:HG2	1:B:29:PHE:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:HIS:NE2	1:C:35:LYS:HE3	2.32	0.44
1:E:85:TYR:O	1:E:89:GLU:HG3	2.17	0.44
1:F:50:PHE:CD1	1:F:117:PRO:HG3	2.52	0.44
1:F:69:ILE:O	1:F:73:VAL:HG23	2.17	0.44
1:A:198:TRP:CE3	1:A:256:ILE:HD13	2.51	0.44
1:A:225:ILE:HD13	1:A:245:VAL:HG23	2.00	0.44
1:C:57:VAL:CG1	1:C:58:ALA:H	2.31	0.44
1:C:82:ILE:CG2	1:C:84:THR:HG23	2.47	0.44
1:E:88:VAL:HG22	1:E:233:LEU:HD21	2.00	0.44
1:F:136:ASP:HA	1:F:137:PRO:HD3	1.71	0.44
1:B:170:LEU:N	1:B:170:LEU:CD1	2.81	0.44
1:C:73:VAL:HG11	1:C:79:LYS:CD	2.48	0.44
1:C:167:ILE:CG2	1:C:167:ILE:O	2.65	0.44
1:C:204:VAL:HG12	1:C:216:LEU:CD1	2.48	0.44
1:E:62:GLY:H	1:E:197:ASN:HD21	1.66	0.44
1:E:65:GLY:H	1:E:197:ASN:ND2	2.16	0.44
1:B:128:MET:HE1	1:B:158:GLY:HA3	2.00	0.43
1:D:62:GLY:HA2	1:D:114:VAL:HG12	2.00	0.43
1:D:119:ARG:O	1:D:183:SER:HA	2.19	0.43
1:D:137:PRO:C	1:D:138:LEU:HD12	2.38	0.43
1:D:198:TRP:CE3	1:D:256:ILE:HD13	2.53	0.43
1:C:11:GLY:O	1:C:13:ARG:N	2.50	0.43
1:C:266:GLU:OE2	1:E:252:VAL:HG21	2.18	0.43
1:D:89:GLU:OE2	1:D:99:LEU:HD13	2.18	0.43
1:E:43:ARG:HH11	1:E:107:ASP:HB3	1.83	0.43
1:E:70:TYR:CE2	1:E:97:VAL:HG13	2.52	0.43
1:E:248:ILE:CG2	1:E:252:VAL:HB	2.48	0.43
1:C:48:THR:HB	1:C:84:THR:HG22	2.00	0.43
1:E:61:ASP:HB2	1:E:245:VAL:HG23	2.00	0.43
1:E:115:GLU:OE1	1:E:161:GLU:HG2	2.18	0.43
1:E:187:THR:CG2	1:E:189:GLU:O	2.67	0.43
1:B:187:THR:HG22	1:B:189:GLU:O	2.18	0.43
1:C:32:ASN:HB3	1:C:189:GLU:OE1	2.18	0.43
1:C:60:THR:HG22	1:C:245:VAL:HB	2.00	0.43
1:C:177:HIS:ND1	3:C:405:HOH:O	2.03	0.43
1:C:266:GLU:HG3	1:E:249:ARG:HD2	1.99	0.43
1:D:1:MET:HG3	1:D:206:GLN:CA	2.47	0.43
1:F:23:ARG:O	1:F:23:ARG:HD3	2.19	0.43
1:B:168:ARG:HG3	1:B:168:ARG:HH11	1.84	0.43
1:C:61:ASP:HB2	1:C:246:ASP:OD1	2.18	0.43
1:C:29:PHE:CD1	1:C:30:LEU:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:THR:O	1:C:162:ILE:HG13	2.17	0.43
1:D:21:ASP:O	1:D:24:ARG:HB3	2.19	0.43
1:A:16:LEU:HD21	1:F:4:HIS:HD2	1.84	0.43
1:D:160:ASN:OD1	1:D:161:GLU:OE2	2.37	0.43
1:C:99:LEU:CD1	1:C:99:LEU:N	2.78	0.43
1:C:134:LYS:O	1:C:135:ARG:HG2	2.18	0.43
1:D:1:MET:HG3	1:D:206:GLN:N	2.33	0.43
1:F:70:TYR:CE2	1:F:97:VAL:HG13	2.54	0.43
1:D:233:LEU:HD12	1:D:233:LEU:HA	1.81	0.42
1:F:177:HIS:HB2	1:F:181:ILE:HD12	2.01	0.42
1:E:255:GLY:O	1:E:259:LEU:HB2	2.18	0.42
1:D:177:HIS:HB2	1:D:181:ILE:HD12	2.00	0.42
1:E:195:VAL:O	1:E:196:SER:C	2.58	0.42
1:F:228:ILE:HG23	1:F:233:LEU:HB2	2.01	0.42
1:A:154:GLY:H	1:A:187:THR:HG21	1.84	0.42
1:B:249:ARG:NH1	1:D:269:LEU:HD13	2.34	0.42
1:C:44:VAL:CG1	1:C:79:LYS:HD3	2.47	0.42
1:C:81:GLU:HB2	1:C:82:ILE:H	1.50	0.42
1:C:85:TYR:OH	1:C:138:LEU:HD13	2.19	0.42
1:C:110:LEU:HD12	1:C:151:PRO:O	2.19	0.42
1:C:120:ALA:C	1:C:122:ASP:H	2.23	0.42
1:D:242:ALA:HA	1:D:243:PRO:HD3	1.82	0.42
1:E:158:GLY:N	1:E:161:GLU:OE2	2.52	0.42
1:A:55:MET:CE	1:A:239:LYS:HB3	2.49	0.42
1:B:249:ARG:NH1	1:D:269:LEU:CD1	2.82	0.42
1:C:84:THR:HG21	1:C:88:VAL:HG11	2.02	0.42
1:C:184:VAL:HG12	1:C:184:VAL:O	2.18	0.42
1:E:23:ARG:HG2	1:E:29:PHE:CE2	2.55	0.42
1:F:187:THR:HG22	1:F:189:GLU:O	2.20	0.42
1:F:234:ILE:HG23	1:F:235:ASP:N	2.34	0.42
1:A:261:LYS:HD3	1:D:223:ARG:HD3	2.01	0.42
1:B:177:HIS:O	1:B:178:GLY:C	2.58	0.42
1:C:105:PRO:O	1:C:108:TYR:N	2.45	0.42
1:E:37:PHE:HA	1:E:110:LEU:CD2	2.49	0.42
1:A:157:ASP:CB	1:A:193:SER:O	2.68	0.42
1:B:128:MET:CB	3:B:414:HOH:O	2.68	0.42
1:F:41:LEU:O	1:F:42:GLU:C	2.58	0.42
1:C:102:THR:N	1:C:103:PRO:CD	2.82	0.42
1:D:38:LEU:H	1:D:38:LEU:HD22	1.83	0.42
1:D:119:ARG:NH1	3:D:418:HOH:O	2.51	0.42
1:F:152:THR:HG22	1:F:188:ASP:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:VAL:C	1:C:75:MET:N	2.73	0.42
1:E:69:ILE:O	1:E:73:VAL:HG23	2.20	0.42
1:F:184:VAL:O	1:F:184:VAL:HG12	2.19	0.42
1:C:44:VAL:H	1:C:79:LYS:CB	2.32	0.41
1:C:129:SER:O	1:C:130:ALA:HB3	2.20	0.41
1:C:235:ASP:HB3	1:C:238:SER:HB3	2.02	0.41
1:F:91:ALA:HB1	1:F:228:ILE:HG12	2.00	0.41
1:F:187:THR:HG21	1:F:189:GLU:O	2.20	0.41
1:B:5:LEU:N	1:B:5:LEU:CD2	2.83	0.41
1:C:62:GLY:N	1:C:197:ASN:ND2	2.48	0.41
1:D:187:THR:HG22	1:D:189:GLU:N	2.33	0.41
1:E:93:GLU:N	1:E:94:PRO:CD	2.82	0.41
1:B:5:LEU:HD12	1:B:259:LEU:HD13	2.00	0.41
1:B:144:LYS:O	1:B:147:ALA:HB3	2.21	0.41
1:D:111:ILE:HG22	1:D:142:PHE:CE2	2.55	0.41
1:F:189:GLU:HA	1:F:189:GLU:OE1	2.21	0.41
1:B:8:THR:CG2	1:B:8:THR:O	2.67	0.41
1:E:102:THR:N	1:E:103:PRO:CD	2.83	0.41
1:F:48:THR:CG2	1:F:66:ALA:HB2	2.49	0.41
1:C:202:GLY:O	1:C:205:ALA:HB3	2.19	0.41
1:E:250:LEU:O	1:E:254:GLU:HG3	2.20	0.41
1:A:43:ARG:H	1:A:109:SER:HB3	1.86	0.41
1:D:177:HIS:O	1:D:181:ILE:HB	2.21	0.41
1:E:201:TYR:N	1:E:201:TYR:CD1	2.88	0.41
1:A:45:LEU:HD22	1:A:46:ILE:N	2.35	0.41
1:E:157:ASP:HB2	1:E:193:SER:O	2.20	0.41
1:C:2:ILE:HD13	1:C:205:ALA:CB	2.51	0.41
1:C:264:VAL:O	1:C:266:GLU:N	2.53	0.41
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.95	0.41
1:D:87:GLU:O	1:D:90:LYS:HB3	2.20	0.41
1:D:166:LYS:O	1:D:166:LYS:HG2	2.21	0.41
1:E:47:VAL:HG21	1:E:142:PHE:HE1	1.86	0.41
1:E:237:VAL:O	1:E:239:LYS:HG3	2.21	0.41
1:F:53:PRO:HA	1:F:54:PRO:HA	1.78	0.41
1:B:128:MET:HA	1:B:128:MET:HE2	2.03	0.41
1:C:40:ASN:C	1:C:42:GLU:H	2.24	0.41
1:C:50:PHE:CE1	1:C:117:PRO:HG3	2.56	0.41
1:C:262:ALA:O	1:C:264:VAL:N	2.54	0.41
1:D:64:PRO:HG3	1:D:228:ILE:HD12	2.01	0.41
1:D:125:TYR:CE2	1:D:137:PRO:HB3	2.55	0.41
1:D:160:ASN:OD1	1:D:160:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:LEU:HD12	1:D:260:LEU:HA	1.98	0.41
1:E:172:VAL:HA	1:E:178:GLY:HA3	2.03	0.41
1:E:187:THR:HG21	1:E:189:GLU:O	2.21	0.41
1:C:10:ILE:O	1:C:10:ILE:CG2	2.64	0.41
1:C:150:ILE:CG2	1:C:151:PRO:HD2	2.51	0.41
1:C:203:LEU:HD23	1:C:203:LEU:O	2.20	0.41
1:C:45:LEU:HA	1:C:45:LEU:HD12	1.89	0.40
1:C:103:PRO:HB2	1:C:108:TYR:HE2	1.86	0.40
1:B:63:PRO:HB2	1:B:64:PRO:HD3	2.03	0.40
1:C:209:ILE:O	1:C:211:VAL:N	2.53	0.40
1:D:91:ALA:HB2	1:D:231:ALA:HB3	2.03	0.40
1:E:225:ILE:O	1:E:228:ILE:HG22	2.21	0.40
1:B:50:PHE:CE2	1:B:133:ILE:HD11	2.55	0.40
1:E:56:MET:CE	1:E:134:LYS:HB2	2.52	0.40
1:F:148:LEU:HD12	1:F:148:LEU:HA	1.92	0.40
1:B:187:THR:HG21	1:B:189:GLU:O	2.22	0.40
1:D:93:GLU:N	1:D:94:PRO:CD	2.84	0.40
1:E:76:LEU:HD21	1:E:211:VAL:HG21	2.03	0.40
1:A:54:PRO:O	1:A:56:MET:HG2	2.22	0.40
1:A:90:LYS:HD2	1:A:90:LYS:HA	1.92	0.40
1:A:198:TRP:CZ3	1:A:256:ILE:CD1	3.05	0.40
1:A:252:VAL:CG2	1:F:266:GLU:HG3	2.52	0.40
1:C:44:VAL:HA	1:C:110:LEU:O	2.22	0.40
1:C:167:ILE:HG22	1:C:170:LEU:HB2	2.00	0.40
1:D:93:GLU:HG2	1:D:94:PRO:HD3	2.02	0.40
1:D:198:TRP:CZ2	1:D:256:ILE:HD12	2.57	0.40
1:E:50:PHE:O	1:E:59:GLU:HG2	2.21	0.40
1:F:20:LEU:HD12	1:F:20:LEU:HA	1.87	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	256/269 (95%)	235 (92%)	21 (8%)	0	100 100
1	B	263/269 (98%)	233 (89%)	27 (10%)	3 (1%)	14 34
1	C	267/269 (99%)	205 (77%)	44 (16%)	18 (7%)	1 1
1	D	267/269 (99%)	236 (88%)	29 (11%)	2 (1%)	22 46
1	E	254/269 (94%)	219 (86%)	30 (12%)	5 (2%)	7 19
1	F	267/269 (99%)	248 (93%)	19 (7%)	0	100 100
All	All	1574/1614 (98%)	1376 (87%)	170 (11%)	28 (2%)	8 21

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	ASP
1	C	12	ASN
1	C	168	ARG
1	C	213	ARG
1	D	2	ILE
1	E	181	ILE
1	B	12	ASN
1	C	96	GLY
1	C	210	GLU
1	E	36	MET
1	E	135	ARG
1	E	140	GLY
1	C	42	GLU
1	C	80	ALA
1	C	81	GLU
1	C	82	ILE
1	C	121	ALA
1	C	265	ASP
1	E	35	LYS
1	C	76	LEU
1	C	106	GLU
1	C	214	ASN
1	D	166	LYS
1	C	41	LEU
1	C	105	PRO
1	B	141	ILE
1	C	212	GLY
1	C	94	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/218 (96%)	195 (93%)	14 (7%)	16	37
1	B	212/218 (97%)	197 (93%)	15 (7%)	14	34
1	C	218/218 (100%)	205 (94%)	13 (6%)	19	42
1	D	218/218 (100%)	200 (92%)	18 (8%)	11	25
1	E	207/218 (95%)	191 (92%)	16 (8%)	13	30
1	F	218/218 (100%)	205 (94%)	13 (6%)	19	42
All	All	1282/1308 (98%)	1193 (93%)	89 (7%)	15	35

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	20	LEU
1	A	45	LEU
1	A	48	THR
1	A	55	MET
1	A	92	LEU
1	A	99	LEU
1	A	127	SER
1	A	146	ARG
1	A	170	LEU
1	A	203	LEU
1	A	211	VAL
1	A	222	ARG
1	A	251	MET
1	B	16	LEU
1	B	23	ARG
1	B	38	LEU
1	B	45	LEU
1	B	55	MET
1	B	83	LEU
1	B	92	LEU
1	B	93	GLU

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Mol	Chain	Res	Type
1	B	106	GLU
1	B	222	ARG
1	B	234	ILE
1	B	240	THR
1	B	245	VAL
1	B	256	ILE
1	B	259	LEU
1	C	23	ARG
1	C	38	LEU
1	C	55	MET
1	C	110	LEU
1	C	135	ARG
1	C	164	MET
1	C	168	ARG
1	C	203	LEU
1	C	210	GLU
1	C	213	ARG
1	C	245	VAL
1	C	259	LEU
1	C	265	ASP
1	D	1	MET
1	D	9	ASP
1	D	13	ARG
1	D	20	LEU
1	D	23	ARG
1	D	26	ASN
1	D	45	LEU
1	D	48	THR
1	D	55	MET
1	D	83	LEU
1	D	84	THR
1	D	92	LEU
1	D	97	VAL
1	D	143	LEU
1	D	203	LEU
1	D	233	LEU
1	D	258	GLU
1	D	260	LEU
1	E	20	LEU
1	E	21	ASP
1	E	23	ARG
1	E	38	LEU

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Mol	Chain	Res	Type
1	E	45	LEU
1	E	83	LEU
1	E	84	THR
1	E	106	GLU
1	E	139	ASP
1	E	181	ILE
1	E	203	LEU
1	E	223	ARG
1	E	240	THR
1	E	245	VAL
1	E	259	LEU
1	E	265	ASP
1	F	20	LEU
1	F	23	ARG
1	F	45	LEU
1	F	55	MET
1	F	74	GLU
1	F	83	LEU
1	F	129	SER
1	F	148	LEU
1	F	203	LEU
1	F	210	GLU
1	F	234	ILE
1	F	245	VAL
1	F	258	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	B	197	ASN
1	C	197	ASN
1	C	253	HIS
1	D	7	ASN
1	D	26	ASN
1	D	197	ASN
1	D	206	GLN
1	E	197	ASN
1	F	40	ASN
1	F	197	ASN
1	F	253	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 38 ligands modelled in this entry, 38 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	258/269 (95%)	-0.21	2 (0%) 86 87	23, 37, 53, 72	0
1	B	265/269 (98%)	-0.15	2 (0%) 86 87	25, 44, 70, 96	0
1	C	269/269 (100%)	0.52	18 (6%) 17 16	41, 66, 90, 103	0
1	D	269/269 (100%)	-0.15	2 (0%) 87 89	23, 45, 64, 81	0
1	E	256/269 (95%)	0.90	42 (16%) 1 1	41, 70, 83, 89	0
1	F	269/269 (100%)	-0.23	1 (0%) 92 93	20, 40, 56, 74	0
All	All	1586/1614 (98%)	0.11	67 (4%) 36 35	20, 48, 81, 103	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	141	ILE	8.2
1	D	1	MET	6.0
1	C	79	LYS	5.1
1	E	139	ASP	5.1
1	E	84	THR	4.5
1	E	125	TYR	4.4
1	C	81	GLU	4.3
1	E	88	VAL	4.1
1	E	255	GLY	3.8
1	E	112	ILE	3.6
1	C	92	LEU	3.6
1	E	85	TYR	3.6
1	E	101	ARG	3.5
1	E	57	VAL	3.4
1	A	101	ARG	3.2
1	E	69	ILE	3.2
1	E	52	ILE	3.2
1	C	67	LEU	3.1
1	C	74	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	135	ARG	3.0
1	E	68	ALA	3.0
1	E	202	GLY	3.0
1	E	260	LEU	2.9
1	E	58	ALA	2.9
1	E	137	PRO	2.9
1	E	82	ILE	2.9
1	B	5	LEU	2.9
1	C	225	ILE	2.8
1	E	131	LEU	2.8
1	E	42	GLU	2.8
1	E	140	GLY	2.8
1	C	147	ALA	2.8
1	E	45	LEU	2.7
1	E	55	MET	2.7
1	D	4	HIS	2.7
1	C	217	GLU	2.7
1	F	101	ARG	2.6
1	C	228	ILE	2.6
1	E	138	LEU	2.5
1	C	76	LEU	2.5
1	E	153	ILE	2.5
1	C	213	ARG	2.4
1	A	269	LEU	2.4
1	E	53	PRO	2.4
1	B	101	ARG	2.4
1	E	133	ILE	2.4
1	C	95	PHE	2.4
1	E	81	GLU	2.3
1	E	145	ALA	2.3
1	E	97	VAL	2.3
1	E	136	ASP	2.3
1	C	234	ILE	2.3
1	E	269	LEU	2.2
1	C	90	LYS	2.2
1	E	134	LYS	2.2
1	E	205	ALA	2.2
1	E	83	LEU	2.1
1	E	251	MET	2.1
1	C	70	TYR	2.1
1	E	259	LEU	2.1
1	E	232	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	256	ILE	2.1
1	C	91	ALA	2.1
1	C	98	SER	2.1
1	E	47	VAL	2.1
1	E	198	TRP	2.1
1	C	13	ARG	2.1

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	307	1/1	0.85	0.05	104,104,104,104	0
2	ZN	F	302	1/1	0.89	0.14	112,112,112,112	0
2	ZN	E	306	1/1	0.90	0.10	102,102,102,102	0
2	ZN	E	308	1/1	0.92	0.07	117,117,117,117	0
2	ZN	B	306	1/1	0.94	0.15	70,70,70,70	0
2	ZN	A	304	1/1	0.95	0.17	89,89,89,89	0
2	ZN	F	307	1/1	0.95	0.07	87,87,87,87	0
2	ZN	F	301	1/1	0.96	0.05	107,107,107,107	0
2	ZN	D	301	1/1	0.96	0.14	84,84,84,84	0
2	ZN	E	304	1/1	0.96	0.07	94,94,94,94	0
2	ZN	C	301	1/1	0.97	0.15	56,56,56,56	0
2	ZN	B	304	1/1	0.97	0.17	72,72,72,72	0
2	ZN	B	307	1/1	0.98	0.14	64,64,64,64	0
2	ZN	B	305	1/1	0.98	0.06	99,99,99,99	0
2	ZN	C	303	1/1	0.98	0.13	67,67,67,67	0
2	ZN	A	305	1/1	0.98	0.22	61,61,61,61	0
2	ZN	E	302	1/1	0.98	0.10	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	E	303	1/1	0.98	0.07	74,74,74,74	0
2	ZN	D	303	1/1	0.99	0.17	56,56,56,56	0
2	ZN	D	304	1/1	0.99	0.20	41,41,41,41	0
2	ZN	E	301	1/1	0.99	0.15	59,59,59,59	0
2	ZN	A	302	1/1	0.99	0.11	41,41,41,41	0
2	ZN	A	306	1/1	0.99	0.17	47,47,47,47	0
2	ZN	A	303	1/1	0.99	0.17	28,28,28,28	0
2	ZN	E	305	1/1	0.99	0.17	50,50,50,50	0
2	ZN	B	302	1/1	0.99	0.14	54,54,54,54	0
2	ZN	E	307	1/1	0.99	0.15	97,97,97,97	0
2	ZN	C	302	1/1	0.99	0.19	51,51,51,51	0
2	ZN	B	303	1/1	0.99	0.13	43,43,43,43	0
2	ZN	C	304	1/1	0.99	0.17	51,51,51,51	0
2	ZN	F	303	1/1	0.99	0.16	41,41,41,41	0
2	ZN	F	304	1/1	0.99	0.16	29,29,29,29	0
2	ZN	F	305	1/1	0.99	0.15	38,38,38,38	0
2	ZN	F	306	1/1	0.99	0.10	51,51,51,51	0
2	ZN	A	301	1/1	0.99	0.20	33,33,33,33	0
2	ZN	B	301	1/1	1.00	0.14	37,37,37,37	0
2	ZN	D	302	1/1	1.00	0.17	32,32,32,32	0
2	ZN	D	305	1/1	1.00	0.18	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.