Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 01:48 PM EDT

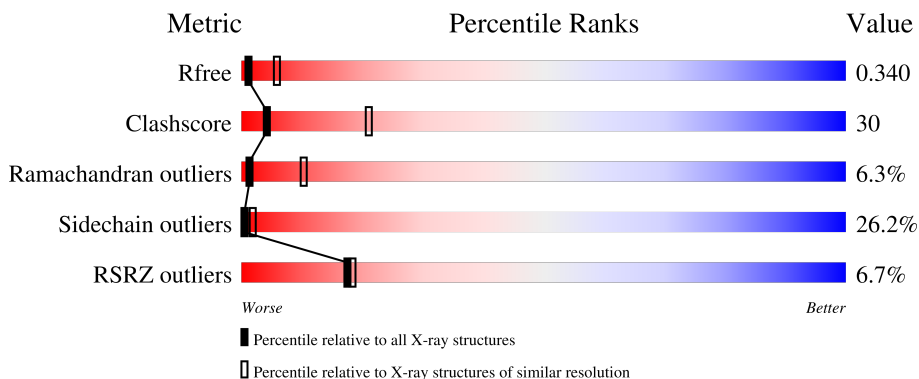|		
PDB ID	:	4HYG
Title	:	Structure of a presenilin family intramembrane aspartate protease in C222 space group
Authors	:	Li, X.; Dang, S.; Yan, C.; Wang, J.; Shi, Y.
Deposited on	:	2012-11-13
Resolution	:	3.32 Å(reported)

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 3.32 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	Percentile Ranks	Value
Rfree		0.340
Clashscore		30
Ramachandran outliers		6.3%
Sidechain outliers		26.2%
RSRZ outliers		6.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	301	3% — 30% / 40% / 11% • 18%
1	B	301	5% — 31% / 37% / 12% • 18%
1	C	301	6% — 34% / 34% / 9% • 21%
1	D	301	7% — 33% / 34% / 11% • 21%

2 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 7115 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	247	Total	C	N	O	S	0	0	0
			1810	1226	277	296	11			
1	C	238	Total	C	N	O	S	0	0	0
			1763	1197	267	288	11			
1	D	237	Total	C	N	O	S	0	0	0
			1740	1180	264	285	11			

There are 20 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
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

3 Residue-property plots ⓘ

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: Putative uncharacterized protein
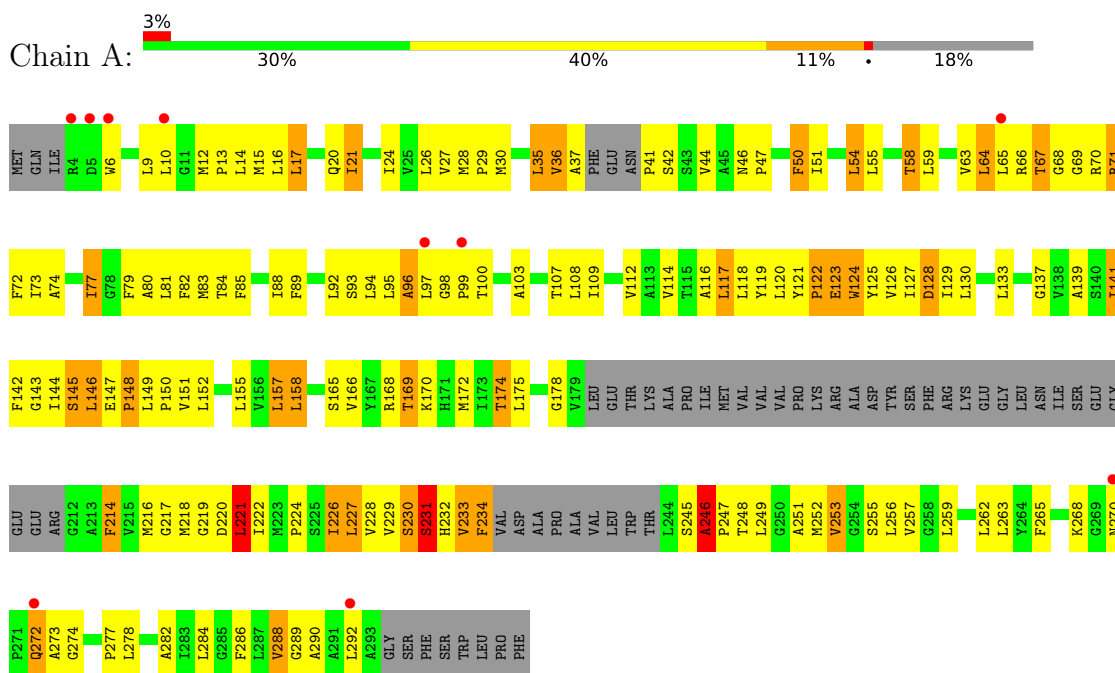
• Molecule 1: Putative uncharacterized protein
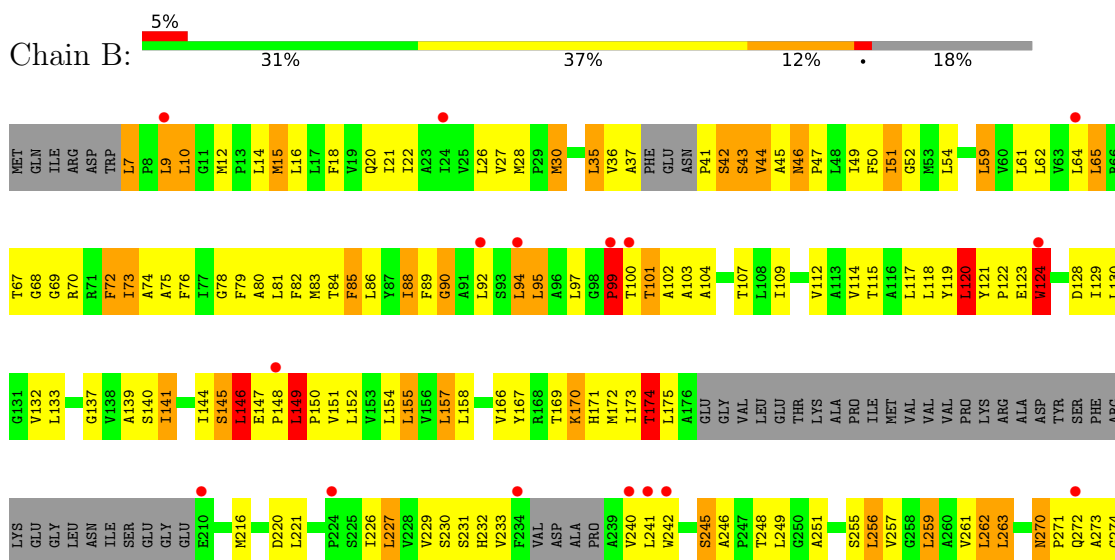
• Molecule 1: Putative uncharacterized protein

• Molecule 1: Putative uncharacterized protein

4 Data and refinement statistics ⓘ

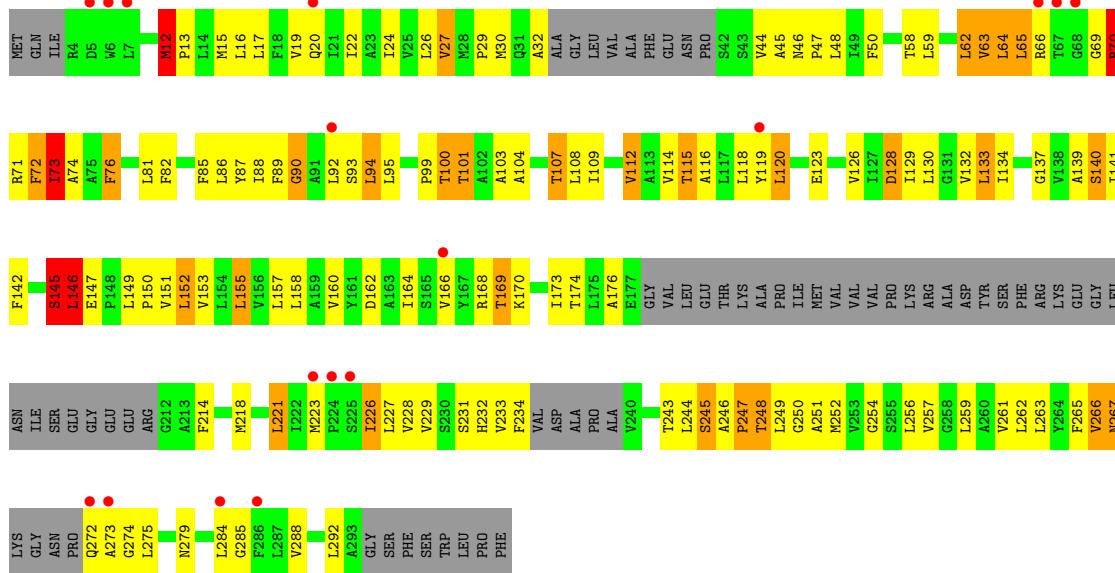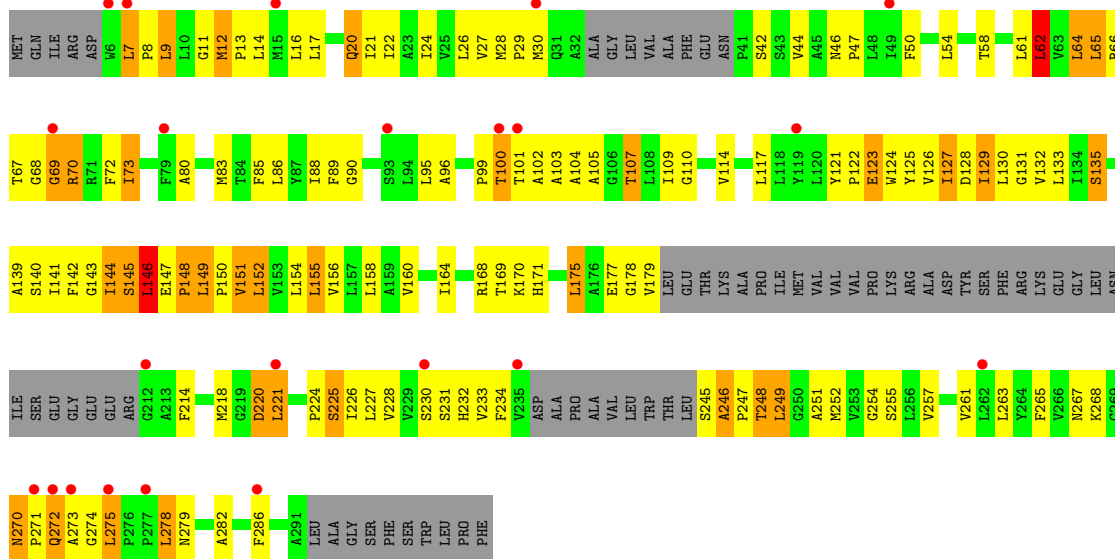| Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	168.30Å　201.89Å　117.53Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	49.11　–　3.32	Depositor
	49.11　–　3.32	EDS
% Data completeness (in resolution range)	82.0 (49.11-3.32)	Depositor
	82.4 (49.11-3.32)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.298　,　0.344	Depositor
	0.301　,　0.340	DCC
R_{free} test set	1260 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	111.9	Xtriage
Anisotropy	1.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 145.3	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	7115	wwPDB-VP
Average B, all atoms (Å^2)	165.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.56	0/1839	0.84	1/2511 (0.0%)
1	B	0.52	0/1847	0.87	3/2523 (0.1%)
1	C	0.51	0/1799	0.82	0/2457
1	D	0.53	0/1777	0.86	3/2427 (0.1%)
All	All	0.53	0/7262	0.85	7/9918 (0.1%)

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	5
1	B	0	3
1	C	0	2
1	D	0	1
All	All	0	11

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	120	LEU	CA-CB-CG	8.27	134.33	115.30
1	B	35	LEU	CA-CB-CG	8.20	134.15	115.30
1	D	146	LEU	CB-CG-CD1	5.87	120.98	111.00
1	B	59	LEU	CA-CB-CG	5.57	128.10	115.30
1	D	249	LEU	CA-CB-CG	5.40	127.72	115.30
1	D	62	LEU	CA-CB-CG	-5.35	102.99	115.30
1	A	221	LEU	CA-CB-CG	5.30	127.49	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	A	146	LEU	Peptide
1	A	246	ALA	Peptide
1	A	272	GLN	Peptide
1	B	145	SER	Peptide
1	B	146	LEU	Peptide
1	B	99	PRO	Peptide
1	C	145	SER	Peptide
1	C	146	LEU	Peptide
1	D	146	LEU	Peptide

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	1802	0	1949	123	0
1	B	1810	0	1965	109	0
1	C	1763	0	1903	95	0
1	D	1740	0	1881	119	0
All	All	7115	0	7698	437	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 30.

All (437) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ALA:HA	1:B:249:LEU:HD12	1.43	1.00
1:D:139:ALA:HA	1:D:226:ILE:HG12	1.53	0.89
1:A:36:VAL:HG12	1:A:37:ALA:H	1.40	0.87
1:D:265:PHE:HB3	1:D:271:PRO:HG2	1.56	0.87
1:D:228:VAL:HG22	1:D:251:ALA:HB1	1.58	0.86
1:B:146:LEU:HD12	1:B:147:GLU:HG2	1.57	0.85
1:C:12:MET:H	1:C:13:PRO:HD2	1.41	0.85
1:C:90:GLY:HA2	1:C:107:THR:HG21	1.57	0.85
1:A:63:VAL:O	1:A:67:THR:OG1	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:THR:OG1	1:C:101:THR:N	2.04	0.84
1:C:74:ALA:O	1:C:119:TYR:OH	1.97	0.83
1:D:220:ASP:HB2	1:D:275:LEU:HD12	1.59	0.83
1:D:151:VAL:HG13	1:D:227:LEU:HD13	1.59	0.83
1:B:85:PHE:HE1	1:B:133:LEU:HD23	1.44	0.81
1:D:263:LEU:O	1:D:267:ASN:ND2	2.13	0.81
1:D:275:LEU:HD13	1:D:278:LEU:HG	1.65	0.79
1:C:263:LEU:O	1:C:267:ASN:ND2	2.17	0.78
1:D:147:GLU:HB3	1:D:148:PRO:HD2	1.65	0.77
1:D:29:PRO:HB3	1:D:95:LEU:HG	1.66	0.77
1:C:88:ILE:O	1:C:92:LEU:HB2	1.85	0.76
1:B:36:VAL:HG12	1:B:37:ALA:H	1.51	0.75
1:D:151:VAL:HG22	1:D:227:LEU:HD22	1.68	0.75
1:A:42:SER:HB2	1:A:146:LEU:HD12	1.67	0.75
1:D:246:ALA:HB3	1:D:248:THR:HB	1.68	0.74
1:C:88:ILE:HA	1:C:92:LEU:HD12	1.70	0.74
1:D:154:LEU:HD23	1:D:227:LEU:HD11	1.71	0.73
1:A:36:VAL:HG13	1:A:145:SER:HA	1.71	0.73
1:B:61:LEU:HA	1:B:64:LEU:HD12	1.71	0.72
1:C:26:LEU:HD22	1:C:92:LEU:HD13	1.70	0.72
1:B:100:THR:OG1	1:B:101:THR:N	2.19	0.72
1:A:253:VAL:HA	1:A:256:LEU:HD12	1.71	0.72
1:A:262:LEU:HD23	1:A:277:PRO:HG2	1.71	0.72
1:B:26:LEU:HD22	1:B:92:LEU:HB3	1.71	0.72
1:B:82:PHE:HA	1:B:115:THR:HG21	1.72	0.72
1:A:65:LEU:HD23	1:A:73:ILE:HD13	1.73	0.71
1:C:71:ARG:O	1:C:73:ILE:N	2.23	0.71
1:A:124:TRP:HA	1:A:127:ILE:HG12	1.71	0.70
1:C:71:ARG:C	1:C:73:ILE:H	1.93	0.70
1:D:16:LEU:HA	1:D:221:LEU:HD11	1.72	0.70
1:D:146:LEU:O	1:D:230:SER:OG	2.06	0.70
1:A:148:PRO:O	1:A:151:VAL:N	2.24	0.70
1:A:41:PRO:C	1:A:146:LEU:HG	2.12	0.70
1:D:88:ILE:HG21	1:D:133:LEU:HD21	1.73	0.70
1:C:118:LEU:HD12	1:C:130:LEU:HD12	1.73	0.70
1:D:131:GLY:O	1:D:135:SER:OG	2.09	0.69
1:B:43:SER:O	1:B:46:ASN:HB2	1.91	0.69
1:C:16:LEU:HA	1:C:221:LEU:HD11	1.74	0.69
1:D:148:PRO:O	1:D:151:VAL:N	2.26	0.68
1:A:246:ALA:HB1	1:A:247:PRO:HD2	1.76	0.68
1:C:247:PRO:O	1:C:250:GLY:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HD12	1:A:130:LEU:HD12	1.76	0.68
1:B:280:GLY:O	1:B:284:LEU:HG	1.94	0.68
1:B:171:HIS:HA	1:B:174:THR:HG23	1.76	0.67
1:B:169:THR:HA	1:B:172:MET:HB2	1.74	0.67
1:D:100:THR:HB	1:D:103:ALA:HB3	1.76	0.67
1:A:218:MET:O	1:A:221:LEU:HB3	1.95	0.67
1:B:139:ALA:HA	1:B:226:ILE:HD11	1.76	0.67
1:D:65:LEU:O	1:D:69:GLY:N	2.28	0.67
1:A:74:ALA:O	1:A:119:TYR:OH	2.13	0.66
1:A:59:LEU:HD23	1:B:72:PHE:CZ	2.30	0.66
1:A:17:LEU:HD21	1:A:256:LEU:HD11	1.76	0.66
1:A:30:MET:HE2	1:A:144:ILE:HD12	1.78	0.66
1:D:142:PHE:HB2	1:D:226:ILE:HD13	1.78	0.66
1:D:155:LEU:HD22	1:D:279:ASN:ND2	2.09	0.66
1:D:251:ALA:HB2	1:D:286:PHE:HB2	1.77	0.66
1:B:251:ALA:HB2	1:B:286:PHE:HB2	1.77	0.66
1:B:9:LEU:HD12	1:B:10:LEU:HG	1.78	0.65
1:C:69:GLY:H	1:C:73:ILE:HG22	1.62	0.65
1:B:51:ILE:HD11	1:B:158:LEU:HD21	1.78	0.65
1:B:173:ILE:O	1:B:175:LEU:N	2.29	0.65
1:C:254:GLY:HA3	1:C:285:GLY:HA3	1.79	0.64
1:D:170:LYS:HZ2	1:D:270:ASN:ND2	1.95	0.64
1:D:143:GLY:HA2	1:D:230:SER:HB2	1.78	0.64
1:D:272:GLN:HE22	1:D:275:LEU:H	1.45	0.63
1:A:123:GLU:HB3	1:A:125:TYR:CE2	2.33	0.63
1:D:151:VAL:CG2	1:D:227:LEU:HD22	2.29	0.63
1:A:143:GLY:HA3	1:A:229:VAL:HB	1.80	0.63
1:C:85:PHE:HE1	1:C:133:LEU:HD22	1.64	0.63
1:C:103:ALA:O	1:C:107:THR:HG23	1.99	0.63
1:B:94:LEU:HD11	1:B:100:THR:HA	1.81	0.63
1:B:262:LEU:HD23	1:B:263:LEU:HD23	1.81	0.63
1:C:146:LEU:HG	1:C:147:GLU:OE2	1.99	0.62
1:C:94:LEU:HD11	1:C:104:ALA:HA	1.79	0.62
1:D:68:GLY:O	1:D:70:ARG:N	2.32	0.62
1:B:118:LEU:HD12	1:B:130:LEU:HD12	1.80	0.62
1:C:29:PRO:HG2	1:C:92:LEU:HD22	1.81	0.62
1:C:71:ARG:HA	1:C:74:ALA:HB3	1.82	0.62
1:C:90:GLY:O	1:C:94:LEU:N	2.23	0.61
1:A:69:GLY:HA2	1:A:72:PHE:HB3	1.82	0.61
1:B:129:ILE:HG22	1:B:130:LEU:HD23	1.82	0.61
1:A:142:PHE:HB2	1:A:226:ILE:CD1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLY:O	1:A:100:THR:N	2.34	0.61
1:B:47:PRO:O	1:B:50:PHE:HB3	2.00	0.61
1:A:147:GLU:HB3	1:A:148:PRO:HD2	1.83	0.61
1:B:120:LEU:HD23	1:B:121:TYR:N	2.16	0.61
1:B:95:LEU:HD22	1:B:99:PRO:HB3	1.82	0.60
1:A:51:ILE:HG22	1:B:79:PHE:CE2	2.36	0.60
1:A:89:PHE:HB3	1:A:107:THR:HB	1.82	0.60
1:C:146:LEU:HG	1:C:147:GLU:CD	2.22	0.60
1:A:165:SER:O	1:A:169:THR:HG23	2.01	0.60
1:A:36:VAL:CG1	1:A:37:ALA:H	2.13	0.60
1:A:166:VAL:HG21	1:A:273:ALA:HA	1.82	0.60
1:D:155:LEU:CD2	1:D:227:LEU:HD12	2.32	0.59
1:A:36:VAL:HG12	1:A:37:ALA:N	2.14	0.59
1:D:224:PRO:HG3	1:D:278:LEU:HD12	1.85	0.59
1:B:30:MET:SD	1:B:141:ILE:HG12	2.42	0.59
1:A:142:PHE:HB2	1:A:226:ILE:HD11	1.84	0.59
1:C:162:ASP:OD2	1:C:275:LEU:HG	2.03	0.59
1:D:110:GLY:O	1:D:114:VAL:HG23	2.02	0.59
1:D:246:ALA:HB1	1:D:247:PRO:HD2	1.85	0.59
1:C:273:ALA:HB3	1:C:274:GLY:HA2	1.85	0.59
1:C:243:THR:O	1:C:245:SER:N	2.30	0.59
1:D:129:ILE:HD13	1:D:130:LEU:HD23	1.85	0.59
1:C:116:ALA:O	1:C:120:LEU:HG	2.02	0.58
1:C:19:VAL:HG21	1:C:221:LEU:HG	1.85	0.58
1:D:151:VAL:HG13	1:D:227:LEU:HB3	1.86	0.58
1:B:21:ILE:HG22	1:B:22:ILE:HD13	1.85	0.58
1:D:122:PRO:HB2	1:D:127:ILE:HG13	1.84	0.58
1:D:170:LYS:HD3	1:D:270:ASN:HB2	1.86	0.57
1:D:89:PHE:HZ	1:D:114:VAL:HG21	1.68	0.57
1:D:275:LEU:HD22	1:D:278:LEU:HD23	1.87	0.57
1:A:54:LEU:O	1:A:58:THR:HG23	2.05	0.57
1:D:254:GLY:HA3	1:D:282:ALA:HA	1.85	0.57
1:A:24:ILE:HA	1:A:27:VAL:HG23	1.87	0.57
1:A:42:SER:N	1:A:146:LEU:HG	2.19	0.56
1:B:145:SER:O	1:B:146:LEU:HB2	2.05	0.56
1:B:166:VAL:O	1:B:170:LYS:HB2	2.06	0.56
1:B:281:GLY:HA2	1:B:284:LEU:HD12	1.86	0.56
1:C:45:ALA:HA	1:C:48:LEU:HD12	1.87	0.56
1:D:170:LYS:NZ	1:D:270:ASN:ND2	2.53	0.56
1:D:272:GLN:NE2	1:D:275:LEU:H	2.04	0.56
1:D:155:LEU:HG	1:D:227:LEU:HD12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:HD23	1:D:72:PHE:CE2	2.41	0.56
1:A:259:LEU:HB2	1:A:278:LEU:HD11	1.87	0.56
1:D:24:ILE:O	1:D:27:VAL:HB	2.05	0.56
1:C:257:VAL:O	1:C:261:VAL:HG23	2.06	0.55
1:D:151:VAL:CG1	1:D:227:LEU:HB3	2.37	0.55
1:D:17:LEU:HA	1:D:20:GLN:HG3	1.88	0.55
1:B:65:LEU:HG	1:B:73:ILE:HD13	1.88	0.55
1:B:227:LEU:HD11	1:B:283:ILE:HG12	1.88	0.55
1:D:148:PRO:HD3	1:D:230:SER:O	2.06	0.55
1:C:100:THR:O	1:C:104:ALA:N	2.34	0.55
1:D:155:LEU:HD23	1:D:227:LEU:HD12	1.89	0.54
1:A:229:VAL:O	1:A:231:SER:N	2.39	0.54
1:B:26:LEU:HD13	1:B:92:LEU:HD13	1.89	0.54
1:B:41:PRO:C	1:B:146:LEU:HG	2.27	0.54
1:B:82:PHE:CZ	1:B:112:VAL:HG23	2.42	0.54
1:B:88:ILE:O	1:B:92:LEU:HB2	2.07	0.54
1:D:64:LEU:HD13	1:D:72:PHE:HE2	1.72	0.54
1:C:99:PRO:HB2	1:C:100:THR:HG22	1.89	0.54
1:B:74:ALA:O	1:B:119:TYR:OH	2.26	0.54
1:A:42:SER:HA	1:A:146:LEU:HB3	1.88	0.54
1:C:12:MET:N	1:C:13:PRO:HD2	2.19	0.54
1:A:251:ALA:HB2	1:A:286:PHE:HB2	1.89	0.54
1:D:54:LEU:O	1:D:58:THR:HG23	2.07	0.54
1:D:90:GLY:HA2	1:D:107:THR:HG21	1.89	0.54
1:A:73:ILE:O	1:A:77:ILE:HG12	2.07	0.54
1:A:255:SER:HB2	1:A:282:ALA:HB2	1.88	0.54
1:B:73:ILE:HA	1:B:76:PHE:HB3	1.90	0.54
1:A:36:VAL:HG22	1:A:144:ILE:HG22	1.89	0.54
1:D:89:PHE:CZ	1:D:114:VAL:HG21	2.43	0.54
1:A:20:GLN:CD	1:A:252:MET:HG2	2.29	0.53
1:C:86:LEU:HD21	1:C:108:LEU:HD12	1.90	0.53
1:B:85:PHE:CE1	1:B:133:LEU:HD23	2.35	0.53
1:C:128:ASP:N	1:C:128:ASP:OD1	2.41	0.53
1:D:143:GLY:N	1:D:226:ILE:HG23	2.24	0.53
1:A:97:LEU:HB2	1:A:103:ALA:HB2	1.91	0.53
1:A:170:LYS:O	1:A:174:THR:HG23	2.09	0.53
1:A:68:GLY:HA3	1:A:73:ILE:HD11	1.91	0.53
1:B:16:LEU:O	1:B:20:GLN:HG3	2.09	0.53
1:A:93:SER:HA	1:A:96:ALA:HB3	1.90	0.52
1:B:94:LEU:O	1:B:99:PRO:HA	2.08	0.52
1:A:262:LEU:HD21	1:A:274:GLY:HA2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:ASN:OD1	1:D:271:PRO:HD3	2.09	0.52
1:C:24:ILE:HD11	1:C:228:VAL:HG12	1.90	0.52
1:D:151:VAL:HG13	1:D:227:LEU:CD1	2.36	0.52
1:A:288:VAL:O	1:A:292:LEU:HG	2.09	0.52
1:B:241:LEU:HA	1:B:245:SER:H	1.75	0.52
1:C:76:PHE:CD1	1:C:76:PHE:C	2.83	0.52
1:A:69:GLY:CA	1:A:72:PHE:HB3	2.40	0.52
1:B:173:ILE:C	1:B:175:LEU:H	2.13	0.52
1:C:247:PRO:O	1:C:249:LEU:N	2.42	0.52
1:D:11:GLY:O	1:D:14:LEU:HB3	2.10	0.52
1:C:59:LEU:HD23	1:D:72:PHE:CZ	2.45	0.52
1:A:151:VAL:HG11	1:A:227:LEU:HB2	1.90	0.52
1:A:146:LEU:HD13	1:A:147:GLU:OE2	2.08	0.52
1:A:30:MET:HE1	1:A:141:ILE:HA	1.92	0.52
1:B:155:LEU:HB3	1:B:283:ILE:HD11	1.92	0.52
1:C:29:PRO:HG2	1:C:92:LEU:CD2	2.39	0.52
1:A:121:TYR:HA	1:A:124:TRP:HZ2	1.75	0.51
1:C:44:VAL:HA	1:C:150:PRO:HG3	1.90	0.51
1:C:69:GLY:H	1:C:73:ILE:CG2	2.23	0.51
1:D:139:ALA:HA	1:D:226:ILE:CG1	2.32	0.51
1:B:75:ALA:O	1:B:78:GLY:N	2.43	0.51
1:D:7:LEU:HB2	1:D:8:PRO:HD3	1.92	0.51
1:A:122:PRO:HD2	1:A:124:TRP:CE2	2.45	0.51
1:A:24:ILE:O	1:A:27:VAL:N	2.42	0.51
1:A:121:TYR:HA	1:A:124:TRP:CZ2	2.45	0.51
1:C:24:ILE:O	1:C:27:VAL:N	2.43	0.51
1:C:24:ILE:O	1:C:27:VAL:HG12	2.11	0.51
1:B:88:ILE:HD11	1:B:137:GLY:HA3	1.92	0.50
1:C:145:SER:O	1:C:146:LEU:HB2	2.10	0.50
1:A:128:ASP:OD1	1:A:128:ASP:N	2.44	0.50
1:B:88:ILE:HA	1:B:92:LEU:HD12	1.94	0.50
1:B:18:PHE:O	1:B:22:ILE:HG12	2.11	0.50
1:D:122:PRO:CB	1:D:127:ILE:HG13	2.40	0.50
1:B:140:SER:HA	1:B:229:VAL:HG21	1.93	0.50
1:D:21:ILE:HG22	1:D:22:ILE:HD13	1.92	0.50
1:A:219:GLY:O	1:A:222:ILE:HB	2.12	0.50
1:D:47:PRO:O	1:D:50:PHE:HB3	2.12	0.50
1:D:128:ASP:O	1:D:132:VAL:HG23	2.11	0.50
1:B:259:LEU:HB2	1:B:278:LEU:HD23	1.93	0.50
1:D:272:GLN:H	1:D:273:ALA:HA	1.77	0.49
1:D:80:ALA:HA	1:D:83:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:SER:OG	1:A:147:GLU:HB2	2.11	0.49
1:B:231:SER:HB2	1:B:286:PHE:CE1	2.48	0.49
1:B:82:PHE:CE1	1:B:112:VAL:HG23	2.47	0.49
1:B:89:PHE:HB3	1:B:107:THR:HB	1.94	0.49
1:D:42:SER:H	1:D:146:LEU:CD1	2.26	0.49
1:A:114:VAL:O	1:A:117:LEU:HB3	2.11	0.49
1:B:139:ALA:HA	1:B:226:ILE:CD1	2.41	0.49
1:A:28:MET:HG3	1:A:95:LEU:HD22	1.95	0.49
1:C:247:PRO:HG2	1:C:248:THR:H	1.78	0.49
1:D:103:ALA:O	1:D:107:THR:HG23	2.12	0.49
1:C:243:THR:C	1:C:245:SER:H	2.14	0.48
1:B:94:LEU:HD13	1:B:104:ALA:N	2.29	0.48
1:C:142:PHE:HB2	1:C:226:ILE:HG12	1.96	0.48
1:D:160:VAL:O	1:D:164:ILE:HG12	2.13	0.48
1:D:20:GLN:NE2	1:D:225:SER:OG	2.44	0.48
1:A:30:MET:HB3	1:A:35:LEU:HD22	1.94	0.48
1:A:123:GLU:HB2	1:A:126:VAL:HG23	1.96	0.48
1:B:44:VAL:HG12	1:B:150:PRO:HA	1.96	0.48
1:D:227:LEU:N	1:D:227:LEU:HD23	2.28	0.48
1:D:270:ASN:OD1	1:D:270:ASN:N	2.44	0.48
1:C:85:PHE:CD2	1:C:115:THR:HG23	2.49	0.48
1:D:69:GLY:O	1:D:70:ARG:HG3	2.13	0.48
1:B:30:MET:HG2	1:B:92:LEU:CD2	2.44	0.47
1:B:50:PHE:CE1	1:B:154:LEU:HD21	2.49	0.47
1:D:220:ASP:HB2	1:D:275:LEU:CD1	2.39	0.47
1:A:15:MET:HB3	1:A:221:LEU:HD21	1.95	0.47
1:A:59:LEU:HB2	1:B:72:PHE:CE1	2.49	0.47
1:C:76:PHE:C	1:C:76:PHE:HD1	2.16	0.47
1:C:139:ALA:HA	1:C:226:ILE:HG13	1.96	0.47
1:D:228:VAL:HG22	1:D:251:ALA:CB	2.36	0.47
1:B:27:VAL:HG13	1:B:144:ILE:HD11	1.97	0.47
1:C:129:ILE:HG22	1:C:130:LEU:HD23	1.95	0.47
1:C:142:PHE:HB2	1:C:226:ILE:CD1	2.45	0.47
1:B:256:LEU:HD22	1:B:256:LEU:HA	1.76	0.47
1:D:226:ILE:HG22	1:D:227:LEU:HD23	1.95	0.47
1:B:45:ALA:O	1:B:49:ILE:HG13	2.14	0.47
1:C:71:ARG:C	1:C:73:ILE:N	2.64	0.47
1:D:42:SER:H	1:D:146:LEU:HD11	1.79	0.47
1:D:26:LEU:O	1:D:30:MET:HB2	2.14	0.47
1:D:175:LEU:HG	1:D:179:VAL:O	2.14	0.47
1:B:97:LEU:HD13	1:B:103:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:GLN:N	1:D:273:ALA:HB2	2.30	0.47
1:C:12:MET:H	1:C:13:PRO:CD	2.21	0.47
1:D:125:TYR:O	1:D:129:ILE:HG22	2.14	0.47
1:A:265:PHE:HB3	1:A:272:GLN:OE1	2.15	0.47
1:D:42:SER:HA	1:D:146:LEU:HG	1.96	0.47
1:D:142:PHE:HB2	1:D:226:ILE:CD1	2.44	0.47
1:A:16:LEU:HD23	1:A:256:LEU:HD23	1.96	0.46
1:D:145:SER:O	1:D:146:LEU:HD13	2.15	0.46
1:B:149:LEU:HB3	1:B:150:PRO:HD3	1.96	0.46
1:C:64:LEU:HD21	1:C:73:ILE:HA	1.95	0.46
1:C:123:GLU:H	1:C:126:VAL:HB	1.79	0.46
1:C:243:THR:OG1	1:C:246:ALA:HB3	2.15	0.46
1:D:65:LEU:O	1:D:65:LEU:HD12	2.15	0.46
1:B:51:ILE:HG22	1:B:52:GLY:N	2.29	0.46
1:A:26:LEU:C	1:A:29:PRO:HD2	2.36	0.46
1:A:64:LEU:HD21	1:A:73:ILE:HA	1.97	0.46
1:B:69:GLY:O	1:B:73:ILE:HG22	2.15	0.46
1:C:82:PHE:CE1	1:C:112:VAL:HG23	2.51	0.46
1:D:255:SER:HA	1:D:278:LEU:HD13	1.96	0.46
1:A:231:SER:OG	1:A:248:THR:HG21	2.15	0.46
1:B:62:LEU:O	1:B:65:LEU:N	2.48	0.46
1:C:85:PHE:HD2	1:C:115:THR:HG23	1.80	0.46
1:C:87:TYR:N	1:C:87:TYR:CD1	2.84	0.46
1:A:94:LEU:O	1:A:98:GLY:HA2	2.15	0.46
1:B:82:PHE:CA	1:B:115:THR:HG21	2.45	0.46
1:D:170:LYS:HZ3	1:D:270:ASN:CG	2.18	0.46
1:B:90:GLY:HA2	1:B:107:THR:OG1	2.16	0.46
1:B:90:GLY:O	1:B:94:LEU:HB3	2.16	0.46
1:C:88:ILE:HD12	1:C:134:ILE:HD13	1.98	0.46
1:A:30:MET:CE	1:A:141:ILE:HG12	2.45	0.46
1:C:151:VAL:HG12	1:C:227:LEU:HD23	1.97	0.46
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.78	0.46
1:D:147:GLU:HA	1:D:230:SER:OG	2.14	0.46
1:B:100:THR:HG1	1:B:101:THR:H	1.61	0.46
1:B:173:ILE:C	1:B:175:LEU:N	2.69	0.46
1:A:249:LEU:O	1:A:252:MET:N	2.49	0.46
1:C:139:ALA:O	1:C:226:ILE:HG13	2.16	0.45
1:D:65:LEU:HA	1:D:73:ILE:HD12	1.98	0.45
1:D:171:HIS:CE1	1:D:175:LEU:HD13	2.51	0.45
1:B:36:VAL:HG12	1:B:37:ALA:N	2.26	0.45
1:A:224:PRO:HG3	1:A:278:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:MET:O	1:B:86:LEU:HB2	2.16	0.45
1:C:22:ILE:O	1:C:26:LEU:HG	2.16	0.45
1:A:71:ARG:HB2	1:A:71:ARG:NH1	2.31	0.45
1:B:101:THR:OG1	1:B:102:ALA:N	2.50	0.45
1:B:270:ASN:N	1:B:271:PRO:CD	2.80	0.45
1:D:12:MET:N	1:D:13:PRO:HD2	2.32	0.45
1:D:220:ASP:O	1:D:224:PRO:HD3	2.16	0.45
1:C:146:LEU:HG	1:C:147:GLU:OE1	2.17	0.45
1:D:83:MET:O	1:D:86:LEU:HB2	2.17	0.45
1:B:290:ALA:C	1:B:292:LEU:H	2.20	0.45
1:D:125:TYR:CE2	1:D:126:VAL:HG23	2.52	0.45
1:B:155:LEU:HB3	1:B:279:ASN:HD21	1.80	0.45
1:D:155:LEU:CG	1:D:227:LEU:HD12	2.46	0.45
1:A:85:PHE:CE1	1:A:133:LEU:HD23	2.51	0.45
1:A:108:LEU:O	1:A:112:VAL:HG23	2.17	0.45
1:B:130:LEU:HD23	1:B:130:LEU:N	2.32	0.45
1:C:252:MET:HE2	1:C:252:MET:HB2	1.80	0.45
1:D:214:PHE:CD1	1:D:218:MET:HB3	2.52	0.45
1:A:146:LEU:HD12	1:A:147:GLU:HG2	1.98	0.45
1:C:87:TYR:HD1	1:C:87:TYR:H	1.65	0.45
1:B:148:PRO:HG3	1:B:230:SER:O	2.17	0.44
1:D:214:PHE:CE1	1:D:218:MET:HB3	2.52	0.44
1:A:17:LEU:O	1:A:21:ILE:HD13	2.17	0.44
1:A:17:LEU:CD2	1:A:256:LEU:HD11	2.44	0.44
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.87	0.44
1:A:214:PHE:CE1	1:A:218:MET:HB3	2.52	0.44
1:A:218:MET:HG3	1:A:219:GLY:N	2.31	0.44
1:D:28:MET:HB3	1:D:29:PRO:HD3	1.98	0.44
1:A:157:LEU:HD21	1:B:82:PHE:CE2	2.52	0.44
1:B:30:MET:HG2	1:B:92:LEU:HD21	1.99	0.44
1:B:100:THR:O	1:B:101:THR:OG1	2.35	0.44
1:A:82:PHE:HE1	1:A:112:VAL:HG22	1.83	0.44
1:A:265:PHE:O	1:A:268:LYS:HG2	2.16	0.44
1:B:83:MET:HE2	1:B:83:MET:HB3	1.81	0.44
1:C:248:THR:O	1:C:251:ALA:HB3	2.17	0.44
1:B:80:ALA:O	1:B:84:THR:HG23	2.17	0.44
1:D:44:VAL:HG12	1:D:150:PRO:HA	2.00	0.44
1:D:101:THR:OG1	1:D:102:ALA:N	2.50	0.44
1:D:152:LEU:HA	1:D:152:LEU:HD22	1.59	0.44
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.83	0.44
1:C:85:PHE:CE1	1:C:133:LEU:HD22	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:THR:O	1:C:103:ALA:N	2.51	0.44
1:A:10:LEU:HD23	1:A:10:LEU:HA	1.72	0.44
1:A:47:PRO:O	1:A:50:PHE:HB3	2.18	0.44
1:B:233:VAL:HG12	1:B:233:VAL:O	2.17	0.44
1:A:227:LEU:O	1:A:231:SER:HB3	2.18	0.43
1:A:227:LEU:O	1:A:227:LEU:HG	2.19	0.43
1:B:124:TRP:O	1:B:128:ASP:OD1	2.35	0.43
1:C:63:VAL:CG2	1:D:67:THR:HB	2.48	0.43
1:D:62:LEU:HD12	1:D:62:LEU:HA	1.61	0.43
1:A:149:LEU:HB3	1:A:150:PRO:HD3	2.00	0.43
1:B:97:LEU:HD13	1:B:103:ALA:CB	2.48	0.43
1:C:29:PRO:HA	1:C:32:ALA:HB3	2.00	0.43
1:D:170:LYS:NZ	1:D:270:ASN:CG	2.72	0.43
1:D:105:ALA:O	1:D:109:ILE:HG12	2.18	0.43
1:D:273:ALA:HA	1:D:274:GLY:HA2	1.57	0.43
1:C:70:ARG:HA	1:C:70:ARG:HD3	1.58	0.43
1:C:152:LEU:HD22	1:C:152:LEU:HA	1.77	0.43
1:C:160:VAL:O	1:C:164:ILE:HG12	2.19	0.43
1:D:27:VAL:HG13	1:D:144:ILE:HD11	2.00	0.43
1:A:13:PRO:HD3	1:A:259:LEU:HD21	1.99	0.43
1:B:61:LEU:O	1:B:64:LEU:HB2	2.18	0.43
1:B:242:TRP:CD1	1:B:246:ALA:HB2	2.54	0.43
1:A:217:GLY:O	1:A:220:ASP:N	2.51	0.43
1:B:242:TRP:HB2	1:B:246:ALA:HB2	2.00	0.43
1:C:155:LEU:HD22	1:C:279:ASN:ND2	2.33	0.43
1:A:16:LEU:HA	1:A:221:LEU:CD1	2.49	0.43
1:A:68:GLY:HA2	1:A:69:GLY:HA3	1.60	0.43
1:A:88:ILE:O	1:A:92:LEU:HG	2.19	0.43
1:A:109:ILE:HD13	1:A:109:ILE:HA	1.85	0.43
1:B:42:SER:N	1:B:146:LEU:HG	2.34	0.43
1:D:100:THR:HG21	1:D:104:ALA:HB2	2.01	0.43
1:D:149:LEU:HB3	1:D:150:PRO:HD3	2.01	0.43
1:D:254:GLY:HA2	1:D:257:VAL:HG12	2.00	0.43
1:A:158:LEU:HD22	1:A:158:LEU:HA	1.85	0.43
1:B:289:GLY:HA2	1:B:292:LEU:HD12	1.99	0.43
1:A:168:ARG:HH12	1:A:169:THR:HG22	1.83	0.42
1:A:231:SER:HA	1:A:234:PHE:HD2	1.83	0.42
1:C:231:SER:HB3	1:C:248:THR:HG22	2.01	0.42
1:A:146:LEU:HD13	1:A:146:LEU:HA	1.84	0.42
1:C:90:GLY:HA2	1:C:107:THR:CG2	2.40	0.42
1:B:229:VAL:O	1:B:232:HIS:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:HB2	1:D:72:PHE:CE1	2.54	0.42
1:A:116:ALA:O	1:A:120:LEU:HG	2.19	0.42
1:A:289:GLY:HA2	1:A:292:LEU:HD12	2.01	0.42
1:A:246:ALA:HB1	1:A:247:PRO:CD	2.48	0.42
1:B:155:LEU:CB	1:B:283:ILE:HD11	2.49	0.42
1:A:168:ARG:NH1	1:A:168:ARG:HB3	2.35	0.42
1:A:50:PHE:CD1	1:A:50:PHE:C	2.92	0.42
1:B:255:SER:HB3	1:B:282:ALA:HB2	2.01	0.42
1:C:114:VAL:HG13	1:C:130:LEU:HD13	2.01	0.42
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.79	0.42
1:A:20:GLN:OE1	1:A:252:MET:HG2	2.20	0.42
1:A:144:ILE:HA	1:A:233:VAL:HG21	2.00	0.42
1:B:9:LEU:H	1:B:9:LEU:HG	1.67	0.42
1:C:169:THR:O	1:C:173:ILE:HD12	2.20	0.42
1:D:9:LEU:H	1:D:9:LEU:HG	1.56	0.42
1:D:147:GLU:CB	1:D:148:PRO:HD2	2.44	0.42
1:B:94:LEU:CD1	1:B:100:THR:HA	2.50	0.42
1:C:88:ILE:HD11	1:C:137:GLY:HA3	2.01	0.42
1:A:16:LEU:HD23	1:A:256:LEU:CD2	2.50	0.41
1:C:15:MET:HG2	1:C:132:VAL:HG21	2.02	0.41
1:C:62:LEU:O	1:C:65:LEU:N	2.53	0.41
1:A:26:LEU:O	1:A:29:PRO:HD2	2.20	0.41
1:D:170:LYS:HD3	1:D:270:ASN:CB	2.50	0.41
1:A:117:LEU:HD22	1:A:122:PRO:HB3	2.03	0.41
1:A:59:LEU:HD23	1:B:72:PHE:CE2	2.54	0.41
1:A:290:ALA:C	1:A:292:LEU:H	2.24	0.41
1:C:266:VAL:HG22	1:C:272:GLN:HG2	2.02	0.41
1:A:88:ILE:HD11	1:A:137:GLY:HA3	2.03	0.41
1:A:85:PHE:HE1	1:A:133:LEU:HD23	1.84	0.41
1:A:151:VAL:CG1	1:A:227:LEU:HB2	2.51	0.41
1:A:220:ASP:OD1	1:A:220:ASP:C	2.58	0.41
1:B:149:LEU:HD22	1:B:149:LEU:HA	1.86	0.41
1:C:94:LEU:HD23	1:C:99:PRO:HA	2.03	0.41
1:B:15:MET:HG2	1:B:132:VAL:CG2	2.50	0.41
1:B:68:GLY:HA3	1:B:69:GLY:HA2	1.80	0.41
1:C:262:LEU:HD12	1:C:262:LEU:HA	1.77	0.41
1:A:148:PRO:O	1:A:149:LEU:C	2.59	0.41
1:A:278:LEU:HD13	1:A:278:LEU:HA	1.89	0.41
1:C:20:GLN:CD	1:C:252:MET:HG2	2.40	0.41
1:A:30:MET:HE2	1:A:30:MET:HB2	1.81	0.41
1:B:7:LEU:HA	1:B:7:LEU:HD22	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:PRO:HB3	1:D:95:LEU:CG	2.44	0.41
1:A:80:ALA:O	1:A:84:THR:HG23	2.20	0.41
1:A:139:ALA:O	1:A:226:ILE:HG13	2.21	0.41
1:B:157:LEU:HA	1:B:157:LEU:HD22	1.81	0.41
1:D:89:PHE:HB3	1:D:107:THR:HA	2.03	0.41
1:A:147:GLU:HA	1:A:230:SER:OG	2.21	0.40
1:B:26:LEU:HD22	1:B:92:LEU:CB	2.48	0.40
1:B:89:PHE:HZ	1:B:114:VAL:HG21	1.86	0.40
1:D:155:LEU:HD22	1:D:279:ASN:HD21	1.86	0.40
1:D:232:HIS:HE1	1:D:245:SER:O	2.04	0.40
1:D:123:GLU:O	1:D:125:TYR:N	2.54	0.40
1:D:177:GLU:OE1	1:D:177:GLU:N	2.54	0.40
1:B:151:VAL:HG12	1:B:227:LEU:HG	2.03	0.40
1:C:233:VAL:HG12	1:C:234:PHE:CD2	2.56	0.40
1:D:147:GLU:HB3	1:D:148:PRO:CD	2.45	0.40
1:C:47:PRO:O	1:C:50:PHE:HB3	2.21	0.40
1:C:140:SER:HA	1:C:229:VAL:HG21	2.04	0.40
1:C:142:PHE:HB2	1:C:226:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	238/301 (79%)	196 (82%)	30 (13%)	12 (5%)	2	14
1	B	239/301 (79%)	198 (83%)	24 (10%)	17 (7%)	1	8
1	C	228/301 (76%)	188 (82%)	25 (11%)	15 (7%)	1	9
1	D	229/301 (76%)	191 (83%)	23 (10%)	15 (7%)	1	9
All	All	934/1204 (78%)	773 (83%)	102 (11%)	59 (6%)	1	10

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	VAL
1	A	99	PRO
1	A	122	PRO
1	A	246	ALA
1	B	42	SER
1	B	43	SER
1	B	70	ARG
1	B	72	PHE
1	B	99	PRO
1	B	123	GLU
1	B	149	LEU
1	B	174	THR
1	C	120	LEU
1	C	248	THR
1	D	124	TRP
1	D	148	PRO
1	D	275	LEU
1	A	35	LEU
1	A	96	ALA
1	A	231	SER
1	B	101	THR
1	B	122	PRO
1	B	124	TRP
1	B	146	LEU
1	B	274	GLY
1	C	72	PHE
1	C	89	PHE
1	C	93	SER
1	C	146	LEU
1	C	245	SER
1	D	69	GLY
1	D	96	ALA
1	D	178	GLY
1	D	268	LYS
1	A	148	PRO
1	A	178	GLY
1	A	230	SER
1	B	277	PRO
1	C	12	MET
1	C	70	ARG
1	C	244	LEU
1	D	7	LEU
1	D	99	PRO

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Mol	Chain	Res	Type
1	A	6	TRP
1	B	90	GLY
1	B	240	VAL
1	B	273	ALA
1	C	101	THR
1	D	121	TYR
1	D	123	GLU
1	D	234	PHE
1	C	176	ALA
1	D	246	ALA
1	C	73	ILE
1	D	70	ARG
1	C	90	GLY
1	A	270	ASN
1	D	233	VAL
1	C	247	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	188/236 (80%)	140 (74%)	48 (26%)	0	2
1	B	189/236 (80%)	137 (72%)	52 (28%)	0	1
1	C	185/236 (78%)	132 (71%)	53 (29%)	0	1
1	D	183/236 (78%)	141 (77%)	42 (23%)	1	3
All	All	745/944 (79%)	550 (74%)	195 (26%)	0	2

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	12	MET
1	A	14	LEU
1	A	17	LEU
1	A	21	ILE

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Mol	Chain	Res	Type
1	A	44	VAL
1	A	46	ASN
1	A	50	PHE
1	A	54	LEU
1	A	55	LEU
1	A	58	THR
1	A	64	LEU
1	A	66	ARG
1	A	67	THR
1	A	70	ARG
1	A	71	ARG
1	A	77	ILE
1	A	79	PHE
1	A	83	MET
1	A	117	LEU
1	A	123	GLU
1	A	128	ASP
1	A	129	ILE
1	A	141	ILE
1	A	152	LEU
1	A	155	LEU
1	A	157	LEU
1	A	158	LEU
1	A	169	THR
1	A	172	MET
1	A	174	THR
1	A	175	LEU
1	A	214	PHE
1	A	216	MET
1	A	221	LEU
1	A	226	ILE
1	A	227	LEU
1	A	228	VAL
1	A	231	SER
1	A	232	HIS
1	A	233	VAL
1	A	234	PHE
1	A	245	SER
1	A	253	VAL
1	A	257	VAL
1	A	263	LEU
1	A	284	LEU

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Mol	Chain	Res	Type
1	A	288	VAL
1	B	7	LEU
1	B	9	LEU
1	B	10	LEU
1	B	12	MET
1	B	14	LEU
1	B	15	MET
1	B	28	MET
1	B	30	MET
1	B	35	LEU
1	B	44	VAL
1	B	46	ASN
1	B	51	ILE
1	B	54	LEU
1	B	59	LEU
1	B	65	LEU
1	B	67	THR
1	B	73	ILE
1	B	81	LEU
1	B	85	PHE
1	B	88	ILE
1	B	94	LEU
1	B	95	LEU
1	B	109	ILE
1	B	117	LEU
1	B	120	LEU
1	B	124	TRP
1	B	141	ILE
1	B	146	LEU
1	B	149	LEU
1	B	152	LEU
1	B	155	LEU
1	B	157	LEU
1	B	167	TYR
1	B	170	LYS
1	B	174	THR
1	B	216	MET
1	B	220	ASP
1	B	221	LEU
1	B	227	LEU
1	B	245	SER
1	B	248	THR

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Mol	Chain	Res	Type
1	B	256	LEU
1	B	257	VAL
1	B	259	LEU
1	B	261	VAL
1	B	262	LEU
1	B	263	LEU
1	B	270	ASN
1	B	272	GLN
1	B	278	LEU
1	B	279	ASN
1	B	288	VAL
1	C	12	MET
1	C	17	LEU
1	C	27	VAL
1	C	30	MET
1	C	46	ASN
1	C	58	THR
1	C	62	LEU
1	C	63	VAL
1	C	64	LEU
1	C	65	LEU
1	C	66	ARG
1	C	70	ARG
1	C	72	PHE
1	C	73	ILE
1	C	76	PHE
1	C	81	LEU
1	C	94	LEU
1	C	95	LEU
1	C	100	THR
1	C	107	THR
1	C	109	ILE
1	C	112	VAL
1	C	115	THR
1	C	128	ASP
1	C	133	LEU
1	C	140	SER
1	C	141	ILE
1	C	145	SER
1	C	146	LEU
1	C	149	LEU
1	C	152	LEU

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Mol	Chain	Res	Type
1	C	153	VAL
1	C	155	LEU
1	C	157	LEU
1	C	158	LEU
1	C	166	VAL
1	C	168	ARG
1	C	169	THR
1	C	170	LYS
1	C	174	THR
1	C	214	PHE
1	C	218	MET
1	C	221	LEU
1	C	223	MET
1	C	226	ILE
1	C	232	HIS
1	C	259	LEU
1	C	265	PHE
1	C	266	VAL
1	C	267	ASN
1	C	284	LEU
1	C	288	VAL
1	C	292	LEU
1	D	9	LEU
1	D	12	MET
1	D	20	GLN
1	D	46	ASN
1	D	61	LEU
1	D	62	LEU
1	D	64	LEU
1	D	65	LEU
1	D	66	ARG
1	D	73	ILE
1	D	85	PHE
1	D	100	THR
1	D	107	THR
1	D	117	LEU
1	D	127	ILE
1	D	129	ILE
1	D	135	SER
1	D	140	SER
1	D	141	ILE
1	D	144	ILE

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Mol	Chain	Res	Type
1	D	145	SER
1	D	146	LEU
1	D	149	LEU
1	D	151	VAL
1	D	152	LEU
1	D	155	LEU
1	D	156	VAL
1	D	158	LEU
1	D	168	ARG
1	D	169	THR
1	D	175	LEU
1	D	220	ASP
1	D	221	LEU
1	D	225	SER
1	D	231	SER
1	D	248	THR
1	D	249	LEU
1	D	252	MET
1	D	261	VAL
1	D	270	ASN
1	D	272	GLN
1	D	278	LEU

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

Mol	Chain	Res	Type
1	A	267	ASN
1	B	279	ASN
1	D	20	GLN
1	D	232	HIS
1	D	270	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	246/301 (81%)	0.06	10 (4%)	37	36	105, 136, 202, 270	0
1	B	247/301 (82%)	0.05	16 (6%)	18	19	91, 145, 212, 269	0
1	C	238/301 (79%)	0.20	17 (7%)	16	17	108, 165, 239, 404	0
1	D	237/301 (78%)	0.36	22 (9%)	8	9	140, 183, 267, 341	0
All	All	968/1204 (80%)	0.17	65 (6%)	17	18	91, 158, 233, 404	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	6	TRP	15.3
1	C	6	TRP	8.8
1	C	224	PRO	6.5
1	A	5	ASP	5.8
1	B	272	GLN	5.8
1	B	242	TRP	5.7
1	D	212	GLY	5.4
1	B	224	PRO	5.4
1	B	210	GLU	5.3
1	A	65	LEU	4.9
1	D	30	MET	4.8
1	D	15	MET	4.7
1	A	6	TRP	4.3
1	D	272	GLN	4.1
1	D	262	LEU	4.1
1	D	235	VAL	4.0
1	A	4	ARG	3.9
1	D	271	PRO	3.6
1	B	9	LEU	3.4
1	D	286	PHE	3.3
1	B	240	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	68	GLY	3.3
1	D	100	THR	3.2
1	B	99	PRO	3.1
1	C	273	ALA	3.1
1	D	273	ALA	3.1
1	B	94	LEU	3.0
1	D	93	SER	2.9
1	D	101	THR	2.9
1	D	119	TYR	2.9
1	C	284	LEU	2.9
1	B	234	PHE	2.8
1	A	292	LEU	2.8
1	B	24	ILE	2.8
1	D	69	GLY	2.8
1	A	270	ASN	2.7
1	C	225	SER	2.6
1	D	79	PHE	2.6
1	C	5	ASP	2.6
1	D	275	LEU	2.6
1	A	99	PRO	2.6
1	C	20	GLN	2.5
1	D	277	PRO	2.5
1	B	100	THR	2.5
1	D	7	LEU	2.4
1	D	230	SER	2.4
1	B	64	LEU	2.4
1	B	241	LEU	2.3
1	C	223	MET	2.3
1	C	166	VAL	2.3
1	D	221	LEU	2.3
1	C	92	LEU	2.3
1	C	286	PHE	2.3
1	A	272	GLN	2.2
1	B	92	LEU	2.2
1	D	49	ILE	2.2
1	C	272	GLN	2.2
1	B	148	PRO	2.2
1	C	67	THR	2.1
1	C	66	ARG	2.1
1	C	7	LEU	2.1
1	B	124	TRP	2.0
1	A	10	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	97	LEU	2.0
1	C	119	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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.