Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:21 PM GMT

PDB ID	:	4HYC
Title	:	Structure of a presenilin family intramembrane aspartate protease in P2 space group
Authors	:	Li, X.; Dang, S.; Yan, C.; Wang, J.; Shi, Y.
Deposited on	:	2012-11-13
Resolution	:	3.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

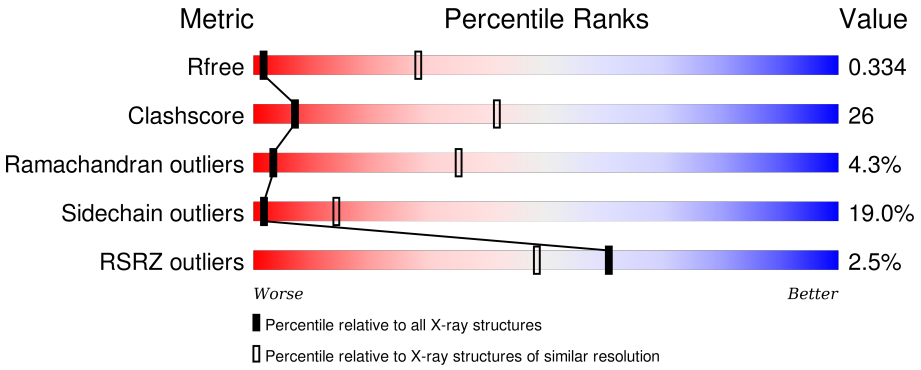
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1011 (4.38-3.54)
Clashscore	102246	1025 (4.32-3.60)
Ramachandran outliers	100387	1008 (4.34-3.58)
Sidechain outliers	100360	1027 (4.36-3.56)
RSRZ outliers	91569	1015 (4.38-3.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	301	38% 36% 7% 18%
1	B	301	40% 32% 9% 18%
1	C	301	40% 34% 7% 18%
1	D	301	36% 37% 9% 18%
1	E	301	42% 31% 9% 18%

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Mol	Chain	Length	Quality of chain
1	F	301	3% 37% 35% 9% 18%
1	G	301	% 37% 36% 9% 18%
1	H	301	5% 40% 34% 8% 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14416 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	B	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	C	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	D	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	E	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	F	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	G	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			
1	H	246	Total	C	N	O	S	0	0	0
			1802	1219	276	296	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	ASN	ASP	ENGINEERED MUTATION	UNP A3CWV0
A	42	SER	GLU	ENGINEERED MUTATION	UNP A3CWV0
A	147	GLU	ALA	ENGINEERED MUTATION	UNP A3CWV0
A	148	PRO	VAL	ENGINEERED MUTATION	UNP A3CWV0
A	229	VAL	ALA	ENGINEERED MUTATION	UNP A3CWV0
B	40	ASN	ASP	ENGINEERED MUTATION	UNP A3CWV0
B	42	SER	GLU	ENGINEERED MUTATION	UNP A3CWV0
B	147	GLU	ALA	ENGINEERED MUTATION	UNP A3CWV0
B	148	PRO	VAL	ENGINEERED MUTATION	UNP A3CWV0
B	229	VAL	ALA	ENGINEERED MUTATION	UNP A3CWV0
C	40	ASN	ASP	ENGINEERED MUTATION	UNP A3CWV0
C	42	SER	GLU	ENGINEERED MUTATION	UNP A3CWV0
C	147	GLU	ALA	ENGINEERED MUTATION	UNP A3CWV0

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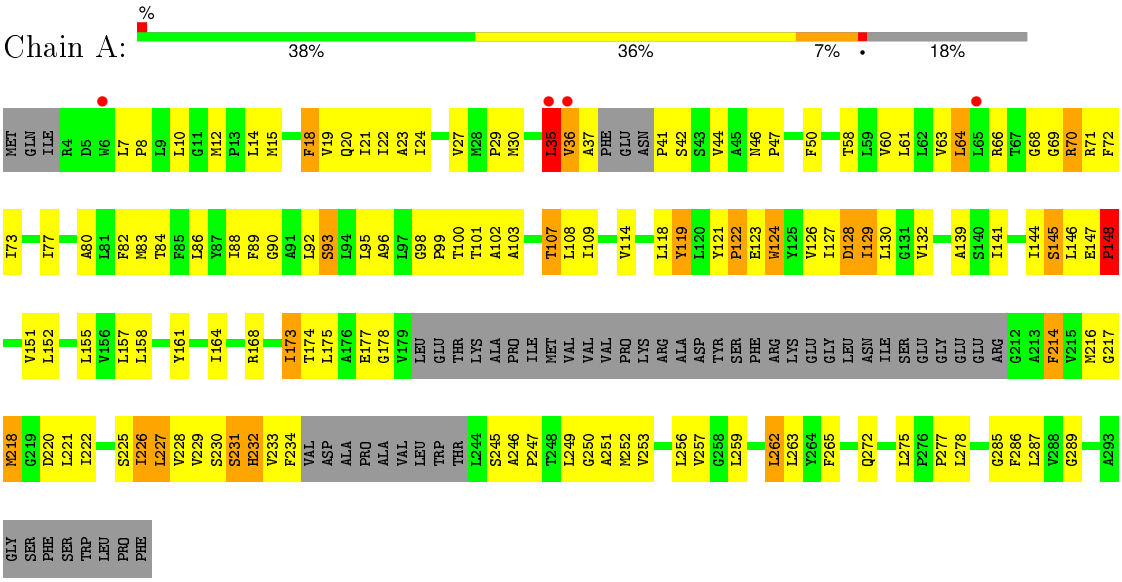
Chain	Residue	Modelled	Actual	Comment	Reference
C	148	PRO	VAL	ENGINEERED MUTATION	UNP A3CWV0
C	229	VAL	ALA	ENGINEERED MUTATION	UNP A3CWV0
D	40	ASN	ASP	ENGINEERED MUTATION	UNP A3CWV0
D	42	SER	GLU	ENGINEERED MUTATION	UNP A3CWV0
D	147	GLU	ALA	ENGINEERED MUTATION	UNP A3CWV0
D	148	PRO	VAL	ENGINEERED MUTATION	UNP A3CWV0
D	229	VAL	ALA	ENGINEERED MUTATION	UNP A3CWV0
E	40	ASN	ASP	ENGINEERED MUTATION	UNP A3CWV0
E	42	SER	GLU	ENGINEERED MUTATION	UNP A3CWV0
E	147	GLU	ALA	ENGINEERED MUTATION	UNP A3CWV0
E	148	PRO	VAL	ENGINEERED MUTATION	UNP A3CWV0
E	229	VAL	ALA	ENGINEERED MUTATION	UNP A3CWV0
F	40	ASN	ASP	ENGINEERED MUTATION	UNP A3CWV0
F	42	SER	GLU	ENGINEERED MUTATION	UNP A3CWV0
F	147	GLU	ALA	ENGINEERED MUTATION	UNP A3CWV0
F	148	PRO	VAL	ENGINEERED MUTATION	UNP A3CWV0
F	229	VAL	ALA	ENGINEERED MUTATION	UNP A3CWV0
G	40	ASN	ASP	ENGINEERED MUTATION	UNP A3CWV0
G	42	SER	GLU	ENGINEERED MUTATION	UNP A3CWV0
G	147	GLU	ALA	ENGINEERED MUTATION	UNP A3CWV0
G	148	PRO	VAL	ENGINEERED MUTATION	UNP A3CWV0
G	229	VAL	ALA	ENGINEERED MUTATION	UNP A3CWV0
H	40	ASN	ASP	ENGINEERED MUTATION	UNP A3CWV0
H	42	SER	GLU	ENGINEERED MUTATION	UNP A3CWV0
H	147	GLU	ALA	ENGINEERED MUTATION	UNP A3CWV0
H	148	PRO	VAL	ENGINEERED MUTATION	UNP A3CWV0
H	229	VAL	ALA	ENGINEERED MUTATION	UNP A3CWV0

3 Residue-property plots (i)

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

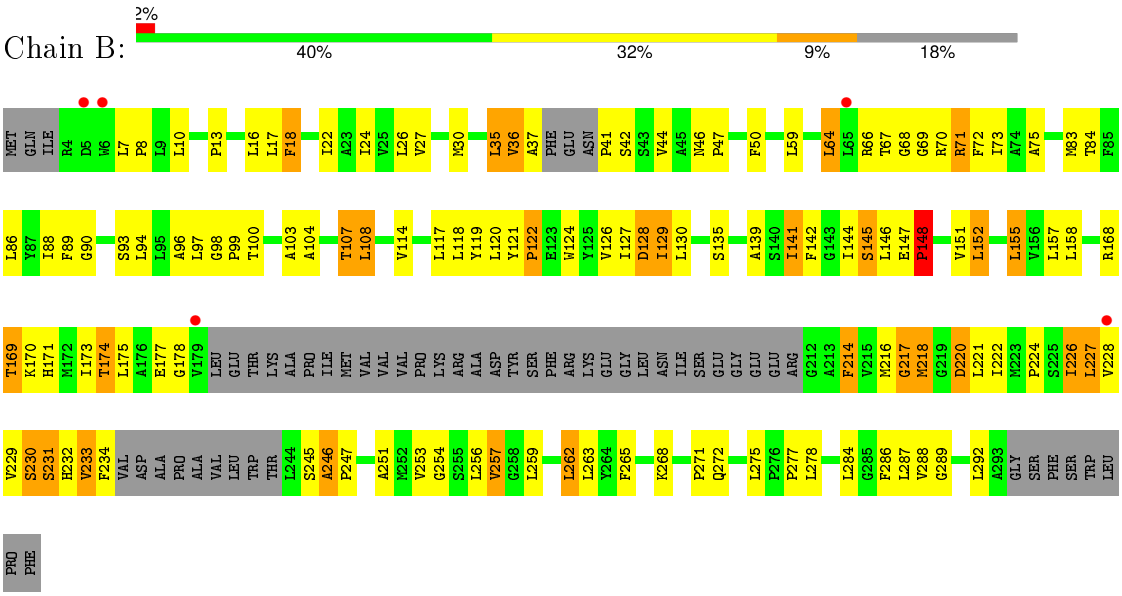
- Molecule 1: Putative uncharacterized protein

Chain A:



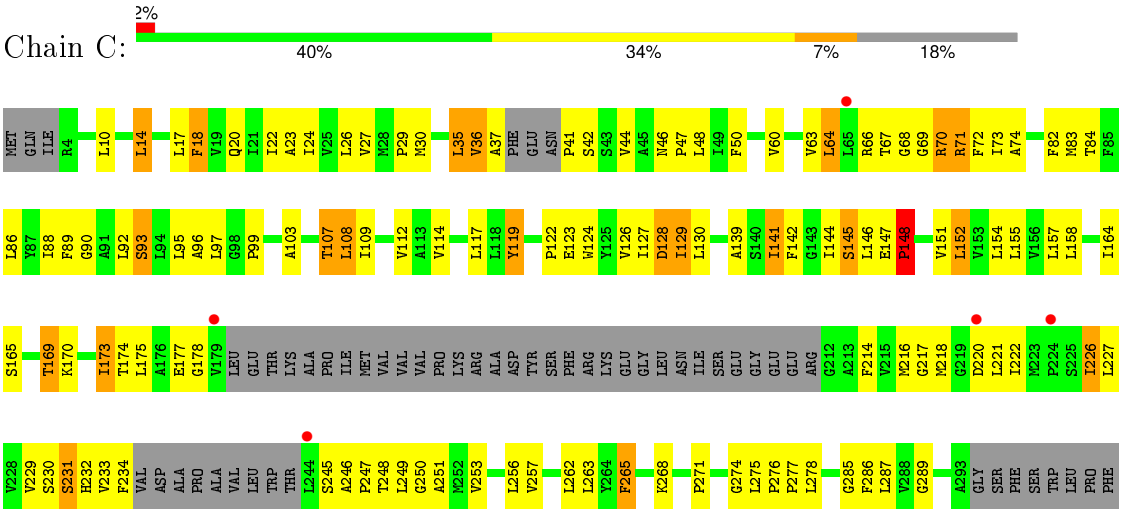
- Molecule 1: Putative uncharacterized protein

Chain B:



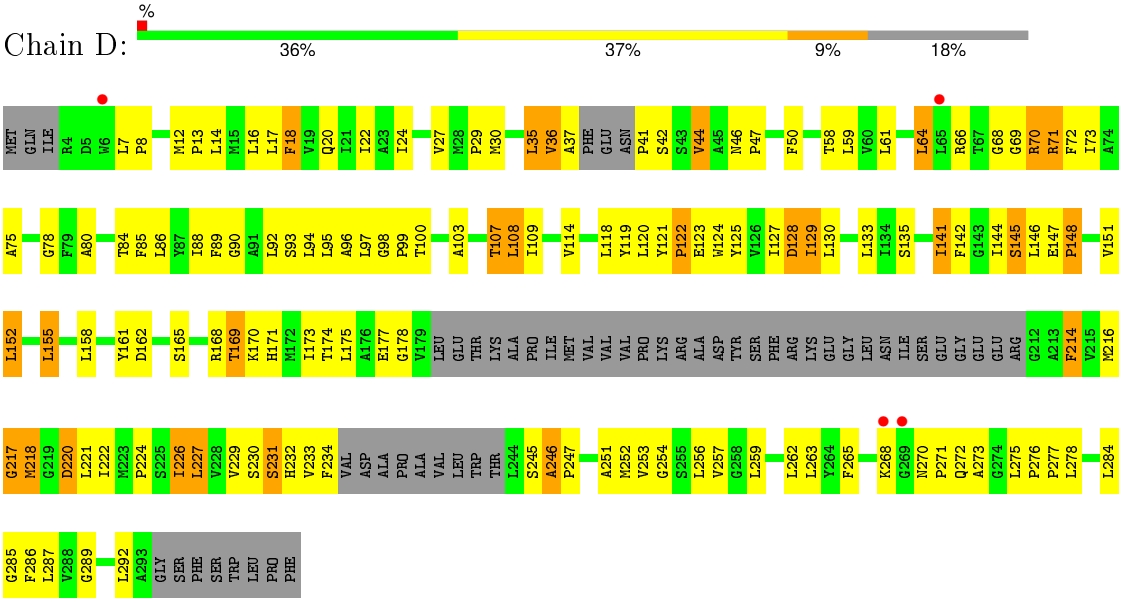
- Molecule 1: Putative uncharacterized protein

Chain C:



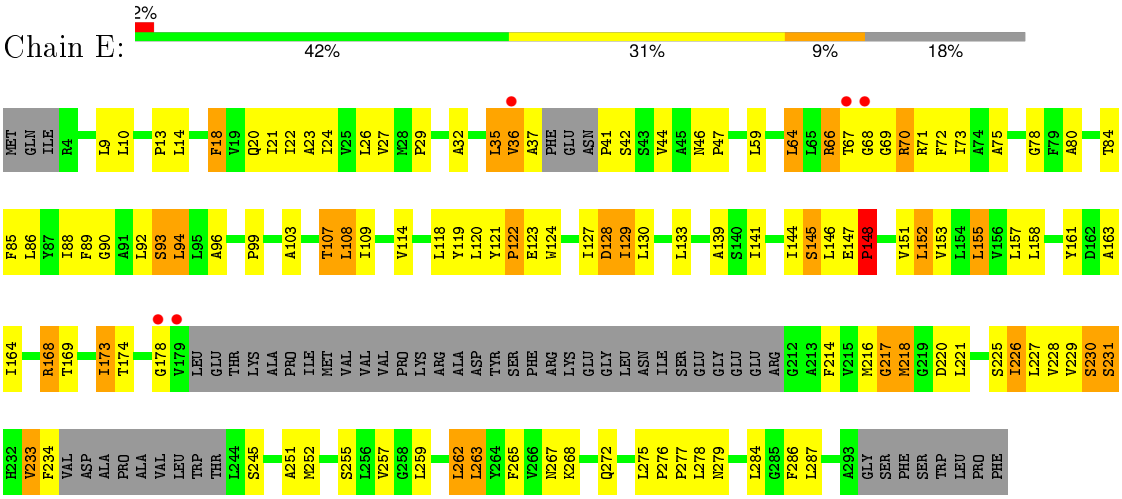
• Molecule 1: Putative uncharacterized protein

Chain D:



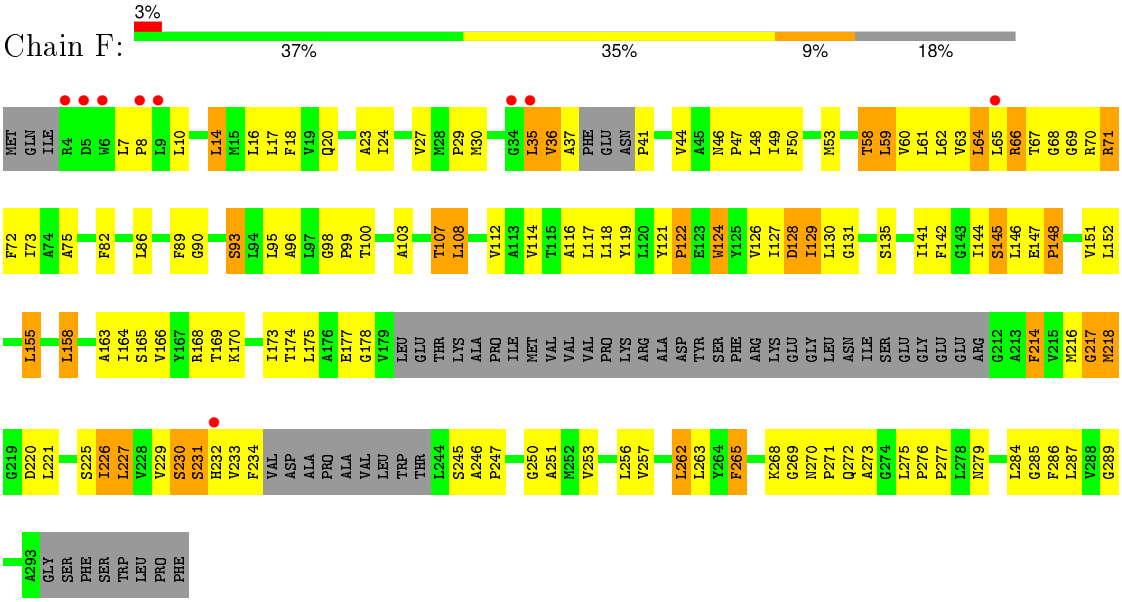
• Molecule 1: Putative uncharacterized protein

Chain E:



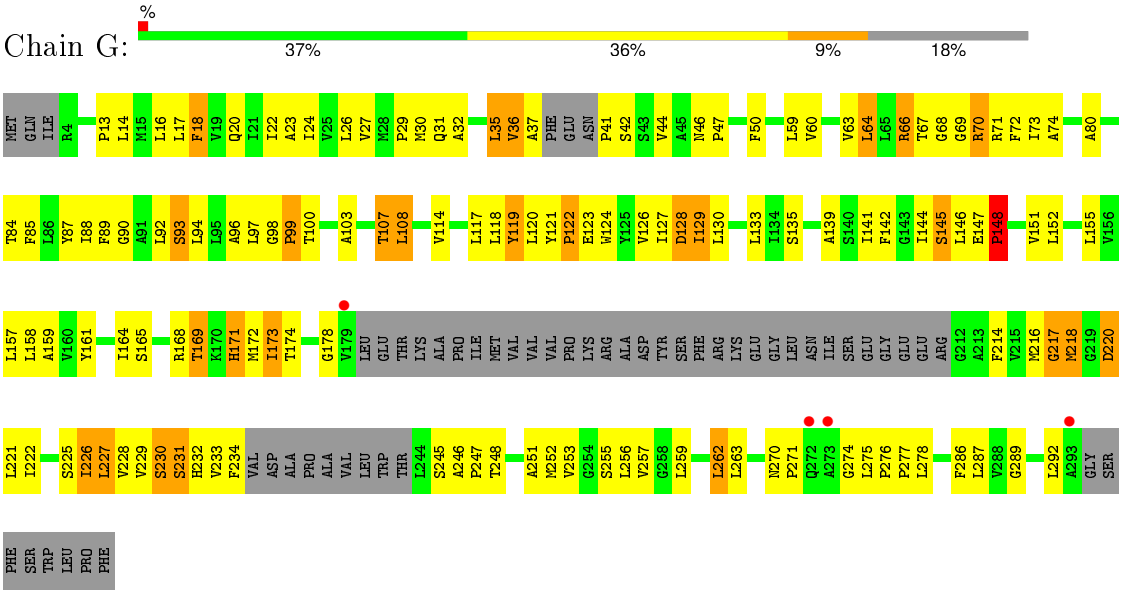
• Molecule 1: Putative uncharacterized protein

Chain F:



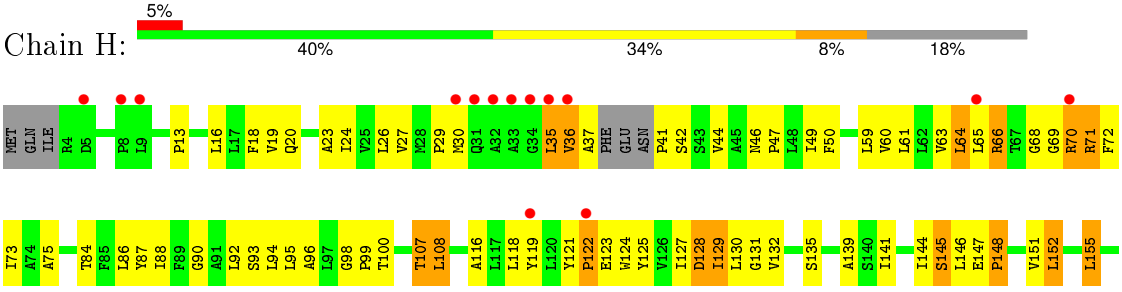
• Molecule 1: Putative uncharacterized protein

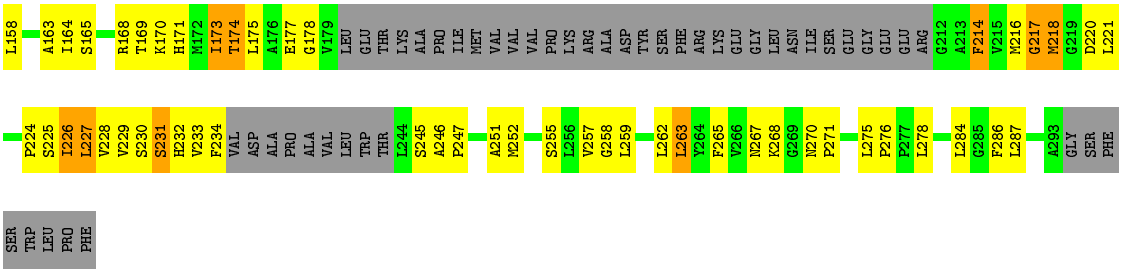
Chain G:



• Molecule 1: Putative uncharacterized protein

Chain H:




L158
A163
I164
S165
R168
T169
K170
H171
M172
I173
T174
L175
A176
E177
G178
V179
LEU
GLU
THR
LYS
ALA
PRO
ILE
MET
VAL
VAL
VAL
PRO
LYS
ARG
ALA
ASP
TYR
SER
PHE
ARG
LYS
GLU
GLY
LEU
ASN
ILE
SER
GLU
GLY
GLU
GLU
ARG
G212
A213
F214
V215
M216
G217
M218
G219
D220
L221
P224
S225
I226
L227
V228
V229
S230
S231
H232
V233
F234
VAL
ASP
ALA
PRO
ALA
VAL
LEU
TRP
THR
L244
S245
A246
P247
A251
M252
S255
L256
V257
G258
L259
L262
L263
Y264
F265
V266
N267
K268
G269
N270
P271
L275
P276
P277
L278
L284
G285
F286
L287
A293
GLY
SER
PHE
SER
TRP
LEU
PRO
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.22Å 115.83Å 137.17Å 90.00° 100.59° 90.00°	Depositor
Resolution (Å)	40.16 – 3.95 40.16 – 3.95	Depositor EDS
% Data completeness (in resolution range)	78.3 (40.16-3.95) 78.5 (40.16-3.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.308 , 0.341 0.306 , 0.334	Depositor DCC
R_{free} test set	1339 reflections (4.93%)	DCC
Wilson B-factor (Å^2)	123.3	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 77.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 27265 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14416	wwPDB-VP
Average B, all atoms (Å^2)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.42	0/1839	0.68	0/2511
1	B	0.44	0/1839	0.68	0/2511
1	C	0.43	0/1839	0.69	0/2511
1	D	0.43	0/1839	0.68	0/2511
1	E	0.44	0/1839	0.71	0/2511
1	F	0.42	0/1839	0.68	1/2511 (0.0%)
1	G	0.44	0/1839	0.71	0/2511
1	H	0.40	0/1839	0.65	1/2511 (0.0%)
All	All	0.43	0/14712	0.69	2/20088 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	2
1	G	0	1
1	H	0	1
All	All	0	11

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	59	LEU	CA-CB-CG	5.51	127.97	115.30
1	H	59	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	TRP	Peptide
1	A	145	SER	Peptide
1	B	145	SER	Peptide
1	C	124	TRP	Peptide
1	C	145	SER	Peptide
1	D	145	SER	Peptide
1	E	145	SER	Peptide
1	F	124	TRP	Peptide
1	F	145	SER	Peptide
1	G	145	SER	Peptide
1	H	145	SER	Peptide

5.2 Too-close contacts (i)

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	1802	0	1949	109	0
1	B	1802	0	1949	98	0
1	C	1802	0	1949	101	0
1	D	1802	0	1949	109	0
1	E	1802	0	1949	100	0
1	F	1802	0	1949	109	0
1	G	1802	0	1949	101	0
1	H	1802	0	1949	103	0
All	All	14416	0	15592	789	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 26.

All (789) 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:A:36:VAL:CG2	1:A:144:ILE:HG22	1.28	1.64
1:C:36:VAL:CG2	1:C:144:ILE:HG22	1.30	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:VAL:CG2	1:F:144:ILE:HG22	1.51	1.40
1:A:36:VAL:HG13	1:A:145:SER:CA	1.59	1.32
1:H:36:VAL:CG2	1:H:144:ILE:HG22	1.63	1.29
1:A:36:VAL:CG1	1:A:145:SER:HA	1.64	1.27
1:C:36:VAL:CG1	1:C:145:SER:HA	1.65	1.26
1:C:36:VAL:HG13	1:C:145:SER:CA	1.64	1.26
1:C:36:VAL:CG2	1:C:144:ILE:CG2	2.18	1.21
1:A:36:VAL:CG2	1:A:144:ILE:CG2	2.19	1.20
1:H:36:VAL:HG13	1:H:145:SER:CA	1.71	1.20
1:E:36:VAL:CG1	1:E:37:ALA:H	1.52	1.19
1:F:36:VAL:HG13	1:F:145:SER:CA	1.71	1.18
1:D:36:VAL:HG12	1:D:37:ALA:N	1.50	1.18
1:H:36:VAL:CG1	1:H:145:SER:HA	1.73	1.18
1:A:36:VAL:CG1	1:A:37:ALA:H	1.56	1.17
1:B:36:VAL:HG12	1:B:37:ALA:N	1.54	1.17
1:A:36:VAL:HG12	1:A:37:ALA:N	1.53	1.17
1:E:36:VAL:HG12	1:E:37:ALA:N	1.47	1.17
1:E:36:VAL:CG2	1:E:144:ILE:HG22	1.75	1.16
1:B:36:VAL:CG2	1:B:144:ILE:HG22	1.76	1.15
1:C:36:VAL:CG1	1:C:37:ALA:H	1.56	1.15
1:D:36:VAL:CG1	1:D:37:ALA:H	1.51	1.15
1:F:36:VAL:HG12	1:F:37:ALA:N	1.58	1.14
1:B:36:VAL:HG13	1:B:145:SER:CA	1.77	1.14
1:B:36:VAL:CG1	1:B:37:ALA:H	1.56	1.14
1:C:36:VAL:HG12	1:C:37:ALA:N	1.54	1.13
1:C:36:VAL:HG22	1:C:144:ILE:CG2	1.78	1.13
1:H:36:VAL:HG12	1:H:37:ALA:N	1.55	1.12
1:H:36:VAL:CG1	1:H:37:ALA:H	1.58	1.12
1:F:36:VAL:CG1	1:F:145:SER:HA	1.78	1.12
1:D:36:VAL:HG13	1:D:145:SER:HA	1.32	1.11
1:B:36:VAL:HG13	1:B:145:SER:HA	1.11	1.10
1:A:36:VAL:HG21	1:A:144:ILE:HG22	1.31	1.08
1:F:36:VAL:CG1	1:F:37:ALA:H	1.62	1.07
1:G:36:VAL:HG12	1:G:37:ALA:N	1.57	1.07
1:B:36:VAL:HG22	1:B:144:ILE:HG22	1.09	1.04
1:A:36:VAL:HG22	1:A:144:ILE:HG22	1.05	1.04
1:E:36:VAL:HG22	1:E:144:ILE:HG22	1.07	1.04
1:G:36:VAL:CG1	1:G:37:ALA:H	1.62	1.04
1:F:36:VAL:HG22	1:F:144:ILE:CG2	1.88	1.03
1:B:289:GLY:HA2	1:B:292:LEU:HD12	1.41	1.01
1:E:36:VAL:HG13	1:E:145:SER:HA	1.40	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:VAL:CG2	1:F:144:ILE:CG2	2.38	1.00
1:A:36:VAL:HG13	1:A:145:SER:HA	1.00	0.99
1:B:36:VAL:CG1	1:B:145:SER:HA	1.93	0.99
1:G:36:VAL:HG13	1:G:145:SER:HA	1.41	0.98
1:H:36:VAL:HG22	1:H:144:ILE:CG2	1.94	0.96
1:C:36:VAL:HG23	1:C:144:ILE:HG22	1.44	0.96
1:H:36:VAL:HG22	1:H:144:ILE:HG22	0.97	0.95
1:E:36:VAL:HG22	1:E:144:ILE:CG2	1.98	0.92
1:B:36:VAL:HG13	1:B:145:SER:CB	1.98	0.92
1:G:36:VAL:HG12	1:G:37:ALA:H	0.76	0.92
1:F:36:VAL:HG22	1:F:144:ILE:HG22	0.92	0.91
1:F:36:VAL:HG12	1:F:37:ALA:H	0.74	0.90
1:F:64:LEU:HD11	1:F:73:ILE:HG23	1.52	0.90
1:A:36:VAL:HG13	1:A:145:SER:CB	2.02	0.89
1:F:36:VAL:HG13	1:F:145:SER:HA	0.90	0.88
1:H:64:LEU:HD11	1:H:73:ILE:HG23	1.55	0.86
1:H:36:VAL:CG2	1:H:144:ILE:CG2	2.50	0.86
1:H:36:VAL:HG12	1:H:37:ALA:H	0.71	0.85
1:C:36:VAL:HG22	1:C:144:ILE:HG22	0.84	0.84
1:E:36:VAL:HG13	1:E:145:SER:CA	2.08	0.84
1:A:36:VAL:HG22	1:A:144:ILE:CG2	1.93	0.84
1:G:36:VAL:HG22	1:G:144:ILE:HG22	1.59	0.83
1:F:64:LEU:HD21	1:F:73:ILE:HA	1.59	0.83
1:C:36:VAL:HG12	1:C:37:ALA:H	0.69	0.81
1:D:36:VAL:HG13	1:D:145:SER:CA	2.09	0.80
1:B:36:VAL:HG12	1:B:37:ALA:H	0.69	0.80
1:G:36:VAL:HG13	1:G:145:SER:CA	2.11	0.80
1:E:36:VAL:CG2	1:E:144:ILE:CG2	2.56	0.79
1:A:36:VAL:HG12	1:A:37:ALA:H	0.69	0.79
1:D:36:VAL:HG22	1:D:144:ILE:HG22	1.63	0.79
1:B:135:SER:HA	1:B:222:ILE:HD11	1.65	0.79
1:E:36:VAL:HG12	1:E:37:ALA:H	0.65	0.79
1:F:116:ALA:HA	1:G:164:ILE:HD11	1.65	0.78
1:C:70:ARG:HH22	1:D:169:THR:HG22	1.50	0.77
1:C:17:LEU:HD21	1:C:256:LEU:HD11	1.68	0.76
1:A:36:VAL:HG23	1:A:144:ILE:HG22	1.62	0.76
1:B:41:PRO:C	1:B:146:LEU:HG	2.05	0.76
1:A:64:LEU:HD11	1:A:73:ILE:HG23	1.67	0.75
1:F:30:MET:HE1	1:F:141:ILE:HA	1.66	0.75
1:B:30:MET:HE1	1:B:141:ILE:HA	1.69	0.74
1:D:289:GLY:HA2	1:D:292:LEU:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:ARG:O	1:F:75:ALA:N	2.21	0.74
1:D:135:SER:HA	1:D:222:ILE:HD11	1.70	0.73
1:B:120:LEU:HD21	1:C:164:ILE:HG12	1.69	0.73
1:B:289:GLY:HA2	1:B:292:LEU:CD1	2.18	0.73
1:C:64:LEU:HD11	1:C:73:ILE:HG23	1.70	0.73
1:D:36:VAL:HG12	1:D:37:ALA:H	0.65	0.73
1:H:64:LEU:HD21	1:H:73:ILE:HA	1.71	0.73
1:C:220:ASP:HB2	1:C:275:LEU:HD21	1.71	0.72
1:H:36:VAL:HG11	1:H:146:LEU:CD2	2.19	0.72
1:G:36:VAL:HG13	1:G:145:SER:CB	2.20	0.72
1:E:120:LEU:HD21	1:F:164:ILE:HG12	1.72	0.72
1:B:246:ALA:HB1	1:B:247:PRO:HD2	1.72	0.71
1:F:128:ASP:OD2	1:F:128:ASP:N	2.21	0.71
1:F:36:VAL:HG23	1:F:144:ILE:HG22	1.65	0.70
1:A:251:ALA:HB2	1:A:286:PHE:HB2	1.71	0.70
1:H:71:ARG:O	1:H:75:ALA:N	2.23	0.70
1:D:36:VAL:HG11	1:D:146:LEU:CD2	2.22	0.70
1:C:36:VAL:HG23	1:C:144:ILE:CG2	2.07	0.70
1:F:20:GLN:HG2	1:F:225:SER:HB2	1.73	0.70
1:D:42:SER:HA	1:D:146:LEU:HB3	1.71	0.70
1:E:118:LEU:HD12	1:E:130:LEU:HD12	1.74	0.69
1:B:36:VAL:CG2	1:B:144:ILE:CG2	2.63	0.69
1:A:64:LEU:HD21	1:A:73:ILE:HA	1.74	0.68
1:G:128:ASP:N	1:G:128:ASP:OD2	2.24	0.68
1:A:68:GLY:HA3	1:A:73:ILE:HD11	1.75	0.68
1:F:262:LEU:HD23	1:F:277:PRO:HG2	1.74	0.68
1:H:29:PRO:HB3	1:H:95:LEU:HD22	1.76	0.68
1:F:36:VAL:HG13	1:F:145:SER:CB	2.24	0.68
1:C:30:MET:HE1	1:C:141:ILE:HA	1.75	0.67
1:A:36:VAL:HG21	1:A:144:ILE:CG2	2.07	0.67
1:H:36:VAL:HG11	1:H:146:LEU:HD22	1.74	0.67
1:E:36:VAL:CG1	1:E:145:SER:HA	2.23	0.67
1:D:24:ILE:HA	1:D:27:VAL:HG23	1.76	0.67
1:C:128:ASP:OD2	1:C:128:ASP:N	2.21	0.67
1:C:129:ILE:HG22	1:C:130:LEU:HD23	1.76	0.67
1:G:36:VAL:CG1	1:G:37:ALA:N	2.34	0.67
1:B:24:ILE:HA	1:B:27:VAL:HG23	1.76	0.67
1:B:170:LYS:NZ	1:B:271:PRO:HG2	2.10	0.67
1:E:70:ARG:NH2	1:F:168:ARG:HH22	1.93	0.67
1:H:128:ASP:OD2	1:H:128:ASP:N	2.23	0.66
1:H:36:VAL:HG13	1:H:145:SER:HA	0.81	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:SER:HA	1:A:146:LEU:HB3	1.76	0.66
1:D:41:PRO:C	1:D:146:LEU:HG	2.15	0.66
1:D:36:VAL:CG2	1:D:144:ILE:HG22	2.25	0.66
1:B:42:SER:HA	1:B:146:LEU:HB3	1.76	0.66
1:H:20:GLN:O	1:H:24:ILE:HG12	1.96	0.66
1:H:30:MET:HE1	1:H:141:ILE:HA	1.77	0.65
1:F:129:ILE:HG22	1:F:130:LEU:HD23	1.77	0.65
1:C:36:VAL:HG22	1:C:144:ILE:C	2.15	0.65
1:B:36:VAL:CG1	1:B:37:ALA:N	2.30	0.65
1:A:36:VAL:HG11	1:A:145:SER:HA	1.73	0.65
1:F:68:GLY:HA3	1:F:73:ILE:HD11	1.78	0.65
1:A:229:VAL:O	1:A:231:SER:N	2.30	0.65
1:B:17:LEU:HD21	1:B:256:LEU:HD11	1.78	0.65
1:G:66:ARG:HH22	1:H:66:ARG:HD3	1.62	0.65
1:A:164:ILE:HG12	1:D:120:LEU:HD21	1.79	0.65
1:F:117:LEU:HD11	1:F:126:VAL:HG11	1.76	0.65
1:H:90:GLY:HA2	1:H:107:THR:HG21	1.79	0.65
1:E:121:TYR:HA	1:E:124:TRP:CZ2	2.32	0.64
1:A:29:PRO:HB3	1:A:95:LEU:HB2	1.79	0.64
1:C:251:ALA:HB2	1:C:286:PHE:HB2	1.78	0.64
1:D:36:VAL:HG13	1:D:145:SER:CB	2.28	0.64
1:G:84:THR:O	1:G:88:ILE:HG12	1.98	0.64
1:A:24:ILE:HD13	1:A:229:VAL:HG22	1.79	0.64
1:G:74:ALA:O	1:G:119:TYR:OH	2.15	0.63
1:B:64:LEU:HD11	1:B:73:ILE:HG23	1.81	0.63
1:D:84:THR:O	1:D:88:ILE:HG12	1.98	0.63
1:E:262:LEU:HD23	1:E:277:PRO:HG2	1.78	0.63
1:H:20:GLN:HG2	1:H:225:SER:HB2	1.81	0.63
1:E:128:ASP:OD2	1:E:128:ASP:N	2.26	0.63
1:B:128:ASP:N	1:B:128:ASP:OD2	2.27	0.63
1:A:47:PRO:O	1:A:50:PHE:HB3	1.99	0.62
1:D:151:VAL:HG12	1:D:227:LEU:HD12	1.79	0.62
1:G:148:PRO:O	1:G:151:VAL:N	2.32	0.62
1:E:121:TYR:HA	1:E:124:TRP:HZ2	1.65	0.62
1:D:97:LEU:HB2	1:D:103:ALA:HB2	1.80	0.62
1:B:83:MET:HG2	1:C:48:LEU:HD23	1.81	0.62
1:G:120:LEU:HD21	1:H:164:ILE:HG12	1.82	0.62
1:D:128:ASP:OD2	1:D:128:ASP:N	2.31	0.62
1:A:36:VAL:HG23	1:A:144:ILE:CG2	2.24	0.62
1:C:262:LEU:HD23	1:C:277:PRO:HG2	1.82	0.62
1:E:36:VAL:CG1	1:E:37:ALA:N	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:MET:HB3	1:D:35:LEU:HD22	1.82	0.61
1:D:36:VAL:CG1	1:D:37:ALA:N	2.26	0.61
1:D:262:LEU:HD23	1:D:277:PRO:HG2	1.82	0.61
1:G:36:VAL:CG2	1:G:144:ILE:HG22	2.29	0.61
1:A:168:ARG:HH12	1:D:70:ARG:NH2	1.98	0.61
1:H:275:LEU:O	1:H:278:LEU:N	2.33	0.61
1:F:36:VAL:HG23	1:F:144:ILE:CG2	2.26	0.61
1:E:41:PRO:C	1:E:146:LEU:HG	2.21	0.61
1:D:118:LEU:HD12	1:D:130:LEU:HD12	1.83	0.61
1:G:64:LEU:HD11	1:G:73:ILE:HG23	1.83	0.61
1:A:129:ILE:HG22	1:A:130:LEU:HD23	1.82	0.61
1:A:20:GLN:HG2	1:A:225:SER:HB2	1.83	0.60
1:A:128:ASP:OD2	1:A:128:ASP:N	2.23	0.60
1:C:148:PRO:O	1:C:151:VAL:N	2.35	0.60
1:C:64:LEU:HD21	1:C:73:ILE:HA	1.83	0.60
1:D:229:VAL:O	1:D:231:SER:N	2.34	0.60
1:E:229:VAL:O	1:E:231:SER:N	2.35	0.60
1:G:31:GLN:HG3	1:G:144:ILE:HD13	1.83	0.60
1:D:246:ALA:HB1	1:D:247:PRO:HD2	1.83	0.60
1:G:29:PRO:O	1:G:32:ALA:HB3	2.00	0.60
1:C:97:LEU:HB2	1:C:103:ALA:HB2	1.84	0.60
1:F:90:GLY:HA2	1:F:107:THR:HG21	1.83	0.60
1:C:72:PHE:CZ	1:D:59:LEU:HD23	2.36	0.60
1:B:71:ARG:O	1:B:75:ALA:N	2.34	0.60
1:E:129:ILE:HG22	1:E:130:LEU:HD23	1.84	0.60
1:E:24:ILE:HD13	1:E:229:VAL:HG22	1.84	0.60
1:C:47:PRO:O	1:C:50:PHE:HB3	2.01	0.60
1:G:147:GLU:HB3	1:G:148:PRO:HD2	1.84	0.60
1:F:17:LEU:HD21	1:F:256:LEU:HD11	1.84	0.59
1:C:117:LEU:HD11	1:C:126:VAL:HG11	1.84	0.59
1:D:64:LEU:HD11	1:D:73:ILE:HG23	1.84	0.59
1:D:253:VAL:HA	1:D:256:LEU:HD12	1.82	0.59
1:G:41:PRO:C	1:G:146:LEU:HG	2.23	0.59
1:G:70:ARG:HH22	1:H:169:THR:HG22	1.67	0.59
1:D:36:VAL:CG1	1:D:145:SER:HA	2.20	0.59
1:A:41:PRO:C	1:A:146:LEU:HG	2.22	0.59
1:E:36:VAL:HG13	1:E:145:SER:CB	2.32	0.59
1:D:165:SER:O	1:D:169:THR:HG23	2.02	0.59
1:A:253:VAL:HA	1:A:256:LEU:HD12	1.84	0.59
1:D:86:LEU:HD21	1:D:108:LEU:HA	1.84	0.59
1:G:24:ILE:HD13	1:G:229:VAL:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:129:ILE:HG22	1:H:130:LEU:HD23	1.84	0.58
1:E:148:PRO:O	1:E:151:VAL:N	2.36	0.58
1:E:163:ALA:HB2	1:E:276:PRO:HG2	1.84	0.58
1:G:42:SER:HA	1:G:146:LEU:HB3	1.84	0.58
1:F:124:TRP:CE3	1:F:127:ILE:HG13	2.39	0.58
1:H:148:PRO:O	1:H:151:VAL:N	2.37	0.58
1:F:30:MET:HB3	1:F:35:LEU:HD22	1.86	0.58
1:D:217:GLY:O	1:D:220:ASP:N	2.37	0.58
1:B:265:PHE:O	1:B:268:LYS:HG2	2.03	0.58
1:E:86:LEU:HD21	1:E:108:LEU:HA	1.86	0.57
1:H:61:LEU:O	1:H:64:LEU:HB3	2.03	0.57
1:B:86:LEU:HD21	1:B:108:LEU:HA	1.84	0.57
1:E:24:ILE:HA	1:E:27:VAL:HG23	1.87	0.57
1:C:229:VAL:O	1:C:231:SER:N	2.37	0.57
1:D:275:LEU:O	1:D:278:LEU:N	2.38	0.57
1:H:36:VAL:CG1	1:H:146:LEU:CD2	2.82	0.57
1:F:253:VAL:HA	1:F:256:LEU:HD12	1.86	0.57
1:D:171:HIS:HA	1:D:174:THR:HG22	1.87	0.57
1:H:36:VAL:CG1	1:H:146:LEU:HD22	2.34	0.57
1:H:86:LEU:HD21	1:H:108:LEU:HA	1.86	0.57
1:G:251:ALA:HB2	1:G:286:PHE:HB2	1.86	0.57
1:B:148:PRO:O	1:B:151:VAL:N	2.38	0.57
1:G:13:PRO:HB3	1:G:259:LEU:HD22	1.87	0.57
1:H:68:GLY:HA3	1:H:73:ILE:HD11	1.86	0.57
1:C:23:ALA:O	1:C:27:VAL:HG23	2.04	0.57
1:G:229:VAL:O	1:G:231:SER:N	2.36	0.56
1:F:147:GLU:HB3	1:F:148:PRO:HD2	1.86	0.56
1:C:68:GLY:HA3	1:C:73:ILE:HD11	1.87	0.56
1:E:164:ILE:HD11	1:H:116:ALA:HA	1.87	0.56
1:A:228:VAL:HG21	1:A:252:MET:HG3	1.87	0.56
1:H:19:VAL:HG22	1:H:132:VAL:HA	1.88	0.56
1:H:24:ILE:HA	1:H:27:VAL:HG23	1.86	0.56
1:D:129:ILE:HG22	1:D:130:LEU:HD23	1.87	0.56
1:C:93:SER:HB3	1:C:107:THR:HG22	1.88	0.56
1:A:247:PRO:O	1:A:289:GLY:HA3	2.04	0.56
1:B:262:LEU:HD23	1:B:277:PRO:HG2	1.88	0.56
1:F:36:VAL:HG11	1:F:146:LEU:CD2	2.35	0.56
1:E:20:GLN:O	1:E:24:ILE:HG12	2.06	0.56
1:G:36:VAL:HG13	1:G:145:SER:OG	2.06	0.56
1:D:148:PRO:O	1:D:151:VAL:N	2.38	0.56
1:A:148:PRO:O	1:A:151:VAL:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:MET:HB3	1:B:35:LEU:HD22	1.87	0.56
1:C:253:VAL:HA	1:C:256:LEU:HD12	1.88	0.56
1:E:84:THR:O	1:E:88:ILE:HG12	2.05	0.56
1:G:253:VAL:HA	1:G:256:LEU:HD12	1.88	0.56
1:C:36:VAL:HG11	1:C:146:LEU:HD22	1.88	0.56
1:C:71:ARG:NH1	1:D:161:TYR:OH	2.39	0.56
1:H:42:SER:HB2	1:H:147:GLU:HG2	1.87	0.56
1:G:70:ARG:NH2	1:H:168:ARG:HH12	2.03	0.56
1:B:84:THR:O	1:B:88:ILE:HG12	2.05	0.56
1:H:124:TRP:HA	1:H:127:ILE:HG12	1.87	0.55
1:G:35:LEU:O	1:G:36:VAL:HB	2.07	0.55
1:E:64:LEU:HD11	1:E:73:ILE:HG23	1.88	0.55
1:G:124:TRP:HA	1:G:127:ILE:HG12	1.88	0.55
1:A:265:PHE:HB3	1:A:272:GLN:OE1	2.06	0.55
1:E:29:PRO:O	1:E:32:ALA:HB3	2.06	0.55
1:B:253:VAL:HA	1:B:256:LEU:HD12	1.89	0.55
1:D:90:GLY:HA2	1:D:107:THR:HG21	1.88	0.55
1:B:18:PHE:O	1:B:22:ILE:HG12	2.07	0.55
1:B:121:TYR:HD1	1:B:124:TRP:HZ2	1.55	0.55
1:F:251:ALA:HB2	1:F:286:PHE:HB2	1.88	0.55
1:C:74:ALA:O	1:C:119:TYR:OH	2.21	0.55
1:H:246:ALA:HB1	1:H:247:PRO:HD2	1.89	0.55
1:E:70:ARG:HH12	1:F:169:THR:HG21	1.72	0.55
1:F:148:PRO:O	1:F:151:VAL:N	2.40	0.55
1:A:36:VAL:CG1	1:A:37:ALA:N	2.29	0.55
1:A:218:MET:HA	1:A:221:LEU:HB3	1.89	0.55
1:F:170:LYS:NZ	1:F:271:PRO:HG2	2.23	0.54
1:E:72:PHE:HZ	1:F:59:LEU:HB2	1.71	0.54
1:E:66:ARG:HH22	1:F:66:ARG:HD3	1.72	0.54
1:E:225:SER:HA	1:E:228:VAL:HB	1.89	0.54
1:E:90:GLY:HA2	1:E:107:THR:HG21	1.89	0.54
1:D:254:GLY:HA3	1:D:285:GLY:HA3	1.89	0.54
1:A:72:PHE:CZ	1:B:59:LEU:HD23	2.42	0.54
1:F:121:TYR:HD1	1:F:124:TRP:HZ2	1.53	0.54
1:D:170:LYS:NZ	1:D:271:PRO:HG2	2.22	0.54
1:F:36:VAL:HG11	1:F:146:LEU:HD22	1.89	0.54
1:C:42:SER:HB2	1:C:147:GLU:HG2	1.88	0.54
1:H:147:GLU:HB3	1:H:148:PRO:HD2	1.89	0.54
1:F:61:LEU:O	1:F:64:LEU:HB3	2.07	0.54
1:B:64:LEU:HD21	1:B:73:ILE:HA	1.89	0.54
1:B:151:VAL:HG12	1:B:227:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:117:LEU:HD11	1:G:126:VAL:HG11	1.89	0.54
1:E:70:ARG:HH21	1:F:168:ARG:HH22	1.55	0.54
1:F:16:LEU:HA	1:F:221:LEU:HD11	1.89	0.54
1:E:251:ALA:HB2	1:E:286:PHE:HB2	1.89	0.54
1:D:29:PRO:HB3	1:D:95:LEU:HD22	1.90	0.54
1:H:86:LEU:CD2	1:H:108:LEU:HA	2.38	0.54
1:C:83:MET:O	1:C:86:LEU:HB2	2.08	0.54
1:F:36:VAL:CG1	1:F:37:ALA:N	2.35	0.54
1:E:42:SER:HA	1:E:146:LEU:HB3	1.90	0.54
1:B:170:LYS:HZ1	1:B:271:PRO:HG2	1.73	0.53
1:C:44:VAL:O	1:C:47:PRO:HD2	2.08	0.53
1:D:13:PRO:HB3	1:D:259:LEU:HD22	1.89	0.53
1:B:251:ALA:HB2	1:B:286:PHE:HB2	1.89	0.53
1:D:265:PHE:O	1:D:268:LYS:HG2	2.09	0.53
1:E:64:LEU:HD21	1:E:73:ILE:HA	1.90	0.53
1:A:123:GLU:HB2	1:A:126:VAL:HG23	1.91	0.53
1:F:218:MET:HA	1:F:221:LEU:HB3	1.90	0.53
1:G:246:ALA:HB1	1:G:247:PRO:HD2	1.91	0.53
1:B:289:GLY:CA	1:B:292:LEU:HD12	2.27	0.53
1:A:24:ILE:HA	1:A:27:VAL:HG23	1.89	0.53
1:A:218:MET:O	1:A:222:ILE:HG13	2.09	0.53
1:B:97:LEU:HB2	1:B:103:ALA:HB2	1.91	0.53
1:G:94:LEU:HD22	1:G:99:PRO:HA	1.89	0.53
1:A:90:GLY:HA2	1:A:107:THR:HG21	1.91	0.53
1:H:16:LEU:HA	1:H:221:LEU:HD11	1.90	0.53
1:G:23:ALA:O	1:G:27:VAL:HG23	2.09	0.53
1:H:170:LYS:NZ	1:H:271:PRO:HG2	2.24	0.53
1:B:229:VAL:O	1:B:231:SER:N	2.42	0.53
1:G:129:ILE:HG22	1:G:130:LEU:HD23	1.90	0.53
1:D:68:GLY:HA3	1:D:73:ILE:HD11	1.92	0.52
1:B:90:GLY:HA2	1:B:107:THR:HG21	1.91	0.52
1:A:147:GLU:HB3	1:A:148:PRO:HD2	1.90	0.52
1:F:60:VAL:O	1:F:63:VAL:HG12	2.09	0.52
1:D:121:TYR:HA	1:D:124:TRP:CZ2	2.44	0.52
1:D:147:GLU:HB3	1:D:148:PRO:HD2	1.92	0.52
1:D:121:TYR:HD1	1:D:124:TRP:HZ2	1.58	0.52
1:B:275:LEU:O	1:B:278:LEU:N	2.42	0.52
1:A:30:MET:HE1	1:A:141:ILE:HA	1.92	0.52
1:H:127:ILE:HG22	1:H:214:PHE:HE2	1.75	0.52
1:A:18:PHE:O	1:A:22:ILE:HG12	2.10	0.52
1:H:36:VAL:CG1	1:H:37:ALA:N	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:60:VAL:O	1:H:63:VAL:HG12	2.10	0.52
1:E:168:ARG:HH12	1:H:70:ARG:HH12	1.57	0.52
1:G:90:GLY:HA2	1:G:107:THR:HG21	1.91	0.52
1:A:89:PHE:HD1	1:A:92:LEU:HD12	1.75	0.52
1:C:142:PHE:HA	1:C:145:SER:HB3	1.90	0.52
1:C:42:SER:HA	1:C:146:LEU:HB3	1.91	0.52
1:F:118:LEU:HD12	1:F:130:LEU:HD12	1.92	0.52
1:B:16:LEU:HA	1:B:221:LEU:HD11	1.92	0.52
1:H:42:SER:HA	1:H:146:LEU:HB3	1.91	0.52
1:G:80:ALA:O	1:G:84:THR:HG23	2.10	0.52
1:D:265:PHE:HB3	1:D:272:GLN:OE1	2.09	0.52
1:H:163:ALA:HB2	1:H:276:PRO:HG2	1.92	0.52
1:B:36:VAL:CG1	1:B:145:SER:CB	2.82	0.52
1:B:217:GLY:O	1:B:220:ASP:N	2.43	0.52
1:F:131:GLY:O	1:F:135:SER:OG	2.16	0.52
1:G:97:LEU:HB2	1:G:103:ALA:HB2	1.92	0.52
1:C:35:LEU:O	1:C:36:VAL:HB	2.09	0.51
1:F:23:ALA:O	1:F:27:VAL:HG23	2.10	0.51
1:E:265:PHE:HB3	1:E:272:GLN:OE1	2.09	0.51
1:D:30:MET:HE1	1:D:141:ILE:HA	1.92	0.51
1:C:36:VAL:CG1	1:C:37:ALA:N	2.30	0.51
1:A:93:SER:OG	1:A:103:ALA:HB1	2.11	0.51
1:H:118:LEU:HD12	1:H:130:LEU:HD12	1.92	0.51
1:H:36:VAL:HG13	1:H:145:SER:CB	2.40	0.51
1:E:44:VAL:O	1:E:47:PRO:HD2	2.09	0.51
1:A:127:ILE:HG22	1:A:214:PHE:HE2	1.75	0.51
1:A:36:VAL:HG13	1:A:145:SER:N	2.22	0.51
1:C:70:ARG:NH2	1:D:168:ARG:HH12	2.08	0.51
1:H:90:GLY:O	1:H:94:LEU:HB2	2.10	0.51
1:H:36:VAL:HG23	1:H:144:ILE:HG22	1.81	0.51
1:C:123:GLU:HB2	1:C:126:VAL:HG23	1.93	0.51
1:H:218:MET:HA	1:H:221:LEU:HB3	1.93	0.51
1:B:68:GLY:HA3	1:B:73:ILE:HD11	1.92	0.51
1:A:168:ARG:HH12	1:D:70:ARG:HH22	1.58	0.51
1:D:98:GLY:O	1:D:100:THR:N	2.43	0.51
1:D:20:GLN:CD	1:D:252:MET:HG2	2.31	0.51
1:G:20:GLN:CD	1:G:252:MET:HG2	2.32	0.51
1:G:17:LEU:HD21	1:G:256:LEU:HD11	1.93	0.51
1:E:93:SER:HB3	1:E:107:THR:HG22	1.93	0.51
1:C:84:THR:O	1:C:88:ILE:HG12	2.10	0.51
1:F:247:PRO:O	1:F:289:GLY:HA3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:217:GLY:O	1:E:220:ASP:N	2.43	0.50
1:B:7:LEU:HB2	1:B:8:PRO:HD3	1.93	0.50
1:A:246:ALA:HB1	1:A:247:PRO:HD2	1.92	0.50
1:F:170:LYS:HZ1	1:F:271:PRO:HG2	1.77	0.50
1:C:41:PRO:C	1:C:146:LEU:HG	2.32	0.50
1:F:165:SER:O	1:F:169:THR:HG23	2.12	0.50
1:C:89:PHE:HD1	1:C:92:LEU:HD12	1.76	0.50
1:E:263:LEU:O	1:E:267:ASN:HB2	2.11	0.50
1:B:89:PHE:HZ	1:B:114:VAL:HG21	1.76	0.50
1:E:89:PHE:HZ	1:E:114:VAL:HG21	1.75	0.50
1:B:288:VAL:O	1:B:292:LEU:HG	2.11	0.50
1:E:161:TYR:OH	1:H:71:ARG:NH1	2.45	0.50
1:F:268:LYS:HG3	1:F:269:GLY:O	2.12	0.50
1:F:89:PHE:HZ	1:F:114:VAL:HG21	1.76	0.50
1:B:35:LEU:O	1:B:36:VAL:HB	2.12	0.50
1:B:117:LEU:HD11	1:B:126:VAL:HG11	1.94	0.50
1:H:217:GLY:O	1:H:220:ASP:N	2.45	0.50
1:H:98:GLY:O	1:H:100:THR:N	2.44	0.50
1:A:30:MET:HE2	1:A:144:ILE:HD12	1.93	0.50
1:A:44:VAL:O	1:A:47:PRO:HD2	2.12	0.50
1:D:7:LEU:HB2	1:D:8:PRO:HD3	1.94	0.50
1:A:70:ARG:HH22	1:B:169:THR:HG22	1.76	0.50
1:B:13:PRO:HB3	1:B:259:LEU:HD22	1.93	0.50
1:E:35:LEU:O	1:E:36:VAL:HB	2.12	0.49
1:H:265:PHE:O	1:H:268:LYS:HG2	2.12	0.49
1:H:41:PRO:C	1:H:146:LEU:HG	2.32	0.49
1:E:265:PHE:O	1:E:268:LYS:HG2	2.11	0.49
1:E:220:ASP:OD2	1:E:221:LEU:N	2.45	0.49
1:F:35:LEU:O	1:F:36:VAL:HB	2.12	0.49
1:E:20:GLN:CD	1:E:252:MET:HG2	2.33	0.49
1:H:229:VAL:O	1:H:231:SER:N	2.45	0.49
1:G:88:ILE:O	1:G:92:LEU:HG	2.13	0.49
1:H:122:PRO:HD2	1:H:124:TRP:CZ2	2.48	0.49
1:A:262:LEU:HD23	1:A:277:PRO:HG2	1.93	0.49
1:C:147:GLU:HB3	1:C:148:PRO:HD2	1.93	0.49
1:E:122:PRO:HD2	1:E:124:TRP:CE2	2.47	0.49
1:G:41:PRO:N	1:G:146:LEU:HG	2.26	0.49
1:A:121:TYR:HD1	1:A:124:TRP:HZ2	1.59	0.49
1:C:93:SER:OG	1:C:103:ALA:HB1	2.13	0.49
1:D:124:TRP:HA	1:D:127:ILE:HG12	1.95	0.49
1:B:118:LEU:HD12	1:B:130:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:CD1	1:B:126:VAL:HG11	2.43	0.49
1:C:26:LEU:O	1:C:30:MET:HG3	2.13	0.49
1:D:41:PRO:O	1:D:146:LEU:HG	2.13	0.49
1:B:268:LYS:HE2	1:B:272:GLN:HE22	1.77	0.49
1:G:24:ILE:HA	1:G:27:VAL:HG23	1.95	0.49
1:B:155:LEU:HD11	1:B:224:PRO:HA	1.95	0.49
1:F:82:PHE:CZ	1:G:157:LEU:HD11	2.48	0.49
1:A:68:GLY:HA2	1:A:69:GLY:HA3	1.62	0.48
1:A:231:SER:OG	1:A:232:HIS:N	2.45	0.48
1:E:59:LEU:HD23	1:H:72:PHE:CZ	2.48	0.48
1:F:44:VAL:O	1:F:47:PRO:HD2	2.13	0.48
1:G:139:ALA:HA	1:G:226:ILE:HD12	1.95	0.48
1:C:36:VAL:CG1	1:C:146:LEU:HD22	2.43	0.48
1:E:147:GLU:HB3	1:E:148:PRO:HD2	1.95	0.48
1:G:118:LEU:HD12	1:G:130:LEU:HD12	1.95	0.48
1:B:230:SER:HA	1:B:233:VAL:HG12	1.94	0.48
1:D:251:ALA:HB2	1:D:286:PHE:HB2	1.95	0.48
1:A:35:LEU:O	1:A:36:VAL:HB	2.14	0.48
1:C:262:LEU:HD21	1:C:274:GLY:HA2	1.96	0.48
1:C:29:PRO:HB3	1:C:95:LEU:HB2	1.94	0.48
1:A:93:SER:HB3	1:A:107:THR:HG22	1.95	0.48
1:F:246:ALA:HB1	1:F:247:PRO:HD2	1.95	0.48
1:C:14:LEU:O	1:C:18:PHE:HB2	2.14	0.48
1:D:35:LEU:O	1:D:36:VAL:HB	2.13	0.48
1:E:89:PHE:CZ	1:E:114:VAL:HG21	2.49	0.48
1:H:121:TYR:HA	1:H:124:TRP:CZ2	2.49	0.48
1:C:139:ALA:HA	1:C:226:ILE:HD12	1.96	0.48
1:F:20:GLN:O	1:F:24:ILE:HG12	2.13	0.48
1:F:265:PHE:O	1:F:268:LYS:HG2	2.14	0.48
1:C:249:LEU:O	1:C:253:VAL:HG22	2.14	0.48
1:E:86:LEU:CD1	1:F:48:LEU:HD21	2.43	0.48
1:G:142:PHE:HB2	1:G:226:ILE:HD11	1.96	0.48
1:G:275:LEU:HB2	1:G:276:PRO:HD3	1.96	0.48
1:G:159:ALA:HB1	1:G:276:PRO:HG3	1.95	0.48
1:F:86:LEU:CD2	1:F:108:LEU:HA	2.44	0.48
1:C:142:PHE:HB2	1:C:226:ILE:CD1	2.44	0.47
1:B:30:MET:HE2	1:B:144:ILE:HD12	1.96	0.47
1:G:18:PHE:O	1:G:22:ILE:HG12	2.14	0.47
1:C:165:SER:O	1:C:169:THR:HG23	2.13	0.47
1:B:47:PRO:O	1:B:50:PHE:HB3	2.14	0.47
1:G:30:MET:HE1	1:G:141:ILE:HA	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:LEU:HB2	1:C:276:PRO:HD3	1.95	0.47
1:H:251:ALA:HB2	1:H:286:PHE:HB2	1.96	0.47
1:D:218:MET:HA	1:D:221:LEU:HB3	1.96	0.47
1:D:17:LEU:HD21	1:D:256:LEU:HD11	1.95	0.47
1:F:29:PRO:HB3	1:F:95:LEU:HD22	1.96	0.47
1:F:36:VAL:HG22	1:F:144:ILE:C	2.35	0.47
1:D:24:ILE:O	1:D:27:VAL:N	2.46	0.47
1:B:152:LEU:HA	1:B:152:LEU:HD22	1.77	0.47
1:H:228:VAL:HG21	1:H:252:MET:HG3	1.96	0.47
1:F:24:ILE:HD13	1:F:229:VAL:HG22	1.97	0.47
1:F:71:ARG:HG2	1:G:168:ARG:HH22	1.79	0.47
1:F:151:VAL:HG12	1:F:227:LEU:HD12	1.96	0.47
1:D:170:LYS:HZ2	1:D:271:PRO:HG2	1.78	0.47
1:F:89:PHE:CZ	1:F:114:VAL:HG21	2.49	0.47
1:H:151:VAL:HG12	1:H:227:LEU:HD12	1.97	0.47
1:E:68:GLY:HA3	1:E:73:ILE:HD11	1.97	0.47
1:D:18:PHE:O	1:D:22:ILE:HG12	2.15	0.47
1:B:16:LEU:HD23	1:B:256:LEU:HD23	1.97	0.47
1:G:20:GLN:O	1:G:24:ILE:HG12	2.14	0.47
1:A:139:ALA:HA	1:A:226:ILE:HD12	1.96	0.47
1:F:68:GLY:HA2	1:F:69:GLY:HA3	1.57	0.47
1:E:26:LEU:C	1:E:29:PRO:HD2	2.36	0.47
1:G:246:ALA:C	1:G:248:THR:H	2.19	0.47
1:C:265:PHE:O	1:C:268:LYS:HG2	2.15	0.47
1:B:10:LEU:HD23	1:B:10:LEU:HA	1.83	0.47
1:H:284:LEU:HD23	1:H:284:LEU:HA	1.71	0.47
1:F:24:ILE:HA	1:F:27:VAL:HG23	1.98	0.46
1:A:161:TYR:OH	1:D:71:ARG:NH1	2.48	0.46
1:F:72:PHE:CZ	1:G:59:LEU:HD23	2.50	0.46
1:E:66:ARG:HH22	1:F:66:ARG:CD	2.27	0.46
1:B:114:VAL:HG13	1:B:130:LEU:HD13	1.96	0.46
1:D:142:PHE:HB2	1:D:226:ILE:HD11	1.97	0.46
1:G:142:PHE:HB2	1:G:226:ILE:CD1	2.45	0.46
1:D:92:LEU:HD23	1:D:92:LEU:HA	1.70	0.46
1:B:24:ILE:O	1:B:27:VAL:N	2.45	0.46
1:E:230:SER:HA	1:E:233:VAL:HG12	1.98	0.46
1:G:60:VAL:HA	1:G:63:VAL:HG12	1.97	0.46
1:F:41:PRO:N	1:F:146:LEU:HG	2.31	0.46
1:D:89:PHE:HZ	1:D:114:VAL:HG21	1.80	0.46
1:G:26:LEU:C	1:G:29:PRO:HD2	2.36	0.46
1:C:89:PHE:CD1	1:C:92:LEU:HD12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ILE:HG22	1:B:130:LEU:HD23	1.97	0.46
1:F:142:PHE:HB2	1:F:226:ILE:CD1	2.46	0.46
1:E:275:LEU:HB2	1:E:276:PRO:HD3	1.97	0.46
1:B:127:ILE:HG22	1:B:214:PHE:HE2	1.81	0.46
1:F:250:GLY:O	1:F:285:GLY:HA3	2.15	0.46
1:F:284:LEU:HA	1:F:284:LEU:HD23	1.68	0.46
1:A:84:THR:O	1:A:88:ILE:HG12	2.15	0.46
1:C:68:GLY:HA2	1:C:69:GLY:HA3	1.63	0.46
1:A:42:SER:HB2	1:A:146:LEU:HD12	1.98	0.46
1:H:47:PRO:O	1:H:50:PHE:HB3	2.16	0.46
1:G:66:ARG:HH22	1:H:66:ARG:CD	2.29	0.46
1:C:20:GLN:O	1:C:24:ILE:HG12	2.16	0.46
1:H:121:TYR:HA	1:H:124:TRP:HZ2	1.81	0.46
1:A:220:ASP:HB2	1:A:275:LEU:HD21	1.98	0.46
1:B:139:ALA:O	1:B:226:ILE:HG13	2.15	0.46
1:B:142:PHE:HB2	1:B:226:ILE:HG12	1.98	0.46
1:F:98:GLY:O	1:F:100:THR:N	2.49	0.46
1:G:47:PRO:O	1:G:50:PHE:HB3	2.15	0.46
1:H:84:THR:O	1:H:88:ILE:HG12	2.16	0.46
1:C:24:ILE:HA	1:C:27:VAL:HG23	1.98	0.45
1:D:71:ARG:O	1:D:75:ALA:N	2.45	0.45
1:E:10:LEU:HD23	1:E:10:LEU:HA	1.76	0.45
1:A:82:PHE:CZ	1:B:157:LEU:HD11	2.51	0.45
1:C:218:MET:HA	1:C:221:LEU:HB3	1.98	0.45
1:C:72:PHE:HZ	1:D:59:LEU:HD23	1.79	0.45
1:A:121:TYR:HA	1:A:124:TRP:CZ2	2.50	0.45
1:C:82:PHE:HE1	1:C:112:VAL:HA	1.80	0.45
1:G:217:GLY:O	1:G:220:ASP:N	2.49	0.45
1:C:18:PHE:O	1:C:22:ILE:HG12	2.17	0.45
1:G:98:GLY:O	1:G:100:THR:N	2.48	0.45
1:A:58:THR:HG1	1:D:72:PHE:HE1	1.62	0.45
1:B:124:TRP:HA	1:B:127:ILE:HG12	1.98	0.45
1:F:49:ILE:O	1:F:53:MET:HG2	2.16	0.45
1:E:85:PHE:HE1	1:E:133:LEU:HD23	1.82	0.45
1:F:217:GLY:O	1:F:220:ASP:N	2.49	0.45
1:F:10:LEU:O	1:F:14:LEU:HB2	2.16	0.45
1:C:36:VAL:HG13	1:C:145:SER:HA	0.71	0.45
1:E:122:PRO:HD2	1:E:124:TRP:CZ2	2.51	0.45
1:A:15:MET:O	1:A:19:VAL:HG23	2.17	0.45
1:C:89:PHE:HZ	1:C:114:VAL:HG21	1.81	0.45
1:B:122:PRO:HD2	1:B:124:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:PRO:HB2	1:D:123:GLU:H	1.57	0.45
1:D:121:TYR:HA	1:D:124:TRP:HZ2	1.80	0.45
1:E:75:ALA:O	1:E:78:GLY:N	2.50	0.45
1:D:155:LEU:HD11	1:D:224:PRO:HA	1.98	0.45
1:C:26:LEU:C	1:C:29:PRO:HD2	2.37	0.45
1:G:122:PRO:HB2	1:G:123:GLU:H	1.60	0.45
1:B:157:LEU:HA	1:B:157:LEU:HD12	1.84	0.45
1:C:36:VAL:HG11	1:C:146:LEU:CD2	2.46	0.45
1:F:93:SER:OG	1:F:103:ALA:HB1	2.16	0.45
1:D:90:GLY:O	1:D:94:LEU:HB2	2.17	0.45
1:G:171:HIS:CE1	1:G:172:MET:HG3	2.52	0.45
1:C:42:SER:OG	1:C:147:GLU:HB2	2.17	0.45
1:F:64:LEU:HD13	1:F:65:LEU:N	2.32	0.45
1:H:68:GLY:HA2	1:H:69:GLY:HA3	1.60	0.45
1:D:20:GLN:NE2	1:D:252:MET:HG2	2.32	0.45
1:C:90:GLY:HA2	1:C:107:THR:HG21	1.99	0.45
1:A:121:TYR:HA	1:A:122:PRO:HD2	1.82	0.45
1:F:72:PHE:CE2	1:G:59:LEU:HD23	2.52	0.45
1:F:142:PHE:HB2	1:F:226:ILE:HD11	1.99	0.45
1:H:30:MET:HB3	1:H:35:LEU:HD22	1.99	0.44
1:H:35:LEU:O	1:H:36:VAL:HB	2.17	0.44
1:E:86:LEU:HD12	1:F:48:LEU:HD21	1.98	0.44
1:B:147:GLU:HB3	1:B:148:PRO:HD2	1.99	0.44
1:D:123:GLU:HB3	1:D:125:TYR:CE2	2.52	0.44
1:A:121:TYR:HA	1:A:124:TRP:HZ2	1.82	0.44
1:D:36:VAL:CG1	1:D:146:LEU:CD2	2.94	0.44
1:A:64:LEU:HD23	1:A:72:PHE:CE2	2.52	0.44
1:H:23:ALA:O	1:H:27:VAL:HG23	2.17	0.44
1:E:13:PRO:HB3	1:E:259:LEU:HD22	1.99	0.44
1:H:86:LEU:HD23	1:H:86:LEU:HA	1.79	0.44
1:D:127:ILE:HG22	1:D:214:PHE:HE2	1.82	0.44
1:A:89:PHE:HZ	1:A:114:VAL:HG21	1.82	0.44
1:H:13:PRO:HD3	1:H:259:LEU:HD21	1.98	0.44
1:D:35:LEU:HB3	1:D:36:VAL:H	1.63	0.44
1:E:90:GLY:O	1:E:94:LEU:HB2	2.17	0.44
1:E:220:ASP:C	1:E:220:ASP:OD2	2.56	0.44
1:A:61:LEU:O	1:A:64:LEU:HB3	2.17	0.44
1:D:68:GLY:HA2	1:D:69:GLY:HA3	1.73	0.44
1:D:16:LEU:HD23	1:D:256:LEU:HD23	1.98	0.44
1:D:220:ASP:C	1:D:220:ASP:OD2	2.56	0.44
1:C:107:THR:OG1	1:C:108:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:PRO:HD3	1:F:230:SER:O	2.17	0.44
1:H:217:GLY:O	1:H:220:ASP:OD2	2.35	0.44
1:B:98:GLY:O	1:B:100:THR:N	2.50	0.44
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.76	0.44
1:F:24:ILE:O	1:F:27:VAL:N	2.47	0.44
1:C:218:MET:O	1:C:222:ILE:HG13	2.16	0.44
1:B:220:ASP:OD2	1:B:221:LEU:N	2.50	0.44
1:G:148:PRO:HD3	1:G:230:SER:O	2.18	0.44
1:H:152:LEU:HA	1:H:152:LEU:HD22	1.80	0.44
1:G:173:ILE:HA	1:G:173:ILE:HD12	1.67	0.44
1:C:173:ILE:HA	1:C:173:ILE:HD12	1.82	0.44
1:G:262:LEU:HD23	1:G:277:PRO:HG2	2.00	0.44
1:C:60:VAL:HA	1:C:63:VAL:HG12	1.99	0.44
1:E:41:PRO:N	1:E:146:LEU:HG	2.33	0.44
1:G:69:GLY:CA	1:G:72:PHE:HB3	2.48	0.44
1:H:220:ASP:OD2	1:H:221:LEU:N	2.51	0.44
1:E:139:ALA:HA	1:E:226:ILE:HD12	2.00	0.44
1:G:225:SER:HA	1:G:228:VAL:HB	1.99	0.44
1:A:275:LEU:O	1:A:278:LEU:N	2.51	0.44
1:F:270:ASN:HA	1:F:271:PRO:HD2	1.78	0.44
1:H:155:LEU:HD11	1:H:224:PRO:HA	1.99	0.44
1:B:284:LEU:HA	1:B:284:LEU:HD23	1.78	0.44
1:G:16:LEU:HA	1:G:221:LEU:HD11	1.98	0.44
1:B:17:LEU:HA	1:B:17:LEU:HD23	1.71	0.43
1:H:124:TRP:CE3	1:H:127:ILE:HG13	2.53	0.43
1:D:270:ASN:HA	1:D:271:PRO:HD2	1.87	0.43
1:A:173:ILE:HA	1:A:173:ILE:HD12	1.80	0.43
1:C:152:LEU:HA	1:C:152:LEU:HD22	1.89	0.43
1:G:85:PHE:HE1	1:G:133:LEU:HD23	1.82	0.43
1:F:166:VAL:HG21	1:F:273:ALA:HA	2.00	0.43
1:D:20:GLN:O	1:D:24:ILE:HG12	2.18	0.43
1:E:89:PHE:HD1	1:E:92:LEU:HD12	1.81	0.43
1:A:14:LEU:O	1:A:18:PHE:HB2	2.18	0.43
1:F:82:PHE:HE1	1:F:112:VAL:HA	1.84	0.43
1:G:218:MET:HA	1:G:221:LEU:HB3	1.98	0.43
1:B:246:ALA:HB1	1:B:247:PRO:CD	2.46	0.43
1:F:122:PRO:HD2	1:F:124:TRP:CE2	2.53	0.43
1:F:47:PRO:O	1:F:50:PHE:HB3	2.19	0.43
1:H:42:SER:OG	1:H:147:GLU:HB2	2.17	0.43
1:B:220:ASP:C	1:B:220:ASP:OD2	2.55	0.43
1:A:44:VAL:C	1:A:47:PRO:HD2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HD23	1:A:119:TYR:HD1	1.83	0.43
1:A:129:ILE:O	1:A:132:VAL:HB	2.18	0.43
1:G:24:ILE:O	1:G:27:VAL:HB	2.18	0.43
1:A:151:VAL:HG12	1:A:227:LEU:HD12	2.01	0.43
1:H:171:HIS:HA	1:H:174:THR:HG23	2.00	0.43
1:G:289:GLY:HA2	1:G:292:LEU:HD12	2.00	0.43
1:E:109:ILE:HD13	1:E:109:ILE:HA	1.71	0.43
1:G:36:VAL:CG1	1:G:145:SER:OG	2.65	0.43
1:C:17:LEU:CD2	1:C:256:LEU:HD11	2.45	0.43
1:B:94:LEU:HD21	1:B:104:ALA:HB2	2.00	0.43
1:E:93:SER:OG	1:E:103:ALA:HB1	2.18	0.43
1:D:58:THR:O	1:D:61:LEU:N	2.51	0.43
1:C:10:LEU:HD23	1:C:10:LEU:HA	1.81	0.43
1:H:139:ALA:HA	1:H:226:ILE:HD12	2.00	0.43
1:G:36:VAL:HA	1:G:145:SER:HB2	2.00	0.43
1:A:29:PRO:CB	1:A:95:LEU:HB2	2.46	0.43
1:A:249:LEU:O	1:A:253:VAL:HG22	2.19	0.43
1:C:247:PRO:HB2	1:C:289:GLY:HA3	2.01	0.43
1:B:89:PHE:CZ	1:B:114:VAL:HG21	2.53	0.43
1:E:18:PHE:O	1:E:22:ILE:HG12	2.19	0.43
1:F:127:ILE:HG22	1:F:214:PHE:HE2	1.84	0.43
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.73	0.43
1:A:89:PHE:CD1	1:A:92:LEU:HD12	2.54	0.43
1:E:218:MET:HA	1:E:221:LEU:HB3	2.00	0.43
1:F:265:PHE:HB3	1:F:272:GLN:OE1	2.19	0.43
1:A:250:GLY:O	1:A:285:GLY:HA3	2.18	0.43
1:C:170:LYS:NZ	1:C:271:PRO:HG2	2.32	0.43
1:D:109:ILE:HA	1:D:109:ILE:HD13	1.79	0.43
1:A:124:TRP:CE3	1:A:127:ILE:HG13	2.54	0.43
1:D:152:LEU:HA	1:D:152:LEU:HD22	1.85	0.43
1:C:30:MET:HE2	1:C:144:ILE:HD12	1.99	0.43
1:D:121:TYR:HD1	1:D:124:TRP:CZ2	2.35	0.43
1:E:168:ARG:NH1	1:H:70:ARG:HH22	2.17	0.43
1:G:165:SER:O	1:G:169:THR:HG23	2.19	0.43
1:E:121:TYR:C	1:E:124:TRP:HE1	2.22	0.43
1:H:275:LEU:HD23	1:H:275:LEU:HA	1.78	0.43
1:E:252:MET:O	1:E:255:SER:HB3	2.19	0.43
1:H:252:MET:O	1:H:255:SER:HB3	2.18	0.43
1:B:171:HIS:O	1:B:174:THR:HG23	2.19	0.43
1:A:7:LEU:HB2	1:A:8:PRO:HD3	2.01	0.43
1:H:165:SER:O	1:H:169:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:THR:OG1	1:B:108:LEU:N	2.51	0.42
1:G:262:LEU:HD21	1:G:274:GLY:HA2	2.00	0.42
1:D:44:VAL:O	1:D:47:PRO:HD2	2.18	0.42
1:D:80:ALA:O	1:D:84:THR:HG23	2.19	0.42
1:D:220:ASP:OD2	1:D:221:LEU:N	2.52	0.42
1:A:259:LEU:HB2	1:A:278:LEU:HD11	2.01	0.42
1:C:250:GLY:O	1:C:285:GLY:HA3	2.19	0.42
1:D:162:ASP:OD2	1:D:273:ALA:HB1	2.19	0.42
1:G:64:LEU:HD21	1:G:73:ILE:HA	2.01	0.42
1:E:80:ALA:O	1:E:84:THR:HG23	2.18	0.42
1:A:214:PHE:HD1	1:A:214:PHE:HA	1.66	0.42
1:D:47:PRO:O	1:D:50:PHE:HB3	2.20	0.42
1:D:247:PRO:O	1:D:289:GLY:HA3	2.19	0.42
1:A:23:ALA:O	1:A:27:VAL:HG23	2.19	0.42
1:E:68:GLY:HA2	1:E:69:GLY:HA3	1.69	0.42
1:A:70:ARG:NH2	1:B:168:ARG:HH12	2.17	0.42
1:B:44:VAL:O	1:B:47:PRO:HD2	2.20	0.42
1:B:90:GLY:O	1:B:94:LEU:HB2	2.19	0.42
1:C:231:SER:OG	1:C:248:THR:HG21	2.19	0.42
1:A:60:VAL:HA	1:A:63:VAL:HG12	2.01	0.42
1:E:24:ILE:O	1:E:27:VAL:HB	2.19	0.42
1:G:122:PRO:HD2	1:G:124:TRP:CE2	2.55	0.42
1:H:44:VAL:O	1:H:47:PRO:HD2	2.20	0.42
1:A:98:GLY:O	1:A:100:THR:N	2.53	0.42
1:H:24:ILE:O	1:H:27:VAL:N	2.51	0.42
1:D:275:LEU:HB2	1:D:276:PRO:HD3	2.00	0.42
1:B:254:GLY:O	1:B:257:VAL:HG12	2.20	0.42
1:G:87:TYR:N	1:G:87:TYR:CD2	2.88	0.42
1:B:218:MET:HA	1:B:221:LEU:HB3	2.01	0.42
1:G:151:VAL:HG12	1:G:227:LEU:HD12	2.01	0.42
1:D:114:VAL:HG13	1:D:130:LEU:HD13	2.02	0.42
1:E:217:GLY:O	1:E:220:ASP:OD2	2.38	0.42
1:E:284:LEU:HD23	1:E:284:LEU:HA	1.84	0.42
1:A:10:LEU:HA	1:A:10:LEU:HD23	1.75	0.42
1:D:36:VAL:HG13	1:D:145:SER:OG	2.19	0.42
1:A:15:MET:SD	1:A:128:ASP:HB3	2.60	0.42
1:D:259:LEU:HA	1:D:278:LEU:HD21	2.02	0.42
1:B:121:TYR:HA	1:B:124:TRP:CZ2	2.54	0.42
1:H:270:ASN:HA	1:H:271:PRO:HD2	1.84	0.42
1:F:163:ALA:HB2	1:F:276:PRO:HG2	2.01	0.42
1:E:23:ALA:O	1:E:27:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:TYR:HA	1:G:124:TRP:CZ2	2.55	0.42
1:E:155:LEU:HD22	1:E:279:ASN:ND2	2.35	0.42
1:F:71:ARG:NH1	1:G:161:TYR:OH	2.52	0.41
1:C:246:ALA:C	1:C:248:THR:H	2.22	0.41
1:D:122:PRO:HD2	1:D:124:TRP:CE2	2.55	0.41
1:F:220:ASP:HB2	1:F:275:LEU:HD21	2.02	0.41
1:E:21:ILE:HG22	1:E:22:ILE:HD13	2.02	0.41
1:D:85:PHE:HE1	1:D:133:LEU:HD23	1.85	0.41
1:B:26:LEU:HA	1:B:26:LEU:HD23	1.85	0.41
1:C:142:PHE:HB2	1:C:226:ILE:HG12	2.03	0.41
1:G:168:ARG:CZ	1:G:168:ARG:HB3	2.50	0.41
1:C:129:ILE:HD13	1:C:129:ILE:HA	1.80	0.41
1:E:122:PRO:HB2	1:E:123:GLU:H	1.62	0.41
1:H:258:GLY:HA3	1:H:278:LEU:HA	2.02	0.41
1:A:220:ASP:OD2	1:A:221:LEU:N	2.53	0.41
1:G:44:VAL:O	1:G:47:PRO:HD2	2.20	0.41
1:F:58:THR:O	1:F:62:LEU:HG	2.19	0.41
1:C:109:ILE:HD13	1:C:109:ILE:HA	1.77	0.41
1:D:284:LEU:HD23	1:D:284:LEU:HA	1.75	0.41
1:F:155:LEU:HD22	1:F:279:ASN:ND2	2.36	0.41
1:C:97:LEU:CB	1:C:103:ALA:HB2	2.49	0.41
1:G:89:PHE:HZ	1:G:114:VAL:HG21	1.85	0.41
1:C:142:PHE:HB2	1:C:226:ILE:HD11	2.03	0.41
1:B:68:GLY:HA2	1:B:69:GLY:HA3	1.76	0.41
1:E:139:ALA:O	1:E:226:ILE:HG13	2.21	0.41
1:H:87:TYR:N	1:H:87:TYR:CD2	2.88	0.41
1:C:157:LEU:HD12	1:C:157:LEU:HA	1.81	0.41
1:F:229:VAL:O	1:F:231:SER:N	2.52	0.41
1:C:89:PHE:C	1:C:107:THR:HB	2.40	0.41
1:D:69:GLY:CA	1:D:72:PHE:HB3	2.50	0.41
1:F:158:LEU:HD22	1:F:158:LEU:HA	1.77	0.41
1:F:27:VAL:O	1:F:144:ILE:HD11	2.21	0.41
1:H:26:LEU:C	1:H:29:PRO:HD2	2.40	0.41
1:A:118:LEU:HD12	1:A:130:LEU:HD12	2.03	0.41
1:E:259:LEU:HB2	1:E:278:LEU:HD11	2.03	0.41
1:C:246:ALA:HB1	1:C:247:PRO:HD2	2.01	0.41
1:D:75:ALA:O	1:D:78:GLY:N	2.54	0.41
1:G:220:ASP:OD2	1:G:220:ASP:C	2.58	0.41
1:G:135:SER:HA	1:G:222:ILE:HD11	2.01	0.41
1:H:131:GLY:O	1:H:135:SER:OG	2.19	0.41
1:A:129:ILE:HD13	1:A:129:ILE:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:PRO:HD2	1:H:124:TRP:CE2	2.55	0.41
1:G:68:GLY:HA3	1:G:73:ILE:HD11	2.02	0.41
1:D:107:THR:OG1	1:D:108:LEU:N	2.54	0.41
1:A:21:ILE:HG22	1:A:22:ILE:HD13	2.02	0.41
1:A:121:TYR:HD1	1:A:124:TRP:CZ2	2.38	0.41
1:C:127:ILE:HD12	1:C:127:ILE:HG23	1.83	0.41
1:H:64:LEU:HD13	1:H:65:LEU:N	2.36	0.41
1:A:64:LEU:HD23	1:A:72:PHE:HE2	1.85	0.41
1:C:50:PHE:HD2	1:C:154:LEU:HD13	1.86	0.41
1:D:69:GLY:HA2	1:D:72:PHE:HB3	2.01	0.41
1:G:93:SER:OG	1:G:103:ALA:HB1	2.21	0.41
1:H:263:LEU:O	1:H:267:ASN:ND2	2.48	0.41
1:H:92:LEU:HA	1:H:92:LEU:HD23	1.90	0.41
1:E:152:LEU:HD22	1:E:152:LEU:HA	1.91	0.41
1:F:41:PRO:C	1:F:146:LEU:HG	2.41	0.41
1:F:17:LEU:HD23	1:F:17:LEU:HA	1.76	0.41
1:G:252:MET:O	1:G:255:SER:HB3	2.22	0.41
1:A:80:ALA:O	1:A:84:THR:HG23	2.21	0.41
1:H:123:GLU:HB3	1:H:125:TYR:CE2	2.56	0.41
1:F:36:VAL:CG1	1:F:146:LEU:CD2	2.99	0.40
1:C:220:ASP:OD2	1:C:221:LEU:N	2.53	0.40
1:G:68:GLY:HA2	1:G:69:GLY:HA3	1.76	0.40
1:D:278:LEU:HA	1:D:278:LEU:HD13	1.89	0.40
1:E:88:ILE:O	1:E:92:LEU:HG	2.21	0.40
1:F:66:ARG:NH1	1:F:67:THR:OG1	2.54	0.40
1:A:101:THR:OG1	1:A:102:ALA:N	2.54	0.40
1:E:173:ILE:HD12	1:E:173:ILE:HA	1.61	0.40
1:H:173:ILE:HD12	1:H:173:ILE:HA	1.81	0.40
1:A:109:ILE:HD13	1:A:109:ILE:HA	1.71	0.40
1:B:36:VAL:HG13	1:B:145:SER:OG	2.21	0.40
1:A:24:ILE:O	1:A:27:VAL:N	2.54	0.40
1:E:275:LEU:O	1:E:278:LEU:N	2.53	0.40
1:A:151:VAL:HG11	1:A:227:LEU:HA	2.04	0.40
1:D:142:PHE:HB2	1:D:226:ILE:CD1	2.50	0.40
1:F:7:LEU:HB2	1:F:8:PRO:HD3	2.03	0.40
1:C:278:LEU:HD13	1:C:278:LEU:HA	1.93	0.40
1:G:30:MET:HE3	1:G:35:LEU:HD23	2.03	0.40
1:E:124:TRP:HA	1:E:127:ILE:HG12	2.02	0.40
1:G:85:PHE:CE1	1:G:133:LEU:HD23	2.56	0.40
1:E:153:VAL:O	1:E:157:LEU:HB2	2.22	0.40
1:B:69:GLY:CA	1:B:72:PHE:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:LEU:HD23	1:F:256:LEU:HD23	2.02	0.40
1:G:259:LEU:HB2	1:G:278:LEU:HD11	2.02	0.40
1:H:19:VAL:HG23	1:H:132:VAL:HG22	2.02	0.40
1:E:85:PHE:CE1	1:E:133:LEU:HD23	2.55	0.40
1:G:270:ASN:HA	1:G:271:PRO:HD2	1.87	0.40
1:G:107:THR:OG1	1:G:108:LEU:N	2.55	0.40
1:E:9:LEU:HA	1:E:9:LEU:HD23	1.80	0.40
1:A:83:MET:O	1:A:86:LEU:HB2	2.20	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	238/301 (79%)	202 (85%)	26 (11%)	10 (4%)	3	35
1	B	238/301 (79%)	196 (82%)	31 (13%)	11 (5%)	3	33
1	C	238/301 (79%)	201 (84%)	27 (11%)	10 (4%)	3	35
1	D	238/301 (79%)	198 (83%)	29 (12%)	11 (5%)	3	33
1	E	238/301 (79%)	198 (83%)	30 (13%)	10 (4%)	3	35
1	F	238/301 (79%)	199 (84%)	29 (12%)	10 (4%)	3	35
1	G	238/301 (79%)	198 (83%)	30 (13%)	10 (4%)	3	35
1	H	238/301 (79%)	198 (83%)	30 (13%)	10 (4%)	3	35
All	All	1904/2408 (79%)	1590 (84%)	232 (12%)	82 (4%)	3	35

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	96	ALA

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Mol	Chain	Res	Type
1	A	230	SER
1	B	36	VAL
1	B	96	ALA
1	B	148	PRO
1	B	230	SER
1	C	36	VAL
1	C	96	ALA
1	C	148	PRO
1	C	230	SER
1	D	36	VAL
1	D	96	ALA
1	D	148	PRO
1	D	230	SER
1	E	36	VAL
1	E	96	ALA
1	E	230	SER
1	F	36	VAL
1	F	96	ALA
1	F	230	SER
1	G	36	VAL
1	G	96	ALA
1	G	148	PRO
1	G	230	SER
1	H	36	VAL
1	H	96	ALA
1	H	230	SER
1	A	122	PRO
1	A	148	PRO
1	A	217	GLY
1	A	231	SER
1	B	122	PRO
1	B	231	SER
1	C	122	PRO
1	D	35	LEU
1	D	122	PRO
1	E	99	PRO
1	E	122	PRO
1	E	148	PRO
1	E	231	SER
1	F	122	PRO
1	F	148	PRO
1	F	217	GLY

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Mol	Chain	Res	Type
1	F	231	SER
1	G	122	PRO
1	G	231	SER
1	H	122	PRO
1	H	148	PRO
1	H	217	GLY
1	H	231	SER
1	A	99	PRO
1	A	178	GLY
1	B	35	LEU
1	B	99	PRO
1	B	217	GLY
1	C	35	LEU
1	C	178	GLY
1	C	217	GLY
1	C	231	SER
1	D	99	PRO
1	D	217	GLY
1	D	231	SER
1	E	35	LEU
1	F	35	LEU
1	F	99	PRO
1	F	178	GLY
1	G	35	LEU
1	G	99	PRO
1	G	217	GLY
1	H	99	PRO
1	H	178	GLY
1	A	35	LEU
1	B	178	GLY
1	D	178	GLY
1	E	178	GLY
1	E	217	GLY
1	G	178	GLY
1	H	35	LEU
1	C	99	PRO
1	B	246	ALA
1	D	246	ALA

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	188/236 (80%)	152 (81%)	36 (19%)	2	14
1	B	188/236 (80%)	150 (80%)	38 (20%)	1	12
1	C	188/236 (80%)	152 (81%)	36 (19%)	2	14
1	D	188/236 (80%)	152 (81%)	36 (19%)	2	14
1	E	188/236 (80%)	152 (81%)	36 (19%)	2	14
1	F	188/236 (80%)	153 (81%)	35 (19%)	2	15
1	G	188/236 (80%)	152 (81%)	36 (19%)	2	14
1	H	188/236 (80%)	155 (82%)	33 (18%)	2	18
All	All	1504/1888 (80%)	1218 (81%)	286 (19%)	2	14

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

Mol	Chain	Res	Type
1	A	12	MET
1	A	18	PHE
1	A	35	LEU
1	A	46	ASN
1	A	64	LEU
1	A	66	ARG
1	A	70	ARG
1	A	71	ARG
1	A	77	ILE
1	A	93	SER
1	A	107	THR
1	A	108	LEU
1	A	119	TYR
1	A	128	ASP
1	A	129	ILE
1	A	148	PRO
1	A	152	LEU
1	A	155	LEU
1	A	158	LEU

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Mol	Chain	Res	Type
1	A	173	ILE
1	A	174	THR
1	A	175	LEU
1	A	177	GLU
1	A	214	PHE
1	A	216	MET
1	A	218	MET
1	A	226	ILE
1	A	227	LEU
1	A	232	HIS
1	A	233	VAL
1	A	234	PHE
1	A	245	SER
1	A	257	VAL
1	A	262	LEU
1	A	263	LEU
1	A	287	LEU
1	B	18	PHE
1	B	46	ASN
1	B	64	LEU
1	B	66	ARG
1	B	67	THR
1	B	70	ARG
1	B	71	ARG
1	B	93	SER
1	B	107	THR
1	B	108	LEU
1	B	119	TYR
1	B	128	ASP
1	B	129	ILE
1	B	141	ILE
1	B	148	PRO
1	B	152	LEU
1	B	155	LEU
1	B	158	LEU
1	B	169	THR
1	B	173	ILE
1	B	174	THR
1	B	175	LEU
1	B	177	GLU
1	B	214	PHE
1	B	216	MET

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Mol	Chain	Res	Type
1	B	218	MET
1	B	220	ASP
1	B	226	ILE
1	B	227	LEU
1	B	228	VAL
1	B	232	HIS
1	B	233	VAL
1	B	234	PHE
1	B	245	SER
1	B	257	VAL
1	B	262	LEU
1	B	263	LEU
1	B	287	LEU
1	C	14	LEU
1	C	18	PHE
1	C	46	ASN
1	C	64	LEU
1	C	66	ARG
1	C	67	THR
1	C	70	ARG
1	C	71	ARG
1	C	93	SER
1	C	107	THR
1	C	108	LEU
1	C	119	TYR
1	C	128	ASP
1	C	129	ILE
1	C	141	ILE
1	C	148	PRO
1	C	152	LEU
1	C	155	LEU
1	C	158	LEU
1	C	169	THR
1	C	173	ILE
1	C	174	THR
1	C	175	LEU
1	C	177	GLU
1	C	214	PHE
1	C	216	MET
1	C	226	ILE
1	C	227	LEU
1	C	232	HIS

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Mol	Chain	Res	Type
1	C	233	VAL
1	C	234	PHE
1	C	245	SER
1	C	257	VAL
1	C	263	LEU
1	C	265	PHE
1	C	287	LEU
1	D	12	MET
1	D	14	LEU
1	D	18	PHE
1	D	44	VAL
1	D	46	ASN
1	D	64	LEU
1	D	66	ARG
1	D	70	ARG
1	D	71	ARG
1	D	93	SER
1	D	107	THR
1	D	108	LEU
1	D	119	TYR
1	D	128	ASP
1	D	129	ILE
1	D	141	ILE
1	D	152	LEU
1	D	155	LEU
1	D	158	LEU
1	D	169	THR
1	D	173	ILE
1	D	175	LEU
1	D	177	GLU
1	D	214	PHE
1	D	216	MET
1	D	218	MET
1	D	220	ASP
1	D	226	ILE
1	D	227	LEU
1	D	232	HIS
1	D	233	VAL
1	D	234	PHE
1	D	245	SER
1	D	257	VAL
1	D	263	LEU

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Mol	Chain	Res	Type
1	D	287	LEU
1	E	14	LEU
1	E	18	PHE
1	E	46	ASN
1	E	64	LEU
1	E	66	ARG
1	E	67	THR
1	E	70	ARG
1	E	71	ARG
1	E	93	SER
1	E	94	LEU
1	E	107	THR
1	E	108	LEU
1	E	119	TYR
1	E	128	ASP
1	E	129	ILE
1	E	141	ILE
1	E	148	PRO
1	E	152	LEU
1	E	155	LEU
1	E	158	LEU
1	E	168	ARG
1	E	169	THR
1	E	173	ILE
1	E	174	THR
1	E	214	PHE
1	E	216	MET
1	E	218	MET
1	E	226	ILE
1	E	227	LEU
1	E	233	VAL
1	E	234	PHE
1	E	245	SER
1	E	257	VAL
1	E	262	LEU
1	E	263	LEU
1	E	287	LEU
1	F	14	LEU
1	F	18	PHE
1	F	46	ASN
1	F	58	THR
1	F	64	LEU

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Mol	Chain	Res	Type
1	F	66	ARG
1	F	70	ARG
1	F	71	ARG
1	F	93	SER
1	F	107	THR
1	F	108	LEU
1	F	119	TYR
1	F	128	ASP
1	F	129	ILE
1	F	152	LEU
1	F	155	LEU
1	F	158	LEU
1	F	173	ILE
1	F	174	THR
1	F	175	LEU
1	F	177	GLU
1	F	214	PHE
1	F	216	MET
1	F	218	MET
1	F	226	ILE
1	F	227	LEU
1	F	232	HIS
1	F	233	VAL
1	F	234	PHE
1	F	245	SER
1	F	257	VAL
1	F	262	LEU
1	F	263	LEU
1	F	265	PHE
1	F	287	LEU
1	G	14	LEU
1	G	18	PHE
1	G	46	ASN
1	G	64	LEU
1	G	66	ARG
1	G	67	THR
1	G	70	ARG
1	G	71	ARG
1	G	93	SER
1	G	107	THR
1	G	108	LEU
1	G	119	TYR

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Mol	Chain	Res	Type
1	G	128	ASP
1	G	129	ILE
1	G	148	PRO
1	G	152	LEU
1	G	155	LEU
1	G	158	LEU
1	G	169	THR
1	G	171	HIS
1	G	173	ILE
1	G	174	THR
1	G	214	PHE
1	G	216	MET
1	G	218	MET
1	G	220	ASP
1	G	226	ILE
1	G	227	LEU
1	G	232	HIS
1	G	233	VAL
1	G	234	PHE
1	G	245	SER
1	G	257	VAL
1	G	262	LEU
1	G	263	LEU
1	G	287	LEU
1	H	18	PHE
1	H	46	ASN
1	H	49	ILE
1	H	64	LEU
1	H	66	ARG
1	H	70	ARG
1	H	71	ARG
1	H	93	SER
1	H	107	THR
1	H	108	LEU
1	H	119	TYR
1	H	128	ASP
1	H	129	ILE
1	H	152	LEU
1	H	155	LEU
1	H	158	LEU
1	H	173	ILE
1	H	174	THR

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Mol	Chain	Res	Type
1	H	175	LEU
1	H	177	GLU
1	H	214	PHE
1	H	216	MET
1	H	218	MET
1	H	226	ILE
1	H	227	LEU
1	H	232	HIS
1	H	233	VAL
1	H	234	PHE
1	H	245	SER
1	H	257	VAL
1	H	262	LEU
1	H	263	LEU
1	H	287	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	171	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers

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	246/301 (81%)	-0.38	4 (1%)	74	63	81, 117, 188, 281	0
1	B	246/301 (81%)	-0.27	5 (2%)	68	57	92, 120, 194, 266	0
1	C	246/301 (81%)	-0.33	5 (2%)	68	57	81, 117, 194, 279	0
1	D	246/301 (81%)	-0.27	4 (1%)	74	63	99, 124, 189, 250	0
1	E	246/301 (81%)	-0.23	5 (2%)	68	57	86, 137, 203, 289	0
1	F	246/301 (81%)	-0.24	9 (3%)	45	34	108, 150, 221, 269	0
1	G	246/301 (81%)	-0.31	4 (1%)	74	63	83, 126, 197, 287	0
1	H	246/301 (81%)	-0.12	14 (5%)	27	19	142, 173, 247, 299	0
All	All	1968/2408 (81%)	-0.27	50 (2%)	61	48	81, 133, 210, 299	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	35	LEU	14.0
1	H	34	GLY	7.4
1	F	35	LEU	6.8
1	E	179	VAL	5.5
1	E	68	GLY	4.8
1	B	6	TRP	4.5
1	G	273	ALA	4.5
1	G	272	GLN	4.3
1	H	122	PRO	4.3
1	A	35	LEU	4.1
1	B	65	LEU	4.0
1	F	65	LEU	3.8
1	H	33	ALA	3.7
1	E	67	THR	3.6
1	G	293	ALA	3.6
1	C	244	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	70	ARG	3.4
1	H	119	TYR	3.4
1	D	269	GLY	3.1
1	D	6	TRP	3.1
1	F	5	ASP	3.0
1	G	179	VAL	3.0
1	H	65	LEU	2.9
1	F	8	PRO	2.8
1	E	178	GLY	2.8
1	A	6	TRP	2.8
1	F	232	HIS	2.7
1	H	32	ALA	2.7
1	C	220	ASP	2.6
1	F	6	TRP	2.6
1	C	65	LEU	2.4
1	B	179	VAL	2.4
1	A	65	LEU	2.4
1	H	31	GLN	2.4
1	H	36	VAL	2.4
1	F	34	GLY	2.3
1	F	4	ARG	2.3
1	A	36	VAL	2.3
1	H	5	ASP	2.3
1	C	224	PRO	2.2
1	E	36	VAL	2.2
1	H	9	LEU	2.2
1	D	65	LEU	2.1
1	B	5	ASP	2.1
1	D	268	LYS	2.1
1	C	179	VAL	2.1
1	H	30	MET	2.0
1	B	228	VAL	2.0
1	H	8	PRO	2.0
1	F	9	LEU	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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.